Evaluated Gas Phase Basicities and Proton Affinities of Molecules: An Update

Edward P. L. Hunter and Sharon G. Lias

Physical and Chemical Properties Division, Chemical Science and Technology Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-0001

Received August 11, 1997; revised manuscript received 23 March 1998

The available data on gas-phase basicities and proton affinities of approximately 1700 molecular, radical and atomic neutral species are evaluated and compiled. Tables of the data are sorted (1) according to empirical formula and (2) according to evaluated gas basicity. This publication constitutes an update of a similar evaluation published in 1984.

[S0047-2689(98)00203-7]

Key words: enthalpy; entropy; gas basicity; Gibbs energy; ion-molecule reactions; proton affinity; protonation entropy; proton transfer.

Contents

List of Tables

1. Introduction

1.1. Dedication to Professor Robert W. Taft

This evaluation of gas basicity and proton affinity data is dedicated to the late Professor Robert W. Taft, whose research led to the early determination of an extensive scale of gas-phase basicity data. The existence of this comprehensive body of internally consistent, interlocking experimental measurements in a very real sense made it possible to tie together and evaluate data from a wide variety of sources generated by various experimental techniques. We are indebted to Professor Taft for pioneering this type of research, and for demonstrating its scientific interest and importance.

1.2. Background

This publication is an update and revision of the evaluation of the scale of gas phase basicity/proton affinity data carried out in this laboratory, and published in 1984.[1] Prior to its appearance, there had been a number of reviews of the field[2–8] and two unevaluated compilations,[9,10] but no single reference had presented a comprehensive collection of data on gas phase proton affinities evaluated for internal consistency. The 1984 evaluation has been proven to be sufficiently useful that it is still widely cited, and current publications often compare new data to data in the proton affinity scale as presented there (the so-called "NBS (National Bureau of Standards) Scale"). However, in the intervening years, a large amount of new data has appeared in the literature, so the so-called "NBS Scale" is seriously out-of-date, missing data for about 900 compounds. In addition, recent studies include several seminal publications, both experimental and theoretical, which present information indicating that portions of the scale as presented in the 1984 publication are incorrect, and therefore in need of re-evaluation.

1.3. Definitions

The gas basicity and proton affinity of a species (molecule, radical, or atom), M, are defined in terms of the hypothetical gas-phase reaction:

$$M(g)+H^+(g)\rightarrow MH^+(g). \tag{1}$$

The gas basicity of M at temperature T, GB(M,T), is the negative of the Gibbs free energy change for this reaction:

$$GB(M,T)\equiv -\Delta G^0_{Rn1}(T). \tag{2}$$

Thermochemical quantities having a subscript Rn followed by an integer means that the quantity is associated with the reaction or process indicated by the integer. The proton affinity, PA(M,T), is the negative of the corresponding enthalpy change:

$$PA(M,T)\equiv -\Delta H^0_{Rn1}(T) = \Delta_f H^0(M,T)+\Delta_f H^0(H^+,T)-\Delta_f H^0(MH^+,T). \tag{3}$$

The corresponding entropy change can be expressed in terms of absolute entropies of the species involved:

$$\Delta S^0_{Rn1}(T)=S^0(MH^+,T)-S^0(M,T)-S^0(H^+,T) \tag{4}$$

$$=\Delta S_p(M,T)-S^0(H^+,T), \tag{5}$$

where ΔS_p(M,T) is defined as the entropy of protonation of M:

$$\Delta S_p(M,T)\equiv S^0(MH^+,T)-S^0(M,T). \tag{6}$$

Since the defining process is understood to always involve gaseous species, the phase designations for the species indicated in reaction (1) are dropped when indicating those species in thermochemical quantities. The relationship between gas basicity, proton affinity and entropy of protonation is obtained by combining Eqs. (2), (3) and (5) to give

$$GB(M,T)=PA(M,T)+T[\Delta S_p(M,T)-S^0(H^+,T)]. \tag{7}$$

2. Sources of Proton Affinity/Gas Basicity Data

Most of the published data on gas phase basicities/proton affinities of molecules are derived from measurements which lead to *relative* scales of basicities/proton affinities, but do not provide *absolute* values for these quantities. Absolute values are assigned to the entire relative thermochemical scales using data for molecules whose position in the relative scale has been established, and for which absolute values of enthalpies of formation of both M and MH^+ are known from other measurements. Thus the evaluation of the basicity/proton affinity scales has three components: (1) an evaluation of the thermochemical data leading to the scale of *relative* gas basicities; (2) an evaluation of measured entropy changes for proton transfer reactions, or an estimation of entropy changes for species for which experimental data are not available, followed by the generation of the scale of *relative* proton affinities, and (3) the evaluation of data leading to the assignment of absolute values to the scales. Before describing the evaluation of these scales, we first describe briefly the methods by which absolute values of proton affinity and relative values of gas basicity are obtained.

2.1. Absolute Proton Affinity Values

2.1.1. Ionization Threshold Measurements

Experiments in which the enthalpy of formation of MH^+ is determined lead directly to values for the proton affinity when combined with the value for the enthalpy of formation of the corresponding neutral molecule, M. If MH is a sufficiently stable species that it can be introduced into a mass spectrometer or be generated *in situ*, or if MH^+ is formed as a product ion from the fragmentation of some larger molecular species, absolute values for the enthalpy of formation can be obtained, either by determining the ionization energy of MH:

$$MH\rightarrow MH^+ + e^- \tag{8}$$

or the appearance energy of MH^+ from a larger molecule, MNH:

$$MNH\rightarrow MH^+ + N + e^-. \tag{9}$$

Since the thermochemical scales provide data on *relative* proton affinities, it is necessary to assign absolute proton affinity values to the entire scale. This is only possible if an absolute proton affinity can be reliably assigned to one or more molecules in the scale. Absolute values for proton affinities can be derived from Eq. (3) by simply inserting available values for enthalpies of formation of M(g), MH^+(g), and H^+(g) when these are all known. Unfortunately, there are relatively few species for which this is possible.

Enthalpies of formation of all relevant species are known for the lower members of the homologous series when M is

an olefin and MH^+ an alkyl ion. For this reason, the proton affinities of ethylene, propene, and isobutene have often been used as the basis for assigning absolute values to the proton affinity scale,[1] and were considered to be reliable anchors. However, as will be discussed below, new results indicate some changes are necessary; for example, the accepted value for the enthalpy of formation of the tert-butyl cation has changed based on new measurements, and the positions of ethylene and propene in the basicity scale are not necessarily as well established as previously thought.

2.1.2. Absolute Values of Proton Affinities from Theoretical Calculations

It has been shown that standard *ab initio* molecular orbital calculations at the G2 level of theory[11] consistently yield values of proton affinities within 10 kJ mol^{-1} of experimental values, which is usually within error limits of the latter. In a recent paper, Smith and Radom[12] reported computed proton affinity values for 31 molecules over an energy range of about 500 kJ mol^{-1}, that is, values that effectively spanned most of the experimental scale reported from equilibrium constant determinations. Further work by East, Smith and Radom[13] provides a set of theoretically predicted values of entropy changes associated with protonation of these molecules. In view of the difficulties in pinning down values to be assigned to species in an experimentally derived thermochemical scale (which may display "shifts" over time, for various reasons discussed elsewhere in this paper), the data from these papers provided an invaluable guide to the evaluation of the proton affinity data presented here.

2.2. Relative Gas Basicity/Proton Affinity Values

2.2.1. Gas Phase Equilibrium Constant Data

Most of the data presented here are based on measurements of the equilibrium constants of gas phase proton transfer reactions between M and a reference species, R, at a single temperature:

$$RH^- + M \rightleftharpoons MH^- + R, \tag{10}$$

where:

$$-R_g T \ln K_{Rn10} = \Delta G^0_{Rn10} = \Delta H^0_{Rn10} - T\Delta S^0_{Rn10}, \tag{11}$$

and R_g is the universal gas constant. The equilibrium constant for reaction (10) is obtained from a mass spectrometric observation of the relative abundances of the ions, RH^- and MH^-, in a mixture of compounds R and M of known composition:

$$K_{Rn10} = \{[MH^-]/[RH^-]\} \cdot \{[R]/[M]\}. \tag{12}$$

When the ratio of ions is observed under conditions such that thermodynamic equilibrium has been attained, the resulting value for the equilibrium constant of reaction (10) directly provides a value for the Gibbs free energy change of reaction at temperature T. We note that reaction (10) can be resolved into reaction (1) and an analogous process in which M is replaced by R, namely:

$$R(g) + H^+(g) \rightarrow RH^+(g). \tag{13}$$

The gas basicity, proton affinity and protonation entropy of R in reaction (13) are similarly defined as for M in Eqs. (2)–(7) in which M is replaced by R. Then, the Gibbs free energy change of reaction (10) is equal to the relative gas phase basicities of compounds R and M, $\Delta GB(M,R,T)$, at the temperature T, i.e.,

$$-\Delta G^0_{Rn10}(T) = GB(M,T) - GB(R,T) \equiv \Delta GB(M,R,T). \tag{14}$$

Scales of relative gas phase basicities derived from equilibrium constant determinations can lead to a quantitative scale of relative proton affinities, $\Delta PA(M,R)$, only if the entropy change of reaction (10), or the relative protonation entropy, $\Delta\Delta S_p(M,R)$, is known or can be reliably estimated.

$$-\Delta H^0_{Rn10} = PA(M,T) - PA(R,T) \equiv \Delta PA(M,R), \tag{15}$$

$$\Delta S^0_{Rn10} = \Delta S_p(M,T) - \Delta S_p(R,T) \equiv \Delta\Delta S_p(M,R). \tag{16}$$

The reader should note that the definitions of relative proton affinities and relative protonation entropies do not show an explicit temperature dependence, even though the quantities involved in their definitions do show such explicit dependence. Unlike relative gas basicity, relative proton affinities and relative protonation entropies are quite temperature independent; more about this feature is explained in Section 2.3.

Some of the data available and presented here are based on measurements of K_{Rn10} over a range of temperatures. When such data are treated in a van't Hoff manner, i.e., when $\ln K_{Rn10}$ is plotted against T^{-1}, then values of ΔH^0_{Rn10} and ΔS^0_{Rn10} can, in principle, be derived directly from the slope and intercept of the fitted line, respectively,

$$\ln K_{Rn10} = -\Delta H^0_{Rn10}/R_g T + \Delta S^0_{Rn10}/R_g. \tag{17}$$

In the van't Hoff treatment, the values of ΔH^0_{Rn10} and ΔS^0_{Rn10} are considered to be constants over the temperature range for which K_{Rn10} is measured (see Sec. 2.3.).

In the 1984 evaluation,[1] proton affinity values were derived from the scale of gas basicities using calculated entropy changes derived from standard statistical mechanics treatments. In most cases, the estimates were based on the simplifying assumption that the protonation entropy of M in reaction (1) can be approximated adequately by the temperature independent expression:

$$\Delta S_p(M) = R_g \ln[\sigma(M)/\sigma(MH^-)], \tag{18}$$

where $\sigma(M)$ and $\sigma(MH^-)$ are the rotational symmetry numbers of M and MH^-.

For the present evaluation, extensive thermochemical ladders from two laboratories[14–16] were available which included determinations of equilibrium constants over a range of temperatures, i.e., which included entropy change determinations. However, as discussed below in the description of the evaluation procedures, there was poor agreement between the entropy change measurements from different labo-

ratories: this was taken as an indication that inherent experimental problems make such determinations unreliable. Therefore, instead of using the (inconsistent) experimental data directly, or resorting to the use of Eq. (18), a procedure was adopted which incorporates an analysis of the data for the entire thermochemical ladder at different temperatures, and the imposition of a requirement that the entropy changes be reasonable and internally consistent.

Most measurements of proton transfer equilibrium constants have been carried out using one of three types of mass spectrometers which operate in very different pressure regimes: an ion cyclotron resonance spectrometer[17(a)] (ICR, $\sim 10^{-4}$ Pa, 1 Torr=133.3224 Pa), a high pressure mass spectrometer[17(b)] (HPMS, 100–1000 Pa), or a flowing afterglow[17(c)] apparatus (FA, 100–1000 Pa). Questions have been raised about whether thermodynamic equilibrium is in fact attained at the low pressures of an ICR experiment (in spite of the long reaction times employed); the generally good agreement between thermochemical scales determined through ICR experiments and those from higher pressure HPMS and FA measurements argues in favor of the validity of the ICR scales.

2.2.2. Relative Gas Basicities from Bracketing Experiments

In some cases, measurements of proton transfer equilibrium constants are difficult or impossible. This happens when M is an unstable molecule, or in systems where MH^+ undergoes fast reactions with M, or a reaction other than proton transfer with R, see reaction (10). In these cases, upper and lower bounds of the basicity can usually be estimated through the technique known as "bracketing." The ion MH^+ is reacted with a series of molecules, R_1 and R_2 in reactions (19) and (20), and the occurrence or nonoccurrence of proton transfer is noted:

$$MH^+ + R_1 \rightarrow \text{no proton transfer}, \tag{19}$$

$$MH^+ + R_2 \rightarrow R_2H^+ + M. \tag{20}$$

Under the assumption that proton transfer will be observed only if the reaction is associated with a negative value of the Gibbs free energy change, the basicity of M is taken to be between the basicities of R_1 and R_2. Note that since it is the Gibbs free energy change that determines whether proton transfer occurs, the quantity that is bracketed is the gas basicity and not necessarily the proton affinity.

Results obtained from bracketing experiments are generally less reliable than those obtained from other types of experiments because of numerous possible complications. For example, exothermic proton transfer reactions sometimes do not occur if there is an energetically favorable alternate channel open to the reactants. If there are several isomeric structures of the species involved in reactions (19) or (20), the observed proton transfer reaction may be accompanied by a rearrangement of those species in the reaction complex to more stable structures; in this case, the observed "bracketing" does not reflect the thermochemistry of the expected proton transfer reaction.

2.2.3. Relative Proton Affinity Data from the "Kinetic Method"

Another often-used approach is based on the observation of the collision-induced dissociation of proton-bound dimer ions, here written as $M \cdot H^+ \cdot R$, formed in association reactions:

$$M \cdot H^+ \cdot R \rightarrow MH^+ + R \tag{21}$$

$$\rightarrow RH^+ + M. \tag{22}$$

A semi-quantitative relationship[18,19] between the ratios of the two product ions and the relative proton affinities has been developed, and can be used to derive relative proton affinity values of M and R provided the entropy changes associated with processes (21) and (22) are similar. Clearly, the ratio of rate coefficients for reactions (21) and (22) is equal to the ratio of the product ions, $[MH^+]/[RH^+]$. Applying an Arrhenius-type relationship to each of the unimolecular decompositions yields

$$\ln\{[MH^+]/[RH^+]\} = \ln\{k_{Rn21}/k_{Rn22}\} = (E_{Rn22} - E_{Rn21})/R_gT, \tag{23}$$

where the E's are the activation energies of the reactions, and the familiar frequency factors or A factors cancel out if the entropy changes for reactions (21) and (22) are similar. If it is assumed that the reverse of reactions of (21) and (22) occur with no activation barriers, then $E_{Rn22} - E_{Rn21} = \Delta PA(M,R)$, which can be substituted into Eq. (23), yielding

$$\ln\{[MH^+]/[RH^+]\} = \Delta PA(M,R)/R_gT. \tag{24}$$

Measuring and plotting the ratio in Eq. (24) against the proton affinities of a series of reference molecules, R, results in a straight line if the temperature is effectively constant. The proton affinity of M is determined from where the line intercepts the PA axis. The value of PA(M) determined by this method depends on the PA values used for each of the reference bases, R, which are being re-evaluated. For this reason, data obtained by this method are tabulated in this compilation as if they were "bracketed" by the PA values of the nearest bases below and above where the plotted line crosses zero.

2.2.4. Relative Gas Basicity/Proton Affinity Data from the "Thermokinetic Method"

Still another approach developed recently to determine gas basicity or proton affinity information uses a correlation observed between the measured reaction efficiency (RE) of a process like reaction (25) and the corresponding Gibbs free energy change[20]

$$MH^+ + B \rightarrow M + BH^+. \tag{25}$$

The observed correlation is expressed as

$$RE = k_{Rn25}/k_{coll} = [1 + \exp(\Delta G^0_{Rn25} + \Delta G^0_d)/R_gT]^{-1}, \tag{26}$$

where k_{Rn25} and k_{coll} are the experimental and collision[21] rate coefficients, respectively, for reaction (25), ΔG^0_{Rn25} is the

standard free energy change and ΔG_a^0 is an "apparent" energy barrier for reaction (25). Substituting $GB(M,T) - GB(B,T)$ for ΔG_{Rn25}^0 into Eq. (26) yields:

$$RE = (1 + \exp\{[GB(M,T) - GB(B,T) + \Delta G_a^0]/R_gT\})^{-1}. \quad (27)$$

By measuring and plotting the reaction efficiency of MH^+ with a series of bases, B, of known gas basicity, the gas basicity of M, $GB(M,T)$, can be evaluated.

This method appears to be well suited to the study of unstable or labile molecules, M, but whose protonated ions, MH^+, can be generated from a suitable precursor and whose reactivity with a series of bases can be measured. An example is the recent measurement[22] of the proton affinity of the imine $CH_2{=}NH$. This molecule is not stable enough to permit an equilibrium type measurement but its protonated ion, $CH_2{=}NH_2^+$, could be generated in the gas phase by α-cleavage of amine radical cations according to:

$$CH_3CH_2NH_2^{+\cdot} \rightarrow CH_2{=}NH_2^+ + CH_3\cdot \quad (28)$$

Clearly, values for $GB(M,T)$ obtained by this correlation depend upon values used for the gas basicities of the series of reference bases, which are being re-evaluated here. As the values for the reference bases change, $GB(M,T)$ must be re-determined from a plot of Eq. (27). For this reason, data obtained by this method are tabulated in this compilation as if they were bracketed by the GB values of the nearest bases below and above that of M.

2.2.5. Other Sources of Relative Proton Affinity Data

Quantitative information about relative proton affinities has also been obtained through the determination of the energy barrier associated with endothermic proton transfer reactions through an Arrhenius treatment of the temperature dependence of the rate coefficients. Also, determinations of the equilibrium constants of association reactions:

$$AH^+ + B \rightarrow ABH^+ \quad (29)$$

can give values for enthalpies of formation of the product ion, ABH^+, provided the enthalpies of formation of AH^+ and B are known; if the enthalpy of formation of AB is also known, its proton affinity can be derived.

2.3. Remarks Concerning Temperature Dependence of Proton Affinities and Protonation Entropies

The experimental determinations of proton affinities and protonation entropies that are derived from equilibrium proton transfer measurements were performed at various temperatures mostly at or above 298 K and below 700 K. A valid question may be how do *absolute* proton affinities and protonation entropies vary with temperature. Differentiating Eq. (3) with respect to temperature gives

$$\partial PA(M)/\partial T = -\partial \Delta H_{Rn1}^0/\partial T = C_p(H^+) - C_p(M) - C_p(MH^+), \quad (30)$$

where the C_p's are the molar heat capacities at constant pressure of the parenthetically indicated species. At room temperature and above, $C_p(H^+)$ is assumed to have the classical value of $(5/2)R_g$, while $C_p(MH^+)$ will be close to but greater than $C_p(M)$. Thus, the difference in absolute proton affinity of M at 298 and 600 K will be less than 6.2 kJ mol^{-1} but still a nontrivial temperature dependence.

The *relative* proton affinities, $\Delta PA(M,R)$, of a pair of molecules M and R in reaction (10), or the enthalpy change of reaction (10), is essentially temperature independent, i.e.,

$$-\Delta H_{Rn10}^0(T_1) = PA(M,T_1) - PA(R,T_1) \approx -\Delta H_{Rn10}^0(T_2) = PA(M,T_2) - PA(R,T_2). \quad (31)$$

This follows from what was found above about the temperature dependence of an individual molecule, but can be shown more formally by differentiating Eq. (15) with respect to temperature

$$\partial \Delta PA(M,R)/\partial T = -\partial \Delta H_{Rn10}^0/\partial T = C_p(RH^+) + C_p(M) - C_p(MH^+) - C_p(R) \quad (32)$$

and noting that because of the structural similarities of reactants and products the heat capacity terms of Eq. (32) will essentially cancel to zero. When a relative proton affinity is derived from a van't Hoff analysis of a proton transfer equilibrium over a suitable temperature range, it is safe to assume that ΔH_{Rn10}^0 is independent of temperature over that range. The above discussion suggests that the temperature independence of ΔH_{Rn10}^0 can be safely assumed throughout the range $298\ K \leq T \leq 600\ K$. This feature is actually a generally observed phenomenon for reactions in which the number of reactants and products is the same, as is the case for proton transfer reactions. Similar considerations also apply to relative protonation entropies, i.e.,

$$\Delta S_{Rn10}(T_1) = \Delta S_p(M,T_1) - \Delta S_p(R,T_1) \approx \Delta S_{Rn10}(T_2) = \Delta S_p(M,T_2) - \Delta S_p(R,T_2). \quad (33)$$

This is the reason that the relative proton affinities $[\Delta PA(M,R)]$ and relative protonation entropies $[\Delta\Delta S_p(M,R)]$, defined by Eqs. (15) and (16), are not written as being explicitly temperature dependent. Thus, in those instances where this evaluation relies on relative proton affinity data that are derived from a van't Hoff analysis [Eq. (17)] over a temperature range that may be far removed from 298 K, within the uncertainty of such measurements, it is considered appropriate to apply the derived relative proton affinity to the 298 K PA value of molecule R to deduce a 298 K PA value of molecule M according to Eq. (15). Likewise for the relative entropy of protonation. In this evaluation, the proton affinity scale uses as its primary anchor point the 298 K proton affinity value for NH_3. In Table 1, which lists the

TABLE A. Bases whose proton affinities were determined absolutely or derived from the procedure described in Sec. 5

Base	Reg. No.	GB(298)[a]	PA(298)[a]	$\Delta S_p(298)$[b]
$(CH_3)_3N$	75-50-3	918.1	948.9	5.6
pyridine	110-86-1	898.1	930.0	2.0
$(CH_3)_2NH$	124-40-3	896.5	929.5	−2.0
$C_2H_5NH_2$	75-04-7	878.0	912.0	−5.1
CH_3NH_2	74-89-5	864.5	899.0	−7
NH_3	7664-41-7	819.0	853.6	−6.4
CH_2CO	463-51-4	793.6	825.3	2.4
$(CH_3)_2CO$	67-64-1	782.1	812.0	8.7
$(CH_3)_2CCH_2$	115-11-7	775.6	802.1	20.0
$(CH_3)_2O$	115-10-6	764.5	792.0	16.5
C_2H_5CN	107-12-0	763.0	794.1	4.7
$C_6H_5CH_3$	108-88-3	756.3	784.0	16
CH_2CHCN	107-13-1	753.7	784.7	4.9
$HCOOCH_3$	107-31-3	751.5	782.5	5.0
CH_3CN	75-05-8	748.0	779.2	4.3
CH_3CHO	75-07-0	736.5	768.5	1.5
CH_3OH	67-56-1	724.5	754.3	9
CH_3CHCH_2	115-07-1	722.7	751.6	12
CH_2O	50-00-0	683.3	712.9	9.5
H_2S	7783-06-4	673.8	705	4.3
H_2O	7732-18-5	660.0	691.0	5.0
CS_2	75-15-0	657.7	681.9	28
CH_2CH_2	74-85-1	651.5	680.5	11.5
CO	630-08-0	562.8	594.0	4.2
CO_2	124-38-9	515.8	540.5	26

[a]In units of kJ mol^{-1}.
[b]In units of J (mol K)$^{-1}$.

evaluated gas basicity, proton affinity and protonation entropy of each molecule considered, all these quantities are therefore referred to a temperature of 298 K. If, however, the present evaluation is used to compute a value of $\Delta H_f(MH^+,T)$ using Eq. (3) at a temperature different than 298 K, the above mentioned temperature dependence of the proton affinity of M will have to be considered.

3. Evaluation of Absolute Proton Affinities from Ionization Threshold Measurements

The proton affinity of a species, M, can be determined *absolutely* if all of the enthalpies of formation indicated in Eq. (3) are known. Values of ΔH_f(M,298 K) are reliably known for a number of species, M, as well as the proton's enthalpy of formation [$\Delta H_f(H^+,298\ K)=1530$ kJ mol^{-1}]. Values for $\Delta H_f(MH^+,298\ K)$ are known for a much smaller set of MH^+; they are mainly derived from ionization threshold measurements according to reactions (8) or (9). Here in Sec. 3 is a description of experiments that lead to values of $\Delta H_f(MH^+,298\ K)$ and thus to absolute values of PA(M, 298 K) for ten molecules that are independent of equilibrium thermochemical scales and depend only on auxiliary thermochemical data for precursor and product molecules, i.e., for the MNH and N species in reaction (9), respectively. In all cases in this section, the most recent and reliable values of the auxiliary data are used, which may differ from that used in the original papers. The absolute proton affinity values for these 10 compounds, along with their gas basicities and entropies of protonation, are summarized in Table A. Table A also contains the same data for 15 other molecules whose values have been evaluated by the procedure described in Sec. 5.

3.1. Ketene: CH_2CO

The PA(CH_2CO) is defined by the enthalpy change of the reaction:

$$CH_2CO+H^+\rightarrow CH_3CO^+. \quad (34)$$

Traeger *et al.*,[23] have measured appearance energies for the acetyl cation, CH_3CO^+, formed by photoionization of a series of methyl ketones and have determined an enthalpy of formation for the acetyl cation as $\Delta_fH^0(CH_3CO^+,298\ K)=(657.0\pm1.5)$ kJ mol^{-1}. Taking $\Delta_fH^0(CH_2CO,298\ K)$[24] $=(-47.7\pm2.5)$ kJ mol^{-1} yields PA(CH_2CO,298 K) $=(825.3\pm3)$ kJ mol^{-1} and is the selected value for this evaluation.

For comparison, Smith and Radom[12] have calculated a 298 K PA value for ketene as 825.0 kJ mol^{-1}, indistinguishable from the photoionization value. The selected value for the entropy of protonation comes from East *et al.*,[13] who calculate $\Delta S_p(CH_2CO,298\ K)=2.4$ J (mol K)$^{-1}$. The selected value for GB(CH_2CO,298 K)$=(793.6\pm3)$ kJ mol^{-1}.

3.2. Isobutene: $(CH_3)_2CCH_2$

The proton affinity of isobutene is defined by the enthalpy change associated with the reaction:

$$(CH_3)_2CCH_2+H^-\rightarrow \text{tert-}C_4H_9^+. \quad (35)$$

It was recognized in the 1984 scale of gas basicities/proton affinities[1] that the enthalpy of formation of tert-$C_4H_9^+$ was not as well established as that for ethyl or sec-propyl cations, and so the PA of isobutene was in need of additional corroborating evidence. The value cited for the enthalpy of formation of tert-$C_4H_9^+$ in the earlier publication[1] was 694 kJ mol^{-1}, based on several apparently consistent pieces of data (appearance energy measurements, an ionization energy for the tert-butyl radical, and a chloride ion transfer equilibrium constant). However, in each instance, there is some uncertainty, usually in the supporting thermochemical data. Indeed, one of the reasons for updating this gas basicity/proton affinity scale is due to the recognition that the proton affinity span between isobutene and NH_3 was not as indicated in the 1984 scale. This discrepancy was first noted by Meot-Ner(Mautner) and Sieck[14] and confirmed by Szulejko and McMahon.[15]

The first indication that it was the proton affinity of isobutene that was in need of significant revision came from the calculations of Smith and Radom,[12] whose *ab initio* results put PA[$(CH_3)_2CCH_2$,298 K]=802.1 kJ mol^{-1}. The first experimental verification that the proton affinity of isobutene needed revision came from the extensive thermochemical ladder of Szulejko and McMahon,[15] in which the proton affinity of CO was used as the anchor point. Since then two

more recent determinations of $\Delta_f H^0(\text{tert-}C_4H_9^+,298\text{ K})$ have appeared that are consistent with each other and with the present thermochemical scale. Keister *et al.*[25] measured $\Delta_f H^0(\text{tert-}C_4H_9^+,298\text{ K})=(711\pm3.6)$ kJ mol^{-1} by dissociative ionization of a supersonically cooled beam of tert-butyl iodide using the photoelectron photoion coincidence technique. Most of the uncertainty in their result comes from the uncertainty in $\Delta_f H^0(\text{tert-}C_4H_9I,298\text{ K})$[26]$=(-72.0\pm3.3)$ kJ mol^{-1}. Traeger[27] used threshold photoionization mass spectrometry and measured $\Delta_f H^0(\text{tert-}C_4H_9^+,298\text{ K})=(711.4\pm1.1)$ kJ mol^{-1} from the appearance energies of tert-$C_4H_9^+$ from isobutane, neopentane and tert-butyl iodide, in excellent agreement with the Keister *et al.* results. Using the average of these experimental estimates for $\Delta_f H^0(\text{tert-}C_4H_9^+,298\text{ K})$ and using $\Delta_f H^0[(CH_3)_2CCH_2,298\text{ K}]$[26]$=(-16.9\pm0.9)$ kJ mol^{-1} yields $PA[(CH_3)_2CCH_2,298\text{ K}]=(802.1\pm1.4)$ kJ mol^{-1}, which is in excellent agreement with the calculations of Smith and Radom[12] and is the selected value in this compilation. For $\Delta S_p[(CH_3)_2CCH_2,298\text{ K}]$, an average of various experimental determinations and a value calculated by East *et al.*[13] is used and assigned 20 J (mol K)$^{-1}$, which sets $GB[(CH_3)_2CCH_2,298\text{ K}]=(775.6\pm1.2)$ kJ mol^{-1}.

As indicated by Traeger,[27] accepting these new values of $PA[(CH_3)_2CCH_2,298\text{ K}]$ and $\Delta_f H^0(\text{tert-}C_4H_9^+,298\text{ K})$ requires some changes in the accepted enthalpy of formation of the tert-butyl radical or of its ionization energy. More recent estimates of $\Delta_f H^0(\text{tert-}C_4H_9,298\text{ K})$ put that value at (46.0 ± 2.5)[28] kJ mol^{-1} and at (51.3 ± 1.8)[29] kJ mol^{-1}. At the time of the 1984 evaluation,[1] this value was considered to vary from 35 to 44 kJ mol^{-1}.

3.3. Acetaldehyde: CH_3CHO

The proton affinity of acetaldehyde is defined as the enthalpy change associated with the reaction:

$$CH_3CHO+H^+\rightarrow CH_3CHOH^+. \qquad (36)$$

Ruscic and Berkowitz[30] have determined the 0 K appearance energy of CH_3CHOH^+ from C_2H_5OH as (10.801 ± 0.005) eV using photoionization mass spectrometry. Assuming that the thermal $(H^0_{298}-H^0_0)$ correction needed for CH_3CHOH^+ is intermediate between that for CH_3CHO and C_2H_5OH, they derive a value of $\Delta_f H^0(CH_3CHOH^+,298\text{ K})\leq(595.4\pm0.4)$ kJ mol^{-1} $[(142.3\pm0.1)$ kcal mol$^{-1}]$. These authors[30] comment further on the inequalities by saying "Although this is rigorously a lower limit, it is very likely close to the true value, since it is based on an appearance potential of a first fragment resulting from a simple bond cleavage." Bogan *et al.*[31] also determined the appearance energy of CH_3CHOH^+ from C_2H_5OH as 10.81 eV using a discharge flow photoionization mass spectrometer, in close agreement with Ruscic and Berkowitz.[30] Accepting $\Delta_f H^0(CH_3CHO,298\text{ K})$[26]$=(-166.1\pm0.5)$ kJ mol^{-1} gives $PA(CH_3CHO,298\text{ K})=(768.5\pm1.6)$ kJ mol^{-1} and is taken as the selected value for this evaluation.

Smith and Radom[12] have calculated a 298 K proton affinity value for CH_3CHO of 770.2 kJ mol^{-1}, in good agreement with the experimental values above. East *et al.*[13] calculate a $\Delta S_p(CH_3CHO,298\text{ K})=1.5$ J (mol K)$^{-1}$. Using as selected values the experimental results for proton affinity[30,31] and the theoretical value[13] for the entropy of protonation of CH_3CHO puts $GB(CH_3CHO,298\text{ K})=(736.5\pm1.6)$ kJ mol^{-1}.

3.4. Propene: CH_3CHCH_2

The proton affinity of $CH_3CH=CH_2$ is defined as the enthalpy change for the reaction:

$$CH_3CHCH_2+H^+\rightarrow \text{sec-}C_3H_7^+. \qquad (37)$$

Rosenstock *et al.*[32] determined appearance energies for sec-$C_3H_7^+$ from 2-C_3H_7Br and 2-C_3H_7I as (10.42 ± 0.01) eV and (9.77 ± 0.02) eV, respectively, using the photoelectron photoion coincidence technique. Using $\Delta_f H^0(2\text{-}C_3H_7Br,298\text{ K})$[26]$=(-98.3\pm0.9)$ kJ mol^{-1} and $\Delta_f H^0(2\text{-}C_3H_7I,298\text{ K})$[26]$=(41.6\pm1.7)$ kJ mol^{-1} and related thermal corrections[26] yielded the values (799.6 ± 2) kJ mol^{-1} and (798.7 ± 3) kJ mol^{-1}, respectively, for the enthalpy of formation of sec-$C_3H_7^+$ at 298 K formed from 2-C_3H_7Br and 2-C_3H_7I. Baer[33] similarly reported $\Delta_f H^0(\text{sec-}C_3H_7^+,298\text{ K})=(798.3\pm4)$ kJ mol^{-1}. Using $\Delta_f H^0(CH_3CHCH_2,298\text{ K})$[26]$=(20.1\pm0.8)$ kJ mol^{-1} and an average of the above experimental values for $\Delta_f H^0(\text{sec-}C_3H_7^+,298\text{ K})$, yields $PA(CH_3CHCH_2,298\text{ K})=(751.6\pm3)$ kJ mol^{-1} and is the selected value. For comparison, Smith and Radom[12] calculated a 298 K proton affinity for propene of 744.3 kJ mol^{-1}.

For the entropy of protonation, the selected value, $\Delta S_p(CH_3CHCH_2,298\text{ K})=12$ J (mol K)$^{-1}$ comes from East *et al.*[23] Based on these values, the selected gas basicity value is $GB(CH_3CHCH_2,298\text{ K})=(722.7\pm3)$ kJ mol^{-1}.

3.5. Formaldehyde: CH_2O

The proton affinity of formaldehyde is defined by the enthalpy change accompanying the process:

$$CH_2O+H^+\rightarrow CH_2OH^+. \qquad (38)$$

Traeger and Holmes[34] measured an appearance energy of (11.578 ± 0.007) eV for CH_2OH^+ from CH_3OH, resulting in a $\Delta_f H^0(CH_2OH^+,298\text{ K})=(708.5\pm0.8)$ kJ mol^{-1}. Using $\Delta_f H^0(CH_2O,298\text{ K})$[26]$=(-108.8\pm0.8)$ kJ mol^{-1} sets $PA(CH_2O,298\text{ K})=(712.9\pm1.1)$ kJ mol^{-1}. For comparison, Smith and Radom[12] calculated a 298 K proton affinity for formaldehyde of 711.8 kJ mol^{-1}. East *et al.*[13] computed $\Delta S_p(CH_2O,298\text{ K})=9.5$ J (mol K)$^{-1}$. The selected values for this evaluation uses the experimental PA value derived from the appearance energy measurement[34] and the theoretical entropy of protonation[13] which combined gives $GB(CH_2O,298\text{ K})=(683.3\pm1.1)$ kJ mol^{-1}.

3.6. Hydrogen sulfide: H_2S

The proton affinity of H_2S is defined by the enthalpy change for the reaction:

$$H_2S+H^+ \rightarrow H_3S^+. \quad (39)$$

Prest *et al.*[35] and Walters and Blais[36] have determined appearance energies for H_3S^+ from the van der Waals dimer $(H_2S)_2$ as (10.249±0.012) eV and (10.263±0.010) eV, respectively. Using $\Delta_f H^0(H_2S,298\ K)^{37}=(-20.6\pm0.8)$ kJ mol^{-1}, $\Delta_f H^0(HS,298\ K)^{37}=(139.3\pm5)$ kJ mol^{-1}, the thermal corrections[37] for H_2S and HS, taking the dimerization energy in $(H_2S)_2$ as 6 kJ mol^{-1}, and assuming the thermal correction for H_3S^+ is equal to that for the isoelectronic PH_3, results in estimates for $\Delta_f H^0(H_3S^+, 298\ K)$ of (803.8 ±5.2) kJ mol^{-1} and (805.1±5.2) kJ mol^{-1}. Taking the average of these two estimates results in a $PA(H_2S,298\ K)$ $=(705.0+5.3)$ kJ mol^{-1}, and is the selected value. For comparison, Smith and Radom[12] computed a value of 707.7 kJ mol^{-1} for this quantity. The selected value for $\Delta S_p(H_2S,298\ K)=4.3$ J (mol K)$^{-1}$ based on the difference in absolute entropies[37] of PH_3 and H_2S. These correspond to $GB(H_2S,298\ K)=(673.8\pm5.3)$ kJ mol^{-1}.

3.7. Water: H_2O

The proton affinity of H_2O is defined by the reaction:

$$H_2O+H^+ \rightarrow H_3O^+. \quad (40)$$

Ng *et al.*[38] measured an appearance energy of (11.73 ±0.03) eV for H_3O^+ from the van der Waals dimer $(H_2O)_2$. Using $\Delta_f H^0(H_2O,298\ K)^{37}=(-241.8\pm0.04)$ kJ mol^{-1}, $\Delta_f H^0(OH,298\ K)^{37}=(39.0\pm1.2)$ kJ mol^{-1}, thermal corrections for H_2O and OH, a dimerization[39] binding energy of 16 kJ mol^{-1} for $(H_2O)_2$, and approximating the thermal correction for H_3O^+ to be that of NH_3, yields $\Delta_f H^0(H_3O^+,298\ K)=(592.6\pm5)$ kJ mol^{-1}. This leads to a proton affinity value of (695.6±5) kJ mol^{-1}. For comparison, Smith and Radom[12] and Pople and Curtiss[39] calculate values of 688.4 and 691.6 kJ mol^{-1}. Because of the rather large and uncertain binding energy of the van der Waals dimer, the selected value for $PA(H_2O,298\ K)=(691\pm3)$ kJ mol^{-1} is based on the theoretical estimations[12,39] and also on a proton transfer equilibrium measurement.[40] A value of $\Delta S_p(H_2O,298\ K)=5$ J (mol K)$^{-1}$ is selected from East *et al.*,[15] corresponding to a selected $GB(H_2O,298\ K)$ $=(660.0\pm3)$ kJ mol^{-1}.

3.8. Ethene: CH_2CH_2

The proton affinity of ethene is defined according to the enthalpy change:

$$CH_2CH_2+H^+ \rightarrow C_2H_5^+. \quad (41)$$

Ruscic *et al.*[41] determined an adiabatic ionization energy of (8.117±0.008) eV for the ethyl radical. Using a value of $\Delta_f H^0(C_2H_5,298\ K)^{42}=(118.6\pm1.7)$ kJ mol^{-1} and reported vibrational frequencies for the ethyl radical[43] and the ethyl cation[44] for the necessary thermal corrections yields $\Delta_f H^0(C_2H_5^+,298\ K)=(902\pm1.9)$ kJ mol^{-1}. Rosenstock *et al.*[32] using the photoelectron photoion coincidence technique, measured an appearance energy of (10.52±0.01) eV for $C_2H_5^+$ from C_2H_5I. Using a value of $\Delta_f H^0(C_2H_5I,298\ K)=-7.7$ kJ mol^{-1} and thermal corrections for I and C_2H_5I given by Wagman *et al.*[45] and estimating the thermal correction for ethyl cation as indicated above, results in $\Delta_f H^0(C_2H_5^+,298\ K)=(903.1\pm2)$ kJ mol^{-1}. Baer,[33] using the same technique and the same system as Rosenstock *et al.*,[32] obtained an appearance energy of 10.49 eV, resulting in the slightly lower value of $\Delta_f H^0(C_2H_5^+,298\ K)$ $=900.2$ kJ mol^{-1}. Using the average of these three values yields $\Delta_f H^0(C_2H_5^+,298\ K)=(901.8\pm1.5)$ kJ mol^{-1}. Accepting the value $\Delta_f H^0(C_2H_4,298\ K)^{26}=(52.3\pm0.8)$ kJ mol^{-1} yields $PA(C_2H_4,298\ K)=(680.5\pm1.7)$ and is the selected value.

Smith and Radom[12] calculate a 298 K PA value 681.9 kJ mol^{-1}, in good agreement with the experimental values. A value of $\Delta S_p(C_2H_4,298\ K)=11.5$ J (mol K)$^{-1}$ is selected as an average of various experimental determinations and a theoretical value,[13] and $GB(C_2H_4,298\ K)$ $=(651.5\pm1.7)$ kJ mol^{-1}.

3.9. Carbon Monoxide: CO

The proton affinity of CO is specified by the enthalpy change associated with the reaction:

$$CO+H^+ \rightarrow HCO^+. \quad (42)$$

The gas phase protonation thermochemistry of CO is rather unique in that experimental spectroscopic and thermochemical information exists for both CO and the formyl cation (HCO^+). Armed with such data, the PA, GB and ΔS_p of CO can be specified entirely from experimental studies subject only to the uncertainties associated with appearance energy measurements and the thermochemical quantities of relevant precursors. The proton affinity, gas basicity and protonation entropy of CO is an excellent choice to anchor a proton affinity ladder as in fact it was by one of the principal data sets used in this evaluation.[15] Unfortunately, the position of CO in the PA scale is rather near the bottom, separated by a scarcity of molecules for confidently linking it to the upper part of the scale.

Traeger[46] reported an appearance energy of HCO^+ from HCOOH as 12.76 eV from which a value of $\Delta_f H^0(HCO^+,298\ K)=(825.6\pm2.7)$ kJ mol^{-1} is derived. Using $\Delta_f H^0(CO,298\ K)^{47}=(-110.5\pm0.2)$ kJ mol^{-1} results in $PA(CO,298\ K)=(594\pm3)$ kJ mol^{-1}, and is the selected value for this quantity.

Protonated CO has been completely spectroscopically characterized in the microwave and infrared regions. In a microwave measurement, Woods *et al.*[48] observed the $J=0\rightarrow1$ rotational transition at 89,188 MHz. Both Gudeman *et al.*[49] and Amano[50] have reported $\nu_1=3088.7$ cm^{-1}. Kawaguchi *et al.*[51] have measured the doubly degenerate

bending mode at $\nu_2 = 828.2\ cm^{-1}$. Foster *et al.*[52] have reported a value for $\nu_3 = 2183.9\ cm^{-1}$. Each of the vibrational studies have revealed P and R branch structures which prove that HCO^+ is linear and have rotational line separations consistent with each other and with the microwave measurements. From these spectroscopic data for HCO^+ the absolute entropy of HCO^+ can be calculated, yielding the protonation entropy of CO at any temperature. They yield $\Delta S_p(CO,298\ K) = 4.2\ J\ (mol\ K)^{-1}$, which is the selected value for this quantity.

Kormornicki and Dixon[53] report a calculated 298 K proton affinity of CO as 593.1 kJ mol^{-1}, while Smith and Radom[12] report a value 593.0 kJ mol^{-1}, both of which agree well with values derived from the above appearance measurement. East *et al.*[13] report $\Delta S_p(CO,298\ K) = 3.8\ J\ (mol\ K)^{-1}$, close to value determined using spectroscopic data.

3.10. Carbon Dioxide: CO_2

The proton affinity of CO_2 is the enthalpy change associated with the process:

$$CO_2 + H^+ \rightarrow CO_2H^+. \qquad (43)$$

In a photoelectron photoion coincidence measurement, Ruscic *et al.*[54] determined an appearance energy of (12.30 ±0.02) eV for CO_2H^+ from formic acid (HCO_2H). Using a $\Delta_f H^0(HCO_2H,298\ K) = (-378.7 \pm 0.4)$ kJ mol^{-1},[45] and the thermal correction for HCO_2H and estimating the thermal correction for CO_2H^+ using theoretical vibrational frequencies[44,55] yields an estimate of $\Delta_f H^0(CO_2H^+,298\ K) = (596 \pm 2)$ kJ mol^{-1}. This corresponds to $PA(CO_2,298\ K) = (540.5 \pm 2)$ kJ mol^{-1} based on $\Delta_f H^0(CO_2,298\ K)$[47] $= (-393.5 \pm 0.1)$ kJ mol^{-1}. Traeger and Kompe[56] used photoionization mass spectrometry to measure appearance energies of CO_2H^+ from a series of carboxylic acid precursors. As a mean value from their measurements, they arrive at $\Delta_f H^0(CO_2H^+,298\ K) = (600 \pm 3)$ kJ mol^{-1}; specifically, however, the appearance energy of CO_2H^+ from HCO_2H was 12.31 eV, in close agreement with the Ruscic value.

For comparison, Kormornicki and Dixon[53] calculate a PA value of 541.0 kJ mol^{-1} while Smith and Radom[12] calculate 539.3 kJ mol^{-1}, both at 298 K and both close to the experimental value. The selected value of $PA(CO_2,298\ K)$ is (540.5 ± 2) kJ mol^{-1}, based on the above appearance observations. For $\Delta S_p(CO_2,298\ K)$ the value from East *et al.*[13] is chosen, 26 J $(mol\ K)^{-1}$, which puts $GB(CO_2,298\ K) = (515.8 \pm 2)$ kJ mol^{-1}.

4. Evaluation of Thermodynamic Ladders

The proton affinity and gas basicity scales presented here result primarily from an evaluation of a large body of interrelated data comprising a long thermochemical ladder. Since such a thermochemical scale imposes the requirements of internal consistency in three parameters, ΔG^0 (at different temperatures), ΔH^0, and ΔS^0, the evaluation of such data necessarily requires that the complete scale be evaluated as a whole. That is, a compound-by-compound evaluation of the data for individual compounds is not possible, but at the same time, final values for the proton affinities and entropy changes for individual compounds must be consistent with what is known about enthalpies of formation of the relevant ion, MH^+, and molecule, M, as well as with entropy changes for the protonation reaction that would be predicted from statistical mechanics and values (when available) of absolute entropies of the relevant species. In addition, trends in homologous series or compounds of a particular structural type must make sense.

The evaluation of such a body of data, therefore, presents a particular challenge. The strategy followed here, to summarize the discussion briefly, is: (a) to compare directly the data from four extensive gas basicity scales obtained over a long period of time in four different laboratories; (b) to find that nearly all disagreements among the scales consist of relative "contractions" or "expansions" of the scales (which are known to be attributed to problems in temperature measurements in the earlier studies), and to proceed to "standardize" the various scales (i.e., to make appropriate corrections for temperature); (c) to use the recently published theoretical values for proton affinities[12] and entropy changes[13] as a guide to assigning absolute proton affinity values and evaluating entropy changes; and (d) to examine the resulting gas basicity and proton affinity scales compound-by-compound to verify internal consistency and "reasonableness" of all the proton affinity and entropy change values.

The evaluation of gas basicity/proton affinity scales presented here takes as its starting point an evaluation of several extensive thermochemical ladders generated in different laboratories over a wide time range. These are:

(1) **The data of Kebarle–Lau:** The early high pressure mass spectrometric proton transfer equilibrium constant determinations carried out in the laboratory of Kebarle[57–62] and summarized in the 1979 thesis of Lau[63] include only a few entropy change determinations. Comparison of this scale with more recent work (see items 3 and 4, below) indicates that the scale is slightly constricted; if one takes the operating temperature as 650 K rather than 600 K, the scale is expanded [Eq. (11)], bringing it into good agreement with the recent results.

(2) **The data of Taft *et al*:** The large body of work emanating from the ICR laboratory of Taft and collaborators was published in dozens of research papers and summarized by Taft in reviews.[4,8] An updated comprehensive list of these determinations was made available to the present authors by Taft.[64] For the original measurements of gas basicities, the temperature of the ICR cell was not measured, but assumed to be 300 K. Subsequently, it has been determined that in many cases ICR cells thought to operate at "room temperature" were actually operating at higher temperatures. At the time of the 1984 evaluation,[1] Taft had estimated the operating temperature of the ICR cell to be 320 K, so the scale reported there was corrected to that temperature. A recent

paper from that laboratory[65] cites a temperature of 373 K for the operating temperature of the cell. Although the extensive scale of ICR data originated from experiments in which, as we now know, the exact temperature is ill-defined, the great value of this large body of data for multiply interconnected thermochemical steps mitigates in favor of making an attempt to reconstruct the probable temperature. One aspect of the current evaluation involved identifying the probable operating temperature at which the bulk of the earlier data from the Taft laboratory were taken. Therefore, multiple comparisons were made between the data in question and data from equilibrium constant determinations in numerous other laboratories where temperature measurements were carried out at the time of the experiments (including ICR, flowing afterglow, and high pressure mass spectrometry determinations); in general, current analysis indicates that had the operating temperature for the Taft laboratory measurements been (350 ± 5) K for that part of the scale above water, the Gibbs free energy changes measured would match well. Accordingly, in the present evaluation, Gibbs free energy values reported in these early studies[64] (which covered the scale above water) have been corrected [Eq. (11)] by multiplying originally reported Gibbs free energy values by 350/300. The lower portion of the basicity scale was better matched by assuming an operating temperature of 320 K; these conclusions were confirmed by one of the authors of the series of papers from that laboratory.[66]

(3) **The data of Meot-Ner (Mautner)–Sieck:** In 1991, Meot-Ner (Mautner) and Sieck[14] determined a scale of temperature-dependent proton transfer equilibrium constants using high pressure mass spectrometry. This study reported that the span between the proton affinities of isobutene and ammonia was 50.6 kJ mol^{-1}; since this span had been evaluated[1] in 1984 to be 33.5 kJ mol^{-1}, based on the earlier (constricted) scales reported in the literature, the Meot-Ner (Mautner)–Sieck paper gave a strong indication that a re-evaluation of the entire scale was needed. After the appearance of the results by Szulejko and McMahon[15(b)] (see item 4, below), Sieck carefully re-measured certain sections of the scale where there were discrepancies between the two sets of results, getting slightly different results for some equilibrium constants; those revised results[16] have been made available for this evaluation. In particular, the authors found that their thermochemical ladder as originally reported was somewhat expanded in the region of the scale between acetaldehyde and methyl acetate; an adjustment by a factor of 0.87, is recommended by Sieck, and has been adopted in this evaluation.

(4) **The data of Szulejko–McMahon:** Szulejko and McMahon published similar proton affinity scales determining temperature-dependent equilibrium constants in a high pressure mass spectrometer in 1991[15(a)] and 1993.[15(b)] These results confirmed the expansion of the gas basicity/proton affinity scales as reported by Meot-Ner (Mautner) and Sieck.[14]

(5) **The data of Smith–Radom:** Smith and Radom[12] produced a scale of proton affinity values generated by *ab initio* computations. That scale included proton affinity values for 31 molecules over an energy range of about 500 kJ mol^{-1}, that is, values that effectively spanned most of the experimental scale reported from equilibrium constant determinations. The same group[13] has also published a set of theoretically predicted values of entropy changes associated with protonation of these molecules. These data based on theory were used extensively as a tool for the evaluation of the experimental data.

Except for small details, the experimental gas basicity scales at 600 K from the three high pressure mass spectrometry laboratories are in generally good agreement (after making the temperature corrections described above). The scale from the ion cyclotron resonance experiments is in good agreement with the other three sets of results when the temperature difference is taken into account.

However, the proton affinity scales derived from the van't Hoff plots of the three high pressure mass spectrometry data sets[14–16,57–63] are in poor agreement. For this reason, the starting point for the evaluation was *not* the reported proton affinity scales,[14–16,57–63] but rather the 600 and 350 K gas basicity scales which appear to be well established from the good agreement and internal consistency among data generated by Kebarle *et al.*,[57–63] Meot-Ner (Mautner) and Sieck,[14,16] Szuljeko and McMahon,[15] and Taft *et al.*[64,65]

Data on relative gas basicities from other laboratories were related to particular molecules included in these extensive scales, then treated the same as these data to generate proton affinity values. Details of the procedure are described in Sec. 5.

5. Generation of the Scale of Absolute Proton Affinities from the Scale of Relative Gas Basicities

5.1. Evaluation of Entropy Change Data

The current evaluation of proton affinity data relies heavily on data from recent high pressure mass spectrometric studies[14–16] in which entropy changes for individual proton transfer reactions were determined experimentally by measuring the equilibrium constants as a function of temperature. In principle, these studies produce a scale of experimentally derived entropy changes, and hence an experimental scale of proton affinity values. However, from the disagreements between the data sets from Refs. 14 and 16 compared to data from Ref. 15, it was obvious that at least one set of data suffered from undefined experimental problems. Several options were explored by the two sets of researchers to explain the differences; a suggestion, for example, that the Meot-Ner (Mautner)–Sieck data were taken under conditions where the ions underwent too few collisions to be thermally equilibrated was tested, and found not to be the explanation for the discrepancies.

A telling result appears to be the fact that the two laboratories do reproduce one another's scales of Gibbs free energy changes at 600 K. A value for a Gibbs free energy change (relative gas basicity) of a proton transfer reaction is ob-

tained *directly* from the measured equilibrium constant [Eq. (11)], unlike the entropy and enthalpy changes of reaction which require multiple measurements over a wide temperature range [Eq. (17)]. High pressure mass spectrometric van't Hoff plot determinations are performed typically at temperatures between 450 and 650 K. Clustering reactions of protonated molecules with polar neutral molecules frequently occur at the lower end of this temperature range, while pyrolysis and isomerization reactions of molecules and ions may ensue at the upper end. These types of processes, which are difficult to detect and evaluate, may well conspire to perturb the equilibrium constant measurement and yield inaccurate van't Hoff plots, that otherwise appear precise and internally consistent. The Gibbs free energy changes measured at temperatures close to 600 K seem to suffer least from the combined effects of clustering, isomerization, and pyrolysis, judging from the good agreement between the different data sets. ICR experiments, generally carried out at a temperature of about 350 K and at much lower pressures, are apparently not as susceptible to errors resulting from clustering and pyrolysis.

For the above reasons, the entropy changes determined in the high pressure mass spectrometric studies[14–16] were not accepted as the "best" values for relevant entropy changes, although in some cases (where clustering and pyrolysis would be expected to be minimal, and sufficient information to carry out an estimate was missing), the data were used, or consulted in making the final decision.

Entropy changes were instead derived through a combination of (a) estimating the entropy change from Gibbs free energy change determinations and the corresponding calculated enthalpy changes;[12] (b) comparing Gibbs free energy changes measured in a high pressure mass spectrometer with values taken at a lower temperature in an ICR; (c) comparing values derived from the procedures described in (a) and (b) with theoretically-calculated entropy changes[13,67] and with "expected" values from statistical mechanics or from considerations of isoelectronic species. A requirement of "reasonableness" and internal consistency was imposed on all entropy change data adopted in the evaluation. Details are given in Sections 5.2 and 5.3.

5.2. Procedures Followed in Evaluating Absolute Proton Affinities from the Scale of Relative Gas Basicities

The following steps were followed in producing an evaluated proton affinity scale from the composite gas basicity scale. This amounts in large part to carrying out an evaluation of entropy changes for the proton transfer reactions.

(1) The relative gas basicity scales at 600 and 350 K were related to the basicity of ammonia.

$$NH_4^+ + B \rightarrow BH^+ + NH_3, \tag{44}$$

$$\Delta GB(B,NH_3,T) = -\Delta G^0_{Rn44}(T). \tag{45}$$

Ammonia was chosen as the primary anchor for the scale because it was considered that quantum chemical calculations lead to a reliable value for the proton affinity of this molecule. Smith and Radom report computational values of 853.6 kJ mol^{-1} at 298 K and 858.8 kJ mol^{-1} at 600 K (in good agreement with earlier *ab initio* results,[68,69] and also incidentally, with the value of 853.3 kJ mol^{-1} recommended in the previous evaluation[1]).

Furthermore, the entropy change associated with protonation of ammonia can be calculated reliably, since both NH_3 and NH_4^+ have well-known structures and are devoid of complications associated with internal rotors, nonclassical structures, internal solvation, and so on. Therefore, the absolute gas basicity of ammonia at any given temperature can be assigned with high reliability. The entropy change for the half reaction associated with protonation of ammonia is taken as -6.4 J (mol K)$^{-1}$ and -4.5 J (mol K)$^{-1}$ at 298 and 600 K, respectively.

(2) The first set of standards comprising the primary evaluated scale were taken to be the molecules included in the *ab initio* calculations published by Smith and Radom.[12] This scale made up a "ladder" to which all other results could be linked.

(a) Taking results from that publication[12] for the absolute enthalpy changes of reaction (44) for the 31 molecules, and using that "theoretical" proton affinity scale with the corresponding Gibbs free energy changes taken from the experimental scale of relative basicities at 600 K, values for ΔS^0_{Rn44} were calculated. Since the entropy change for the half reaction associated with protonation of ammonia is known, this leads to a value for the entropy change for protonation of molecule B. This value for the entropy change was then evaluated to see if it was reasonable. The requirement of "reasonableness" included not only comparing the derived value of $\Delta S^0_p(B)$ with values predicted from statistical mechanics, or from comparisons with entropy changes derived from absolute entropies of isoelectronic species, but also a comparison, when possible, with entropy changes derived from theoretical calculations.[13,67]

(b) The value of $\Delta G^0_{Rn44}(600\ K)$ and the value derived for ΔS^0_{Rn44} were used to estimate $\Delta G^0_{Rn44}(350\ K)$, assuming that ΔS^0_{Rn44} is independent of temperature. When this value was found to be in agreement with the temperature-corrected experimental values reported by Taft *et al.*[64] to within 4 kJ mol^{-1}, then the proton affinity, gas basicity, and entropy change for protonation of B were considered to be established.

Note that this procedure amounts to using the "reasonableness" of the value for the entropy change, as well as the internal consistency among the different data sets, as a criterion for the correctness of the evaluation. The required overall internal consistency also provides a secondary check on the absolute values adopted for the proton affinities; primary checks are agreements with values derived from absolute enthalpies of formation [Eq. (3)] where possible. This procedure yielded a framework proton affinity/gas basicity ladder including data for 25 molecules, and covering the proton

affinity range from about 540 to 950 kJ mol^{-1}. The gas basicities, entropy changes, and proton affinities used for these compounds are listed in Table A.

(3) Data for other molecules were then referenced to one or more of these primary standards, or to other molecules with well-established gas basicities from the initial reference scales. The extensive gas basicity scales,[14–16,57–65] as well as measurements carried out to elucidate proton affinities of molecules not included in those scales, could all be related to the primary scale. There remained the problem of deriving values for entropy changes for proton transfer to molecules not included in the primary scale of 25 molecules (Table A).

(a) For the compounds in the composite 600 K gas basicity scale[14–16,57–63] which also appear in the 350 K gas basicity scale[64] from the ICR experiments, a value for the entropy change was also derived from the difference in these two points. This derived value was then evaluated for reasonableness and internal consistency with entropy changes assigned to other related molecules in the scale.

(b) When a calculated entropy change was available,[13,67] the derived value was also compared to the calculated value; in most cases there was very good agreement between the values of ΔS^0_p(B) derived from the experimental basicity scales, but when there was a discrepancy, if the "reasonableness" of the entropy change obtained in step (a) was questionable, the theoretical value was chosen.

It should be noted that the evaluation procedure is, in fact, an evaluation of the entire scale of gas basicities/proton affinities (rather than a compound-by-compound evaluation of data for individual compounds), and imposes the requirement of internal consistency not only between scales measured at different temperatures, but also between values for the entropy changes for protonation of the different compounds included in the scales. That is, it is expected that entropy changes for protonation of all structurally similar amines, alcohols, ketones, or aldehydes, for example, should be similar. As mentioned before, most of the discrepancies between the data sets reported by Meot-Ner (Mautner) and Sieck[14,16] and by Szulejko and McMahon[15] disappear when one ignores the reported proton affinity scales (e.g., the entropy change values), and takes as a starting point for the evaluation the gas basicity scales at 600 K.

5.3. Sample Evaluations

(1) The evaluation of the gas basicity/proton affinity of methyl amine, B=CH_3NH_2: The 600 K gas basicity ladders reported by Meot-Ner (Mautner) and Sieck[14] and Szulejko and McMahon[15] give ΔG^0_{Rn44} values of −45 and −46 kJ mol^{-1}, respectively, for reaction (44). The difference between the proton affinity values for methyl amine and for ammonia calculated by Smith and Radom[12] is −47 kJ mol^{-1}. Averaging the two 600 K relative basicity values, these data lead to a value of ΔS^0_{Rn44} = −2.5 J (mol K)$^{-1}$ for the entropy change of the proton transfer between ammonia and methyl amine. Taking a value of −6.4 J (mol K)$^{-1}$ for the entropy change of the half reaction associated with the protonation of ammonia, the entropy change for the half reaction of protonation of methyl amine derived from these results is −9 J (mol K)$^{-1}$. To check if this value is reasonable, first take the difference in the absolute symmetry number corrected entropies of C_2H_6 (the isoelectronic analog of $CH_3NH_3^+$) and CH_3NH_2 at 600 K; this difference is −7.3 J (mol K)$^{-1}$. Taking the derived value of the entropy change of reaction, one predicts a Gibbs free energy change at 350 K for the proton transfer from NH_4^+ to CH_3NH_2 of −46 kJ mol^{-1}. The experimental value from the expanded Taft scale[64] is −44.8 kJ mol^{-1}. Since there is excellent internal agreement among the various gas basicity scales, and the derived value of the entropy change for protonation of methyl amine is reasonable, the data are accepted for the evaluation. Absolute values for the proton affinity and gas basicity are assigned relative to the absolute values selected for ammonia.

(2) The evaluation of the gas basicity/proton affinity of isobutene, B=$(CH_3)_2CCH_2$: Smith and Radom[12] compute a value for the 298 K proton affinity of 802.1 kJ mol^{-1}, leading to an enthalpy change associated with proton transfer from NH_4^+ of ΔH^0_{Rn44}=51.5 kJ mol^{-1}. Meot-Ner (Mautner) and Sieck[14] report a 600 K Gibbs free energy change of 38.5 kJ mol^{-1} for this reaction, but this is in the region of the scale for which Sieck recommends a slightly greater value is 38.8 kJ mol^{-1}. Szulejko and McMahon[15] report a value of 32 kJ mol^{-1} for this quantity. Averaging these two values and calculating a value for ΔS^0_{Rn44} taking the enthalpy change of reaction from the theoretical data, one obtains a value of 26 J (mol K)$^{-1}$ for the protonation entropy of isobutene. Taking the difference in absolute entropies at 298 K of isobutene and $B(CH_3)_3$,[45] the isoelectronic analog of the tert-butyl ion, one estimates that the entropy change for the half reaction should be about 22 J (mol K)$^{-1}$, in reasonably good agreement with the value derived from the data analysis. Using these data, one predicts a value for the 350 K Gibbs free energy change of the proton transfer reaction from ammonia to isobutene of 42.2 kJ mol^{-1}, in close agreement with the value taken from the expanded Taft scale,[64] 42.1 kJ mol^{-1}.

(3) The evaluation of the gas basicity/proton affinity of dimethyl ether, B=$(CH_3)_2O$: Smith and Radom[12] compute a 298 K proton affinity of 792 kJ mol^{-1} for dimethyl ether, which yields a calculated enthalpy change for proton transfer from NH_4^+ of ΔH^0_{Rn44}=61.6 kJ mol^{-1}. The corresponding Gibbs free energy change, averaging the results from Szulejko and McMahon[15] and the adjusted results from Meot-Ner (Mautner) and Sieck,[14] is 45.6 kJ mol^{-1}. Using these values as the enthalpy and Gibbs free energy for reaction (44), a value of ΔS^0_{Rn44}=26.7 J (mol K)$^{-1}$ and $\Delta S_p[(CH_3)_2O]$=20.3 J (mol K)$^{-1}$ is obtained. Combining this ΔS^0_{Rn44} value with the averaged 600 K Gibbs free energy change, one gets a 350 K Gibbs free energy value of

52.3 kJ mol^{-1}, in good agreement with 53.5 kJ mol^{-1} obtained from the expanded Taft scale.[64]

But how reasonable is this value for $\Delta S_p[(CH_3)_2O] = 20.3$ J (mol K)$^{-1}$? The difference in absolute entropies at 298 K between $(CH_3)_2NH$ [the isoelectronic neutral analog of $(CH_3)_2OH^-$] and $(CH_3)_2O$ is about 7 J (mol K)$^{-1}$. For the present evaluation, this is not considered "reasonable" agreement. However, a theoretically predicted value obtained by East *et al.*,[13] gives $\Delta S_p[(CH_3)_2O] = 16.5$ J (mol K)$^{-1}$. For this evaluation, the theoretically predicted value and the value derived from the present procedure is deemed in good agreement. This may indicate something unusual about the protonation of ethers whose entropy of protonation may not be reliably estimated using an isoelectronic neutral analog, e.g., a much lower inversion barrier is expected in the oxonium ion than in the amine.

5.4. Uncertainty of the Proton Affinity Scale

In Sec. 3, the standard uncertainty assigned to the absolute proton affinity of the molecules indicated is the usual root-sum-of-squares combination of individual uncertainties associated with relevant enthalpies of formation and the uncertainty of some key measurement, such as an ionization or an appearance energy. The uncertainty assigned to all of the other molecules in this evaluation is based on our best judgment using all the relevant information and a general knowledge and experience with inter-locking thermochemical scales and is considered to be about 8 kJ mol^{-1}.

5.5. Problems Remaining

As discussed recently by Koppel, Anvia and Taft,[65] the scale of gas basicities is not yet well established in the low basicity region, that is, in the region of the scale below the basicities of compounds such as water and hydrogen sulfide. As pointed out by those authors, measurements made in ion cyclotron resonance spectrometers are internally consistent, but are inconsistent with data taken in high pressure mass spectrometers (which data are themselves internally inconsistent).

Without access to more information, it is not possible at this time to resolve these discrepancies. Therefore, for that part of the scale below propene, many of the suggested gas basicity and proton affinity values are broad averages of rather disparate contributing values or are based somewhat indiscriminately on the most recent measurements.

6. Description of the Tables

Table 1 presents a summary of the evaluated proton affinity and gas basicity data sorted by molecular formula according to the Hill sort scheme.[70] The format is: molecular formula in the Hill format; Chemical Abstracts Registry Number; compound name or semiempirical formula; GB: evaluated value of gas basicity in kJ mol^{-1}; PA: evaluated value of proton affinity in kJ mol^{-1}; ΔS_p: evaluated entropy change for the half reaction: $M \rightarrow MH^+$. The last column gives an indication of the reason for the ΔS_p value assigned to each compound. All of the thermochemical quantities are referred to 298 K. Aside from indicating the reasons for ΔS_p values, references are not given in this table, since cited values may be derived from numerous references; the latter are given in Table 2.

Some of the entries in the second column consist of a Registry Number followed by a colon and a lower-case letter. This indicates that the corresponding molecule has estimates of proton affinity related to different sites of protonation. An example is carbon monoxide (CO) which has two entries as "630-08-0:a" (referring to protonation at C) and "630-0808:b" (referring to protonation at O). Other entries in this column begin with the "#" character followed by a number. These refer to molecules for which a Registry Number could not be found. The number following the "#" character has meaning only as an internal indexing pointer for this compilation.

The bold entries in the GB column indicate values that are derived from bracketing measurements (see Section 2.2.2.). The values so tabulated are the average GB values of the bracketing partners. It is necessary to refer to Table 2 to identify the bracketing partners and to get an indication of what may be the range of values associated with this average. Most reports of bracketing measurements do not indicate the temperature at which the observations are made. Even in cases where temperature is indicated, the tabulated values are averages of GB values referred to 298 K; no temperature corrections are included in such averages.

Some of the entries in the PA and ΔS_p columns contain "NE." This means that the protonation entropy is expected to have a large negative value but which cannot be reliably estimated. Most of the molecules having this entry are large, flexible, polyfunctional molecules, such as polypeptides, for which cyclization of the protonated molecule is expected and for which only a gas basicity value has been reported. It is necessary for such molecules to refer to Table 2 to determine the temperature for which the tabulated GB value refers.

Since the site of protonation and the protonation entropy of functionally similar molecules are expected to be nearly equal, many ΔS_p values are assigned to molecules based on their type. Thus, all tertiary amines have the same ΔS_p values as $(CH_3)_3N$, all symmetrical secondary amines have the same ΔS_p values as $(CH_3)_2NH$ and all unsymmetrical secondary amines have the same ΔS_p values as $(CH_3)_2NH$ adjusted for the difference in rotational symmetry. Similarly, all symmetrical ketones have the same ΔS_p values as acetone; unsymmetrical ketones have the value of symmetrical ketones modified for the symmetry difference. Molecules which protonate at an alkene function and give rise to a free internal rotor are assigned the ΔS_p value of propene. As such, many of the entries under "ΔS_p Reasons" simply give the functional type to which the molecule belongs. Many other molecules do not fall neatly into such categories and their ΔS_p values are assigned based on their rotational symmetry. For these molecules, the entry under "ΔS_p Reasons"

is of the form of Eq. (18). Other molecules give a reason in the form of a reference "squib," which is described in the next section. For these molecules, the cited reference is either the primary source of the assigned value of ΔS_p or contains what is believed to be a reasonable explanation of the value.

For many atomic species in Table 1, column six starts with "rot. est.," followed by a number in parenthesis. This means that the protonation entropy of that atom was approximated as being equal to the rotational entropy, where the diatomic species consist of that atom and hydrogen and has a bond length in nanometers as indicated in parenthesis. The bond length was estimated from the sum of the valence radii of the atom and hydrogen. The vibrational contribution to ΔS_p of these atoms is small and is ignored.

Table 2 presents a complete summary of the gas basicity data from the literature, along with the evaluated values for gas basicities at 298 K, entropy changes and proton affinities; these evaluations are summarized in Table 1 in a format sorted according to molecular formula. The data in Table 2 are presented in order of descending gas basicity. To find detailed experimental data for any particular molecule in Table 2, it is most convenient to first locate the molecule of interest in Table 1, then cross reference to the evaluated gas basicity value to locate the species in Table 2.

The structure of Table 2 can be best explained by actually referring to the table. Each page of Table 2 shows the column headings for the table and tabulated information for a few molecules. To begin with, it should be noted that the headings for the first three columns, along with the seventh, tenth and thirteenth columns, consist of two lines. The upper line of these column headings is in bold-face type while the lower line is in regular type. Meanwhile, the tabulated information is grouped for each individual molecule such that the first (header) row of a group is in bold-face type followed by one or more rows in regular type. The bold-faced column headings [namely, "**[Formula]**," "**Reg No(M)**," "**Base(M)**," "**GB(M)**," "**PA(M)**" and "**ΔS_p(M)**"] are meant to describe only the bold-faced data on the header row of each group of tabulated data. Similarly, the regular type headings on the lower line of the column headings describe the data contained on rows below the header row.

The header row for each grouping contains information about the base of interest, indicated by M in parenthesis and corresponding to the M indicated in reaction (10) and in Eqs. (12), (14), (15), and (16). The first column contains the molecular formula expressed in the Hill format, as indicated from the bold-faced column heading. In the second column is the Chemical Abstracts Registry Number for that base. The third column has either a line formula that is suggestive of the base's structure or a name for the base if its structure is too complicated or would be ambiguous to write as such a formula. The seventh and tenth columns contain, respectively, the *evaluated* gas basicity [GB(M)] and proton affinity [PA(M)] in kJ mol^{-1}; the thirteenth column contains the evaluated entropy of protonation [ΔS_p(M)] in J (mol K)$^{-1}$. These three quantities are all referred to 298 K.

The regular type rows below each header row contain summaries of measurements, calculations or other kinds of data that pertain to the base specified in the header row. The structure of information on these rows is intended to accommodate the fact that the vast majority of data comprising this compilation is derived from proton transfer equilibrium measurements. The data for these types of measurements are given in considerable detail, with reference bases, thermochemical quantities and temperatures specifically noted.

The first column gives identifiers for literature references and are presented in a so-called "squib":

00ABC/DEF,

where 00 gives the year of publication (assumed to be in the twentieth century), ABC are the first three letters of the last name of the first author, and DEF are the first three letters of the last name of the second author. As an example, the publication

Koppel, I. A., Anvia, F., and Taft, R. W., J. Phys. Org. Chem. **7**, 717 (1994).

would be represented in a squib as 94KOP/ANV. The complete citations of all references are given in the References section; references are sorted alphabetically according to the alphabetical part of the squib and then chronologically by year. Each entry is annotated, with experimental information such as type of instrument used, and where relevant, additional information about the study. In the case of bracketing experiments, the annotation will include the identities of bracketing compounds.

The second and third columns [labeled "Reg No(R)" and "Base(R)"] of regular-face rows gives the Chemical Abstracts Registry Number and identity, respectively, of the reference base used in proton transfer equilibrium measurements. The letter R in parenthesis corresponds to the R in reaction (10) and in Eqs. (12), (14), (15), and (16). In cases where the data come from bracketing experiments, the Registry Numbers and identities of both bracketing partners, corresponding to R_1 and R_2 of reactions (19) and (20), are given in these columns, separated by a semicolon. Some indication is given in the third column when the data comes from some other source or type of measurement; more information about these can be found in the references.

The fourth column [T(K)] gives the absolute temperature of those measurements done at a single temperature or the maximum temperature of variable temperature experiments. The fifth column [GB(R)] is the evaluated 298 K gas basicity of the reference base employed. The sixth column [ΔGB(M,R,T)] gives the change in gas basicity *at the temperature, T, indicated in the fourth column*; it is the actual value reported. The algebraic sign of this quantity is made clear by referring to Eqs. (6) and (9) and noting that R refers to the reference base and M refers to the base of interest. The seventh column [regular-face type GB(M)] gives the 298 K gas basicity value for the particular measurement based on the entry in the previous column adjusted to 298 K and the

GB value of the reference. Note that the seventh column is not simply the sum of the previous two columns, but rather is given by the equation:

$$\mathrm{GB(M)} = \mathrm{GB(R)} + \Delta\mathrm{GB(M,R,}T\mathrm{)} - \Delta\Delta S_p\mathrm{(M,R)}(T - 298\ \mathrm{K}), \quad (46)$$

where $\Delta\Delta S_p$(M,R) is given by Eq. (16). Equation (46) is derived from Eqs. (14) and (16), and the familiar equation from thermodynamics:

$$(\partial \Delta G/\partial T)_p = -\Delta S, \quad (47)$$

where the subscript means that the partial differentiation is at constant pressure and where S is considered sufficiently independent of temperature as to be treated as a constant in the integration.

Some of the entries in column 7 show a range of values. These values are the GB values (to the nearest integer) of the bracketing partners indicated in the third column.

In most cases, the derivation of the evaluated gas basicity value given in the first line of an entry will be obvious from an examination of the experimental data listed below the header.

The eighth column [PA(R)] is the evaluated 298 K proton affinity of the reference base employed. The ninth column [ΔPA(M,R)] gives the measured change in proton affinity, and is considered to be independent of temperature and *not* necessarily referred to the temperature given in column 4. The tenth column [regular-face type PA(M)] is the proton affinity of M deduced from the particular measurement; it is the sum of the previous two columns. In the eleventh column [ΔS_p(R)] is the evaluated 298 K entropy of protonation of the reference base. The twelfth column [$\Delta\Delta S_p$(M,R)] shows the measured entropy change. Like the change in proton affinity, this quantity is treated as independent of temperature and not referred to any particular temperature. The last column [ΔS_p(M)] is the sum of the two columns to its left and is the value inferred from this particular measurement.

7. References

[1] S. G. Lias, J. F. Liebman, and R. D. Levin, J. Phys. Chem. Ref. Data **13**, 695 (1984).

[2] D. K. Bohme, "The kinetics and energetics of proton transfer," in *Interactions Between Ions and Molecules*, edited by P. Ausloos (Plenum, New York, 1975), pp. 489–504.

[3] E. M. Arnett, "Proton Transfer and the Solvation of Ammonium Ions," in *Proton Transfer Reactions*, edited by E. F. Caldin and V. Gold (Wiley, New York, 1975), pp. 79–101.

[4] R. W. Taft, "Gas phase proton transfer equilibria," in *Proton Transfer Reactions*, edited by E. F. Caldin and V. Gold (Wiley, New York, 1975), pp. 31–78.

[5] P. Kebarle, Ann. Rev. Phys. Chem. **28**, 445 (1977).

[6] D. H. Aue and M. T. Bowers, "Stabilities of positive ions from equilibrium gas phase basicity measurements," in *Gas Phase Ion Chemistry*, edited by M. T. Bowers (Academic, New York, 1979), pp. 1–51.

[7] C. R. Moylan and J. I. Brauman, Ann. Rev. Phys. Chem. **34**, 187 (1983).

[8] R. W. Taft, Prog. Phys. Org. Chem. **14**, 248 (1983).

[9] R. Walder and J. L. Franklin, Int. J. Mass Spectrom. Ion Phys. **36**, 85 (1980).

[10] K. N. Hartman, S. Lias, P. Ausloos, H. M. Rosenstock, S. S. Schroyer, C. Schmidt, D. Martinsen, and G. W. A. Milne, "A Compendium of Gas Phase Basicity and Proton Affinity Measurements," National Bureau of Standards Internal Report 79-1777 (1979).

[11] L. A. Curtiss, K. Raghavachari, G. W. Trucks, and J. A. Pople, J. Chem. Phys. **94**, 7221 (1991).

[12] B. J. Smith and L. Radom, J. Am. Chem. Soc. **115**, 4885 (1993).

[13] A. L. L. East, B. J. Smith, and L. Radom, J. Am. Chem. Soc. **119**, 9014 (1997).

[14] M. Meot-Ner (Mautner) and L. W. Sieck, J. Am. Chem. Soc. **113**, 4448 (1991).

[15] (a) J. Szulejko and T. B. McMahon, Int. J. Mass Spectrom. Ion Proc. **109**, 279 (1991); (b) J. Szulejko and T. B. McMahon, J. Am. Chem. Soc. **115**, 7841 (1993).

[16] L. W. Sieck, J. Phys. Chem. **101**, 8140 (1997).

[17] (a) P. R. Kemper and M. T. Bowers, in *Techniques for the Study of Ion-Molecule Reactions*, edited by J. M. Farrar and W. H. Saunders, Volume XX of *Techniques of Chemistry* (Wiley Interscience, New York, 1988), p. 1; (b) P. Kebarle, *ibid.* p. 221; (c) N. G. Adams and D. Smith, *ibid.* p. 165.

[18] S. A. McLuckey, D. Cameron, and R. G. Cooks, J. Am. Chem. Soc. **103**, 1313 (1981).

[19] R. G. Cooks, J. S. Patrick, T. Kotiaho, and S. A. McLuckey, Mass Spectrom. Rev. **13**, 287 (1995).

[20] G. Bouchoux, J.-Y. Salpin, and D. Leblanc, Int. J. Mass Spectrom. Ion Processes **153**, 37 (1996).

[21] T. Su and W. J. Chesnavich, J. Chem. Phys. **76**, 5183 (1982).

[22] G. Bouchoux and J.-Y. Salpin, J. Phys. Chem. **100**, 16555 (1996).

[23] J. C. Traeger, R. G. McLoughlin, and A. J. C. Nicholson, J. Am. Chem. Soc. **104**, 5318 (1982).

[24] R. L. Nuttall, A. H. Laufer, and M. V. Kilday, J. Chem. Thermodyn. **3**, 167 (1971).

[25] J. W. Keister, J. S. Riley, and T. Baer, J. Am. Chem. Soc. **115**, 12613 (1993).

[26] J. B. Pedley, R. D. Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, London, 1986).

[27] J. C. Traeger, Rapid Commun. Mass Spectrom. **10**, 119 (1996).

[28] W. Tsang, J. Am. Chem. Soc. **107**, 2872 (1985).

[29] P. W. Seakins, M. J. Pilling, J. T. Niiranen, D. Gutman, and L. N. Krasnoperov, J. Phys. Chem. **96**, 9847 (1992).

[30] B. Ruscic and J. Berkowitz, J. Chem. Phys. **101**, 10936 (1994).

[31] D. J. Bogan, F. L. Nesbitt, L. J. Stief, J. L. Durant, S. C. Kuo, Z. Zhang, and R. B. Klemm, "Photoionization and thermochemical study of radicals and ions derived from ethanol: Theory and experiment," presented at the 13th International Symposium on Gas Kinetics, University College, Dublin, Ireland, Sept. 11–16, 1995.

[32] H. M. Rosenstock, R. Buff, M. A. A. Ferreira, S. G. Lias, A. C. Parr, R. L. Stockbauer, and J. L. Holmes, J. Am. Chem. Soc. **104**, 2337 (1982).

[33] T. Baer, J. Am. Chem. Soc. **102**, 2482 (1980).

[34] J. C. Traeger and J. L. Holmes, J. Phys. Chem. **97**, 3453 (1993).

[35] H. F. Prest, W.-B. Tzang, J. M. Brom, Jr., and C. Y. Ng, J. Am. Chem. Soc. **105**, 7531 (1983).

[36] E. A. Walters and N. C. Blais, J. Chem. Phys. **80**, 3501 (1984).

[37] M. W. Chase, Jr., C. A. Davies, J. R. Downey, Jr., D. J. Frurip, R. A. McDonald, and A. N. Syverud, J. Phys. Chem. Ref. Data **14**, Suppl. 1 (1985).

[38] C. Y. Ng, D. J. Trevor, P. W. Tiedemann, S. T. Ceyer, P. L. Kronebusch, B. H. Mahan, and Y. T. Lee, J. Chem. Phys. **67**, 4235 (1977).

[39] J. A. Pople and L. A. Curtiss, J. Phys. Chem. **91**, 155 (1987).

[40] B. J. McIntosh, N. G. Adams, and D. Smith, Chem. Phys. Lett. **148**, 142 (1988).

[41] B. Ruscic, J. Berkowitz, L. A. Curtiss, and J. A. Pople, J. Chem. Phys. **91**, 114 (1989).

[42] M. Brouard, P. D. Lightfoot, and M. J. Pilling, J. Phys. Chem. **90**, 445 (1986).

[43] J. Pacansky and B. Schraeder, J. Chem. Phys. **78**, 1033 (1983).

[44] D. J. DeFrees and A. D. McLean, J. Chem. Phys. **82**, 333 (1985).

[45] D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, J. Phys. Chem. Ref. Data **11** (1982).

[46] J. C. Traeger, Int. J. Mass Spectrom. Ion Proc. **66**, 271 (1985).

[47] J. D. Cox, D. D. Wagman, and V. A. Medvedev, *CODATA Key Values for Thermodynamics* (Hemisphere, New York, 1984), Chap. 1.

[48] R. C. Woods, T. A. Dixon, R. J. Saykally, and P. G. Szanto, Phys. Rev. Lett. **35**, 1269 (1975).
[49] C. S. Gudeman, M. H. Begemann, J. Pfaff, and R. J. Saykally, Phys. Rev. Lett. **50**, 727 (1983).
[50] T. Amano, J. Chem. Phys. **79**, 3595 (1983).
[51] K. Kawaguchi, C. Yamada, S. Saito, and E. Hirota, J. Chem. Phys. **82**, 1750 (1985).
[52] S. C. Foster, A. R. W. McKellar, and T. J. Sears, J. Chem. Phys. **81**, 578 (1984).
[53] A. Kormornicki and D. A. Dixon, J. Chem. Phys. **97**, 1087 (1992).
[54] B. Ruscic, M. Schwarz, and J. Berkowitz, J. Chem. Phys. **91**, 6772 (1989).
[55] M. J. Frisch, H. F. Schaefer III, and J. S. Binkley, J. Phys. Chem. **89**, 2192 (1985).
[56] J. C. Traeger and B. M. Kompe, Org. Mass Spectrom. **26**, 209 (1991).
[57] P. Kebarle, R. Yamdagni, K. Hiroaka, and T. B. McMahon, Int. J. Mass Spectrom. Ion Phys. **19**, 71 (1976).
[58] Y. K. Lau and P. Kebarle, J. Am. Chem. Soc. **98**, 7452 (1976).
[59] Y. K. Lau, K. Nishizawa, A. Tse, R. S. Brown, and P. Kebarle, J. Am. Chem. Soc. **103**, 6291 (1981).
[60] Y. K. Lau, P. P. S. Saluja, P. Kebarle, and R. W. Alder, J. Am. Chem. Soc. **100**, 7328 (1978).
[61] R. Yamdagni and P. Kebarle, J. Am. Chem. Soc. **95**, 3504 (1973).
[62] R. Yamdagni and P. Kebarle, J. Am. Chem. Soc. **98**, 1320 (1976).
[63] Y. K. Lau, Ph. D. Thesis, University of Alberta, 1979.
[64] R. W. Taft (personal communication with S. G. Lias).
[65] I. A. Koppel, F. Anvia, and R. W. Taft, J. Phys. Org. Chem. **7**, 717 (1994).
[66] J. F. Gal (personal communication, 1987).
[67] D. H. Aue, Dept. of Chemistry, Univ. of California, Santa Barbara (unpublished work, 1996).
[68] R. A. Eades, K. Scanlon, M. R. Ellenberger, D. A. Dixon, and D. S. Marynick, J. Phys. Chem. **84**, 2840 (1980).
[69] D. A. Dixon and S. G. Lias, "Absolute values of gas phase proton affinities and basicities of molecules: A comparison between theory and experiment," in *Molecular Structure and Energetics*, edited by J. F. Liebman and A. Greenberg (VCH, New York, 1987), Vol. 2, pp. 269–314.
[70] E. Hill, J. Am. Chem. Soc. **22**, 478 (1900), or see any Formula Index of *Chemical Abstracts*. In this system, a molecular formula has its constituent chemical element symbols ordered as follows: (a) compounds that contain carbon begin with C which is followed by H if the compound also contains hydrogen and the remaining elements are sorted alphabetically according to the chemical symbol; (b) compounds that lack carbon have their elements sorted alphabetically by element symbols.

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[Ar]	7440-37-1	Ar	346.3	369.2	32	S(HCl)-S(Ar)
[AsF_3]	7784-35-2	AsF_3	**604.2**	636.7	0	Rln(3/3)
[AsH_3]	7784-42-1	AsH_3	712.0	747.9	−11.5	Rln(3/12)
[BHO_2]	13460-50-9	HO-B=O	**730.5**	763.0	0	Rln(1/1)
[BH_3O_3]	10043-35-3	$B(OH)_3$	698.4	728.1	9.1	Rln(3/1)
[B_2H_6]	19287-45-7	B_2H_6	586.0	615	11.5	Rln(4/1)
[$B_3H_5N_3$]	61110-11-0	B-Borazinyl radical	**770.6**	803.0	0	Rln(1/1)
[$B_3H_6N_3$]	6569-51-3	Borazine	772.8	802.5	9.1	Rln(6/2)
[B_4H_8]	12007-71-5	B_4H_8	**752.4**	784.9	0	?
[B_4H_{10}]	18283-93-7	B_4H_{10}	572.5	605	0	?
[B_5H_8]	65930-58-7	B_5H_8	**731.0**	763.4	0	Rln(4/4)
[B_5H_9]	19624-22-7	B_5H_9	**666.9**	699.4	0	?
[BaO]	1304-28-5	BaO	1187.6	1215.4	15.5	89GUR/VEY
[Br]	10097-32-2	Br	531.2	554.4	31	rot est (0.114)
[BrH]	10035-10-6	HBr	557.7	584.2	20	97EAS/SMI
[BrLi]	7550-35-8	LiBr	792.5	819	20	linear-to-bent est.
[$CBrF_3$]	75-63-8	CF_3Br	550.3	580.0	9.1	Rln(3/1)
[CBrN]	506-68-3	BrCN	719.2	749.8	6	nitriles
[CClF]	1691-88-9	CFCl	**740.0**	772.4	0	Rln(1/1)
[$CClF_3$]	75-72-9	CF_3Cl	541.5	571.3	9.1	Rln(3/1)
[CClN]	506-77-4	ClCN	691.5	722.1	6	nitriles
[CCl_2]	1605-72-7	CCl_2	828.5	861	0	Rln(2/2)
[CCl_2S]	463-71-8	Cl_2CS	721.8	752.5	5.8	Rln(2/1)
[CFN]	1495-50-7	FCN	601.3	632	6	nitriles
[CF_2]	2154-59-8	CF_2	732.5	765	0	Rln(2/2)
[CF_2O]	353-50-4	F_2CO	637.0	666.7	9	sym ketones
[CF_3I]	2314-97-8	CF_3I	598.2	628.0	9.1	Rln(3/1)
[CF_3NO]	334-99-6	CF_3NO	**670.8**	703.3	0	Rln(1/1)
[CF_4]	75-73-0	CF_4	503.7	529.3	23.3	average
[CHCl]	2108-20-5	CHCl	**839.9**	874.1	−5.8	Rln(1/2)
[CHF]	13453-52-6	CFH	**763.8**	797.9	−5.8	Rln(1/2)
[CHF_3]	75-46-7	CHF_3	**589.7**	619.5	9.1	Rln(3/1)
[CHF_3O_3S]	1493-13-6	CF_3SO_3H	**666.9**	699.4	0	Rln(1/1)
[CHN]	6914-07-4	HNC	739.8	772.3	0	97EAS/SMI
[CHN]	74-90-8	HCN	681.6	712.9	4	97EAS/SMI
[CHNO]	75-13-8	HNCO	718.8	753	−5.8	Rln(1/2)
[CHNO]	506-85-4	HCNO	725.5	758	0	Rln(1/1)
[CHO]	2597-44-6	HCO	601.8	636	−5.8	Rln(1/2)
[CHO_2]	2564-86-5	•COOH	590.9	623.4	0	89HOL/LOS
[CHP]	6829-52-3	HCP	666.5	699	0	Rln(1/1)
[CH_2Co]	116492-58-1	$CoCH_2$	**905.2**	937.7	0	Rln(2/2)
[CH_2F_2]	75-10-5	CH_2F_2	**589.7**	620.5	5.8	Rln(2/1)
[CH_2F_2Si]	51675-50-4	$F_2Si=CH_2$	**713.4**	742.3	12	propene
[CH_2Fe]	95250-85-4	$FeCH_2$	**905.2**	937.7	0	Rln(2/2)
[CH_2N_2]	420-04-2	NH_2-CN	774.9	805.6	6	nitriles
[CH_2N_2]	334-88-3	CH_2NN	**826.7**	858.9	1	$S(CH_3CN)$-$S(CH_2NN)$
[CH_2O]	50-00-0	$H_2C=O$	683.3	712.9	9.5	97EAS/SMI
[CH_2O]	19710-56-6	HCOH (hydroxymethylene)	**933.4**	965.9	0	Rln(1/1)
[CH_2OS]	40100-16-1	$CH_2=S=O$	**766.4**	798.9	0	Rln(1/1)
[CH_2O_2]	64-18-6	HCOOH	710.3	742.0	2.7	97EAS/SMI
[CH_2S]	865-36-1	$H_2C=S$	**730.5**	759.7	11	97EAS/SMI
[CH_2Se]	6596-50-5	$H_2C=Se$	**734.9**	764.0	11	H_2CS
[CH_2Te]	43309-26-8	$H_2C=Te$	766.8	796	11	H_2CS
[CH_3BO_2]	#1524	CH_3O-B=O	**730.5**	763.0	0	Rln(1/1)
[CH_3Br]	74-83-9	CH_3Br	638.0	664.2	21	isoel analog
[CH_3Cl]	74-87-3	CH_3Cl	621.1	647.3	21	$S(CH_3SH)$-$S(CH_3Cl)$
[CH_3F]	593-53-3	CH_3F	571.5	598.9	17	$S(CH_3OH)$-$S(CH_3F)$
[CH_3I]	74-88-4	CH_3I	665.5	691.7	21	isoel analog
[CH_3N]	2053-29-4	$CH_2=NH$	**818.7**	852.9	−5.8	Rln(1/2)
[CH_3NO]	75-12-7	$HCONH_2$	791.2	822.2	5	amides
[CH_3NO_2]	4812-87-2	$HCOONH_2$	802.2	834.7	0	Rln(1/1)
[CH_3NO_2]	75-52-5	CH_3NO_2	721.6	754.6	1.6	$S(CH_3COOH)$-$S(CH_3NO_2)$
[CH_3NO_2]	624-91-9	CH_3ONO	**766.4**	798.9	0	Rln(1/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[CH_3NO_3]	598-58-3	CH_3ONO_2	**714.8**	733.6	46	94CAC/ATT
[CH_3N_3]	624-90-8	CH_3NNN	800.5	833	0	Rln(1/1)
[CH_3O]	2597-43-5	•CH_2OH	662.5	695	0	?
[CH_3S]	17032-46-1	•CH_2SH	**701.5**	733.9	0	Rln(1/1)
[CH_4]	74-82-8	CH_4	520.6	543.5	32	73HEM/RUN
[CH_4N]	10507-29-6	•CH_2NH_2	**801.6**	832.8	4	$S(CH_3NH_2)$-S(•CH_2NH_2)
[CH_4N_2]	26981-93-1:a	CH_3N=NH at terminal N	812.5	845	0	Rln(1/1)
[CH_4N_2]	26981-93-1:b	CH_3N=NH at interior N	808.5	841	0	Rln(1/1)
[CH_4N_2S]	62-56-6	$SC(NH_2)_2$	863.9	893.7	9	sym ketones
[CH_4O]	67-56-1	CH_3OH	724.5	754.3	9	97EAS/SMI
[CH_4O_3S]	75-75-2	CH_3SO_3H	**728.9**	761.3	0	?
[CH_4S]	74-93-1	CH_3SH	742	773.4	3.5	97EAS/SMI
[CH_5N]	74-89-5	CH_3NH_2	864.5	899.0	−7	97EAS/SMI
[CH_5NO]	67-62-9	CH_3ONH_2	812.3	844.8	0	Rln(1/1)
[CH_5N_3]	113-00-8	$(NH_2)_2C$=NH	949.4	986.3	−14.9	Rln(1/6)
[CH_5P]	593-54-4	CH_3PH_2	817.6	851.5	−5	$S(CH_3SiH_3)$-$S(CH_3PH_2)$
[CH_6N_2]	60-34-4	CH_3NHNH_2	866.4	898.8	0	Rln(1/1)
[CN]	2074-87-5	CN at N	>564	>595	4.2	CO
[CNS]	15941-77-2	NCS	718.5	751	0	Rln(1/1)
[CO]	630-08-0:a	CO at C	562.8	594	4.2	exp. spectra
[CO]	630-08-0:b	CO at O	402.2	426.3	28	85DEF/MCL
[COS]	463-58-1	OCS at S	602.6	628.5	22	avg[CO_2,CS_2]-Rln(2/1)
[COSe]	1603-84-5	OCSe at Se	644.1	670	22	OCS
[COTe]	#1602	OCTe at Te	692.1	718	22	OCS
[CO_2]	124-38-9	CO_2	515.8	540.5	26	97EAS/SMI
[CS]	2944-05-0	CS	760	791.5	3.3	97EAS/SMI
[CS_2]	75-15-0	CS_2	657.7	681.9	28	88MCI/ADA
[CSe]	16674-18-3	CSe at C	800.2	831.8	3	CS
[CSe_2]	506-80-9	CSe_2	700.9	725	28	CS_2
[CTe]	12012-15-6	CTe at C	860.4	892	3	CS
[CTe_2]	12192-34-6	CTe_2	747.8	771	31	CS_2-like
[C_2ClF_3O]	354-32-5	CF_3COCl	649.8	681.6	2	aldehydes
[C_2Cl_3N]	545-06-2	CCl_3CN	692.6	723.2	6	nitriles
[C_2D_6O]	17222-37-6	$(CD_3)_2O$	753.0	780.4	17	sym ethers
[C_2F_3N]	353-85-5	CF_3CN	657.7	688.4	6	nitriles
[C_2F_4O]	354-34-7	CF_3CFO	636.7	668.6	2	aldehydes
[C_2H]	2122-48-7	HCC•	720.8	753	0	Rln(1/1)
[C_2HCl_3O]	75-87-6	CCl_3CHO	690.5	722.3	2	CH_3CHO
[$C_2HCl_3O_2$]	76-03-9	CCl_3COOH	739.1	770.0	5	acids
[C_2HF]	2713-09-9	HCCF	661.3	686	26	HCCH
[C_2HF_3]	359-11-5	C_2F_3H	**666.9**	699.4	0	Rln(1/1)
[C_2HF_3O]	75-90-1	CF_3CHO	653.6	685.5	2	aldehydes
[$C_2HF_3O_2$]	76-05-1	CF_3COOH	680.7	711.7	5	acids
[C_2H_2]	74-86-2	C_2H_2	616.7	641.4	26	AUE
[C_2H_2ClN]	107-14-2	$CClH_2CN$	715.1	745.7	6	nitriles
[$C_2H_2F_2$]	1630-78-0	(E)-CHFCHF	**657.9**	688.6	5.8	Rln(2/1)
[$C_2H_2F_2$]	75-38-7	CH_2=CF_2	705.1	734	12	propene
[C_2H_2O]	463-51-4	CH_2=C=O	793.6	825.3	2.4	97EAS/SMI
[C_2H_2S]	18282-77-4	CH_2=C=S	**795.4**	826.2	5.8	Rln(2/1)
[C_2H_3]	2669-89-8	C_2H_3	**719.8**	755.2	−10	$S(C_2H_4)$-$S(C_2H_3)$+Rln(2) (spin corr)
[$C_2H_3ClO_2$]	79-11-8	$CH_2ClCOOH$	734.5	765.4	5	acids
[$C_2H_3Cl_3O$]	115-20-8	CCl_3CH_2OH	698.9	729.3	7	CH_3OH
[C_2H_3F]	75-02-5	CH_2=CHF	700.1	729	12	propene
[$C_2H_3FO_2$]	144-49-0	CH_2FCOOH	734.5	765.4	5	acids
[$C_2H_3F_3O$]	75-89-8	CF_3CH_2OH	669.9	700.2	7	CH_3OH
[$C_2H_3F_3O$]	421-14-7	CF_3OCH_3	690.0	719.2	11	unsym ethers
[C_2H_3N]	75-05-8	CH_3CN	748	779.2	4.3	$S(CH_3CCH)$-$S(CH_3CN)$
[C_2H_3N]	593-75-9	CH_3NC	806.6	839.1	0.1	HNC
[C_2H_3NO]	624-83-9	CH_3NCO	**732.0**	764.4	0	Rln(1/1)
[C_2H_3NS]	556-64-9	CH_3SCN	**766.1**	796.7	6	nitriles
[C_2H_3NS]	556-61-6	CH_3NCS	766.7	799.2	0	Rln(1/1)
[$C_2H_3N_3$]	288-88-0	1,2,4-Triazole	855.9	886.0	8	pyridines+Rln(2/1)
[$C_2H_3N_3$]	288-36-8	1,2,3-triazole	847.4	879.3	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_2H_3O]	4400-01-5	•CH_2CHO	741.5	774	0	89HOL/LOS
[C_2H_3O]	3170-69-2	CH_3CO•	620.5	653	0	89HOL/LOS
[$C_2H_3O_2$]	#1498	•CH_2COOH	737.5	770	0	89HOL/LOS
[C_2H_4]	74-85-1	$CH_2=CH_2$	651.5	680.5	11.5	AUE; 97EAS/SMI
[$C_2H_4F_2O$]	359-13-7	CF_2HCH_2OH	697.0	727.4	7	CH_3OH
[$C_2H_4F_3N$]	753-90-2	$CF_3CH_2NH_2$	812.9	846.8	−5	CH_3NH_2
[$C_2H_4N_2$]	540-61-4	$NCCH_2NH_2$	791.0	824.9	−5	CH_3NH_2
[C_2H_4O]	75-21-8	c-C_2H_4O	745.3	774.2	12	AUE
[C_2H_4O]	75-07-0	CH_3CHO	736.5	768.5	1.5	97EAS/SMI
[$C_2H_4O_2$]	64-19-7	CH_3COOH	752.8	783.7	5	acids
[$C_2H_4O_2$]	107-31-3	$HCOOCH_3$	751.5	782.5	5	97EAS/SMI
[C_2H_4S]	420-12-2	c-C_2H_4S(Thiirane)	777.6	807.4	9	sym sulfides
[C_2H_5]	2025-56-1	C_2H_5•	583.5	616	0	?
[C_2H_5Br]	74-96-4	C_2H_5Br	**669.7**	696.2	20	C_2H_5Cl
[C_2H_5BrO]	540-51-2	$BrCH_2CH_2OH$	**735.7**	766.1	7	CH_3OH
[C_2H_5Cl]	75-00-3	C_2H_5Cl	**666.9**	693.4	20	$S(C_2H_5SH)$-$S(C_2H_5Cl)$
[C_2H_5ClO]	107-07-3	$ClCH_2CH_2OH$	**735.7**	766.1	7	CH_3OH
[C_2H_5F]	353-36-6	C_2H_5F	**655.8**	683.4	16	$S(C_2H_5OH)$-$S(C_2H_5F)$
[C_2H_5FO]	371-62-0	FCH_2CH_2OH	**685.2**	715.6	7	CH_3OH
[C_2H_5FSi]	125413-85-6	$F(CH_3)Si=CH_2$	**742.2**	771.1	12	propene
[$C_2H_5F_2N$]	430-67-1	$CF_2HCH_2NH_2$	836.6	870.5	−5.1	CH_3NH_2
[C_2H_5I]	75-03-6	C_2H_5I	**698.3**	724.8	20	ethyl halides
[C_2H_5N]	593-67-9	$CH_2=CHNH_2$	**866.5**	898.9	0	Rln(1/1)
[C_2H_5N]	151-56-4	Aziridine	872.5	905.5	−2	$(CH_3)_2NH$
[C_2H_5N]	20729-41-3	$CH_3CH=NH$	**852.6**	885.1	0	Rln(1/1)
[C_2H_5N]	1761-67-7	$CH_2=NCH_3$	**852.1**	884.6	0	Rln(1/1)
[C_2H_5NO]	123-39-7	$HCONHCH_3$	820.3	851.3	5	amides
[C_2H_5NO]	60-35-5	CH_3CONH_2	832.6	863.6	5	amides
[$C_2H_5NO_2$]	79-24-3	$C_2H_5NO_2$	733.2	765.7	0	?
[$C_2H_5NO_2$]	56-40-6	glycine	852.2	886.5	−6	CH_3NH_2
[$C_2H_5NO_2$]	546-88-3	Acetamide,N-hydroxy	823.0	854.0	5	amides
[$C_2H_5NO_2$]	109-95-5	C_2H_5ONO	**786.4**	818.9	0	Rln(1/1)
[C_2H_5NS]	62-55-5	CH_3CSNH_2	852.8	884.6	2	unsym ketones
[$C_2H_5N_3$]	871-31-8	CH_3CH_2NNN	845.5	878	0	Rln(1/1)
[C_2H_6O]	4422-54-2	•CH_2CH_2OH	712.5	745	0	89HOL/LOS
[C_2H_6O]	16520-04-0	•CH_2OCH_3	**723.6**	756.1	0	Rln(1/1)
[C_2H_6O]	2348-46-1	$CH_3CH(•)OH$	**687.7**	720.1	0	Rln(1/1)
[C_2H_5P]	6569-82-0	c-C_2H_4PH	768.3	802.5	−5.8	Rln(1/2)
[C_2H_6]	74-84-0	C_2H_6	569.9	596.3	20	94CAR/SCH
[$C_2H_6B_4$]	20693-67-8	1,6-$C_2B_4H_6$	**834.8**	863.8	11.5	Rln(4/1)
[C_2H_6FN]	406-34-8	$CH_2FCH_2NH_2$	858.0	892.0	−5	CH_3NH_2
[C_2H_6Hg]	593-74-8	$(CH_3)_2Hg$	**740.8**	771.6	5.8	Rln(2/1)
[C_2H_6N]	#804	•$CH_2CH_2NH_2$	854.5	887	0	89HOL/LOS
[$C_2H_6N_2$]	143-37-3	$CH_3C(=NH)NH_2$	938.2	970.7	0	Rln(1/1)
[$C_2H_6N_2$]	4143-41-3	(E)-$CH_3N=NCH_3$	834.4	865.1	5.8	Rln(2/1)
[$C_2H_6N_2O$]	598-41-4	$H_2NCH_2CONH_2$ (glycinamide)	**882.3**	NE	NE	not estimated
[$C_2H_6N_2O_2$]	4164-28-7	$(CH_3)_2NNO_2$	795.8	828.3	0	?
[C_2H_6O]	64-17-5	C_2H_5OH	746	776.4	7	CH_3OH
[C_2H_6O]	115-10-6	$(CH_3)_2O$	764.5	792	16.5	97EAS/SMI
[C_2H_6OS]	67-68-5	$(CH_3)_2SO$	853.7	884.4	5.8	Rln(2/1)
[$C_2H_6O_2$]	107-21-1	$HOCH_2CH_2OH$	773.6	815.9	−33	95CHE/STO
[C_2H_6S]	75-18-3	$(CH_3)_2S$	801.2	830.9	9.1	97EAS/SMI
[C_2H_6S]	75-08-1	C_2H_5SH	758.4	789.6	4	CH_3SH
[$C_2H_6S_2$]	624-92-0	CH_3SSCH_3	**782.8**	815.3	0	Rln(1/1)
[C_2H-B_5]	20693-69-0	2,4-C_2B_5H-	**665.0**	697.4	0	Rln(1/1)
[C_2H-N]	75-04-7	$C_2H_5NH_2$	878	912.0	−5.1	97EAS/SMI
[C_2H-N]	124-40-3	$(CH_3)_2NH$	896.5	929.5	−2	97EAS/SMI
[C_2H-NO]	141-43-5	$NH_2(CH_2)_2OH$	896.8	930.3	−3.3	80MAC/HAM
[C_2H-O$_3$P]	868-85-9	$(CH_3O)_2PHO$	**862.4**	894.8	0	Rln(1/1)
[C_2H-P]	676-59-5	$(CH_3)_2PH$	877.9	912.0	−5.8	Rln(1/2)
[$C_2H_6N_2$]	57-14-7	$(CH_3)_2NNH_2$	894.7	927.1	0	Rln(1/1)
[$C_2H_8N_2$]	107-15-3	1,2-Diaminoethane	912.5	951.6	−22.1	80MAC/HAM
[C_2N_2]	460-19-5	NC-CN	645.8	674.7	11.8	nitriles=Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_2O]	12071-23-7	CCO	747.0	774.7	16	93MAC/SUD
[C_2S]	12602-41-4	C_2S	840.7	869.6	12	92MAC/SUD
[C_3]	12075-35-3	C_3	**736.3**	767.0	5.8	Rln(2/1)
[C_3F_5N]	422-04-8	C_2F_5CN	661.3	692.0	6	nitriles
[C_3F_6O]	684-16-2	$(CF_3)_2CO$	639.7	670.4	5.8	Rln(2/1)
[C_3HN]	1070-71-9	HCC-CN	720.5	751.2	6	nitriles
[C_3HNO]	145798-71-6	HNCCCO	828.5	861	0	?
[C_3HNO]	4452-08-8	NCCHCO	751.5	784	0	Rln(1/1)
[C_3HN_3]	290-87-9	1,3,5-Triazine	819.6	848.8	11	pyridines+Rln(6/2)
[C_3H_2]	16165-40-5	cyclopropenylidene	915.9	951.1	−9.1	Rln(2/6)
[$C_3H_2F_4O$]	360-52-1	CF_2HCOCF_2H	669.0	698.8	9	sym ketones
[$C_3H_2F_6O$]	920-66-1	$(CF_3)_2CHOH$	656.2	686.6	7	CH_3OH
[$C_3H_2N_2$]	109-77-3	$CH_2(CN)_2$	694.1	723.0	12	nitriles+Rln(2/1)
[$C_3H_2N_4O_4$]	38858-89-8	3,5-dinitropyrazole	727.5	759.4	2	pyridines
[C_3H_3]	2932-78-7	$HCCCH_2$•	708.5	741	0	89HOL/LOS
[C_3H_3]	28933-84-8	c-C_3H_3•	**701.8**	734.3	0	Rln(2/2)
[$C_3H_3ClN_2$]	15965-31-8	4-Cl-pyrazole	834.9	868.5	−3.8	pyridines+Rln(1/2)
[$C_3H_3Cl_3O$]	918-00-3	CCl_3COCH_3	736.3	768.3	1.5	CH_3CHO
[$C_3H_3FN_2$]	35277-02-2	4-fluoropyrazole	829.4	863.0	−4	pyridines+Rln(1/2)
[$C_3H_3F_3O$]	421-50-1	CF_3COCH_3	692.0	723.9	2	unsym ketones
[$C_3H_3F_3OS$]	41879-94-1	CF_3COSCH_3	734.3	765.2	5	esters
[$C_3H_3F_3O_2$]	431-47-0	CF_3COOCH_3	709.6	740.5	5	acids
[$C_3H_3F_3O_2$]	32042-38-9	$HCOOCH_2CF_3$	714.6	745.5	5	acids
[C_3H_3N]	107-13-1	CH_2=CHCN	753.7	784.7	4.9	97EAS/SMI
[C_3H_3NO]	631-57-2	CH_3COCN	716.2	746.9	6	nitriles
[C_3H_3NO]	288-42-6	oxazole	844.5	876.4	2	pyridines
[C_3H_3NO]	288-14-2	Isooxazole	816.8	848.6	2	pyridines
[$C_3H_3NO_2$]	17640-15-2	CH_3COOCN	714.7	745.7	5	esters
[C_3H_3NS]	288-47-1	thiazole	872.1	904	2	pyridines
[$C_3H_3N_3O$]	2075-46-9	4-NO_2-pyrazole	788.7	822.2	−3.8	pyridines+Rln(1/2)
[$C_3H_3N_3O_2$]	26621-44-3	3(5)-nitropyrazole	789.0	820.8	2	pyridines
[C_3H_4]	463-49-0	H_2C=C=CH_2	745.8	775.3	10	AUE
[C_3H_4]	2781-85-3	Cyclopropene	787.8	818.5	5.8	Rln(2/1)
[C_3H_4]	74-99-7	CH_3CCH	723.0	748	25	AUE
[C_3H_4ClN]	542-76-7	$Cl(CH_2)_2CN$	742.4	773.1	6	nitriles
[$C_3H_4F_2O$]	453-14-5	CFH_2COCFH_2	733.0	762.8	9	(CH3)2CO
[$C_3H_4N_2$]	288-32-4	Imidazole	909.2	942.8	−3.8	pyridines+Rln(1/2)
[$C_3H_4N_2$]	288-13-1	Pyrazole	860.5	894.1	−3.8	pyridines+Rln(1/2)
[$C_3H_4N_2S$]	96-50-4	2-Aminothiazole	898.7	930.6	2	pyridines
[C_3H_4O]	6004-44-0	CH_2CH-CO	803.4	834.1	6	ketene+Rln(3/2)
[C_3H_4O]	107-02-8	CH_2=CHCHO	765.1	797.0	2	CH_3CHO
[$C_3H_4O_3$]	96-49-1	1,3-Dioxolane-2-one	784.4	814.2	9	sym ketones
[C_3H_5]	2417-82-5	c-C_3H_5•	**702.0**	738.9	−14.9	Rln(1/6)
[C_3H_5]	1981-80-2	CH_2-CHCH_2•	707.4	736	13	$S(C_3H_6)$−Rln(2/1)-$S(C_3H_5$•)
[$C_3H_5ClO_2$]	541-41-3	$ClCOOC_2H_5$	733.8	764.8	5	esters
[C_3H_5FO]	430-51-3	CH_3COCH_2F	763.5	795.4	2	unsym ketones
[$C_3H_5FO_2$]	461-64-3	$FCO_2C_2H_5$	726.0	757.0	5	esters
[$C_3H_5F_3O$]	460-43-5	$CF_3CH_2OCH_3$	718.4	747.6	11	unsym ethers
[C_3H_5N]	107-12-0	C_2H_5CN	763.0	794.1	4.7	$S(C_2H_5CCH)$-$S(C_2H_5CN)$
[C_3H_5N]	18295-52-8	vinylimine	**879.7**	912.1	0	Rln(1/1)
[C_3H_5N]	19540-05-7	1-Azabicyclo[1.1.0]butane	856.1	886.9	5.6	$(CH_3)_3N$
[C_3H_5N]	2450-71-7	$HCCCH_2NH_2$	853.5	887.4	−5	$CH_3CH_2NH_2$
[C_3H_5N]	624-79-3	C_2H_5NC	818.9	851.3	0	HNC
[C_3H_5NO]	930-21-2	2-Azetidinone	821.7	852.6	5	amides
[C_3H_5NO]	1738-36-9	CH_3OCH_2CN	727.4	758.1	6	nitriles
[C_3H_5NO]	79-06-1	2-propenamide	839.8	870.7	5	amides
[C_3H_5NS]	35120-10-6	CH_3SCH_2CN	754.1	784.8	6	nitriles
[$C_3H_5N_3$]	1820-80-0	3(5)-aminopyrazole	889.6	921.5	2	pyridines
[$C_3H_5N_3$]	28466-26-4	4-NH2-pyrazole	874.0	907.6	−3.8	pyridines+Rln(1/2)
[C_3H_5O]	3122-07-4	•CH_2COCH_3	787.5	820	0	89HOL/LOS
[$C_3H_5O_2$]	#1324	•CH_2COOCH_3	783.5	816	0	89HOL/LOS
[$C_3H_5O_3P$]	279-53-8	2,6,7-Trioxa-1-phosphabicyclo[2.2.1]heptane	770.6	803.1	0	Rln(1/1)
[C_3H_6]	115-07-1	$CH_3CH=CH_2$	722.7	751.6	12	97EAS/SMI

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_3H_6]$	75-19-4	c-C_3H_6	722.2	750.3	14.9	Rln(6/1)
$[C_3H_6ClNO]$	96-30-0	$ClCON(CH_3)_2$	814.8	845.8	5	amides
$[C_3H_6F_3N]$	460-39-9	$CF_3CH_2CH_2NH_2$	853.2	887.2	−5	$CH_3CH_2NH_2$
$[C_3H_6F_3N]$	2730-67-8	$CF_3CH_2NHCH_3$	848.0	881.1	−2	$(CH_3)_2NH$
$[C_3H_6F_3N]$	677-41-8	$CF_3N(CH_3)_2$	772.2	803.0	5.6	$(CH_3)_3N$
$[C_3H_6N_2]$	1467-79-4	$(CH_3)_2NCN$	821.4	852.1	6	nitriles
$[C_3H_6N_2]$	151-18-8	$H_2N(CH_2)_2CN$	832.5	866.4	−5	CH_3NH_2
$[C_3H_6N_2]$	5616-32-0	CH_3NHCH_2CN	830.7	863.8	−2	CH_3NH_2
$[C_3H_6N_2S]$	96-45-7	2-imidazolinethione	891.2	921.9	5.8	Rln(2/1)
$[C_3H_6O]$	107-25-5	CH_2=CH-OCH_3	830.3	859.2	12	propene
$[C_3H_6O]$	75-56-9	2-Methyloxirane	772.7	803.3	6	oxirane-Rln(2/1)
$[C_3H_6O]$	503-30-0	c-C_3H_6O(Oxetane)	773.9	801.3	17	sym ethers
$[C_3H_6O]$	123-38-6	C_2H_5CHO	754.0	786.0	1.5	CH_3CHO
$[C_3H_6O]$	67-64-1	$(CH_3)_2CO$	782.1	812	8.7	97EAS/SMI
$[C_3H_6OS]$	21119-13-1	$CH_3C(=S)OCH_3$	816.5	846.0	10	CH_2S
$[C_3H_6OS]$	1534-08-3	$CH_3C(=O)SCH_3$	798.0	829.0	5	esters
$[C_3H_6OS_2]$	19708-81-7	$CH_3OC(S)SCH_3$	830.8	862.6	2	unsym ketones
$[C_3H_6O_2]$	109-94-4	$HCO_2C_2H_5$	768.4	799.4	5	esters
$[C_3H_6O_2]$	79-20-9	$CH_3CO_2CH_3$	790.7	821.6	5	esters
$[C_3H_6O_2]$	79-09-4	C_2H_5COOH	766.2	797.2	5	esters
$[C_3H_6O_3]$	616-38-6	$(CH_3O)_2CO$	799.2	830.2	5	acids
$[C_3H_6S]$	1822-74-8	CH_2=CH-SCH_3	829.3	858.2	12	propene
$[C_3H_6S]$	287-27-4	Thietane	805.0	834.8	9	sym sulfides
$[C_3H_6S]$	1072-43-1	2-Methylthiirane	801.5	833.3	2	thiirane-Rln(2/1)
$[C_3H_6S_2]$	2168-84-5	$CH_3C(=S)SCH_3$	831.5	860.7	11	CH_2S
$[C_3H_6Se]$	76573-19-8	CH_2=CH-$SeCH_3$	822.0	850.9	12	propene
$[C_3H_7]$	2025-55-0	i-C_3H_7•	638.9	671.4	0	?
$[C_3H_7N]$	765-30-0	c-$C_3H_5NH_2$	869.9	904.7	−7.9	$S(C_3H_5CH_3)$-$S(C_3H_5NH_2)$
$[C_3H_7N]$	503-29-7	Azetidine	908.6	943.4	−7.8	$(CH_3)_2NH$+Rln(1/2)
$[C_3H_7N]$	1072-44-2	N-Methylaziridine	904.1	934.8	5.6	$(CH_3)_3N$
$[C_3H_7N]$	75-55-8	2-Methylaziridine	892.1	925.1	−2	$(CH_3)_2NH$
$[C_3H_7N]$	107-11-9	H_2C=$CHCH_2NH_2$	875.5	909.5	−5.1	CH_3NH_2
$[C_3H_7N]$	38697-07-3	$(CH_3)_2C$=NH	**898.2**	932.3	−5.8	Rln(1/2)
$[C_3H_7N]$	4427-28-5	CH_2=$C(CH_3)NH_2$	909.3	941.8	0	Rln(1/1)
$[C_3H_7NO]$	68-12-2	$(CH_3)_2NCHO$	856.6	887.5	5	amides
$[C_3H_7NO]$	79-05-0	$C_2H_5CONH_2$	845.3	876.2	5	amides
$[C_3H_7NO]$	79-16-3	Acetamide, N-methyl	857.6	888.5	5	amides
$[C_3H_7NO_2]$	56-41-7	L-alanine	867.7	901.6	−5	CH_3NH_2
$[C_3H_7NO_2]$	5806-90-6	Acetamide, N-methoxy	848.0	879.0	5	amides
$[C_3H_7NO_2]$	541-42-4	i-C_3H_7ONO	**813.0**	845.5	0	Rln(1/1)
$[C_3H_7NO_2]$	107-97-1	Sarcosine	888.7	921.2	0	Rln(1/1)
$[C_3H_7NO_2]$	13115-24-7	Acetamide, N-hydroxy-N-methyl	845.3	876.2	5	amides
$[C_3H_7NO_2S]$	52-90-4	L-Cysteine	869.3	903.2	−5	CH_3NH_2
$[C_3H_7NO_3]$	56-45-1	L-Serine	880.7	914.6	−5	CH_3NH_2
$[C_3H_7NS]$	758-16-7	$(CH_3)_2NC(=S)H$	875.5	906.4	5	amides
$[C_3H_7O]$	31594-81-7	•$CH_2CH_2CH_2OH$	703.5	736	0	89HOL/LOS
$[C_3H_7O_3P]$	3741-36-4	2-Methoxy-1,3,2-dioxaphospholane	862.7	895.1	0	Rln(1/1)
$[C_3H_8]$	74-98-6	C_3H_8	607.8	625.7	49	75HIR/KEB
$[C_3H_8FN]$	462-41-9	$FCH_2CH_2CH_2NH_2$	886.9	920.9	−5	$CH_3CH_2NH_2$
$[C_3H_8Ge]$	82064-99-1	$(CH_3)_2Ge$=CH_2	822.2	851.1	12	propene
$[C_3H_8N_2O]$	96-31-1	$OC(NHCH_3)_2$	873.5	903.3	9	sym ketones
$[C_3H_8N_2S]$	534-13-4	$SC(NHCH_3)_2$	895.1	926.0	5	amides
$[C_3H_8O]$	67-63-0	i-C_3H_7-OH	762.6	793.0	7	CH_3OH
$[C_3H_8O]$	71-23-8	n-C_3H_7-OH	756.1	786.5	7	CH_3OH
$[C_3H_8O]$	540-67-0	$CH_3OC_2H_5$	781.2	808.6	17	unsym ethers
$[C_3H_8O_2]$	109-86-4	$CH_3OCH_2CH_2OH$	729.8	768.8	−22	1,2-diaminoethane
$[C_3H_8O_2]$	504-63-2	$HO(CH_2)_3OH$	825.9	876.2	−60	95CHE/STO
$[C_3H_8O_3]$	56-81-5	$HOCH_2CH(OH)CH_2OH$	820	874.8	−75	80MAU/HAM
$[C_3H_8Pb]$	82065-01-8	$(CH_3)_2Pb$=CH_2	911.5	938.0	20	$(CH_3)_2C$=CH_2
$[C_3H_8S]$	75-33-2	i-C_3H_7-SH	772.3	803.6	4	CH_3SH
$[C_3H_8S]$	107-03-9	n-C_3H_7-SH	763.6	794.9	4	CH_3SH
$[C_3H_8S]$	624-89-5	$CH_3SC_2H_5$	815.3	846.5	4	unsym sulfides
$[C_3H_8Si]$	4112-23-6	$(CH_3)_2Si$=CH_2	921.0	947.5	20	$(CH_3)_2C$=CH_2

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_3H_8Sn]$	82065-00-7	$(CH_3)_2Sn{=}CH_2$	867.1	893.6	20	$(CH_3)_2C{=}CH_2$
$[C_3H_9As]$	593-88-4	$(CH_3)_3As$	864.9	897.3	0	Rln(3/3)
$[C_3H_9B_3O]$	121-43-7	$B(OCH_3)_3$	**783.4**	815.8	0	Rln(1/1)
$[C_3H_9N]$	75-50-3	$(CH_3)_3N$	918.1	948.9	5.6	97EAS/SMI
$[C_3H_9N]$	107-10-8	$n\text{-}C_3H_7NH_2$	883.9	917.8	−5	CH_3NH_2
$[C_3H_9N]$	624-78-2	$(CH_3)(C_2H_5)NH$	909.2	942.2	−2	$(CH_3)_2NH$
$[C_3H_9N]$	75-31-0	$i\text{-}C_3H_7NH_2$	889.0	923.8	−8	CH_3NH_2
$[C_3H_9NO]$	156-87-6	$NH_2(CH_2)_3OH$	917.3	962.5	−43	80MAU/HAM
$[C_3H_9NO]$	109-85-3	$CH_3OCH_2CH_2NH_2$	894.6	928.6	−5.1	CH_3NH_2
$[C_3H_9NO]$	1184-78-7	$(CH_3)_3NO$	953.5	983.2	9.1	Rln(3/1)
$[C_3H_9OP]$	676-96-0	$OP(CH_3)_3$	880.0	909.7	9.1	Rln(3/1)
$[C_3H_9O_3P]$	121-45-9	$P(OCH_3)_3$	899.9	929.7	9.1	Rln(3/1)
$[C_3H_9O_3PS]$	152-18-1	$SP(OCH_3)_3$	853.9	883.6	9.1	Rln(3/1)
$[C_3H_9O_4P]$	512-56-1	$OP(OCH_3)_3$	860.8	890.6	9.1	Rln(3/1)
$[C_3H_9P]$	594-09-2	$(CH_3)_3P$	926.3	958.8	0	Rln(3/3)
$[C_3H_{10}N_2]$	109-76-2	1,3-Diaminopropane	940.0	987.0	−49	80MAU/HAM
$[C_3H_{10}OSi]$	1066-40-6	Silanol, trimethyl	**781.5**	814.0	0	Rln(1/1)
$[C_3O]$	11127-17-6	CCCO	847.7	880.2	0	Rln(1/1)
$[C_3S]$	109545-35-9	C_3S	900.5	933	0	Rln(1/1)
$[C_4F_7N]$	375-00-8	C_3F_7CN	662.6	693.2	6	nitriles
$[C_4HF_9O]$	2378-02-1	$(CF_3)_3COH$	646.7	676.8	8	CH_3OH
$[C_4H_2]$	460-12-8	HCC-CCH	712.8	737.2	27	AUE
$[C_4H_2F_9N]$	2809-92-9	$(CF_3)_3CNH_2$	752.9	783.7	5.6	$(CH_3)_3N$
$[C_4H_3NO]$	145355-49-3	CH_3NCCCO	887.5	920	0	?
$[C_4H_3NO]$	57681-10-4	$NCC(CH_3)CO$	765.5	798	0	Rln(1/1)
$[C_4H_4F_4O_2]$	1683-88-1	$CF_3COOCH_2CH_2F$	704.7	735.7	5	acids
$[C_4H_4F_6O]$	333-36-8	$(CF_3CH_2)_2O$	674.9	702.3	17	sym ethers
$[C_4H_4F_6O]$	1515-14-6	$(CF_3)_2C(CH_3)OH$	660.9	691.2	7	CH_3OH
$[C_4H_4N_2]$	290-37-9	Pyrazine	847.0	877.1	7.8	pyridines+Rln(4/2)
$[C_4H_4N_2]$	289-80-5	Pyridazine	877.1	907.2	7.8	pyridines+Rln(2/1)
$[C_4H_4N_2]$	289-95-2	Pyrimidine	855.7	885.8	7.8	pyridines+Rln(2/1)
$[C_4H_4N_2O]$	557-01-7	2(1H)-Pyrimidinone	**841.7**	872.7	5	amides
$[C_4H_4N_2O_2]$	66-22-8	Uracil	**841.7**	872.7	5	amides
$[C_4H_4N_2S_2]$	2001-93-6	Dithiouracil	**880.5**	911.4	5	amides
$[C_4H_4N_4O_4]$	32683-48-0	1-methyl-3,5-dinitropyrazole	757.0	788.8	2	pyridines
$[C_4H_4O]$	110-00-9	Furan	770.9	803.4	0	Rln(1/1),
$[C_4H_4S]$	110-02-1	Thiophene	784.3	815.0	5.8	Rln(2/1)
$[C_4H_5Cl_3O_2]$	515-84-4	$CCl_3COOC_2H_5$	759.4	790.4	5	esters
$[C_4H_5F_3O_2]$	383-63-1	$CF_3CO_2C_2H_5$	727.9	758.8	5	esters
$[C_4H_5F_9N]$	407-01-2	$(CF_3CH_2)_2NH$	805.1	838.1	−2	$(CH_3)_2NH$
$[C_4H_5N]$	5500-21-0	$c\text{-}C_3H_5CN$	777.5	808.2	6	nitriles
$[C_4H_5N]$	109-97-7	pyrrole	843.8	875.4	2.8	97EAS/SMI
$[C_4H_5NO_2]$	623-49-4	$NCCOOC_2H_5$	714.7	745.7	5	acids
$[C_4H_5NS]$	3581-87-1	2-Methylthiazole	898.7	930.6	?	pyridines
$[C_4H_5N_3O]$	71-30-7	Cytosine	918	949.9	2	pyridines
$[C_4H_5N_3O_2]$	54210-33-2	1-methyl-5-nitropyrazole	818.4	850.3	2	pyridines
$[C_4H_5N_3O_2]$	54210-32-1	1-methyl-3-nitropyrazole	815.7	847.6	2	pyridines
$[C_4H_5N_3O_2]$	3034-42-2	1-Methyl-5-nitroimidazole	863.5	895.3	2	pyridines
$[C_4H_6]$	590-19-2	$CH_2{=}C{=}CHCH_3$	**749.8**	778.9	11	AUE
$[C_4H_6]$	822-35-5	Cyclobutene	753.6	784.4	5.8	Rln(2/1)
$[C_4H_6]$	3100-04-7	1-Methylcyclopropene	826.9	856.0	11	?
$[C_4H_6]$	503-17-3	$CH_3\text{-}CC\text{-}CH_3$	745.1	775.8	5.8	Rln(2/1)
$[C_4H_6]$	106-99-0	$CH_2{=}CHCH{=}CH_2$	757.6	783.4	22	propene+Rln(2/1)
$[C_4H_6F_3NO]$	1547-87-1	$CF_3CON(CH_3)_2$	818.0	849.0	5	amides
$[C_4H_6N_2]$	7554-65-6	4-methylpyrazole	873.4	906.8	−3	pyridines+Rln(1/2)
$[C_4H_6N_2]$	822-36-6	4-Methylimidazole	920.9	952.8	2	pyridines
$[C_4H_6N_2]$	693-98-1	2-Methylimidazole	929.6	963.4	−4	pyridines+Rln(1/2)
$[C_4H_6N_2]$	616-47-7	1-methylimidazole	927.7	959.6	2	pyridines
$[C_4H_6N_2]$	930-36-9	1-methylpyrazole	880.1	912.0	2	pyridines
$[C_4H_6N_2]$	1453-58-3	3(5)-methylpyrazole	874.2	906.0	2	pyridines
$[C_4H_6N_2O]$	16703-51-8	$(CH_3)_2NCOCN$	797.1	829.0	2	unsym ketones
$[C_4H_6O]$	78-85-3	$CH_2{=}C(CH_3)CHO$	776.8	808.7	2	CH_3CHO
$[C_4H_6O]$	4170-30-3	$CH_3CH{=}CHCHO$	799.0	830.8	2	CH_3CHO

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_4H_8O]	1708-29-8	2,5-Dihydrofuran	796	823.4	17	sym ethers
[C_4H_6O]	78-94-4	CH_2=CHCOCH$_3$	802.8	834.7	2	unsym ketones
[C_4H_6O]	1191-95-3	cyclobutanone	772.7	802.5	9	sym ketones
[C_4H_8O]	1191-99-7	2,3-Dihydrofuran	834.4	866.9	0	Rln(1/1)
[$C_4H_6O_2$]	79-41-4	$CH_3C(=CH_2)COOH$	785.7	816.7	5	acids
[$C_4H_6O_2$]	431-03-8	$CH_3COCOCH_3$	770.1	801.9	2	unsym ketones
[$C_4H_6O_2$]	96-48-0	γ-Butyrolactone	808.1	840.0	2	unsym ketones
[$C_4H_6O_2$]	108-05-4	$CH_3COOCH=CH_2$	782.9	813.9	5	esters
[$C_4H_6O_2$]	96-33-3	CH_2=CHCOOCH$_3$	794.8	825.8	5	esters
[$C_4H_6O_2$]	543-75-9	Dihydro-1,4-dioxin	792.8	823.5	5.8	Rln(2/1)
[$C_4H_6O_2$]	1759-53-1	Cyclopropane carboxylic acid	**790.4**	821.4	5	acids
[$C_4H_6O_2$]	107-93-7	(E)-CH_3CH=CHCOOH	793	824.0	5	acids
[C_4H_7]	15157-95-6	CH_2=C(CH_3)CH_2•	747.3	778	6	S(i-C_4H_8)+spin-S(C_4H_7•)
[C_4H_7]	#1452	CH_3CH=$CHCH_2$•	**754.4**	785.1	6	S(2-C_4H_8)+spin-S(C_4H_7•)
[$C_4H_7F_2NO$]	667-50-5	$CF_2HCON(CH_3)_2$	833.1	864.1	5	amides
[$C_4H_7F_3O$]	461-24-5	$C_2H_5OCH_2CF_3$	735.0	762.4	17	$(CH_3)_2O$
[$C_4H_7F_3S$]	5187-62-2	$CF_3CH_2SC_2H_5$	766.4	797.6	4	unsym sulfides
[C_4H_7N]	109-74-0	n-C_3H_7CN	767.7	798.4	6	nitriles
[C_4H_7N]	78-82-0	i-C_3H_7CN	772.8	803.6	5.7	S(i-PrCCH)-S(i-PrCN)
[C_4H_7N]	627-36-1	i-C_3H_7NC	**824.3**	856.8	0	HNC
[C_4H_7NO]	79-39-0	2-propenamide, 2-methyl-	849.4	880.4	5	amides
[C_4H_7NO]	23350-58-5	2-butenamide	856.1	887.1	5	amides
[C_4H_7NO]	2679-13-2	N-methyl-2-azetidinone	851.3	882.2	5	amides
[$C_4H_7NO_4$]	56-84-8	L-aspartic acid	875	908.9	−5	CH_3NH_2
[$C_4H_7N_3$]	1192-21-8	1-methyl-5-aminopyrazole	917.6	949.5	2	pyridines
[$C_4H_7N_3$]	1904-31-0	1-methyl-3-aminopyrazole	905.5	937.4	2	pyridines
[$C_4H_7N_3$]	39687-97-3	N′-cyano-N,N-dimethyl formamidine	857.3	889.7	0	Rln(1/1)
[$C_4H_7O_2$]	4598-47-4	1,4-Dioxyl radical	770.7	803.2	0	Rln(1/1)
[$C_4H_7O_3P$]	61580-09-4	4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.1]heptane	791.5	823.9	0	?
[$C_4H_7O_3P$]	280-45-5	2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane	836.4	868.8	0	Rln(3/3)
[C_4H_8]	624-64-6	E-CH_3CH=$CHCH_3$	719.9	747	18	propene+Rln(2/1)
[C_4H_8]	115-11-7	$(CH_3)_2C$=CH_2	775.6	802.1	20	97EAS/SMI
[$C_4H_8Cl_3N$]	36726-94-0	$CCl_3CH_2N(CH_3)_2$	882.0	912.8	5.6	$(CH_3)_3N$
[$C_4H_8F_3N$]	819-46-5	$CF_3(CH_2)_3NH_2$	869.6	903.5	−5	CH_3NH_2
[$C_4H_8F_3N$]	819-06-7	$CF_3CH_2N(CH_3)_2$	871.9	902.7	5.6	$(CH_3)_3N$
[$C_4H_8N_2$]	926-64-7	$NCCH_2N(CH_3)_2$	853.7	884.5	5.6	$(CH_3)_3N$
[$C_4H_8N_2$]	1606-49-1	1,4,5,6-tetrahydropyrimdine	967.8	1002.0	−5.8	Rln(1/2)
[$C_4H_8N_2O_3$]	70-47-3	L-Asparagine	891.5	929	−17	80MAU/HAM
[$C_4H_8N_2O_3$]	556-50-3	diglycine	882	NE	NE	not estimated
[C_4H_8O]	109-92-2	$C_2H_5OCH=CH_2$	840.4	870.1	9.5	91MAU/SIE
[C_4H_8O]	109-99-9	Tetrahydrofuran	794.7	822.1	17	sym ethers
[C_4H_8O]	78-84-2	i-C_3H_7CHO	765.5	797.3	2	CH_3CHO
[C_4H_8O]	78-93-3	$CH_3COC_2H_5$	795.5	827.3	2	unsym ketones
[C_4H_8O]	116-11-0	CH_2=C(CH_3)OCH_3	866.1	894.9	12	propene
[C_4H_8O]	123-72-8	n-C_3H_7CHO	760.8	792.7	2	CH_3CHO
[C_4H_8OS]	926-67-0	$CH_3C(S)OC_2H_5$	831.8	863.6	2	unsym ketones
[$C_4H_8O_2$]	625-55-8	$HCOOCH(CH_3)_2$	780.3	811.3	5	esters
[$C_4H_8O_2$]	123-91-1	1,4-Dioxane	770.0	797.4	17	sym ethers
[$C_4H_8O_2$]	505-22-6	1,3-Dioxane	796.2	825.4	11	unsym ethers
[$C_4H_8O_2$]	141-78-6	$CH_3CO_2C_2H_5$	804.7	835.7	5	esters
[$C_4H_8O_2$]	110-74-7	HCO_2(n-C_3H_7)	773.9	804.9	5	esters
[$C_4H_8O_2$]	554-12-1	$C_2H_5COOCH_3$	799.2	830.2	5	esters
[$C_4H_8O_2$]	922-69-0	CH_2=C(OCH_3)$_2$	928.1	957.0	12	propene
[$C_4H_8O_2S$]	38103-96-7	$C_2H_5S(OCH_3)CO$	802.9	833.9	5	esters
[$C_4H_8O_3$]	623-53-0	$C_2H_5OCOOCH_3$	810.8	842.7	2	unsym ketones
[C_4H_8S]	110-01-0	c-C_4H_8S	819.3	849.1	9	sym sulfides
[C_4H_8S]	7594-44-7	CH_2=C(CH_3)-SCH_3	859.7	888.6	12	propene
[$C_4H_8S_2$]	51102-74-0	CH_2=C(SCH_3)$_2$	902.2	931.1	12	propene
[C_4H_8Se]	114659-08-4	CH_2=C(CH_3)-$SeCH_3$	850.5	879.4	12	propene
[$C_4H_8Se_2$]	99030-02-1	CH_2=C($SeCH_3$)$_2$	**892.6**	921.5	12	propene
[C_4H_9N]	1190-79-0	CH_3CH=NC_2H_5	909.4	941.9	0	Rln(1/1)
[C_4H_9N]	123-75-1	Pyrrolidine	915.3	948.3	−2	$(CH_3)_2NH$
[C_4H_9N]	5763-87-1	$(CH_3)_2NCH=CH_2$	**924.4**	956.8	0	Rln(1/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_4H_9N]$	2878-14-0	$CH_2=C(CH_3)CH_2NH_2$	883.5	917.5	−5	$CH_3CH_2NH_2$
$[C_4H_9N]$	4923-79-9	Azetidine, N-methyl-	851.7	882.5	5.6	$(CH_3)_3N$
$[C_4H_9NO]$	110-91-8	Morpholine	891.2	924.3	−2	$(CH_3)_2NH$
$[C_4H_9NO]$	1187-58-2	$C_2H_5CONHCH_3$	889.4	920.4	5	amides
$[C_4H_9NO]$	563-83-7	$i\text{-}C_3H_7CONH_2$	846.7	878.6	2	amides
$[C_4H_9NO]$	625-50-3	Acetamide, N-ethyl-	867.0	898.0	5	amides
$[C_4H_9NO]$	127-19-5	Dimethylacetamide	877.0	908.0	5	amides
$[C_4H_9NO]$	6281-94-3	$n\text{-}C_3H_7NHCHO$	847.4	878.4	5	amides
$[C_4H_9NOS]$	16703-45-0	$CH_3OC(S)N(CH_3)_2$	869.0	900.0	5	amides
$[C_4H_9NO_2]$	105-40-8	$CH_3NHCOOC_2H_5$	857.8	888.8	5	esters
$[C_4H_9NO_2]$	7541-16-4	$(CH_3)_2NCOOCH_3$	847.3	878.3	5	esters
$[C_4H_9NO_2]$	540-80-7	$t\text{-}C_4H_9ONO$	**831.4**	863.9	0	CH_3ONO
$[C_4H_9NO_3]$	72-19-5	L-threonine	888.5	922.5	−5	CH_3NH_2
$[C_4H_9NS]$	631-67-4	$CH_3C(S)N(CH_3)_2$	894.4	925.3	5	amides
$[C_4H_9O_3P]$	31121-06-9	2-Methoxy-1,3,2-dioxa-phosphorinane	892.8	925.3	0	Rln(1/1)
$[C_4H_{10}]$	75-28-5	$iso\text{-}C_4H_{10}$	671.3	677.8	87	76HIR/KEB
$[C_4H_{10}N_2]$	110-85-0	Piperazine	914.7	943.7	11.5	Rln(4/1)
$[C_4H_{10}N_2]$	1609-01-4	$(CH_3)_2N\ CH{-}N\ CH_3$	970.0	1002.5	0	Rln(1/1)
$[C_4H_{10}N_2]$	4901-75-1	$c\text{-}C(CH_3)(C_2H_5)NHNH$	871.3	903.8	0	Rln(1/1)
$[C_4H_{10}N_2]$	110-70-3	$CH_3NHCH_2CH_2NHCH_3$	946.9	989.2	−33	80MAU/HAM
$[C_4H_{10}N_2O]$	139033-03-7	$(CH_3)_2N\text{-}CH{=}N\text{-}OCH_3$	915.8	948.3	0	Rln(1/1)
$[C_4H_{10}O]$	78-92-2	$CH_3CH_2CH(OH)CH_3$	784.6	815	7	CH_3OH
$[C_4H_{10}O]$	71-36-3	$n\text{-}C_4H_9OH$	758.9	789.2	7	CH_3OH
$[C_4H_{10}O]$	78-83-1	$i\text{-}C_4H_9OH$	762.2	793.7	3	$S(i\text{-}C_4H_9NH_2)$-S(i-
$[C_4H_{10}O]$	75-65-0	$t\text{-}C_4H_9OH$	772.2	802.6	7	CH_3OH
$[C_4H_{10}O]$	598-53-8	$(CH_3)_2CHOCH_3$	797.1	826.3	11	unsym ethers
$[C_4H_{10}O]$	557-17-5	$n\text{-}C_3H_7OCH_3$	785.7	814.9	11	unsym ethers
$[C_4H_{10}O]$	60-29-7	$(C_2H_5)_2O$	801	828.4	17	sym ethers
$[C_4H_{10}O_2]$	110-71-4	$CH_3OCH_2CH_2OCH_3$	820.2	858.0	−18	84SHA/BLA; 83MAU
$[C_4H_{10}O_2]$	110-63-4	$HO(CH_2)_4OH$	854.9	915.6	−95	80MAU/HAM
$[C_4H_{10}O_3]$	3068-00-6	$HOCH_2CH(OH)CH_2CH_2OH$	841	905.9	−109	86SUN/KUL
$[C_4H_{10}S]$	513-53-1	$CH_3CH_2CH(SH)CH_3$	781.7	813	4	unsym sulfides
$[C_4H_{10}S]$	109-79-5	$n\text{-}C_4H_9SH$	770.5	801.7	4	CH_3SH
$[C_4H_{10}S]$	352-93-2	$(C_2H_5)_2S$	827.0	856.7	9	sym sulfides
$[C_4H_{10}S]$	75-66-1	$t\text{-}C_4H_9SH$	785.1	816.4	4	CH_3SH
$[C_4H_{10}S]$	513-44-0	$i\text{-}C_4H_9SH$	771.4	802.6	4	CH_3SH
$[C_4H_{11}N]$	4747-21-1	$CH_3NH(i\text{-}C_3H_7)$	919.4	952.4	−2	$(CH_3)_2NH$
$[C_4H_{11}N]$	109-73-9	$n\text{-}C_4H_9NH_2$	886.6	921.5	−8	$S(C_5H_{12})$-S(n-$BuNH_2$)+Rln2
$[C_4H_{11}N]$	75-64-9	$t\text{-}C_4H_9NH_2$	899.9	934.1	−6	CH_3NH_2
$[C_4H_{11}N]$	13952-84-6	$sec\text{-}C_4H_9NH_2$	895.7	929.7	−5	CH_3NH_2
$[C_4H_{11}N]$	598-56-1	$(CH_3)_2(C_2H_5)N$	929.1	960.1	5.6	$(CH_3)_3N$
$[C_4H_{11}N]$	78-81-9	$i\text{-}C_4H_9NH_2$	890.8	924.8	−5	CH_3NH_2
$[C_4H_{11}N]$	109-89-7	$(C_2H_5)_2NH$	919.4	952.4	−1.9	$(CH_3)_2NH$
$[C_4H_{11}NO]$	13325-10-5	$NH_2(CH_2)_4OH$	932.1	984.5	−67	80MAU/HAM
$[C_4H_{11}NO]$	3710-84-7	$(C_2H_5)_2NOH$	882.2	914.7	0	Rln(1/1)
$[C_4H_{11}NO_2]$	111-42-2	$(HOCH_2CH_2)_2NH$	920	953	−2	$(CH_3)_2NH$
$[C_4H_{12}NOP]$	50663-05-3	$OP(N(CH_3)_2)(CH_3)_2$	903.0	935.5	0	Rln(1/1)
$[C_4H_{12}N_2]$	6415-12-9	$(CH_3)_2NN(CH_3)_2$	917.9	948.7	5.8	Rln(2/1)
$[C_4H_{12}N_2]$	110-60-1	1,4-butanediamine	954.3	1005.6	−63	93CHE/WU; 80MAU/HAM
$[C_4H_{12}OSi]$	1825-61-2	$(CH_3)_3SiOCH_3$	**814.6**	847.0	0	Rln(1/1)
$[C_4H_{12}Sn]$	594-27-4	$(CH_3)_4Sn$	**797.4**	823.7	20.6	Rln(12/1)
$[C_4H_{13}N_2OP]$	3732-86-3	$OP(NH_2)(N(CH_3)_2)_2$	915.0	947.5	0	Rln(1/1)
$[C_4H_{12}OSi_2]$	3277-26-7	$((CH_3)_2SiH)_2O$	**814.6**	845.3	5.8	Rln(2/1)
$[C_4NiO_4]$	13463-39-3	$(CO)_4Ni$	716.0	742.3	20.6	Rln(12/1)
$[C_5F_5N]$	700-16-3	Pentafluoropyridine	733.0	764.9	2	pyridines
$[C_5FeO_5]$	13463-40-6	$(CO)_5Fe$	798.5	833.0	−7	91ALL/CRA
$[C_5HMnO_5]$	16972-33-1	$(CO)_5MnH$	803.0	835.5	0	?
$[C_5H_3ClN_4]$	87-42-3	6-Chloropurine	**841.7**	873.6	2	pyridines
$[C_5H_4BrN]$	626-55-1	3-Br-pyridine	878.2	910.0	2	pyridines
$[C_5H_4BrN]$	109-04-6	2-Br-pyridine	873.0	904.8	2	pyridines
$[C_5H_4BrN]$	1120-87-2	4-Br-pyridine	886.0	917.8	2	pyridines
$[C_5H_4ClN]$	109-09-1	2-Cl-pyridine	869	900.9	2	pyridines
$[C_5H_4ClN]$	626-61-9	4-Cl-pyridine	884.2	916.1	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_5H_4ClN]	626-60-8	3-Cl-pyridine	871.5	903.4	2	pyridines
[C_5H_4ClNO]	1851-22-5	3-chloro-pyridine-1-oxide	869.7	902.2	0	Rln(1/1)
[C_5H_4FN]	372-47-4	3-F-pyridine	870.1	902.0	2	pyridines
[C_5H_4FN]	372-48-5	2-F-pyridine	852.7	884.6	2	pyridines
[C_5H_4FN]	694-52-0	4-F-pyridine	881.2	913.1	2	pyridines
[C_5H_4FNO]	695-37-4	3-fluoro-pyridine-1-oxide	867.6	900.1	0	Rln(1/1)
[$C_5H_4N_2O_3$]	1124-33-0	4-(NO_2)-pyridine-1-oxide	837.3	868.0	5.8	Rln(2/1)
[$C_5H_4N_4$]	120-73-0	Purine	888.2	920.1	2	pyridines
[$C_5H_4N_4O$]	68-94-0	Hypoxanthine	**880.5**	912.3	2	pyridines
[$C_5H_4N_2O_2$]	1122-61-8	4-(NO_2)-pyridine	842.5	874.3	2	pyridines
[C_5H_5]	2143-53-5	c-C_5H_5 radical	**799.1**	831.5	0	Rln(2/2)
[C_5H_5As]	289-31-6	Arsabenzene	752.4	784.8	0	Rln(2/2)
[C_5H_5N]	110-86-1	pyridine	898.1	930	2	pyridines
[C_5H_5NNiO]	12071-73-7	(C_5H_5)NiNO	798.6	827.0	13.4	Rln(5/1)
[C_5H_5NO]	694-59-7	pyridine-1-oxide	892.9	923.6	5.8	Rln(2/1)
[C_5H_5NO]	109-00-2	3-(OH)-pyridine	897.7	929.5	2	pyridines
[$C_5H_5N_5$]	73-24-5	Adenine	912.5	942.8	7	79MAU
[$C_5H_5N_5O$]	73-40-5	Guanine	927.6	959.5	2	pyridines
[C_5H_5P]	289-68-9	Phosphabenzene	785.3	817.7	0	Rln(2/2)
[C_5H_6]	542-92-7	1,3-c-C_5H_6	798.4	821.6	31	AUE
[$C_5H_6N_2$]	504-29-0	2-Pyridinamine	915.3	947.2	2	pyridines
[$C_5H_6N_2$]	462-08-8	3-Pyridinamine	922.6	954.4	2	pyridines
[$C_5H_6N_2$]	504-24-5	4-Pyridinamine	947.8	979.7	2	pyridines
[$C_5H_6N_2O_2$]	65-71-4	Thymine	850.0	880.9	5	amides
[C_5H_6O]	534-22-5	2-methylfuran	833.5	865.9	0	Rln(1/1)
[C_5H_6O]	930-27-8	3-methylfuran	821.5	854.0	0	Rln(1/1)
[C_5H_6S]	554-14-3	2-Methylthiophene	826.5	859.0	0	Rln(1/1)
[$C_5H_7F_3O_2$]	352-23-8	$CF_3CH_2COOC_2H_5$	766.3	797.3	5	esters
[$C_5H_7F_3O_2$]	383-66-4	CF_3CO_2(n-C_3H_7)	732.9	763.9	5	esters
[C_5H_7O]	#1169	•$CH_2CH_2CH_2CH$=CO	**806.2**	838.6	0	?
[C_5H_8]	598-23-2	(CH_3)$_2$CHCCH	787.8	814.9	18	AUE
[C_5H_8]	627-21-4	$C_2H_5CCCH_3$	778.0	810.2	1	2-butyne
[C_5H_8]	693-86-7	c-C_3H_5CH=CH_2	787.5	816.3	12	propene
[C_5H_8]	3907-06-0	3,3-Dimethylcyclopropene	817.1	847.8	5.8	?
[C_5H_8]	2004-70-8	(E)CH_3CH=$CHCH$=CH_2	804.4	834.1	9.1	AUE
[C_5H_8]	1489-60-7	1-Methylcyclobutene	807.3	841.5	−5.8	Rln(1/2)
[C_5H_8]	142-29-0	c-C_5H_8	733.8	766.3	0	Rln(2/2)
[C_5H_8]	78-79-5	CH_2=$CHC(CH_3)$=CH_2	797.6	826.4	12	propene
[$C_5H_8N_2$]	694-31-5	1,5-Dimethylpyrazole	902.8	934.3	3	pyrazole(pyrrole)
[$C_5H_8N_2$]	35520-41-3	trans-dimethylamino acrylonitrile	864.3	896.8	0	Rln(1/1)
[$C_5H_8N_2$]	6338-45-0	1,4-Dimethylimidazole	944.9	976.7	2	pyridines
[$C_5H_8N_2$]	1739-84-0	1,2-Dimethylimidazole	952.6	984.7	2	pyridines
[$C_5H_8N_2$]	694-48-4	1,3-Dimethylpyrazole	902.3	933.9	3	pyrazole(pyrrole)
[$C_5H_8N_2$]	10447-93-5	1,5-Dimethylimidazole	945.8	977.6	2	pyridines
[$C_5H_8N_2$]	1072-68-0	1,4-Dimethylpyrazole	896.8	928.4	3	pyrazole
[$C_5H_8N_2$]	67-51-6	3,5-dimethylpyrazole	900.1	933.5	−3	pyrazole-Rln2
[$C_5H_8N_2$]	2820-37-3	3(5),4-dimethylpyrazole	895.4	927.3	2	pyridines
[C_5H_8O]	107-86-8	3-methyl-2-butenal	825.0	856.9	2	unsym ketones
[C_5H_8O]	814-78-8	CH_3C(=O)C(=CH_2)CH_3	811.3	843.1	2	unsym ketones
[C_5H_8O]	765-43-5	c-$C_3H_5COCH_3$	823	854.9	2	unsym ketones
[C_5H_8O]	110-87-2	2H-Pyran, 3, 4-dihydro-	833.4	865.8	0	Rln(1/1)
[C_5H_8O]	120-92-3	Cyclopentanone	794.0	823.7	9	sym ketones
[C_5H_8O]	625-33-2	CH_3CH=CHC(=O)CH_3	832.5	864.3	2	unsym ketones
[C_5H_8O]	6038-09-1	2-methyl-2-butenal(Z)	812.1	843.9	2	unsym ketones
[C_5H_8O]	34314-83-5	4-Methyl-2,3-dihydrofuran	836.2	868.6	0	?
[C_5H_8O]	1576-87-0	2-pentenal(E)	807.2	839.0	2	aldehydes
[C_5H_8O]	1487-15-6	5-Methyl-2,3-dihydrofuran	877.9	910.3	0	Rln(1/1)
[$C_5H_8O_2$]	565-63-9	(Z)CH_3CH=$C(CH_3)COOH$	791.5	822.5	5	acids
[$C_5H_8O_2$]	623-43-8	CH_3CH=$CHCOOCH_3$	820.4	851.3	5	esters
[$C_5H_8O_2$]	123-54-6	$CH_3COCH_2COCH_3$	836.8	873.5	−14	83MAU
[$C_5H_8O_2$]	13991-37-2	(E)CH_3CH_2CH=$CHCOOH$	792.6	823.6	5	acids
[$C_5H_8O_2$]	3721-95-7	Cyclobutane carboxylic acid	**786.4**	817.4	5	acids
[$C_5H_8O_2$]	80-62-6	CH_2=$C(CH_3)COOCH_3$	800.5	831.4	5	esters
[$C_5H_8O_2$]	2868-37-3	c-$C_3H_5COOCH_3$	811.2	842.1	5	esters

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_5H_8O_2]$	541-47-9	$(CH_3)_2C{=}CHCOOH$	791.9	822.9	5	acids
$[C_5H_9F_3N]$	134166-59-9	$(CH_3)_2N\text{-}CH{=}N\text{-}CH_2CF_3$	933.8	966.2	0	Rln(1/1)
$[C_5H_9N]$	110-59-8	$n\text{-}C_4H_9CN$	771.7	802.4	6	nitriles
$[C_5H_9N]$	7223-38-3	$HCCCH_2N(CH_3)_2$	909.5	940.3	5.6	$(CH_3)_3N$
$[C_5H_9N]$	630-18-2	$t\text{-}C_4H_9CN$	780.2	810.9	6	nitriles
$[C_5H_9N]$	7188-38-7	$t\text{-}C_4H_9NC$	838.3	870.7	0.1	HNC
$[C_5H_9NO]$	5264-35-7	$c\text{-}C_4H_6N(2\text{-}OCH_3)$	925.5	957.9	0	Rln(1/1)
$[C_5H_9NO]$	872-50-4	1-Methyl-2-pyrrolidinone	891.6	923.5	2	unsym ketones
$[C_5H_9NO]$	2141-62-0	$C_2H_5CH(OC_2H_5)CH_2CN$	776.5	807.2	6	nitriles
$[C_5H_9NO]$	2680-03-7	2-propenamide, N,N-dimethyl	873.4	904.3	5	amides
$[C_5H_9NO_2]$	147-85-3	L-proline	886.0	920.5	−7	93LI/HAR
$[C_5H_9NO_3]$	1117-77-7	$CH_3CONHCH_2COOCH_3$	861	892.0	5	amides
$[C_5H_9NO_4]$	56-86-0	L-GlutamicAcid	879.1	913.0	−5	CH_3NH_2
$[C_5H_9N_3]$	134166-58-8	$(CH_3)_2N\text{-}CH{=}N\text{-}CH_2CN$	915.5	948.0	0	Rln(1/1)
$[C_5H_9N_3]$	51-45-6	Histamine	961.9	999.8	−18	histidine
$[C_5H_9O_3P]$	1449-91-8	4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane	**850.3**	882.8	0	Rln(3/3)
$[C_5H_{10}]$	513-35-9	$(CH_3)_2C{=}CHCH_3$	779.9	808.8	12	propene
$[C_5H_{10}N_2]$	2305-59-1	4,4-dimethyl-2-imidazoline	955.7	988.1	0	Rln(1/1)
$[C_5H_{10}N_2O]$	80-73-9	1,3-Dimethyl-2-imidazolidinone	886.0	918.4	0	?
$[C_5H_{10}N_2O_3]$	56-85-9	L-Glutamine	900	937.8	−18	Asparigine
$[C_5H_{10}N_2O_4]$	7361-43-5	ser-gly	**886.4**	NE	NE	not estimated
$[C_5H_{10}N_2O_4]$	687-63-8	gly-ser	**880.9**	NE	NE	not estimated
$[C_5H_{10}O]$	96-47-9	$c\text{-}C_4H_7O(2\text{-}CH_3)$	811.6	840.8	11	unsym ethers
$[C_5H_{10}O]$	96-22-0	$(C_2H_5)_2CO$	807	836.8	9	sym ketones
$[C_5H_{10}O]$	142-68-7	$c\text{-}C_5H_{10}O$	795.4	822.8	17	sym ethers
$[C_5H_{10}O]$	107-87-9	$n\text{-}C_3H_7COCH_3$	800.9	832.7	2	unsym ketone
$[C_5H_{10}O]$	110-62-3	$n\text{-}C_4H_9CHO$	764.8	796.6	2	CH_3CHO
$[C_5H_{10}O]$	4696-26-8	$trans\text{-}CH_3CH{=}CH\text{-}OC_2H_5$	848.0	876.9	12	propene
$[C_5H_{10}O]$	563-80-4	$(i\text{-}C_3H_7)COCH_3$	804.4	836.3	2	unsym ketones
$[C_5H_{10}O]$	928-55-2	$C_2H_5OCH{=}CHCH_3$	847.7	876.6	12	propene
$[C_5H_{10}O]$	557-31-3	$C_2H_5OCH_2CH{=}CH_2$	804.5	833.7	11	unsym ethers
$[C_5H_{10}O_2]$	5057-98-7	cis-1,2-cyclopentanediol	853.1	885.6	0	Rln(1/1)
$[C_5H_{10}O_2]$	623-42-7	$C_3H_7COOCH_3$	805.4	836.4	5	esters
$[C_5H_{10}O_2]$	592-84-7	$HCO_2(n\text{-}C_4H_9)$	775	806.0	5	esters
$[C_5H_{10}O_2]$	108-21-4	isopropyl acetate	805.6	836.6	5	esters
$[C_5H_{10}O_2]$	547-63-7	$i\text{-}C_3H_7COOCH_3$	805.7	836.6	5	esters
$[C_5H_{10}O_2]$	109-60-4	$CH_3COOC_3H_7$	805.6	836.6	5	esters
$[C_5H_{10}S]$	1613-51-0	Tetrahydrothiopyran	826.0	855.8	9	sym sulfides
$[C_5H_{11}N]$	6163-56-0	$CH_3CH{=}CHN(CH_3)_2$	**934.5**	967.0	0	Rln(1/1)
$[C_5H_{11}N]$	1743-55-1	$(CH_3)_2C{=}NC_2H_5$	943.5	976.0	0	Rln(1/1)
$[C_5H_{11}N]$	2155-94-4	$CH_2{=}CHCH_2N(CH_3)_2$	926.8	957.8	5.6	$(CH_3)_3N$
$[C_5H_{11}N]$	120-94-5	N-Methylpyrrolidine	934.8	965.6	5.6	$(CH_3)_3N$
$[C_5H_{11}N]$	110-89-4	Piperidine	921	954.0	−1.9	$(CH_3)_2NH$
$[C_5H_{11}NO]$	754-10-9	$t\text{-}C_4H_9CONH_2$	857.2	889.0	2	amides
$[C_5H_{11}NOS]$	#638	$C_2H_5OC(S)N(CH_3)_2$	880.0	911.0	5	amides
$[C_5H_{11}NO_2]$	72-18-4	L-valine	876.7	910.6	−5	CH_3NH_2
$[C_5H_{11}NO_2]$	687-48-9	$(CH_3)_2NCOOC_2H_5$	865.6	896.6	5	esters
$[C_5H_{11}NO_2S]$	63-68-3	L-Methionine	901.5	935.4	−5	CH_3NH_2
$[C_5H_{12}N_2]$	28504-67-8	$(CH_3)_2N\text{-}C(CH_3){=}NCH_3$	990.8	1023.2	0	Rln(1/1)
$[C_5H_{12}N_2]$	38704-89-1	Pyrazolidine, 1,2-dimethyl	928.6	959.3	5.8	Rln(2/1)
$[C_5H_{12}N_2]$	74119-36-1	$(CH_3)_2N\text{-}CH{=}N\text{-}C_2H_5$	976.3	1008.7	0	Rln(1/1)
$[C_5H_{12}N_2O]$	632-22-4	$[(CH_3)_2N]_2C{=}O$	899.6	930.6	5	amides
$[C_5H_{12}N_2S]$	2782-91-4	$SC[N(CH_3)_2]_2$	916.6	947.6	5	amides
$[C_5H_{12}O]$	625-54-7	$C_2H_5O(i\text{-}C_3H_7)$	813.5	842.7	11	unsym ethers
$[C_5H_{12}O]$	1634-04-4	$t\text{-}C_4H_9OCH_3$	812.4	841.6	11	unsym ethers
$[C_5H_{12}O]$	75-84-3	$neo\text{-}C_5H_{11}OH$	765.2	795.5	7	CH_3OH
$[C_5H_{12}O]$	628-28-4	$n\text{-}C_4H_9OCH_3$	791.2	820.3	11	unsym ethers
$[C_5H_{12}O_2]$	17081-21-9	$CH_3O(CH_2)_3OCH_3$	858.6	897.2	−20.6	83MAU
$[C_5H_{12}S]$	1679-08-9	$neo\text{-}C_5H_{11}SH$	778.2	809.5	4	CH_3SH
$[C_5H_{12}Si]$	754-05-2	$(CH_3)_3SiCH{=}CH_2$	804.1	833	12	propene
$[C_5H_{13}N]$	5813-64-9	$neo\text{-}C_5H_{11}NH_2$	894.0	928.3	−6	CH_3NH_2
$[C_5H_{13}N]$	594-39-8	$t\text{-}C_5H_{11}NH_2$	903.6	937.8	−6	CH_3NH_2

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_5H_{13}N]$	996-35-0	$(CH_3)_2(i\text{-}C_3H_7)N$	939.6	970.6	5.6	$(CH_3)_3N$
$[C_5H_{13}N]$	926-63-6	$(CH_3)_2(n\text{-}C_3H_7)N$	931.9	962.8	5.6	$(CH_3)_3N$
$[C_5H_{13}N]$	616-39-7	$(CH_3)(C_2H_5)_2N$	940.0	971.0	5.6	$(CH_3)_3N$
$[C_5H_{13}N]$	110-58-7	$n\text{-}C_5H_{11}NH_2$	889.5	923.5	−5	CH_3NH_2
$[C_5H_{13}N]$	19961-27-4	$(C_2H_5)(i\text{-}C_3H_7)NH$	926.7	960.0	−1.9	$(CH_3)_2NH$
$[C_5H_{13}N_2OP]$	16606-18-1	$c\text{-}P(O)CH_3N(CH_3)CH_2CH_2N(CH_3)$	915.0	947.5	0	Rln(1/1)
$[C_5H_{13}N_3]$	80-70-6	$((CH_3)_2N)_2C{=}NH$	997.4	1031.6	−5.8	Rln(1/2)
$[C_5H_{13}N_3]$	32150-27-9	$CH_3C(N(CH_3)_2){=}NN(CH_3)_2$	963.4	995.8	0	Rln(1/1)
$[C_5H_{14}N_2]$	462-94-2	1,5-Diaminopentane	946.2	999.6	−70	80MAU/HAM
$[C_5H_{14}N_2]$	51-80-9	$(CH_3)_2NCH_2N(CH_3)_2$	919.8	952.2	0	$(CH_3)_3N$-Rln2
$[C_5H_{14}N_2]$	109-55-7	$(CH_3)_2N(CH_2)_3NH_2$	975.3	1025.0	−58	80MAU/HAM
$[C_5H_{15}NSi]$	18135-05-2	$(CH_3)_3SiN(CH_3)_2$	936	966.8	5.6	$(CH_3)_3N$
$[C_5H_{15}N_2OP]$	2511-17-3	$OP(N(CH_3)_2)_2(CH_3)$	918.9	951.3	0	Rln(1/1)
$[C_6CrO_6]$	13007-92-6	$(CO)_6Cr$	714.6	739.2	26.4	Rln(24/1)
$[C_6F_6]$	392-56-3	C_6F_6	624.4	648.0	30	aromatics
$[C_6HF_5]$	363-72-4	C_6HF_5	662.7	690.4	16	aromatics
$[C_6H_2F_4]$	551-62-2	$1,2,3,4\text{-}C_6H_2F_4$	672.7	700.4	16	aromatics
$[C_6H_2F_4]$	2367-82-0	$1,2,3,5\text{-}C_6H_2F_4$	719.6	747.3	16	aromatics
$[C_6H_2F_4]$	327-54-8	$1,2,4,5\text{-}C_6H_2F_4$	718.8	746.5	16	aromatics
$[C_6H_3F_3]$	1489-53-8	$1,2,3\text{-}C_6H_3F_3$	696.6	724.3	16	aromatics
$[C_6H_3F_3]$	367-23-7	$1,2,4\text{-}C_6H_3F_3$	699.4	729.5	8	93SZU/MCM
$[C_6H_3F_3]$	372-38-3	$1,3,5\text{-}C_6H_3F_3$	715.4	741.9	20	93SZU/MCM
$[C_6H_3MnO_5]$	13601-24-6	$(CO)_5MnCH_3$	735.4	764.4	11.5	Rln(4/1)
$[C_6H_3O_5Re]$	14524-92-6	$(CO)_5ReCH_3$	745.9	774.9	11.5	Rln(4/1)
$[C_6H_4]$	462-80-6	ortho-benzyne	808.5	841	0	Rln(2/2)
$[C_6H_4FO]$	2145-21-3	4-F-phenoxy	822	854.5	0	?
$[C_6H_4F_2]$	367-11-3	$1,2\text{-}C_6H_4F_2$	703.5	731.2	16	average
$[C_6H_4F_2]$	540-36-3	$1,4\text{-}C_6H_4F_2$	692.8	718.7	22	aromatics
$[C_6H_4F_2]$	372-18-9	$1,3\text{-}C_6H_4F_2$	722	749.7	16	average
$[C_6H_4F_3N]$	368-48-9	$2\text{-}(CF_3)$-pyridine	855.2	887.1	2	pyridines
$[C_6H_4F_3N]$	3796-23-4	$3\text{-}(CF_3)$-pyridine	860.7	892.5	2	pyridines
$[C_6H_4F_3N]$	3796-24-5	$4\text{-}(CF_3)$-pyridine	862.0	893.9	2	pyridines
$[C_6H_4N_2]$	100-70-9	2-Pyridinecarbonitrile	841	872.9	2	pyridines
$[C_6H_4N_2]$	100-48-1	4-Pyridinecarbonitrile	848.8	880.6	2	pyridines
$[C_6H_4N_2]$	100-54-9	3-Pyridinecarbonitrile	845.1	877.0	2	pyridines
$[C_6H_4N_2O]$	14906-59-3	4-cyano-pyridine-1-oxide	842.7	873.4	5.8	Rln(2/1)
$[C_6H_4N_2O]$	14906-64-0	3-cyano-pyridine-1-oxide	847.1	879.6	0	Rln(1/1)
$[C_6H_4O_2]$	106-51-4	p-benzoquinone	**769.3**	799.1	9	96IRI/MAU
$[C_6H_5]$	116139-00-5	$HCCCH_2CH(\bullet)CCH$	716.4	748.9	0	?
$[C_6H_5]$	2396-01-2	phenyl radical	851.5	884	0	Rln(1/1)
$[C_6H_5]$	116138-99-9	$CH_3\text{-}CC\text{-}CC\text{-}CH_2\bullet$	786.6	819.1	0	?
$[C_6H_5Br]$	108-86-1	C_6H_5Br	725.8	754.1	14	C_6H_5Cl
$[C_6H_5Cl]$	108-90-7	C_6H_5Cl	724.6	753.1	13.5	average
$[C_6H_5F]$	462-06-6	C_6H_5F	726.6	755.9	10.5	average
$[C_6H_5NO]$	586-96-9	Nitrosobenzene	**823.6**	854.3	5.8	Rln(2/1)
$[C_6H_5NO]$	872-85-5	4-Pyridinecarboxaldehyde	872.8	904.6	2	pyridines
$[C_6H_5NO_2]$	98-95-3	$C_6H_5NO_2$	769.5	800.3	5.8	Rln(2/1)
$[C_6H_5N_3]$	622-37-7	phenyl azide	787.5	820	0	Rln(1/1)
$[C_6H_5O]$	2122-46-5	C_6H_5O radical	827	857.7	5.8	Rln(2/1)
$[C_6H_6]$	71-43-2	C_6H_6	725.4	750.4	25	97EAS/SMI
$[C_6H_6BrN]$	591-19-5	$3\text{-}BrC_6H_4NH_2$	841.4	873.2	2	anilines
$[C_6H_6ClN]$	18368-63-3	$2\text{-}Cl\text{-}6\text{-}(CH_3)$-pyridine	876.2	908.0	2	pyridines
$[C_6H_6ClN]$	3678-62-4	$2\text{-}Cl\text{-}4\text{-}(CH_3)$-pyridine	889.4	921.2	2	pyridines
$[C_6H_6ClN]$	106-47-8	$4\text{-}ClC_6H_4NH_2$	842.0	873.8	2	anilines
$[C_6H_6ClN]$	108-42-9	$3\text{-}Cl\text{-}C_6H_4NH_2$	836.3	868.1	2	anilines
$[C_6H_6ClNO]$	17228-63-6	6-Chloro-1-methyl-2(1H)pyridinone	885.5	918.5	−1.9	
$[C_6H_6ClNO]$	17228-64-7	$2\text{-}Cl\text{-}6\text{-}(CH_3O)$-pyridine	878.0	909.9	2	pyridines
$[C_6H_6FN]$	371-40-4	$4\text{-}F\text{-}C_6H_4NH_2$	839.7	871.5	2	anilines
$[C_6H_6FN]$	372-19-0	$3\text{-}F\text{-}C_6H_4NH_2$	835.5	867.3	2	anilines
$[C_6H_6IN]$	626-01-7	$3\text{-}I\text{-}C_6H_4NH_2$	846.8	878.7	2	anilines
$[C_6H_6N]$	2348-49-4	C_6H_5NH radical	**917.4**	949.8	0	?
$[C_6H_6N_2O]$	98-92-0	nicotinamide	886.4	918.3	2	pyridines
$[C_6H_6N_2O_2]$	100-01-6	4-Nitroaniline	834.2	866.0	2	anilines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_6H_6N_4]$	2004-03-7	6-Methylpurine	**907.3**	939.2	2	pyridines
$[C_6H_6O]$	6921-27-3	$(HCCCH_2)_2O$	756.5	783.9	17	sym ethers
$[C_6H_6O]$	108-95-2	C_6H_5OH	786.3	817.3	5	$S(C_6H_5NH_2)$-$S(C_6H_5OH)$
$[C_6H_7N]$	6921-28-4	$(HCCCH_2)_2NH$	876.9	910.0	−2	$(CH_3)_2NH$
$[C_6H_7N]$	62-53-3	$C_6H_5NH_2$	850.6	882.5	2	$S(C_6H_5CH_3)$-$S(C_6H_5NH_2)$
$[C_6H_7N]$	109-06-8	2-(CH_3)-pyridine	917.3	949.1	2	pyridines
$[C_6H_7N]$	108-99-6	3-(CH_3)-pyridine	911.6	943.4	2	pyridines
$[C_6H_7N]$	108-89-4	4-(CH_3)-pyridine	915.3	947.2	2	pyridines
$[C_6H_7NO]$	95-55-6	2-$(OH)C_6H_4NH_2$	866.9	898.8	2	anilines
$[C_6H_7NO]$	620-08-6	4-(CH_3O)-pyridine	929.8	961.7	2	pyridines
$[C_6H_7NO]$	591-27-5	3-$(OH)C_6H_4NH_2$	866.9	898.8	2	anilines
$[C_6H_7NO]$	1628-89-3	2-(CH_3O)-pyridine	902.8	934.7	2	pyridines
$[C_6H_7NO]$	7295-76-3	3-(CH_3O)-pyridine	910.9	942.7	2	pyridines
$[C_6H_7NO]$	694-85-9	1-Methyl-2-pyridinone	894.8	925.8	5	amides
$[C_6H_7NO]$	1003-73-2	3-methyl-pyridine-1-oxide	902.8	935.2	0	Rln(1/1)
$[C_6H_7NS]$	18794-33-7	3-(CH_3S)-pyridine	904.7	936.5	2	pyridines
$[C_6H_7NS]$	18438-38-5	2-(CH_3S)-pyridine	906.0	937.8	2	pyridines
$[C_6H_7NS]$	22581-72-2	4-(CH_3S)-pyridine	923.3	955.2	2	pyridines
$[C_6H_8]$	592-57-4	1,3-c-C_6H_8	804.5	837	0	Rln(2/2)
$[C_6H_8]$	628-41-1	1,4-c-C_6H_8	808.0	837	11.5	Rln(4/1)
$[C_6H_8]$	15082-13-0	1-Methyl-3-methylenecyclobutene	856.9	891.0	−5.8	Rln(1/2)
$[C_6H_8N_2]$	95-54-5	1,2-$C_6H_4(NH_2)_2$	865.8	896.5	5.8	Rln(2/1)
$[C_6H_8N_2]$	108-45-2	1,3-$C_6H_4(NH_2)_2$	899.2	929.9	5.8	Rln(2/1)
$[C_6H_8N_2]$	106-50-3	1,4-$C_6H_4(NH_2)_2$	874.0	905.9	2	anilines
$[C_6H_8N_2O]$	1656-48-0	$O(CH_2CH_2CN)_2$	**786.4**	813.8	17	sym ethers
$[C_6H_8N_2O_2]$	37622-90-5	4-(C_2H_5COO)-pyrazole	846.5	880.7	−5.8	Rln(1/2)
$[C_6H_8O]$	625-86-5	2,5-dimethylfuran	835.2	865.9	5.8	Rln(2/1)
$[C_6H_8O]$	20843-07-6	3,4-dimethylfuran	838.3	869.0	5.8	Rln(2/1)
$[C_6H_8O]$	3710-43-8	2,4-dimethylfuran	862.3	894.7	0	Rln(1/1)
$[C_6H_8O]$	6705-50-6	Bicyclo[2.2.1]hept-2-ene,7-oxa-	804.7	837.1	0	Rln(1/1)
$[C_6H_8O_2]$	504-02-9	c-hexane-1,3-dione	849.4	881.2	2	unsym ketones
$[C_6H_8O_2]$	765-87-7	c-hexane-1,2-dione	818.9	849.6	5.8	Rln(2/1)
$[C_6H_8O_2]$	637-88-7	c-hexane-1,4-dione	782.7	812.5	9	sym ketones
$[C_6H_9F_3O_2]$	367-64-6	$CF_3CO_2(n\text{-}C_4H_9)$	733.8	764.8	5	esters
$[C_6H_9N]$	625-84-3	2,5-Dimethylpyrrole	887.1	918.7	3	pyrrole
$[C_6H_9N_3O_2]$	71-00-1	L-histidine	950.2	988	−18	94WU/FEN
$[C_6H_9O_3P]$	281-33-4	2,8,9-Trioxa-1-phosphadamantane	866.8	899.3	0	Rln(3/3)
$[C_6H_{10}]$	1528-30-9	c-C_5H_8=CH_2	803.5	832.4	12	propene
$[C_6H_{10}]$	1501-58-2	1,2-Dimethylcyclobutene	807.3	838.0	5.8	Rln(2/1)
$[C_6H_{10}]$	1118-58-7	CH_3CH=$CHC(CH_3)$=CH_2	836	864.9	12	propene
$[C_6H_{10}]$	764-35-2	2-hexyne	781.1	806.1	25	CH_3CCH
$[C_6H_{10}]$	693-02-7	1-hexyne	774.8	799.8	25	CH_3CCH
$[C_6H_{10}]$	513-81-5	CH_2=$C(CH_3)C(CH_3)$=CH_2	807.8	835.0	17.8	propene+Rln(2/1)
$[C_6H_{10}]$	693-89-0	1-Methylcyclopentene	787.1	816.5	10	?
$[C_6H_{10}]$	4663-22-3	c-$C_3H_5C(CH_3)$=CH_2	842.7	871.6	12	propene
$[C_6H_{10}]$	4549-74-0	CH_3CH=$C(CH_3)CH$=CH_2	823.4	852.3	12	propene
$[C_6H_{10}]$	16906-27-7	1-ethenyl-1-methylcyclopropane	826.9	855.7	12	propene
$[C_6H_{10}]$	3664-56-0	1,3,3-Trimethylcyclopropene	865.9	895.4	10	AUE
$[C_6H_{10}]$	110-83-8	c-C_6H_{10}	752.0	784.5	0	Rln(2/2)
$[C_6H_{10}F_3N]$	657-36-3	4-Trifluoromethylpiperidine	892.0	925.1	−2	$(CH_3)_2NH$
$[C_6H_{10}F_3NO]$	400-59-9	$CF_3CONH(n\text{-}C_4H_9)$	819.4	850.3	5	amides
$[C_6H_{10}N_2]$	1530-87-6	Piperidine, 1-carbonitrile-	846.1	876.7	6	nitriles
$[C_6H_{10}N_2]$	5519-42-6	3,4,5-Trimethylpyrazole	916.0	949.3	−3	pyridines-Rln2
$[C_6H_{10}N_2]$	1072-91-9	1,3,5-Trimethylpyrazole	917.4	949.3	2	pyridines
$[C_6H_{10}N_2]$	4395-98-6	4-Cyanopiperidine	879.2	912.3	−2	$(CH_3)_2NH$
$[C_6H_{10}N_2]$	121508-72-3	$(CH_3)_2N$-CH=N-(2-propynyl)	960.7	993.1	0	Rln(1/1)
$[C_6H_{10}O]$	557-40-4	$(CH_2$=$CHCH_2)_2O$	800.0	827.4	17	sym ethers
$[C_6H_{10}O]$	286-20-4	Cyclohexene oxide	**815.6**	848.1	0	Rln(1/1)
$[C_6H_{10}O]$	1567-72-2	3-methyl-3-penten-2-one(Z)	834.5	866.4	2	unsym ketones
$[C_6H_{10}O]$	108-94-1	cyclohexanone	811.2	841.0	9	sym ketones
$[C_6H_{10}O]$	141-79-7	$(CH_3)_2C$=$CH(C$=$O)CH_3$	846.9	878.7	2	unsym ketones
$[C_6H_{10}O]$	279-49-2	Bicyclo[2.2.1]heptane,7-oxa	816.8	844.2	17	sym ethers
$[C_6H_{10}O]$	4376-23-2	3-hexen-2-one(E)	833.8	865.6	2	unsym ketones

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[$C_6H_{10}O_2$]	3400-45-1	cyclopentane carboxylic acid	**786.4**	817.4	5	acids
[$C_6H_{10}O_2$]	110-13-4	$CH_3COCH_2CH_2COCH_3$	851.8	892.0	−26	83MAU
[$C_6H_{10}O_3$]	22157-30-8	$CH_3C(OCH_3)=CHCOOCH_3$	885.8	916.8	5	esters
[$C_6H_{11}N$]	124-02-7	$(CH_2=CHCH_2)_2NH$	916.3	949.3	−2	$(CH_3)_2NH$
[$C_6H_{11}NO$]	931-20-4	c-C_5H_8N(2-O)1-CH_3	892.6	924.4	2	unsym ketones
[$C_6H_{11}NO$]	6976-91-6	2-propenamide, N,N,2-trimethyl-	880.6	911.5	5	amides
[$C_6H_{11}NO$]	23135-18-4	2-propenamide, N,N-dimethyl-	899.4	930.3	5	amides
[$C_6H_{11}NO$]	4030-18-6	Acetylpyrrolidine	894.4	925.4	5	amides
[$C_6H_{11}NO_3$]	26629-33-4	$CH_3CONHCH(CH_3)COOCH_3$	888.0	938.6	−61	83MAU
[$C_6H_{11}N_3$]	134166-60-2	$(CH_3)_2N$-CH=N-CH_2CH_2CN	948.3	980.8	0	Rln(1/1)
[$C_6H_{11}N_3O_4$]	556-33-2	triglycine	916.8	966.8	−59	93CHE/WU
[C_6H_{12}]	625-27-4	$(CH_3)_2C=CHCH_2CH_3$	783.1	812	12	propene
[C_6H_{12}]	563-79-1	$(CH_3)_2C=C(CH_3)_2$	785.9	813.9	15	$(CH_3)_2C=CH_2$
[C_6H_{12}]	592-41-6	1-hexene	776.3	805.2	12	propene
[C_6H_{12}]	110-82-7	c-C_6H_{12}	**666.9**	686.9	42	C_2H_6; c-C_3H_6
[C_6H_{12}]	922-61-2	$CH_3CH=C(CH_3)C_2H_5$	784.0	812.9	12	propene
[$C_6H_{12}N$]	60598-49-4	$(CH_3)_2N$-CH=N-(2-propenyl)	972.3	1004.8	0	Rln(1/1)
[$C_6H_{12}N_2$]	5397-67-1	1H,5H-pyrazolo[1,2-a]pyrazole, tetrahydro	947.3	978.0	5.8	Rln(2/1)
[$C_6H_{12}N_2$]	280-57-9	1,4-Diazabicyclo[2.2.2]octane	934.6	963.4	12	$(CH_3)_3N$+Rln(6/3)
[$C_6H_{12}N_2$]	133835-16-2	$(CH_3)_2N$-CH=N-(c-propyl)	973.8	1006.2	0	Rln(1/1)
[$C_6H_{12}N_2O_3$]	1948-31-8	di-L-alanine	905.6	NE	NE	not estimated
[$C_6H_{12}N_2O_4$]	6620-95-7	ser-ser	**886.4**	NE	NE	not estimated
[$C_6H_{12}O$]	592-90-5	c-$C_6H_{12}O$(Oxepane)	806.8	834.2	17	sym ethers
[$C_6H_{12}O$]	75-97-8	t-$C_4H_9COCH_3$	808.2	840.1	2	unsym ketones
[$C_6H_{12}O$]	1003-17-4	2,2-Dimethyltetrahydrofuran	818.5	847.7	11	unsym ethers
[$C_6H_{12}O$]	589-38-8	3-hexanone	811.3	843.2	2	unsym ketones
[$C_6H_{12}O_2$]	823-18-7	cis-1,3-cyclohexandiol	849.7	882.2	0	?
[$C_6H_{12}O_2$]	598-98-1	t-C_4H_9-$COOCH_3$	814.2	845.2	5	esters
[$C_6H_{12}O_2$]	5515-64-0	trans-1,3-cyclohexanol	**797.9**	828.6	5.8	Rln(2/1)
[$C_6H_{12}O_2$]	123-42-2	$(CH_3)_2C(OH)CH_2(C=O)CH_3$	791.1	822.9	2	unsym ketones
[$C_6H_{12}O_6$]	26655-34-5	alpha-D-glucose	**778.9**	NE	NE	not estimated
[$C_6H_{12}O_6$]	28905-12-6	beta-D-glucose	**778.9**	NE	NE	not estimated
[$C_6H_{13}N$]	111-49-9	Hexahydroazepine	923.5	956.7	−1.9	$(CH_3)_2NH$
[$C_6H_{13}N$]	626-67-5	1-Methylpiperidine	940.1	971.1	5.6	$(CH_3)_3N$
[$C_6H_{13}N$]	1611-12-7	n-$C_3H_7CH=NC_2H_5$	923.0	955.5	0	Rln(1/1)
[$C_6H_{13}N$]	78733-72-9	$(CH_3)_2NC(CH_3)=CHCH_3$	**972.9**	1005.4	0	Rln(1/1)
[$C_6H_{13}N$]	108-91-8	c-$C_6H_{11}NH_2$	899.6	934.4	−8	$S(C_6H_{11}CH_3)$-
[$C_6H_{13}N$]	6906-32-7	$(CH_3)_2C=CHN(CH_3)_2$	**934.5**	967.0	0	Rln(1/1)
[$C_6H_{13}NO$]	760-79-2	n-$C_3H_7CON(CH_3)_2$	890.8	921.7	5	amides
[$C_6H_{13}NO$]	685-91-6	$CH_3CON(C_3H_8)_2$	894.4	925.4	5	amides
[$C_6H_{13}NO$]	21678-37-5	i-C_3H_7-$CON(CH_3)_2$	891.8	923.7	2	amides
[$C_6H_{13}NO$]	53687-79-9	c-$C_5H_{10}N$(2-OCH_3)	936.7	969.9	−2	$(CH_3)_2NH$
[$C_6H_{13}NO_2$]	61-90-5	L-leucine	880.6	914.6	−5	CH_3NH_2
[$C_6H_{13}NO_2$]	73-32-5	L-isoleucine	**883.5**	917.4	−5	CH_3NH_2
[$C_6H_{13}O_3P$]	7735-82-2	cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane	919.1	951.6	0	Rln(1/1)
[$C_6H_{13}O_3P$]	41821-91-4	trans-2-Methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane	914.1	946.6	0	Rln(1/1)
[$C_6H_{13}P$]	39763-50-3	$(CH_3)_5PCH_3$	936.7	969.4	0	Rln(1/1)
[$C_6H_{14}N_2$]	32150-25-7	$(CH_3)_2N$-CH=N-(n-propyl)	979.2	1011.7	0	Rln(1/1)
[$C_6H_{14}N_2$]	32150-24-6	$(CH_3)_2N$-CH=N-(1-methylethyl)	981.0	1013.5	0	Rln(1/1)
[$C_6H_{14}N_2$]	151328-40-4	$(CH_3)_2N$-$C(CH_3)$=NC_2H_5	996.7	1029.1	0	Rln(1/1)
[$C_6H_{14}N_2$]	26163-37-1	Pyridazine, hexahydro-1,2-dimethyl	935.4	966.1	5.6	$(CH_3)_3N$
[$C_6H_{14}N_2O$]	134166-62-4	$(CH_3)_2N$-CH=N-(2-methoxyethyl)	986.4	1018.9	0	Rln(1/1)
[$C_6H_{14}N_2O_2$]	56-87-1	L-lysine	951.0	996	−42	93CHE/WU
[$C_6H_{14}N_2O_2$]	74-79-3	L-Arginine	1006.6	1051.0	−40	80MAU/HAM
[$C_6H_{14}O$]	108-20-3	(i-C_3H_7)$_2O$	828.1	855.5	17	sym ethers
[$C_6H_{14}O$]	111-43-3	(n-C_3H_7)$_2O$	810.5	837.9	17	sym ethers
[$C_6H_{14}O$]	637-92-3	C_2H_5O(t-C_4H_9)	826.9	856.0	11	unsym ethers
[$C_6H_{14}O$]	1118-00-9	neo-$C_5H_{11}OCH_3$	796.7	825.8	11	unsym ethers
[$C_6H_{14}OSi$]	1833-53-0	$CH_2=C(CH_3)OSi(CH_3)_3$	**898.2**	930.6	0	Rln(1/1)
[$C_6H_{14}O_2$]	13179-96-9	$CH_3O(CH_2)_4OCH_3$	880.6	931.5	−62	84SHA/BLA
[$C_6H_{14}O_2$]	111-96-6	$CH_3(OCH_2CH_2)_2OCH_3$	870.9	918.8	−52	84SHA/BLA; 83MAU

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_6H_{14}S]$	111-47-7	$(n\text{-}C_3H_7)_2S$	834.9	864.7	9	sym sulfides
$[C_6H_{14}S]$	625-80-9	$(i\text{-}C_3H_7)_2S$	846.6	876.4	9	sym sulfides
$[C_6H_{15}N]$	121-44-8	$(C_2H_5)_3N$	951	981.8	5.6	$(CH_3)_3N$
$[C_6H_{15}N]$	142-84-7	$(n\text{-}C_3H_7)_2NH$	929.3	962.3	−1.9	$(CH_3)_2NH$
$[C_6H_{15}N]$	111-26-2	$n\text{-}C_6H_{13}NH_2$	893.5	927.5	−5	CH_3NH_2
$[C_6H_{15}N]$	927-62-8	$(CH_3)_2(n\text{-}C_4H_9)N$	938.2	969.2	5.6	$(CH_3)_3N$
$[C_6H_{15}N]$	921-04-0	$(sec\text{-}C_4H_9)(CH_3)_2N$	945.1	975.9	5.6	$(CH_3)_3N$
$[C_6H_{15}N]$	7239-24-9	$(CH_3)_2(i\text{-}C_4H_9)N$	937.8	968.7	5.6	$(CH_3)_3N$
$[C_6H_{15}N]$	108-18-9	$(i\text{-}C_3H_7)_2NH$	938.6	971.9	−1.9	$(CH_3)_2NH$
$[C_6H_{15}N]$	918-02-5	$(CH_3)_2(t\text{-}C_4H_9)N$	948.6	979.6	5.6	$(CH_3)_3N$
$[C_6H_{15}NO]$	4048-33-3	$NH_2(CH_2)_6OH$	915.7	969.0	−70	80MAU
$[C_6H_{15}N_3]$	13439-84-4	$((CH_3)_2N)_2C{=}NCH_3$	1015.2	1047.7	0	Rln(1/1)
$[C_6H_{15}OP]$	597-50-2	$(C_2H_5)_3PO$	906.8	936.6	9.1	Rln(3/1)
$[C_6H_{15}O_4P]$	78 40 0	$OP(OC_2H_5)_3$	879.6	909.3	9.1	Rln(3/1)
$[C_6H_{15}P]$	554-70-1	$(C_2H_5)_3P$	952.0	984.5	0	Rln(3/3)
$[C_6H_{16}N_2]$	60678-65-1	$(n\text{-}C_3H_7)(CH_3)NN(CH_3)_2$	934.3	966.8	0	Rln(1/1)
$[C_6H_{16}N_2]$	23337-93-1	Hydrazine, 1,2-diethyl-1,2-dimethyl	933.0	963.7	5.8	Rln(2/1)
$[C_6H_{16}N_2]$	110-18-9	$(CH_3)_2N(CH_2)_2N(CH_3)_2$	970.6	1012.8	−33	80MAU/HAM
$[C_6H_{16}N_2]$	124-09-4	1,6-Diaminohexane	946.2	999.5	−70	80MAU/HAM
$[C_6H_{16}N_3OP]$	7778-06-5	$c\text{-}OP\{N(CH_3)_2\}N(CH_3)CH_2CH_2N(CH_3)$	929.3	961.7	0	Rln(1/1)
$[C_6H_{16}OSi]$	597-52-4	$(C_2H_5)_3SiOH$	794.8	822.1	17	88LI/STO
$[C_6H_{17}NSi]$	18182-40-6	$(CH_3)_3SiCH_2N(CH_3)_2$	943.8	974.5	5.6	$(CH_3)_3N$
$[C_6H_{18}N_3OP]$	680-31-9	$OP(N(CH_3)_2)_3$	928.7	958.6	9.1	Rln(3/1)
$[C_6H_{18}N_3P]$	1608-26-0	$P(N(CH_3)_2)_3$	897.7	930.1	0	Rln(1/1)
$[C_6H_{18}N_3PS]$	3732-82-9	$SP(N(CH_3)_2)_3$	912.2	942.0	9.1	Rln(3/1)
$[C_6H_{18}N_3PSe]$	7422-73-3	$SeP(N(CH_3)_2)_3$	904.3	934.1	9.1	Rln(3/1)
$[C_6H_{18}OSi_2]$	107-46-0	$(CH_3)_3SiOSi(CH_3)_3$	816.2	846.4	7.8	87LI/STO
$[C_6MoO_6]$	13939-06-5	$(CO)_6Mo$	738.1	762.6	26.4	Rln(24/1)
$[C_6O_6V]$	20644-87-5	$(CO)_6V$	775.3	799.9	26.4	Rln(24/1)
$[C_6O_6W]$	14040-11-0	$(CO)_6W$	733.4	758.0	26.4	Rln(24/1)
$[C_7H_4N_2O_2]$	619-72-7	$4\text{-}NO_2\text{-}C_6H_4\text{-}CN$	745.1	775.7	6	nitriles
$[C_7H_4N_2O_2]$	619-24-9	$3\text{-}NO_2\text{-}C_6H_4\text{-}CN$	750.7	781.4	6	nitriles
$[C_7H_5ClO]$	587-04-2	$3\text{-}ClC_6H_4CHO$	781.1	813.0	2	CH_3CHO
$[C_7H_5ClO]$	104-88-1	$4\text{-}ClC_6H_4CHO$	799.4	831.3	2	CH_3CHO
$[C_7H_5CrNO_3]$	36312-04-6	$(C_5H_5)Cr(CO)_2NO$	786.7	819.1	0	Rln(1/1)
$[C_7H_5D_3]$	1124-18-1	$C_6H_5CD_3$	762	789.7	16	toluene
$[C_7H_5FO]$	456-48-4	$3\text{-}FC_6H_4CHO$	782.5	814.3	2	aldehydes
$[C_7H_5FO]$	459-57-4	$4\text{-}FC_6H_4CHO$	795.3	827.1	2	aldehydes
$[C_7H_5N]$	100-47-0	C_6H_5CN	780.9	811.5	6	nitriles
$[C_7H_5N]$	931-54-4	C_6H_5NC	**836.0**	868.4	0	Rln(1/1)
$[C_7H_5N]$	2510-22-7	4-ethynyl-pyridine	898.2	930.1	2	pyridines
$[C_7H_5NO]$	273-53-0	benzoxazole	859.8	891.6	2	pyridines
$[C_7H_5NO_3]$	555-16-8	$4\text{-}(NO_2)C_6H_4CHO$	763.2	795.1	2	aldehydes
$[C_7H_5O_2Rh]$	12192-97-1	$(C_5H_5)Rh(CO)_2$	851.8	882.5	5.8	Rln(2/1)
$[C_7H_6ClNO]$	618-48-4	$3\text{-}Cl\text{-}C_6H_4CONH_2$	**846.3**	877.2	5	amides
$[C_7H_6ClNO]$	619-56-7	$4\text{-}Cl\text{-}C_6H_4CONH_2$	**846.3**	877.2	5	amides
$[C_7H_6F]$	2599-73-7	$3\text{-}FC_6H_4CH_2$ radical	**804**	836.5	0	?
$[C_7H_6FNO]$	455-37-8	$3\text{-}F\text{-}C_6H_4CONH_2$	**846.3**	877.2	5	amides
$[C_7H_6FNO]$	824-75-9	$4\text{-}F\text{-}C_6H_4CONH_2$	**846.3**	877.2	5	amides
$[C_7H_6F_3N]$	98-16-8	$3\text{-}CF_3C_6H_4NH_2$	825.1	856.9	2	anilines
$[C_7H_6N_2]$	274-76-0	Imidazo(1,2-a)pyridine	940.3	972.1	2	pyridines
$[C_7H_6N_2]$	271-44-3	1H-Indazole	868.9	900.8	2	pyridines
$[C_7H_6N_2]$	271-63-6	7-Azaindole	908.3	940.2	2	pyridines
$[C_7H_6N_2]$	51-17-2	Benzimidazole	920.5	953.8	−3	pyridine-Rln2
$[C_7H_6N_2]$	2237-30-1	$3\text{-}NH_2\text{-}C_6H_4CN$	810.4	842.3	2	anilines
$[C_7H_6N_2O_3]$	619-80-7	$4\text{-}NO_2\text{-}C_6H_4CONH_2$	**814.4**	845.3	5	amides
$[C_7H_6N_2O_3]$	645-09-0	$3\text{-}NO_2\text{-}C_6H_4CONH_2$	**823.2**	854.2	5	amides
$[C_7H_6O]$	539-80-0	2,4,6-Cycloheptatriene-1-one	**891.0**	920.8	9	sym ketones
$[C_7H_6O]$	502-87-4	4-Methylene-2,5-cyclohexadiene-1-one	894.0	923.8	9	sym ketones
$[C_7H_6O]$	100-52-7	C_6H_5CHO	802.1	834.0	2	CH_3CHO
$[C_7H_6O_2]$	65-85-0	C_6H_5COOH	790.1	821.1	5	acids
$[C_7H_7]$	2154-56-5	$C_6H_5CH_2$	800.7	831.4	6	isoel analog
$[C_7H_7]$	3551-27-7	c-C-H- radical	**800.0**	832.4	0	?

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_7H_7Br]	106-38-7	4-Br-toluene	745.8	775.3	10	aromatics
[C_7H_7Br]	95-46-5	2-Br-toluene	745.8	775.3	10	aromatics
[C_7H_7Br]	591-17-3	3-Br-toluene	752.5	782.0	10	aromatics
[C_7H_7Cl]	95-49-8	2-Cl-toluene	761.1	790.5	10	aromatics
[C_7H_7Cl]	106-43-4	4-Cl-toluene	735.2	762.9	16	aromatics
[C_7H_7Cl]	108-41-8	3-Cl-toluene	754.5	783.9	10	aromatics
[C_7H_7F]	95-52-3	2-F-toluene	743.8	773.3	10	aromatics
[C_7H_7F]	352-70-5	3-F-toluene	756.0	785.4	10	aromatics
[C_7H_7F]	352-32-9	4-CH_3-C_6H_4F	736.1	763.8	16	aromatics
[C_7H_7I]	615-37-2	2-I-toluene	750.8	780.3	10	aromatics
[C_7H_7N]	16118-22-2	$C_6H_5CH{=}NH$	**879.4**	911.9	0	Rln(1/1)
[C_7H_7N]	56911-25-2	2,3-Cyclobutenopyridine	922.0	953.9	2	pyridines
[C_7H_7N]	56911-27-4	3,4-Cyclobutenopyridine	925.6	957.5	2	pyridines
[C_7H_7N]	100-43-6	4-Vinylpyridine	912.3	944.1	2	pyridines
[C_7H_7NO]	350-03-8	3-(CH_3CO)-pyridine	884.3	916.2	2	pyridines
[C_7H_7NO]	1122-54-9	1-(4-Pyridinyl)-ethanone	882.9	914.7	2	pyridines
[C_7H_7NO]	55-21-0	$C_6H_5CONH_2$	**861.2**	892.1	5	amides
[$C_7H_7NO_2$]	118-92-3	2-NH_2-benzoic acid	**869.0**	901.5	0	?
[$C_7H_7NO_2$]	150-13-0	4-NH_2-benzoic acid	**832.3**	864.7	0	?
[$C_7H_7NO_2$]	99-05-8	3-NH_2-benzoic acid	**832.3**	864.7	0	?
[C_7H_7NO]	556-18-3	4-$NH_2C_6H_4CHO$	878.6	910.4	2	anilines
[$C_7H_7NO_2$]	93-60-7	methylnicotinate	893.8	925.6	2	pyridines
[$C_7H_7NO_2$]	14188-94-4	1-(3-pyridinyl-1-oxide)ethanone	880.6	913.1	0	?
[$C_7H_7NO_2$]	99-99-0	4-Nitrotoluene	782.7	815.2	0	?
[$C_7H_7NO_2$]	2459-09-8	Pyridine-4-carboxylic acid, methyl ester	894.7	926.6	2	pyridines
[$C_7H_7NO_3$]	619-73-8	4-NO_2-$C_6H_4CH_2OH$	778.0	810.5	0	86SUN/KUL
[$C_7H_7N_3$]	13351-73-0	1-methylbenzotriazole	898.7	931.2	0	Rln(1/1)
[$C_7H_7N_3$]	16584-00-2	2-methyl-2H-benzotriazole	855.9	890.1	−5.8	Rln(1/2)
[C_7H_7O]	155174-22-4	3-OH-benzyl	853	885.5	0	Rln(1/1)
[C_7H_7O]	3174-48-9	4-Me-phenoxy	852	884.5	0	Rln(1/1)
[C_7H_7O]	88170-17-6	4-OH-benzyl	864	896.5	0	Rln(1/1)
[C_7H_7O]	155174-21-3	2-OH-benzyl	846	878.5	0	Rln(1/1)
[C_7H_7O]	3174-49-0	2-Me-phenoxy	842	874.5	0	Rln(1/1)
[C_7H_7O]	41115-75-7	3-Me-phenoxy	845	877.5	0	Rln(1/1)
[C_7H_8]	108-88-3	$C_6H_5CH_3$	756.3	784.0	16	toluene
[C_7H_8]	121-46-0	Bicyclo[2.2.1]hepta-2,5-diene	820.3	849.3	11.5	Rln(4/1)
[$C_7H_8N_2O$]	3544-24-9	3-NH_2-$C_6H_4CONH_2$	**869.9**	900.9	5	amides
[$C_7H_8N_2O$]	2835-68-9	4-NH_2-$C_6H_4CONH_2$	**896.9**	927.9	5	amides
[$C_7H_8N_2O_2$]	100-15-2	N-Methyl-4-nitroaniline	865.1	891.6	20	anilines
[$C_7H_8N_4$]	27258-04-4	Di(1-pyrazolyl)methane	893.9	924.7	5.8	Rln(2/1)
[C_7H_8O]	694-71-3	Bicyclo[2.2.1]hept-2-ene-7-one	798.3	830.2	2	unsym ketones
[C_7H_8O]	100-51-6	$C_6H_5CH_2OH$	748.0	778.3	7	CH_3OH
[C_7H_8O]	100-66-3	$C_6H_5OCH_3$	807.2	839.6	0	?
[C_7H_8O]	694-98-4	Bicyclo[2.2.1]hept-2-ene-5-one	813.4	845.3	2	unsym ketones
[$C_7H_8O_2$]	1004-36-0	2,6-Dimethyl-4-pyrone	907.3	941.5	−5.8	Rln(1/2)
[$C_7H_8O_2S$]	3112-85-4	$C_6H_5SO_2CH_3$	780.3	812.7	0	Rln(1/1)
[C_7H_8S]	100-68-5	$C_6H_5SCH_3$	843.7	872.6	12	
[C_7H_9N]	95-53-4	2-methylaniline	859.1	890.9	2	anilines
[C_7H_9N]	536-75-4	4-(C_2H_5)-pyridine	919.2	951.1	2	pyridines
[C_7H_9N]	108-48-5	2,6-(CH_3)$_2$-pyridine	931.1	963.0	2	pyridines
[C_7H_9N]	108-44-1	3-$CH_3C_6H_4NH_2$	864.0	895.8	2	anilines
[C_7H_9N]	100-46-9	$C_6H_5CH_2NH_2$	879.4	913.3	−5	CH_3NH_2
[C_7H_9N]	100-71-0	2-(C_2H_5)-pyridine	920.6	952.4	2	pyridines
[C_7H_9N]	589-93-5	2,5-(CH_3)$_2$-pyridine	926.9	958.8	2	pyridines
[C_7H_9N]	108-47-4	2,4-(CH_3)$_2$-pyridine	930.8	962.9	2	pyridines
[C_7H_9N]	583-61-9	2,3-(CH_3)$_2$-pyridine	927.0	958.9	2	pyridines
[C_7H_9N]	100-61-8	$C_6H_5NHCH_3$	890.1	916.6	20	anilines
[C_7H_9N]	591-22-0	3,5-(CH_3)$_2$-pyridine	923.5	955.4	2	pyridines
[C_7H_9N]	106-49-0	4-$CH_3C_6H_4NH_2$	864.8	896.7	2	anilines
[C_7H_9N]	583-58-4	3,4-(CH_3)$_2$-pyridine	925.5	957.3	2	pyridines
[C_7H_9N]	536-78-7	3-(C_2H_5)-pyridine	915.5	947.4	2	pyridines
[C_7H_9NO]	536-90-3	3-$CH_3OC_6H_4NH_2$	881.1	913.0	2	anilines
[C_7H_9NO]	90-04-0	2-$CH_3OC_6H_4NH_2$	873.3	905.2	2	anilines
[C_7H_9NO]	23579-92-2	2-(CH_3OCH_2)-pyridine	926.4	958.3	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_7H_9NO]	104-94-9	4-$CH_3OC_6H_4NH_2$	868.5	900.3	2	anilines
[C_7H_9NS]	1783-81-9	3-$CH_3SC_6H_4NH_2$	870.3	902.1	2	anilines
[C_7H_{10}]	498-66-8	Bicyclo[2.2.1]hept-2-ene	804.0	836.5	0	Rln(1/1)
[$C_7H_{10}ClN$]	#449	3-Chloro-1-azabicyclo[2.2.2]oct-2-ene	916.7	947.5	5.6	$(CH_3)_3N$
[$C_7H_{10}N_2$]	18437-57-5	N,N-Dimethyl-3-pyridinamine	943.1	969.6	20	anilines
[$C_7H_{10}N_2$]	1122-58-3	N,N-Dimethyl-4-pyridinamine	971.1	997.6	20	anilines
[$C_7H_{10}N_2$]	5683-33-0	N,N-Dimethyl-2-pyridinamine	941.6	968.2	20	anilines
[$C_7H_{10}N_2O_2$]	4027-57-0	3(5)-methyl-5(3)-ethoxycarbonylpyrazole	870.8	902.6	2	pyridines
[$C_7H_{10}O$]	10218-02-7	Bicyclo[2.2.1]heptan-7-one	802.4	832.1	9	sym ketones
[$C_7H_{10}O$]	497-38-1	Bicyclo[2.2.1]heptan-2-one	815.5	847.4	2	unsym ketones
[$C_7H_{10}O$]	1121-37-5	(c-$C_3H_5)_2CO$	850.6	880.4	9	sym ketones
[$C_7H_{10}S$]	38381-24-7	(c-$C_3H_5)_2CS$	874.5	904.3	9	sym ketones
[$C_7H_{11}F_2N$]	#524	3,3-Difluoro-1-azabicyclo[2.2.2]octane	904.8	935.5	5.6	$(CH_3)_3N$
[$C_7H_{11}N$]	766-05-2	c-$C_8H_{11}CN$	784.4	815.0	6	nitriles
[$C_7H_{11}N$]	87-62-7	2,6-dimethylaniline	869.8	901.7	2	anilines
[$C_7H_{11}N$]	13929-94-7	1-Azabicyclo[2.2.2]oct-2-ene	938.6	969.4	5.6	$(CH_3)_3N$
[$C_7H_{11}NO$]	3731-38-2	1-Azabicyclo[2.2.2]octan-3-one	905.2	936.0	5.6	$(CH_3)_3N$
[C_7H_{12}]	765-47-9	c-C_5H_6-1,2-$(CH_3)_2$	791.9	822.6	5.8	Rln(2/1)
[C_7H_{12}]	1000-86-8	$(CH_3)_2C{=}CHC(CH_3){=}CH_2$	857.6	886.5	12	propene
[C_7H_{12}]	591-49-1	1-Methylcyclohexene	792.6	825.1	0	?
[$C_7H_{12}BrN$]	#364	3-Bromo-1-azabicyclo[2.2.2]octane	931.8	962.6	5.6	$(CH_3)_3N$
[$C_7H_{12}ClN$]	42332-45-6	3-Chloro-1-azabicyclo[2.2.2]octane	923.5	954.3	5.6	$(CH_3)_3N$
[$C_7H_{12}ClN$]	5960-95-2	1-azabicyclo[2.2.2]-octane, 4-chloro	918.6	949.4	5.6	$(CH_3)_3N$
[$C_7H_{12}ClN$]	96943-88-3	1-azabicyclo[2.2.2]-octane, 2-chloro	920.0	950.8	5.6	$(CH_3)_3N$
[$C_7H_{12}FN$]	#321	3-Fluoro-1-azabicyclo[3.2.1]octane	936.7	967.5	5.6	$(CH_3)_3N$
[$C_7H_{12}N_2$]	3001-72-7	1,5-diazabicyclo[4.3.0]non-5-ene	1005.9	1038.3	0	Rln(1/1)
[$C_7H_{12}N_2$]	45676-04-8	1-t-Butylimidazole	954.9	987.0	2	pyridines
[$C_7H_{12}N_2$]	15802-80-9	3(5)-t-butylpyrazole	891.0	922.8	2	pyridines
[$C_7H_{12}N_2$]	52096-24-9	n-Butylpyrazole	897.3	928.8	3	pyrazole
[$C_7H_{12}N_2O_3$]	704-15-4	gly-pro	**905.6**	NE	NE	not estimated
[$C_7H_{12}N_2O_3$]	2578-57-6	pro-gly	**925.1**	NE	NE	not estimated
[$C_7H_{12}O$]	589-92-4	4-methylcyclohexanone	813.0	844.9	2	unsym ketones
[$C_7H_{12}O$]	502-42-1	cycloheptanone	815.9	845.6	9	sym ketones
[$C_7H_{12}O_2$]	98-89-5	Cyclohexane carboxylic acid	**792.8**	823.8	5	acids
[$C_7H_{13}N$]	100-76-5	1-azabicyclo[2.2.2]-octane	952.5	983.3	5.6	$(CH_3)_3N$
[$C_7H_{13}N$]	7242-92-4	Bicyclo[2.2.1]heptan-2-amine,exo	901.3	935.3	−5	CH_3NH_2
[$C_7H_{13}N$]	31002-73-0	Bicyclo[2.2.1]heptan-2-amine,endo	901.3	935.3	−5	CH_3NH_2
[$C_7H_{13}N_3$]	673-46-1	N_α,N_α-dimethylhistamine	990.1	1022.0	2	pyridines
[$C_7H_{13}N_3$]	5807-14-7	1,5,7-triazabicyclo [4.4.0]dec-5-ene	1022.1	1054.6	0	Rln(1/1)
[$C_7H_{13}N_3O_4$]	3146-40-5	ala-gly-gly	917.8	NE	NE	not estimated
[$C_7H_{13}N_3O_4$]	19729-30-7	gly-gly-ala	914.8	NE	NE	not estimated
[C_7H_{14}]	625-65-0	$(CH_3)_2C{=}CHCH(CH_3)_2$	783.1	812	12	propene
[$C_7H_{14}ClN$]	49665-74-9	c-C_5H_6N,2-CH_2Cl,1-CH_3	934.2	965.0	5.6	$(CH_3)_3N$
[$C_7H_{14}N_2$]	6238-14-8	3-Amino-1-azabicyclo[2.2.2]octane	954.7	985.5	5.6	$(CH_3)_3N$
[$C_7H_{14}N_2$]	6523-29-1	2-Methyl-1,2-diazabicyclo[2.2.2]-octane	938.1	968.9	5.6	$(CH_3)_3N$
[$C_7H_{14}N_2$]	14287-89-9	2,3-diazabicyclo[2.2.1]heptane, 2,3-dimethyl	945.6	978.0	0	Rln(1/1)
[$C_7H_{14}N_2$]	151328-39-1	$(CH_3)_2N$-$C(CH_3){=}N$(c-C_3H_5)	991.7	1024.1	0	Rln(1/1)
[$C_7H_{14}N_2O_3$]	1963-21-9	gly-val	**874.1**	NE	NE	not estimated
[$C_7H_{14}N_2O_3$]	686-43-1	val-gly	**874.1**	NE	NE	not estimated
[$C_7H_{14}O$]	100-49-2	c-$C_6H_{11}CH_2OH$	771.7	802.1	7	CH_3OH
[$C_7H_{14}O$]	931-56-6	c-$C_6H_{11}OCH_3$	811.3	840.5	11	unsym ethers
[$C_7H_{14}O$]	123-19-3	(n-$C_3H_7)_2CO$	815.3	845.0	9	sym ketones
[$C_7H_{14}O$]	565-80-0	(i-$C_3H_7)_2CO$	820.5	850.3	9	sym ketones
[$C_7H_{14}S$]	2550-37-0	c-$C_6H_{11}CH_2SH$	782.4	813.6	4	CH_3SH
[$C_7H_{14}S$]	6572-99-2	Heptamethylenesulfide	830.7	860.5	9	sym sulfides
[$C_7H_{14}S$]	7133-37-1	c-$C_6H_{11}SCH_3$	833.3	864.5	4	unsym sulfides
[$C_7H_{15}N$]	78733-73-0	$(CH_3)_2NC(C_2H_5){=}CHCH_3$	961	991.8	5.6	$(CH_3)_3N$
[$C_7H_{15}N$]	3218-02-8	c-$C_6H_{11}CH_2NH_2$	895.8	926.6	5.6	$(CH_3)_3N$
[$C_7H_{15}NO$]	24331-71-3	t-$C_4H_9CON(CH_3)_2$	895.2	927.1	2	amides
[$C_7H_{16}N_2$]	94793-20-1	$(CH_3)_2N$-$C(CH_3){=}N$(n-C_3H_7)	997.9	1030.3	0	Rln(1/1)
[$C_7H_{16}N_2$]	49840-68-8	1H-1,2-diazepine, hexahydro-1,2-dimethyl	936.1	966.8	5.8	Rln(2/1)
[$C_7H_{16}N_2$]	85599-92-4	$(CH_3)_2N$-CH=N-(1-methylpropyl)	985.7	1018.1	0	Rln(1/1)
[$C_7H_{16}N_2$]	94793-19-8	$(CH_3)_2N$-$C(CH_3){=}N$(i-C_3H_7)	999.2	1031.6	0	Rln(1/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[$C_7H_{16}N_2$]	3717-82-6	$(CH_3)_2N$-CH=N-(n-butyl)	980.5	1013.0	0	Rln(1/1)
[$C_7H_{16}N_2$]	67161-18-6	$(CH_3)_2N$-CH=N-(2-methylpropyl)	982.0	1014.5	0	Rln(1/1)
[$C_7H_{16}N_2$]	23314-06-9	$(CH_3)_2N$-CH=N(t-C_4H_9)	988.3	1020.8	0	Rln(1/1)
[$C_7H_{16}N_2O$]	151328-41-5	$(CH_3)_2N$-C(CH_3)=N$(CH_2)_2OCH_3$	1003.8	1036.2	0	Rln(1/1)
[$C_7H_{16}O$]	17348-59-3	(i-C_3H_7)O(t-C_4H_9)	841.5	870.7	11	unsym ethers
[$C_7H_{16}O_2$]	111-89-7	$CH_3O(CH_2)_5OCH_3$	879.5	931.3	−65	84SHA/BLA
[$C_7H_{17}N$]	57757-60-5	(t-C_5H_{11})$(CH_3)_2N$	951.5	982.5	5.6	$(CH_3)_3N$
[$C_7H_{17}N$]	10076-31-0	$(CH_3)_2$(neo-C_5H_{11})N	939.5	970.5	5.6	$(CH_3)_3N$
[$C_7H_{17}N$]	4458-31-5	$(C_2H_5)_2$(n-C_3H_7)N	947.9	978.8	5.6	$(CH_3)_3N$
[$C_7H_{17}N$]	6006-15-1	(i-C_3H_7)N$(C_2H_5)_2$	965.6	996.4	5.6	$(CH_3)_3N$
[$C_7H_{17}N$]	111-68-2	n-$C_7H_{15}NH_2$	889.3	923.2	−5	$CH_3CH_2NH_2$
[$C_7H_{17}N_3$]	13439-88-8	$((CH_3)_2N)_2C$=NC_2H_5	1019.0	1051.4	0	Rln(1/1)
[$C_7H_{17}N_3$]	101398-58-7	$(CH_3)_2N$-CH=N$(CH_2)_2N(CH_3)_2$	996.4	1028.8	0	Rln(1/1)
[$C_7H_{17}P$]	3405-42-3	(n-$C_3H_7)_2(CH_3)$P	950.9	983.5	0	Rln(1/1)
[$C_7H_{18}N_2$]	60678-73-1	(t-C_4H_9)(CH_3)NN$(CH_3)_2$	936.4	968.8	0	Rln(1/1)
[$C_7H_{18}N_2$]	110-95-2	$(CH_3)_2N(CH_2)_3N(CH_3)_2$	985.4	1035.2	−58	80MAU/HAM
[$C_7H_{18}N_2$]	52598-10-4	(n-C_4H_9)(CH_3)NN$(CH_3)_2$	938.1	970.5	0	Rln(1/1)
[$C_7H_{18}N_2$]	646-19-5	1,7-Diaminoheptane	944.9	998.5	−71	80MAU/HAM
[$C_7H_{19}NSi$]	23138-94-5	$(CH_3)_3Si(CH_2)_2N(CH_3)_2$	949.4	980.4	5.6	$(CH_3)_3N$
[$C_8H_4F_3N$]	368-77-4	3-(CF_3)-C_6H_4-CN	760.8	791.4	6	nitriles
[$C_8H_4F_3N$]	455-18-5	4-(CF_3)-C_6H_4-CN	758.3	787.2	11.8	nitriles+Rln(2/1)
[$C_8H_4N_2$]	626-17-5	1,3-$(CN)_2$-C_6H_4	750.4	779.3	11.8	nitriles+Rln(2/1)
[$C_8H_4N_2$]	623-26-7	1,4-$(CN)_2$-C_6H_4	751.8	779.0	17.5	nitriles+Rln(4/1)
[C_8H_5Cl]	873-73-4	4-Cl-C_6H_4-CCH	801.7	832.4	5.8	Rln(2/1)
[C_8H_5Cl]	766-83-6	3-ClC_6H_4CCH	779.8	812.3	0	Rln(1/1)
[$C_8H_5Cl_3O$]	2902-69-4	$C_6H_5COCCl_3$	787.0	818.9	2	unsym ketones
[C_8H_5F]	2561-17-3	3-FC_6H_4CCH	776.3	808.7	0	Rln(1/1)
[C_8H_5F]	766-98-3	4-FC_6H_4CCH	796.7	827.4	5.8	Rln(2/1)
[$C_8H_5F_3O$]	455-19-6	p-$CF_3C_6H_4$CHO	773.8	805.6	2	CH_3CHO
[$C_8H_5F_3O$]	434-45-7	$C_6H_5COCF_3$	767.4	799.2	2	unsym ketones
[C_8H_5NO]	105-07-7	4-CNC_6H_4CHO	766.3	796.9	6	nitriles
[C_8H_6]	536-74-3	C_6H_5-CCH	801.3	832.0	5.8	Rln(2/1)
[C_8H_6ClN]	64407-07-4	3-(CH_2Cl)-C_6H_4-CN	780.6	811.2	6	nitriles
[C_8H_6ClN]	874-86-2	4-(CH_2Cl)-C_6H_4-CN	782.1	812.8	6	nitriles
[$C_8H_6F_3NO$]	1801-10-1	3-CF_3-$C_6H_4CONH_2$	**836.0**	866.9	5	amides
[$C_8H_6F_3NO$]	1891-90-3	4-CF_3-$C_6H_4CONH_2$	**831.8**	862.8	5	amides
[$C_9H_6N_2$]	253-66-7	Cinnoline	904.4	936.3	2	pyridines
[$C_8H_6N_2$]	91-19-0	Quinoxaline	873.7	903.8	8	pyridines+Rln(2/1)
[C_8H_7Br]	2039-82-9	4-BrC_6H_4CH=CH_2	809.8	838.7	12	propene
[C_8H_7Br]	2039-86-3	3-BrC_6H_4CH=CH_2	793.5	822.4	12	propene
[C_8H_7Cl]	2039-85-2	3-ClC_6H_4CH=CH_2	812.6	841.5	12	propene
[C_8H-ClO]	99-02-5	3-Cl-C_6H_4-$COCH_3$	815.1	846.9	2	unsym ketones
[C_8H-ClO]	99-91-2	4-Cl-C_6H_4-$COCH_3$	824.8	856.6	2	unsym ketones
[C_8H-ClO_2]	2905-65-9	3-Cl-C_6H_4-$COOCH_3$	804.4	835.4	5	esters
[C_8H-ClO_2]	1126-46-1	4-Cl-C_6H_4-$COOCH_3$	811.1	842.1	5	esters
[C_8H-FO]	403-42-9	4-F-C_6H_4-$COCH_3$	826.8	858.6	2	unsym ketones
[C_8H-FO]	455-36-7	3-F-$C_6H_4COCH_3$	813.8	845.7	2	unsym ketones
[C_8H-FO_2]	455-68-5	3-F-C_6H_4-$COOCH_3$	801.9	832.9	5	esters
[C_8H-FO_2]	403-33-8	4-F-C_6H_4-$COOCH_3$	810.3	841.3	5	esters
[C_8H-FO_4S]	124397-38-2	4-SO_2F-C_6H_4-$COOCH_3$	771.6	802.6	5	esters
[C_8H-FO_4S]	124397-36-0	3-SO_2F-C_6H_4-$COOCH_3$	775.1	806.1	5	esters
[C_8H-N]	14235-81-5	4-H_2N-C_6H_4-CCH	882.0	912.7	5.8	Rln(2/1)
[C_8H-N]	140-29-4	Benzyl cyanide	774.8	805.5	6	nitriles
[C_8H-N]	120-72-9	Indole	901.9	933.4	3	pyrrole
[C_8H-NO_2S]	22821-76-7	4-(CH_3SO_2)-C_6H_4-CN	768.0	798.7	6	nitriles
[C_8H-NO_2S]	22821-75-6	3-(CH_3SO_2)-C_6H_4-CN	768.8	799.5	6	nitriles
[C_8H-NO_3]	121-89-1	3-NO_2-C_6H_4-$COCH_3$	794.1	826.0	2	unsym ketones
[C_8H-NO_3]	100-19-6	4-NO_2-C_6H_4-$COCH_3$	792.5	824.3	2	unsym ketones
[C_8H-NO_4]	619-50-1	4-O_2N-C_6H_4-$COOCH_3$	782.3	813.2	5	esters
[C_8H-NO_4]	618-95-1	3-O_2N-C_6H_4-$COOCH_3$	784.7	815.7	5	esters
[C_8H_8]	277-10-1	Cubane	833.6	859.9	20.6	Rln(24/2)
[C_8H_8]	100-42-5	$C_6H_5CHCH_2$	809.2	839.5	7.4	AUE
[C_8H_8]	32796-95-5	1,2-$C_6H_4(CH_3)_2$	**871.7**	898.8	18	propene+Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[C_8H_8]	502-86-3	1,4-$C_6H_4(=CH_2)_2$	**873.5**	900.6	18	propene+Rln(4/2)
[C_8H_8FeO]	12080-06-7	$(C_5H_5)Fe(CO)_2CH_3$	759.5	792.0	0	Rln(1/1)
[$C_8H_8N_2$]	934-37-2	2-Methylimidazo(1,2-a)pyridine	959.0	990.9	2	pyridines
[$C_8H_8N_2$]	933-69-7	5-Methylimidazo(1,2-a)pyridine	955.4	987.4	2	pyridines
[$C_8H_8N_2$]	1632-83-3	1-methylbenzimidazole	935.2	967.0	2	pyridines
[$C_8H_8N_2$]	4838-00-0	2-Methyl-2H-indazole	909.6	941.4	2	pyridines
[$C_8H_8N_2$]	874-39-5	7-Methylimidazo(1,2-a)pyridine	962.7	994.6	2	pyridines
[$C_8H_8N_2$]	13436-48-1	1-methylindazole	890.5	922.4	2	pyridines
[C_8H_8O]	104-87-0	4-$(CH_3)C_6H_4CHO$	820.0	851.8	2	CH_3CHO
[C_8H_8O]	620-23-5	3-$CH_3C_6H_4CHO$	808.1	840.0	2	CH_3CHO
[C_8H_8O]	98-86-2	$C_6H_5COCH_3$	829.3	861.1	2	unsym ketones
[$C_8H_8O_2$]	99-04-7	Benzoic acid, 3-methyl	**798.8**	829.8	5	acids
[$C_8H_8O_2$]	123-11-5	4-$CH_3OC_6H_4CHO$	849.3	881.1	2	aldehydes
[$C_8H_8O_2$]	99-93-4	4-HO-C_6H_4-$COCH_3$	851.9	883.7	2	unsym ketones
[$C_8H_8O_2$]	93-58-3	$C_6H_5CO_2CH_3$	819.5	850.5	5	esters
[$C_8H_8O_2$]	118-90-1	Benzoic acid, 2-methyl	**807.8**	838.8	5	acids
[$C_8H_8O_2$]	591-31-1	3-$CH_3OC_6H_4CHO$	812.2	844.1	2	aldehydes
[$C_8H_8O_2$]	121-71-1	3-HO-C_6H_4-$COCH_3$	831.8	863.6	2	unsym ketones
[$C_8H_8O_2$]	99-94-5	Benzoic acid, 4-methyl	**805.7**	836.7	5	acids
[$C_8H_8O_3$]	19438-10-9	3-HO-C_6H_4-$COOCH_3$	819.1	850.0	5	esters
[$C_8H_8O_3$]	99-76-3	4-HO-C_6H_4-$COOCH_3$	832.5	863.4	5	esters
[C_8H_9]	2348-51-8	$C_6H_5CHCH_3$ radical	**804**	836.5	0	?
[C_8H_9N]	533-35-7	3,4-Cyclopentenopyridine	930.5	962.4	2	pyridines
[C_8H_9N]	533-37-9	2,3-Cyclopentenopyridine	925.6	957.5	2	pyridines
[C_8H_9N]	696-18-4	Aziridine, 1-phenyl	895.7	926.5	5.6	$(CH_3)_3N$
[C_8H_9N]	496-15-1	2,3-Dihydroindole	926.3	957.1	5.6	$(CH_3)_3N$
[C_8H_9NO]	619-55-6	4-CH_3-$C_6H_4CONH_2$	**869.9**	900.9	5	amides
[C_8H_9NO]	618-47-3	3-CH_3-$C_6H_4CONH_2$	**869.9**	900.9	5	amides
[C_8H_9NO]	99-92-3	4-NH_2-C_6H_4-$COCH_3$	877.0	908.8	2	anilines
[$C_8H_9NO_2$]	89-87-2	2,4-Dimethylnitrobenzene	798.5	831.0	0	?
[$C_8H_9NO_2$]	619-45-4	4-NH_2-C_6H_4-$COOCH_3$	853.0	883.9	5	esters
[$C_8H_9NO_2$]	3424-93-9	4-CH_3O-$C_6H_4CONH_2$	**869.4**	900.3	5	amides
[$C_8H_9NO_2$]	5813-86-5	3-CH_3O-$C_6H_4CONH_2$	**869.9**	900.9	5	amides
[C_8H_{10}]	95-47-6	o-Xylene	768.3	796.0	16	aromatics
[C_8H_{10}]	106-42-3	p-Xylene	766.8	794.4	16	aromatics
[C_8H_{10}]	100-41-4	$C_2H_5C_6H_5$	760.3	788.0	16	toluene
[C_8H_{10}]	108-38-3	1,3-$(CH_3)_2$-C_6H_4	786.2	812.1	22	87LI/STO
[$C_8H_{10}ClN$]	698-69-1	4-$ClC_6H_4N(CH_3)_2$	896.4	922.9	20	anilines
[$C_8H_{10}FN$]	403-46-3	4-$FC_6H_4N(CH_3)_2$	898.3	924.8	20	anilines
[$C_8H_{10}F_5NS$]	#696	4-$SF_5C_6H_4N(CH_3)_2$	872.2	898.7	20	anilines
[$C_8H_{10}F_5NS$]	#678	3-$(CH_3)_2NC_6H_4SF_5$	874.5	901.0	20	anilines
[$C_8H_{10}N_2O_2$]	100-23-2	N,N-Dimethyl-4-nitroaniline	870.2	896.7	20	anilines
[$C_8H_{10}N_2O_2$]	619-31-8	3-$(NO_2)C_6H_4N(CH_3)_2$	867.6	894.1	20	anilines
[$C_8H_{10}O$]	538-86-3	$C_6H_5CH_2OCH_3$	787.5	816.7	11	unsym ethers
[$C_8H_{11}ClO$]	17530-69-7	3-Chloro-5,5-dimethylcyclohexen-2-one	836.0	867.9	2	unsym ketones
[$C_8H_{11}N$]	121-69-7	$C_6H_5N(CH_3)_2$	909.2	941.1	2	anilines
[$C_8H_{11}N$]	587-02-0	3-$C_2H_5C_6H_4NH_2$	866.1	897.9	2	anilines
[$C_8H_{11}N$]	64-01-0	$C_6H_5CH_2CH_2NH_2$	902.3	936.2	−5	CH_3NH_2
[$C_8H_{11}N$]	696-30-0	4-(i-C_3H_7)-C_5H_4N	923.8	955.7	2	pyridines
[$C_8H_{11}N$]	622-39-9	2-(C_3H_5)-pyridine	923.8	955.7	2	pyridines
[$C_8H_{11}N$]	75981-47-4	2-(i-C_3H_5)-pyridine	924.6	956.4	2	pyridines
[$C_8H_{11}N$]	103-69-5	$C_6H_5NHC_2H_5$	892.9	924.8	2	anilines
[$C_8H_{11}OP$]	10311-08-7	$(CH_3)_2(C_6H_5)PO$	**876.4**	908.9	0	Rln(1/1)
[$C_8H_{11}P$]	672-66-2	$C_6H_5P(CH_3)_2$	936.8	969.2	0	Rln(1/1)
[C_8H_{12}]	822-93-5	(c-C_3H_5)$_2$C=CH_2	875.8	904.7	12	propene
[C_8H_{12}]	497-35-8	2-Methylenebicyclo[2.2.1]heptane	831.8	860.7	12	propene
[C_8H_{12}]	694-92-8	2-Methylbicyclo[2.2.1]hept-2-ene	812.5	845	0	Rln(1/1)
[$C_8H_{12}F_3N$]	#363	1-Azabicyclo[2.2.2]octane,4-trifluoromethyl-	916.8	947.6	5.6	$(CH_3)_3N$
[$C_8H_{12}N_2$]	26458-78-6	1-azabicyclo[2.2.2]-octane, 4-cyano	902.3	933.1	5.6	$(CH_3)_3N$
[$C_8H_{12}N_2$]	51627-76-0	1-azabicyclo[2.2.2]-octane, 3-cyano	904.6	935.4	5.6	$(CH_3)_3N$
[$C_8H_{12}N_2$]	90196-91-1	1-azabicyclo[2.2.2]-octane, 2-cyano	895.6	926.4	5.6	$(CH_3)_3N$
[$C_8H_{12}N_2$]	99-98-9	4-$H_2NC_6H_4N(CH_3)_2$	928.4	955.0	20	anilines
[$C_8H_{12}N_2O_2$]	5744-40-1	1,3-dimethyl-5-ethoxycarbonylpyrazole	893.1	924.9	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_8H_{12}N_2O_2]$	5744-51-4	1,5-dimethyl-3-ethoxycarbonylpyrazole	901.5	933.4	2	pyridines
$[C_8H_{12}N_4O_3]$	2578-58-7	his-gly	**955.5**	NE	NE	not estimated
$[C_8H_{12}N_4O_3]$	2489-13-6	gly-his	**955.5**	NE	NE	not estimated
$[C_8H_{12}O]$	4694-17-1	5,5-Dimethylcyclohex-2-ene-1-one	837.9	869.8	2	unsym ketones
$[C_8H_{12}O]$	10599-58-3	2,3,4,5-tetramethylfuran	884.8	915.5	5.8	Rln(2/1)
$[C_8H_{13}N]$	#249	1-Azabicyclo[2.2.2]oct-2-ene, 3-methyl	950.8	981.6	5.6	$(CH_3)_3N$
$[C_8H_{13}N]$	22207-84-7	1-Azabicyclo[2.2.2]octane, 3-methylene	946.4	977.2	5.6	$(CH_3)_3N$
$[C_8H_{13}N]$	609-72-3	N,N,2-trimethylaniline	925.3	951.8	20	anilines
$[C_8H_{13}NO]$	873-95-0	3-Amino-5,5-dimethylcyclohex-2-enone	915.9	946.9	5	amide-like
$[C_8H_{14}]$	72014-90-5	$(CH_3)_2C{=}C(CH_3)C(CH_3){=}CH_2$	841.0	869.9	12	propene
$[C_8H_{14}N_2]$	141665-17-0	1-methyl-5-t-butylpyrazole	907.3	939.2	2	pyridines
$[C_8H_{14}N_2]$	141665-16-9	1-methyl-3-t-butylpyrazole	912.5	944.4	2	pyridines
$[C_8H_{14}N_2]$	19616-52-5	1,5-diazabicyclo[4.4.0]dec-6-ene (DBD)	1014.0	1046.4	0	Rln(1/1)
$[C_8H_{14}N_2]$	96440-80-1	3(5)-methyl-5(3)-t-butylpyrazole	914.3	946.2	2	pyridines
$[C_8H_{14}N_2]$	13618-34-3	3,5-diethyl-4-methylpyrazole	919.2	952.8	−4	pyridines+Rln(1/2)
$[C_8H_{14}N_4O_5]$	637-84-3	tetraglycine	928.2	973.8	−44	93CHE/WU
$[C_8H_{14}O]$	502-49-8	cyclooctanone	819.6	849.4	9	sym ketones
$[C_8H_{14}O]$	823-76-7	c-$C_6H_{11}COCH_3$	809.5	841.4	2	unsym ketones
$[C_8H_{14}O_2]$	4630-82-4	c-$C_6H_{11}COOCH_3$	815.3	846.2	5	esters
$[C_8H_{15}N]$	5261-65-4	1-azabicyclo[2.2.2]-octane, 2-methyl	956.1	986.9	5.6	$(CH_3)_3N$
$[C_8H_{15}N]$	45651-41-0	1-azabicyclo[2.2.2]-octane, 4-methyl	948.6	979.4	5.6	$(CH_3)_3N$
$[C_8H_{15}N]$	35079-50-6	1,4,4-$(CH_3)_3$-1,2,3,4-tetrahydropyridine	947.3	979.9	0	estimate
$[C_8H_{15}N]$	695-88-5	1-azabicyclo[2.2.2]-octane, 3-methyl	951.7	982.5	5.6	$(CH_3)_3N$
$[C_8H_{15}NO]$	17997-65-8	cis-3-Aminobicyclo[2.2.2]octan-2-ol	916.2	948.6	0	Rln(1/1)
$[C_8H_{15}NO]$	40335-14-6	trans-3-Aminobicyclo[2.2.2]octan-2-ol	899.2	933.1	−5	CH_3NH_2
$[C_8H_{15}N_3]$	84030-20-6	7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene	1030.2	1062.7	0	Rln(1/1)
$[C_8H_{16}N_2]$	14287-92-4	2,3-diazabicyclo[2.2.2]octane, 2,3-dimethyl	950.0	980.7	5.8	Rln(2/1)
$[C_8H_{16}N_2]$	3661-15-2	Pyridazino[1,2-a]pyridazine, octahydro-	947.9	978.7	5.8	Rln(2/1)
$[C_8H_{16}N_2]$	18389-95-2	1,1′-bipyrrolidine	949.0	979.7	5.8	Rln(2/1)
$[C_8H_{16}N_2O_3]$	3303-45-5	ala-val	**874.1**	NE	NE	not estimated
$[C_8H_{16}N_2O_3]$	27493-61-4	val-ala	**883.5**	NE	NE	not estimated
$[C_8H_{16}N_2O_4]$	13588-94-8	val-ser	**874.1**	NE	NE	not estimated
$[C_8H_{16}O]$	19752-94-4	$C_6H_{11}CH_2OCH_3$	801.6	833.5	2	unsym ketones
$[C_8H_{16}O]$	5857-36-3	i-C_3H_7CO(t-C_4H_9)	825.0	856.9	2	unsym ketones
$[C_8H_{16}O_4]$	294-93-9	12-crown-4	890.5	927.2	−14	84SHA/BLA; 83MAU
$[C_8H_{17}N]$	27644-32-2	N,3,5-Trimethylpiperidine	947.2	978.1	5.6	$(CH_3)_3N$
$[C_8H_{17}N]$	1003-84-5	1,4,4-Trimethylpiperidine	934.7	965.7	5.6	$(CH_3)_3N$
$[C_8H_{17}N]$	98-94-2	c-$C_6H_{11}N(CH_3)_2$	952.6	983.6	5.6	$(CH_3)_3N$
$[C_8H_{17}NO]$	26153-90-2	neo-$C_5H_{11}CON(CH_3)_2$	896.7	927.7	5	amides
$[C_8H_{17}N_3O_3]$	997-62-6	gly-lys	**945.6**	NE	NE	not estimated
$[C_8H_{17}N_3O_3]$	7563-03-3	lys-gly	**946.0**	NE	NE	not estimated
$[C_8H_{17}P]$	#181	$(CH_2)_5PCH_3$	947.2	979.7	0	Rln(1/1)
$[C_8H_{18}N_2]$	112752-57-5	$(CH_3)_2N$-C(C_2H_5)=N(i-C_3H_7)	1004.6	1037.0	0	Rln(1/1)
$[C_8H_{18}N_2]$	133835-17-3	$(CH_3)_2N$-CH=N-(1,1-dimethylpropyl)	989.6	1022.0	0	Rln(1/1)
$[C_8H_{18}N_2]$	94793-23-1	$(CH_3)_2N$-CH=N(n-C_5H_{11})	985.5	1018.0	0	Rln(1/1)
$[C_8H_{18}N_2]$	147350-05-8	$(CH_3)_2N$-C(CH_3)=N(t-C_4H_9)	1005.9	1038.3	0	Rln(1/1)
$[C_8H_{18}O]$	142-96-1	(n-C_4H_9)$_2$O	818.3	845.7	17	sym ethers
$[C_8H_{18}O]$	6163-66-2	(t-C_4H_9)$_2$O	860.0	887.4	17	sym ethers
$[C_8H_{18}O]$	6863-58-7	(sec-C_4H_9)$_2$O	838.5	865.9	17	sym ethers
$[C_8H_{18}O_4]$	112-49-2	$CH_3O[CH_2CH_2O]_3CH_3$	892.4	946.6	−73	84SHA/BLA; 83MAU
$[C_8H_{18}O_5]$	112-60-7	$HO[CH_2CH_2O]_4H$	>910	NE	NE	not estimated
$[C_8H_{18}S]$	544-40-1	(n-C_4H_9)$_2$S	842.1	871.8	9	sym sulfides
$[C_8H_{18}S]$	107-47-1	(t-C_4H_9)$_2$S	864.0	893.8	9	sym sulfides
$[C_8H_{19}N]$	111-86-4	n-$C_8H_{17}NH_2$	895.0	928.9	−5	CH_3NH_2
$[C_8H_{19}N]$	7087-68-5	(i-C_3H_7)$_2$(C_2H_5)N	963.5	994.3	5.6	$(CH_3)_3N$
$[C_8H_{19}N]$	111-92-2	(n-C_4H_9)$_2$NH	935.3	968.5	−1.9	$(CH_3)_2NH$
$[C_8H_{19}N]$	110-96-3	(i-C_4H_9)$_2$NH	925.1	958.1	−1.9	$(CH_3)_2NH$
$[C_8H_{19}N]$	626-23-3	(sec-C_4H_9)$_2$NH	947.5	980.7	−1.9	$(CH_3)_2NH$
$[C_8H_{19}N]$	21981-37-3	(t-C_4H_9)$_2$NH	954.7	987.9	−1.9	$(CH_3)_2NH$
$[C_8H_{20}N_2]$	151328-45-9	$(CH_3)_2NC(CH_3)=N(CH_3)_2N(CH_3)_2$	1016.1	1048.5	0	Rln(1/1)
$[C_8H_{20}N_2]$	29166-71-0	$(CH_3)_2N_2C=N(i\text{-}C_3H_7)$	1023.2	1055.6	0	Rln(1/1)
$[C_8H_{20}N_4]$	139033-04-8	$(CH_3)_2N$-CH=N-$(CH_2)_3N(CH_3)_2$	1010.6	1057.7	−49	$NH_2(CH_2)_3NH_2$
$[C_8H_{21}N_3]$	4267-00-9	$(C_2H_5)_2NN(C_2H_5)_2$	935.3	964.3	11.5	Rln(4/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_8H_{20}N_2]$	23337-88-4	Hydrazine, 1,2-dimethyl-1,2-dipropyl	941.2	971.9	5.8	Rln(2/1)
$[C_8H_{20}N_2]$	111-51-3	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	992.7	1046.3	−71	80MAU/HAM
$[C_8H_{21}NSi]$	28247-29-2	$(CH_3)_3Si(CH_2)_3N(CH_3)_2$	949.4	980.4	5.6	$(CH_3)_3N$
$[C_8H_{21}NSi]$	66365-05-7	$(CH_3)_2(t\text{-}C_4H_9)SiN(CH_3)_2$	938.8	969.8	5.6	$(CH_3)_3N$
$[C_9H_5F_3]$	705-28-2	3-CF_3-C_6H_4-CCH	773.8	806.2	0	Rln(1/1)
$[C_9H_7ClO]$	120136-29-0	3-Cl-4-CH_3O-C_6H_3-CCH	839.5	871.9	0	Rln(1/1)
$[C_9H_7ClS]$	120136-30-3	3-Cl-4-CH_3S-C_6H_3-CCH	836.1	868.6	0	Rln(1/1)
$[C_9H_7FO]$	120136-28-9	3-F-4-CH_3O-C_6H_3-CCH	839.5	871.9	0	Rln(1/1)
$[C_9H_7F_3]$	402-24-4	3-$CF_3C_6H_4CH{=}CH_2$	781.8	810.7	12	propene
$[C_9H_7F_3O]$	709-63-7	4-CF_3-C_6H_4-$COCH_3$	805.0	836.9	2	unsym ketones
$[C_9H_7F_3O]$	349-76-8	3-CF_3-C_6H_4-$COCH_3$	803.7	835.6	2	unsym ketones
$[C_9H_7F_3O_2]$	2967-66-0	3-CF_3-C_6H_4-$COOCH_3$	796.5	827.5	5	esters
$[C_9H_7F_3O_2]$	2557-13-3	4-CF_3-C_6H_4-$COOCH_3$	795.7	826.6	5	esters
$[C_9H_7MnO_3]$	12108-13-3	$(CH_3C_5H_4)Mn(CO)_3$	801.3	833.8	0	Rln(1/1)
$[C_9H_7N]$	91-22-5	Quinoline	921.4	953.2	2	pyridines
$[C_9H_7N]$	119-65-3	Isoquinoline	919.9	951.7	2	pyridines
$[C_9H_7NO]$	1443-80-7	4-CN-C_6H_4-$COCH_3$	795.0	826.8	2	unsym ketones
$[C_9H_7NO]$	6136-68-1	3-CN-C_6H_4-$COCH_3$	795.4	827.2	2	unsym ketones
$[C_9H_7NO]$	1613-37-2	Quinoline-1-oxide	910.8	943.3	0	Rln(1/1)
$[C_9H_7NO_2]$	13531-48-1	3-CN-C_6H_4-$COOCH_3$	786.5	817.4	5	esters
$[C_9H_7NO_2]$	1129-35-7	4-CN-C_6H_4-$COOCH_3$	785.6	816.6	5	esters
$[C_9H_8]$	766-82-5	3-CH_3-C_6H_4-CCH	810.6	843.0	0	Rln(1/1)
$[C_9H_8]$	95-13-6	indene	819.6	848.8	11	91MAU/SIE
$[C_9H_8]$	766-97-2	4-CH_3-C_6H_4-CCH	822.5	853.2	5.8	Rln(2/1)
$[C_9H_8CrO_3]$	41311-89-1	$(C_5H_5)Cr(CO)_3CH_3$	827.3	859.8	0	Rln(1/1)
$[C_9H_8N_2]$	2458-26-6	3(5)-phenylpyrazole	882.3	914.2	2	pyridines
$[C_9H_8N_2]$	10199-68-5	4-(C_6H_5)-pyrazole	871.8	906.0	−5.8	Rln(1/2)
$[C_9H_8O]$	768-60-5	4-CH_3O-C_6H_4-CCH	855.7	886.4	5.8	Rln(2/1)
$[C_9H_8O]$	4265-25-2	2-methylbenzofuran	827.2	859.6	0	?
$[C_9H_8O_3]$	1571-08-0	4-HC(O)-C_6H_4-$COOCH_3$	801.9	832.9	5	esters
$[C_9H_8S]$	56041-85-1	4-CH_3S-C_6H_4-CCH	854.1	886.6	0	?
$[C_9H_9Cl]$	1712-70-5	4-$ClC_6H_4C(CH_3){=}CH_2$	825.4	854.3	12	propene
$[C_9H_9ClOS]$	32467-66-6	3-Cl-4-CH_3S-C_6H_3-$COCH_3$	848.6	880.4	2	unsym ketones
$[C_9H_9ClO_2]$	37612-52-5	3-Cl-4-CH_3O-C_6H_3-$COCH_3$	851.9	883.7	2	unsym ketones
$[C_9H_9ClO_2S]$	105442-23-7	3-Cl-4-CH_3S-C_6H_3-$COOCH_3$	825.4	856.3	5	esters
$[C_9H_9ClO_3]$	37908-98-8	3-Cl-4-CH_3O-C_6H_3-$COOCH_3$	827.5	858.4	5	esters
$[C_9H_9F]$	3825-81-8	3-$FC_6H_4C(CH_3){=}CH_2$	810.8	839.7	12	propene
$[C_9H_9F]$	350-40-3	4-$FC_6H_4C(CH_3){=}CH_2$	833.7	862.6	12	propene
$[C_9H_9N]$	6921-29-5	$(HCCCH_2)_3N$	894.4	925.2	5.6	$(CH_3)_3N$
$[C_9H_9NO_2]$	64416-49-5	3-$(NO_2)C_6H_4C(CH_3){=}CH_2$	783.3	812.2	12	propene
$[C_9H_9NO_2]$	1830-68-8	4-$(NO_2)C_6H_4C(CH_3){=}CH_2$	786.5	815.4	12	propene
$[C_9H_{10}]$	873-49-4	c-C_3H_5-C_6H_5	802.4	834.9	0	Rln(1/1)
$[C_9H_{10}]$	873-66-5	Benzene, trans-(2-methylethenyl)	805.3	834.2	12	propene
$[C_9H_{10}]$	611-15-4	Benzene, 1-ethenyl-2-methyl	826.3	855.2	12	propene
$[C_9H_{10}]$	766-90-5	Benzene, cis-(2-methylethenyl)	807.5	836.4	12	propene
$[C_9H_{10}]$	100-80-1	3-CH_3-C_6H_4-$CH{=}CH_2$	820.5	849.4	12	propene
$[C_9H_{10}]$	622-97-9	4-CH_3-C_6H_4-$CH{=}CH_2$	832.8	861.7	12	propene
$[C_9H_{10}]$	98-83-9	C_6H_5-$C(CH_3){=}CH_2$	835.3	861.2	12	propene
$[C_9H_{10}ClNO]$	14062-80-7	4-Cl-$C_6H_4CON(CH_3)_2$	**896.9**	927.9	5	amides
$[C_9H_{10}ClNO]$	24167-52-0	3-Cl-$C_6H_4CON(CH_3)_2$	**896.9**	927.9	5	amides
$[C_9H_{10}FNO]$	24167-56-4	4-F-$C_6H_4CON(CH_3)_2$	**896.9**	927.9	5	amides
$[C_9H_{10}FNO]$	33322-64-4	3-F-$C_6H_4CON(CH_3)_2$	**896.9**	927.9	5	amides
$[C_9H_{10}F_3N]$	329-00-0	3-$CF_3C_6H_4N(CH_3)_2$	881.8	908.3	20	anilines
$[C_9H_{10}F_3N]$	329-17-9	4-$CF_3C_6H_4N(CH_3)_2$	876.8	903.2	20	anilines
$[C_9H_{10}F_3NS]$	#585	3-$(SCF_3)C_6H_4N(CH_3)_2$	887.7	914.2	20	anilines
$[C_9H_{10}N_2]$	1197-19-9	1,4-$(CH_3)_2NC_6H_2CN$	862.6	889.1	20	anilines
$[C_9H_{10}N_2]$	875-80-9	2,3-Dimethylimidazo(1,2-a)pyridine	966.4	998.2	2	pyridines
$[C_9H_{10}N_2]$	6188-30-3	2,5-Dimethylimidazo(1,2-a)pyridine	964.5	996.4	2	pyridines
$[C_9H_{10}N_2]$	3268-61-9	2,7-Dimethylimidazo(1,2-a)pyridine	968.6	1000.5	2	pyridines
$[C_9H_{10}N_2]$	38803-30-4	3-$(CH_3)_2NC_6H_2CN$	868.1	894.6	20	anilines
$[C_9H_{10}N_2O_3]$	7291-02-3	3-NO_2-$C_6H_2CON(CH_3)_2$	**869.9**	900.9	5	amides
$[C_9H_{10}N_2O_3]$	7291-01-2	4-NO_2-$C_6H_2CON(CH_3)_2$	**869.9**	900.9	5	amides
$[C_9H_{10}O]$	93-55-0	$C_6H_5COC_2H_5$	835.6	867.4	2	unsym ketones
$[C_9H_{10}O]$	103-79-7	$C_6H_5CH_2COCH_3$	810.8	842.6	2	unsym ketones

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_9H_{10}O]$	122-00-9	4-CH_3-C_6H_4-$COCH_3$	843.6	875.5	2	unsym ketones
$[C_9H_{10}O]$	585-74-0	3-CH_3-C_6H_4-$COCH_3$	836.4	868.2	2	unsym ketones
$[C_9H_{10}OS]$	1441-99-2	3-CH_3S-C_6H_4-$COCH_3$	834.7	866.6	2	unsym ketones
$[C_9H_{10}OS]$	1778-09-2	4-CH_3S-C_6H_4-$COCH_3$	856.3	888.2	2	unsym ketones
$[C_9H_{10}O_2]$	99-75-2	4-CH_3-C_6H_4-$COOCH_3$	830.6	861.5	5	esters
$[C_9H_{10}O_2]$	100-06-1	4-CH_3O-C_6H_4-$COCH_3$	863.7	895.6	2	unsym ketones
$[C_9H_{10}O_2]$	586-37-8	3-CH_3O-C_6H_4-$COCH_3$	839.3	871.2	2	unsym ketones
$[C_9H_{10}O_2]$	99-36-5	3-CH_3-C_6H_4-$COOCH_3$	826.8	857.7	5	esters
$[C_9H_{10}O_2]$	89-71-4	2-CH_3-$C_6H_4COOCH_3$	827.3	858.3	5	esters
$[C_9H_{10}O_2S]$	90721-40-7	3-CH_3S-C_6H_4-$COOCH_3$	822.4	853.4	5	esters
$[C_9H_{10}O_2S]$	3795-79-7	4-CH_3S-C_6H_4-$COOCH_3$	833.3	864.3	5	esters
$[C_9H_{10}O_3]$	5368-81-0	3-CH_3O-C_6H_4-$COOCH_3$	825.8	856.7	5	esters
$[C_9H_{10}O_3]$	121-98-2	4-CH_3O-C_6H_4-$COOCH_3$	839.6	870.6	5	esters
$[C_9H_{10}O_4S]$	22821-70-1	4-CH_3SO_2-$C_6H_4COOCH_3$	796.7	827.7	5	esters
$[C_9H_{10}O_4S]$	22821-69-8	3-CH_3SO_2-C_6H_4-$COOCH_3$	799.5	830.5	5	esters
$[C_9H_{11}]$	16804-70-9	$C_6H_5C(CH_3)_2$ radical	**809.7**	842.2	0	Rln(1/1)?
$[C_9H_{11}]$	19019-92-2	$C_6H_5(CHC_2H_5)$ radical	**809.7**	842.2	0	?
$[C_9H_{11}BrN_2]$	119044-60-9	$(CH_3)_2N$-CH=N-(4-bromophenyl)	948.9	981.3	0	Rln(1/1)
$[C_9H_{11}N]$	36556-06-6	Isoquinoline, 5,6,7,8-tetrahydro-	934.7	966.6	2	pyridines
$[C_9H_{11}N]$	1962-08-9	4-$H_2NC_6H_4C(CH_3)=CH_2$	903.3	929.8	20	anilines
$[C_9H_{11}N]$	3334-89-2	Azetidine, 1-phenyl	902.4	933.2	5.6	$(CH_3)_3N$
$[C_9H_{11}N]$	10500-57-9	Quinoline, 5,6,7,8-tetrahydro-	934.1	966.0	2	pyridines
$[C_9H_{11}NO]$	100-10-7	4-$CHOC_6H_4N(CH_3)_2$	898.3	924.8	20	anilines
$[C_9H_{11}NO]$	611-74-5	$C_6H_5CON(CH_3)_2$	901.8	932.7	5	amides
$[C_9H_{11}NO_2]$	603-71-4	2,4,6-Trimethylnitrobenzene	793.1	823.8	5.8	Rln(2/1)
$[C_9H_{11}NO_2]$	63-91-2	L-phenylalanine	888.9	922.9	−5	$CH_3CH_2NH_2$
$[C_9H_{11}NO_3]$	60-18-4	L-tyrosine	892.1	926	−5	CH_3NH_2
$[C_9H_{11}N_3O_2]$	74739-51-8	$(CH_3)_2N$-CH=N-(4-nitrophenyl)	917.8	950.2	0	Rln(1/1)
$[C_9H_{12}]$	108-67-8	1,3,5-$(CH_3)_3$-C_6H_3	808.6	836.2	16.2	86STO/XI
$[C_9H_{12}]$	103-65-1	n-$C_3H_7C_6H_5$	762.4	790.1	16	aromatics
$[C_9H_{12}]$	98-82-8	i-$C_3H_7C_6H_5$	763.9	791.6	16	aromatics
$[C_9H_{12}N_2]$	56687-95-7	$(CH_3)_2N$-CH=N-phenyl	951.3	983.8	0	Rln(1/1)
$[C_9H_{12}N_2]$	494-97-3	3-(2-pyrrolidinyl)pyridine	931.0	964.0	−2	$(CH_3)_2NH$
$[C_9H_{12}N_2O]$	33322-60-0	3-NH_2-$C_6H_4CON(CH_3)_2$	**913.5**	944.4	5	amides
$[C_9H_{12}N_2O]$	6331-71-1	4-NH_2-$C_6H_4CON(CH_3)_2$	**925.9**	956.9	5	amides
$[C_9H_{12}N_2O_4]$	37687-24-4	3,5-diethoxycarbonylpyrazole	849.7	881.6	2	pyridines
$[C_9H_{12}N_2O_6]$	58-96-8	Uridine	916.6	947.6	5	amides
$[C_9H_{12}O_3]$	621-23-8	1,3,5-$C_6H_3(OCH_3)_3$	898.2	926.7	13	aromatics
$[C_9H_{13}N]$	3978-81-2	4-(t-C_4H_9)-pyridine	925.8	957.7	2	pyridines
$[C_9H_{13}N]$	613-97-8	$C_6H_5N(CH_3)(C_2H_5)$	912.4	939.0	20	anilines
$[C_9H_{13}N]$	103-83-3	$C_6H_5CH_2N(CH_3)_2$	937.4	968.4	5.6	$(CH_3)_3N$
$[C_9H_{13}N]$	121-72-2	3-$CH_3C_6H_4N(CH_3)_2$	915.7	942.1	20	anilines
$[C_9H_{13}N]$	5944-41-2	2-(t-C_4H_9)-pyridine	929.8	961.7	2	pyridines
$[C_9H_{13}N]$	99-97-8	4-$CH_3C_6H_4N(CH_3)_2$	918.1	950.0	2	anilines
$[C_9H_{13}N]$	935-28-4	2,6-$(C_2H_5)_2$-pyridine	940.4	972.3	2	pyridines
$[C_9H_{13}NO]$	701-56-4	4-$CH_3OC_6H_4N(CH_3)_2$	922.4	949.1	20	anilines
$[C_9H_{13}NO]$	15799-79-8	3-Methoxy-N,N-dimethylbenzenamine	894.1	920.6	20	anilines
$[C_9H_{13}N_2O_4]$	951-77-9	Deoxycytidine	956.0	988.4	0	Rln(1/1)
$[C_9H_{13}N_3O_5]$	65-46-3	cytidine	950.0	982.5	0	Rln(1/1)
$[C_9H_{14}N_2O_6]$	5627-05-4	5,6-Dihydrouridine	**841.7**	874.2	0	Rln(1/1)
$[C_9H_{14}N_4]$	111062-19-2	1H-dimidazo[1,2-d:2',1'-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro (TTT)	>1049	>1081	0	Rln(1/1)
$[C_9H_{14}O]$	78-59-1	Isophorone	861.6	893.5	2	unsym ketones
$[C_9H_{14}O_2]$	4683-45-8	3-Methoxy-5,5-dimethylcyclohex-2-enone	890.1	922.6	0	?
$[C_9H_{15}N]$	102-70-5	$(CH_2=CHCH_2)_3N$	941.3	972.3	5.6	$(CH_3)_3N$
$[C_9H_{15}N]$	7148-07-4	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	988.4	1019.2	5.6	$(CH_3)_3N$
$[C_9H_{15}N_3O_4]$	14379-76-1	gly-gly-pro	**915.5**	NE	NE	not estimated
$[C_9H_{15}N_3O_4]$	7561-25-3	pro-gly-gly	**925.1**	NE	NE	not estimated
$[C_9H_{15}N_3O_4]$	2441-63-6	gly-pro-gly	**915.5**	NE	NE	not estimated
$[C_9H_{16}N_2]$	6674-22-2	1,8-diazabicyclo [5.4.0]undec-7-ene	1015.5	1047.9	0	Rln(1/1)
$[C_9H_{16}N_2O_4]$	13433-04-0	asp-val	**874.1**	NE	NE	not estimated
$[C_9H_{16}N_2O_4]$	20556-16-5	val-asp	**874.1**	NE	NE	not estimated
$[C_9H_{18}O]$	3350-30-9	c-Nonanone	822.8	852.6	9	sym ketones
$[C_9H_{19}N]$	673-33-6	c-$C_5H_{10}NCH=C(CH_3)_2$	949.4	978.2	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_9H_{17}NO_2]$	#231	3,3-Dimethoxy-1-azabicyclo[2.2.2]octane	954.7	985.7	5.6	$(CH_3)_3N$
$[C_9H_{17}N_3]$	95510-44-4	7-ethyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ETBD)	1035.8	1068.2	0	Rln(1/1)
$[C_9H_{18}NO]$	2564-83-2	2,2,6,6-tetramethyl-1-piperidinyloxy radical	**849.8**	882.3	0	Rln(1/1)
$[C_9H_{17}N_3O_4]$	5874-90-8	tri-L-alanine	924.1	NE	NE	not estimated
$[C_9H_{18}N_2]$	283-58-9	1,5-Diazabicyclo[3.3.3]undecane	940.1	971.1	5.6	$(CH_3)_3N$
$[C_9H_{18}N_2]$	3459-75-4	$(CH_3)_2N$-CH=N-(c-hexyl)	987.9	1020.4	0	Rln(1/1)
$[C_9H_{18}N_2]$	22766-69-4	1-Azabicyclo[2.2.2]octane,4-N,N-dimethylamino-	952.9	983.9	5.6	$(CH_3)_3N$
$[C_9H_{18}O]$	815-24-7	$(t\text{-}C_4H_9)_2CO$	831.5	861.3	9	sym ketones
$[C_9H_{18}O]$	502-56-7	$(n\text{-}C_4H_9)_2CO$	821.9	853.7	2	unsym ketones
$[C_9H_{18}S]$	54396-69-9	$(t\text{-}C_4H_9)_2CS$	852.0	881.8	9	*sym ketones*
$[C_9H_{19}N]$	16607-80-0	$c\text{-}C_6H_{11}CH_2N(CH_3)_2$	944.7	975.6	5.6	$(CH_3)_3N$
$[C_9H_{19}N]$	10315-89-6	N-Isobutylpiperidine	943.5	974.5	5.6	$(CH_3)_3N$
$[C_9H_{19}N]$	768-66-1	2,2,6,6-Tetramethyl-piperidine	953.9	987.0	−1.9	$(CH_3)_2NH$
$[C_9H_{20}N_2]$	85599-94-6	$(CH_3)_2N$-CH=N-(n-hexyl)	984.9	1017.4	0	Rln(1/1)
$[C_9H_{20}N_2]$	151328-44-8	$(CH_3)_2N\text{-}C(C_2H_5)=N(t\text{-}C_4H_9)$	1010.9	1043.3	0	Rln(1/1)
$[C_9H_{20}N_2]$	94793-24-5	$(CH_3)_2N\text{-}C(CH_3)=N(n\text{-}C_5H_{11})$	1002.1	1034.5	0	Rln(1/1)
$[C_9H_{20}N_2]$	151328-42-6	$(C_2H_5)_2N\text{-}C(CH_3)=N(n\text{-}C_3H_7)$	1005.5	1037.9	0	Rln(1/1)
$[C_9H_{21}N]$	102-69-2	$(n\text{-}C_3H_7)_3N$	960.1	991.0	5.6	$(CH_3)_3N$
$[C_9H_{21}N]$	3733-36-6	$(t\text{-}C_4H_9)C(CH_3)_2N(CH_3)_2$	951.4	982.4	5.6	$(CH_3)_3N$
$[C_9H_{21}N]$	58471-09-3	$(t\text{-}C_5H_{11})(t\text{-}C_4H_9)NH$	958.2	991.4	−2	$(CH_3)_2NH$
$[C_9H_{21}N_3]$	34331-58-3	$((CH_3)_2N)_2C=N(t\text{-}C_4H_9)$	1029.4	1061.8	0	Rln(1/1)
$[C_8H_{19}N]$	15673-04-8	$(CH_3)_3C(CH_2)_2N(CH_3)_2$	942.0	973.0	5.6	$(CH_3)_3N$
$[C_9H_{21}N_3]$	151328-47-1	$(CH_3)_2NC(CH_3)=N\text{-}(CH_2)_3N(CH_3)_2$	1030.5	1077.5	−49	80MAU/HAM
$[C_9H_{21}OP]$	17513-58-5	$(i\text{-}C_3H_7)_3PO$	924.5	954.4	9.1	Rln(3/1)
$[C_9H_{21}OP]$	1496-94-2	$OP(n\text{-}C_3H_7)_3$	918.4	948.2	9.1	Rln(3/1)
$[C_9H_{24}N_3OP]$	2327-88-0	$OP(CH_2N(CH_3)_2)_3$	965.2	997.7	0	Rln(1/1)
$[C_{10}H_7CrO_3]$	32984-97-7	$(C_6H_5CH_2)Cr(CO)_3$	819.9	852.4	0	Rln(1/1)
$[C_{10}H_8]$	275-51-4	azulene	896	925.2	11	average
$[C_{10}H_8]$	91-20-3	Naphthalene	779.4	802.9	30	88LI/STO
$[C_{10}H_9F_3]$	55186-75-9	$4\text{-}CF_3C_6H_4C(CH_3)CH_2$	796.6	825.5	12	*propene*
$[C_{10}H_9F_3]$	368-79-6	$3\text{-}CF_3C_6H_4C(CH_3)=CH_2$	794.8	823.7	12	propene
$[C_{10}H_9F_6N]$	34060-81-6	$3,5\text{-}(CF_3)_2C_6H_3N(CH_3)_2$	858.4	884.9	20	anilines
$[C_{10}H_9N]$	134-32-7	1-Naphthalenamine	875.1	907.0	2	anilines
$[C_{10}H_{10}]$	6366-06-9	$3,5\text{-}(CH_3)_2\text{-}C_6H_3CCH$	819.7	850.4	5.8	Rln(2/1)
$[C_{10}H_{10}F_3NO]$	25771-21-5	$4\text{-}CF_3\text{-}C_6H_4CON(CH_3)_2$	**873.5**	904.5	5	amides
$[C_{10}H_{10}F_3NO]$	90238-10-1	$3\text{-}CF_3\text{-}C_6H_4CON(CH_3)_2$	**876.2**	907.1	5	amides
$[C_{10}H_{10}Fe]$	102-54-5	$(C_5H_5)_2Fe$	841.3	863.6	34	average
$[C_{10}H_{10}N_2]$	3463-27-2	1-methyl-5-phenylpyrazole	900.5	932.4	2	pyridines
$[C_{10}H_{10}N_2]$	3463-26-1	1-methyl-3-phenylpyrazole	900.8	932.6	2	pyridines
$[C_{10}H_{10}N_2]$	479-27-6	1,8-Diaminonaphthalene	912.1	944.5	0	?
$[C_{10}H_{10}N_2]$	3347-62-4	3(5)-methyl-5(3)-phenylpyrazole	900.2	932.1	2	pyridines
$[C_{10}H_{10}Ni]$	1271-28-9	$Ni(C_5H_5)_2$	907.3	935.7	13.4	Rln(5/1)
$[C_{10}H_{10}O_2]$	6781-42-6	$3\text{-}CH_3CO\text{-}C_6H_4\text{-}COCH_3$	822.3	852.0	9	sym ketones
$[C_{10}H_{10}O_2]$	1009-61-6	$4\text{-}CH_3CO\text{-}C_6H_4\text{-}COCH_3$	821.0	850.8	9	sym ketones
$[C_{10}H_{10}O_2]$	90843-31-5	1-(2,3-dihydro-5-benzofuranyl)-ethanone	870.7	902.6	2	unsym ketones
$[C_{10}H_{10}O_3]$	13031-43-1	$4\text{-}CH_3COO\text{-}C_6H_4\text{-}COCH_3$	821.3	853.2	2	unsym ketones
$[C_{10}H_{10}O_4]$	1459-93-4	$3\text{-}CH_3COO\text{-}C_6H_4\text{-}COOCH_3$	814.3	843.5	10.8	esters+*Rln(2/1)*
$[C_{10}H_{10}O_4]$	120-61-6	$4\text{-}CH_3COO\text{-}C_6H_4\text{-}COOCH_3$	812.3	843.2	5	esters
$[C_{10}H_{10}Ru]$	1287-13-4	$(C_5H_5)_2Ru$	876.8	899.1	34	$(C_5H_5)_2Fe$
$[C_{10}H_{11}N_3]$	119044-58-5	$(CH_3)_2N$-CH=N-(4-cyanophenyl)	919.8	952.2	0	Rln(1/1)
$[C_{10}H_{12}]$	6921-43-3	Benzene, 1-cyclopropyl-4-methyl-	813.8	846.3	0	?
$[C_{10}H_{12}]$	7399-49-7	Benzene, 1-methyl-2-(1-methylethenyl)-	828.9	857.8	12	propene
$[C_{10}H_{12}]$	27546-46-9	Benzene, 1-cyclopropyl-2-methyl-	807.9	840.4	0	?
$[C_{10}H_{12}]$	1195-32-0	$4\text{-}CH_3C_6H_4C(CH_3)CH_2$	852.9	881.8	12	propene
$[C_{10}H_{12}]$	19714-73-9	Benzene, 1-cyclopropyl-3-methyl-	803.3	835.8	0	?
$[C_{10}H_{12}]$	1124-20-5	Benzene, 3-methyl-3-(1-methylethenyl)-	838.7	867.6	12	propene
$[C_{10}H_{12}]$	119-64-2	1,2,3,4-Tetrahydronaphthalene	782.1	809.7	16	*aromatics*
$[C_{10}H_{12}]$	26444-18-8	$3\text{-}CH_3C_6H_4C(CH_3)=CH_2$	842.4	871.3	12	propene
$[C_{10}H_{12}ClN]$	4280-30-2	Pyrrolidine, 1-(4-chlorophenyl)	906.6	937.4	5.6	$(CH_3)_3N$
$[C_{10}H_{12}NS]$	74362-50-8	$4\text{-}CH_3SC_6H_4C(CH_3)=CH_2$	917.4	946.2	12	propene
$[C_{10}H_{12}N_2]$	34165-19-0	2,3,5-Trimethylimidazo(1,2-a)-pyridine	973.7	1005.5	2	pyridines
$[C_{10}H_{12}O]$	25108-57-0	$3\text{-}CH_3OC_6H_3C(CH_3)=CH_2$	843.7	872.6	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[$C_{10}H_{12}O$]	2142-73-6	2,5-$(CH_3)_2C_6H_3$-$COCH_3$	841.6	873.5	2	unsym ketones
[$C_{10}H_{12}O$]	5379-16-8	3,5-(CH_3)=C_6H_3-$COCH_3$	844.2	876.0	2	unsym ketones
[$C_{10}H_{12}O$]	3637-01-2	3,4-$(CH_3)_2C_6H_3$-$COCH_3$	851.0	882.8	2	unsym ketones
[$C_{10}H_{12}O$]	1712-69-2	4-$CH_3OC_6H_4C(CH_3)$=CH_2	882.2	911.1	12	propene
[$C_{10}H_{12}O$]	2142-76-9	2,6-$(CH_3)_2C_6H_3$-$COCH_3$	825.2	857.0	2	unsym ketones
[$C_{10}H_{12}O$]	89-74-7	2,4-$(CH_3)_2C_6H_3$-$COCH_3$	850.8	882.6	2	unsym ketones
[$C_{10}H_{12}O$]	2142-71-4	2,3-(CH_3)=C_6H_3-$COCH_3$	842.7	874.6	2	unsym ketones
[$C_{10}H_{12}O_2$]	23617-71-2	2,4-$(CH_3)_2$-C_6H_3-$COOCH_3$	837.2	868.2	5	esters
[$C_{10}H_{12}O_2$]	15012-36-9	2,3-$(CH_3)_2$-C_6H_3-$COOCH_3$	832.7	863.6	5	esters
[$C_{10}H_{12}O_2$]	14920-81-1	2,6-$(CH_3)_2$-C_6H_3-$COOCH_3$	824.3	855.3	5	esters
[$C_{10}H_{12}O_2$]	38404-42-1	3,4-$(CH_3)_3$-C_6H_3-CO_2CH_3	837.5	868.5	5	esters
[$C_{10}H_{12}O_2$]	13730-55-7	2,5-(CH_3)2-C_6H_3-$COOCH_3$	833.7	864.7	5	esters
[$C_{10}H_{12}O_2$]	25081-39-4	3,5-$(CH_3)_2$-C_6H_3-$COOCH_3$	833.4	864.3	5	esters
[$C_{10}H_{12}S$]	#838	3-$(CH_3S)C_6H_4C(CH_3)$=CH_2	850.6	879.5	12	propene
[$C_{10}H_{13}N$]	4096-21-3	N-Phenylpyrrolidine	915.1	941.6	20	anilines
[$C_{10}H_{13}NO$]	18992-80-8	3-$(CH_3)_2NC_6H_4COCH_3$	901.5	928.0	20	anilines
[$C_{10}H_{13}NO$]	6935-65-5	3-CH_3-$C_6H_4CON(CH_3)_2$	**896.0**	927.0	5	amides
[$C_{10}H_{13}NO$]	14062-78-3	4-CH_3-$C_6H_4CON(CH_3)_2$	**896.0**	927.0	5	amides
[$C_{10}H_{13}NO$]	2124-31-4	4-[$(CH_3)_2N$]-C_6H_4-$COCH_3$	906.3	932.8	20	anilines
[$C_{10}H_{13}NO_2$]	7290-99-5	3-CH_3O-$C_6H_4CON(CH_3)_2$	**896.0**	927.0	5	amides
[$C_{10}H_{13}NO_2$]	1202-25-1	4-$(CH_3)_2NC_6H_4COOCH_3$	894.1	920.6	20	anilines
[$C_{10}H_{13}NO_2$]	16518-64-2	3-$(CH_3)_2NC_6H_4COOCH_3$	903.8	930.2	20	anilines
[$C_{10}H_{13}NO_2$]	7291-00-1	4-CH_3O-$C_6H_4CON(CH_3)_2$	**917.4**	948.3	5	amides
[$C_{10}H_{13}N_5O_2$]	118-00-3	guanosine	960.9	993.4	0	Rln(1/1)
[$C_{10}H_{13}N_5O_3$]	958-09-8	Deoxyadenosine	959.1	991.5	0	Rln(1/1)
[$C_{10}H_{13}N_5O_4$]	961-07-9	Deoxyguanosine	962.9	995.4	0	Rln(1/1)
[$C_{10}H_{13}N_5O_4$]	58-61-7	adenosine	956.8	989.3	0	Rln(1/1)
[$C_{10}H_{14}$]	527-53-7	1,2,3,5-$(CH_3)_4$-C_6H_2	816.5	845.6	11.4	86STO/XI
[$C_{10}H_{14}$]	104-51-8	n-$C_4H_9C_6H_5$	764.2	791.9	16	aromatics
[$C_{10}H_{14}BrN$]	50638-54-5	N,N,2,6-Tetramethylaniline,4-bromo-	902.9	935.4	0	anilines-restricted
[$C_{10}H_{14}ClN$]	2873-89-4	4-$ClC_6H_4N(C_2H_5)_2$	899.2	931.0	2	anilines
[$C_{10}H_{14}FN$]	14994-35-5	N,N,2,6-Tetramethylaniline,4-fluoro	910.7	943.2	0	anilines-restricted
[$C_{10}H_{14}N_2$]	54-11-5	3-(2-(N-methylpyrrolidinyl))pyridine	932.6	963.4	5.6	$(CH_3)_3N$
[$C_{10}H_{14}N_2$]	119044-57-4	$(CH_3)_2N$-C(C_6H_5)=NCH_3	1000.9	1033.3	0	Rln(1/1)
[$C_{10}H_{14}N_2$]	27159-75-7	$(CH_3)_2N$-CH=N-(phenylmethyl)	981.7	1014.1	0	Rln(1/1)
[$C_{10}H_{14}N_2$]	56638-68-7	$(CH_3)_2N$-CH=N-(4-methylphenyl)	956.1	988.6	0	Rln(1/1)
[$C_{10}H_{14}N_2O$]	59-26-7	N,N-diethylnicotinamide	909.0	940.9	2	pyridines
[$C_{10}H_{14}N_2O_2$]	24558-36-9	N,N,2,6-Tetramethyl-4-nitroaniline	886.0	918.4	0	anilines-restricted
[$C_{10}H_{14}N_2O_2S$]	28809-04-3	S-(2-(4-pyridyl)ethyl)cysteine	>869	NE	NE	not estimated
[$C_{10}H_{14}N_2O_4$]	100852-80-0	1-methyl-3,5-diethoxycarbonylpyrazole	881.5	913.4	2	pyridines
[$C_{10}H_{14}N_2O_5$]	50-89-5	Thymidine	915.9	948.3	0	Rln(1/1)
[$C_{10}H_{14}O_3$]	#997	3-Acetyl-5,5-dimethylcyclohexen-2-one	828.8	861.2	0	Rln(1/1)
[$C_{10}H_{15}N$]	769-06-2	N,N,2,6-Tetramethylaniline	923.2	954.1	5.6	$(CH_3)_3N$
[$C_{10}H_{15}N$]	4913-13-7	3,5-$(CH_3)_2C_6H_3N(CH_3)_2$	924.3	956.1	2	anilines
[$C_{10}H_{15}N$]	91-66-7	$C_6H_5N(C_2H_5)_2$	927.9	959.8	2	anilines
[$C_{10}H_{15}N_5O_4$]	7451-76-5	gly-gly-his	979.5	NE	NE	not estimated
[$C_{10}H_{15}N_5O_4$]	32999-80-7	his-gly-gly	**946.0**	NE	NE	not estimated
[$C_{10}H_{15}N_5O_4$]	7758-33-0	gly-his-gly	**955.5**	NE	NE	not estimated
[$C_{10}H_{20}N_4O_4$]	45214-22-0	gly-lys-gly	**955.5**	NE	NE	not estimated
[$C_{10}H_{16}$]	16609-28-2	1,5,5-Trimethyl-3-methylenecyclohexene	874.2	904.9	6	propene-Rln2
[$C_{10}H_{16}N_2$]	704-01-8	1,2-$(N(CH_3)_2)_2C_6H_4$	950.2	982.6	0	?
[$C_{10}H_{16}N_2O_3$]	20488-28-2	pro-pro	**944.8**	NE	NE	not estimated
[$C_{10}H_{16}N_4$]	111062-21-6	1H-diimidazo[1,2-d:2',1'-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro-1-methyl (MTTT)	>1060	>1091	0	Rln(1/1)
[$C_{10}H_{16}O$]	76-22-2	Camphor	827.3	859.2	2	unsym ketones
[$C_{10}H_{16}S$]	7519-74-6	thiocamphor	852.0	883.9	2	unsym ketones
[$C_{10}H_{17}N$]	768-94-5	Tricyclo[3.3.1.1^{3,7}]decane-1-amine	916.3	948.8	0	Rln(1/1)
[$C_{10}H_{17}NO$]	31039-88-0	3-(N,N-Dimethylamino)-5,5-dimethyl-cyclohex-2-en-1-one	952.9	983.8	5.6	$(CH_3)_3N$
[$C_{10}H_{17}NO$]	33540-02-2	tricyclo[4.4.0.0^{3,8}]decan-4-ol-5-amino, stereoisomer	914.5	947.0	0	?
[$C_{10}H_{17}NO$]	33701-54-1	5-amino-tricyclo[4.4.0.0^{3,8}]decan-4-ol	896.0	928.4	0	?
[$C_{10}H_{17}NO$]	52305-49-4	tricyclo[4.4.0.0^{3,8}]decan-4-ol-5-amino, stereoisomer	916.6	949.0	0	?
[$C_{10}H_{17}N_5O_6$]	7093-67-6	pentaglycine	921	NE	NE	not estimated

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_{10}H_{18}N_2O_3]$	52899-09-9	pro-val	**909.0**	NE	NE	not estimated
$[C_{10}H_{18}N_2O_3]$	20488-27-1	val-pro	**918.8**	NE	NE	not estimated
$[C_{10}H_{18}N_2O_5]$	3062-07-5	val-glu	921	NE	NE	not estimated
$[C_{10}H_{19}N]$	31023-92-4	1-Azabicyclo[3.3.3]undecane (Manxine)	947.7	978.7	5.6	$(CH_3)_3N$
$[C_{10}H_{19}NO]$	29910-43-8	2-Naphthalenol, 3-aminodecahydro-(2,3β,4α, 8$\alpha\beta$)	914.5	947.0	0	?
$[C_{10}H_{19}N_3]$	160172-95-2	7-isopropyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ITBD)	1039.2	1071.6	0	Rln(1/1)
$[C_{10}H_{19}N_3O_4]$	1187-50-4	leu-gly-gly	926.7	NE	NE	not estimated
$[C_{10}H_{19}N_3O_4]$	2576-67-2	gly-leu-gly	921.8	NE	NE	not estimated
$[C_{10}H_{19}N_3O_4]$	14857-82-0	gly-gly-leu	918.1	NE	NE	not estimated
$[C_{10}H_{20}N_2]$	6130-94-5	1,1′-bipiperidine	950.4	981.2	5.8	Rln(2/1)
$[C_{10}H_{20}N_2O_3]$	14486-13-6	met-val	**899.0**	NE	NE	not estimated
$[C_{10}H_{20}N_2O_3]$	14486-09-0	val-met	**909.0**	NE	NE	not estimated
$[C_{10}H_{20}N_2O_3]$	3918-94-3	val-val	**883.5**	NE	NE	not estimated
$[C_{10}H_{20}N_4O_4]$	10236-53-0	gly-gly-lys	**958.6**	NE	NE	not estimated
$[C_{10}H_{20}N_4O_4]$	55488-08-9	lys-gly-gly	**958.6**	NE	NE	not estimated
$[C_{10}H_{20}N_6O_4]$	54944-27-3	gly-gly-arg	1028.5	NE	NE	not estimated
$[C_{10}H_{20}O_5]$	33100-27-5	15-Crown-5	899.7	943.8	−39	84SHA/BLA
$[C_{10}H_{22}N_2]$	107322-35-0	$(CH_3)_2N$-C(C_2H_5)=N(n-C_5H_{11})	1005.5	1037.9	0	Rln(1/1)
$[C_{10}H_{22}N_2]$	94793-26-7	$(CH_3)_2N$-C(CH_3)=N(n-C_6H_{13})	1000.9	1033.3	0	Rln(1/1)
$[C_{10}H_{22}O]$	693-65-2	(n-C_5H_{11})$_2$O	825.3	852.7	17	sym ethers
$[C_{10}H_{22}O_5]$	143-24-8	$CH_3O[CH_2CH_2O]_4CH_3$	897.8	953.8	−79	84SHA/BLA
$[C_{10}H_{22}O_6]$	4792-15-8	$HO[CH_2CH_2O]_5H$	>910	NE	NE	not estimated
$[C_{10}H_{23}N]$	2016-57-1	n-($C_{10}H_{21}$)NH_2	896.5	930.4	−5	CH_3NH_2
$[C_{10}H_{24}N_2]$	68970-05-8	Hydrazine, 1,2-dimethyl-1,2-bis(2-methylpropyl)	949.0	979.7	5.8	Rln(2/1)
$[C_{10}H_{24}N_2]$	116149-14-5	Hydrazine, 1,2-dibutyl-1,2-dimethyl	945.2	975.9	5.8	Rln(2/1)
$[C_{10}H_{24}N_2]$	111-18-2	$(CH_3)_2N(CH_2)_6N(CH_3)_2$	982.2	1035.8	−71	80MAU/HAM
$[C_{11}H_9N]$	939-23-1	4-phenyl-pyridine	907.8	939.7	2	pyridines
$[C_{11}H_{10}]$	91-57-6	2-Methylnaphthalene	802.4	831.9	10	aromatics
$[C_{11}H_{10}]$	90-12-0	1-methylnaphthalene	805.3	834.8	10	aromatics
$[C_{11}H_{12}N_2]$	10250-60-9	1,5-dimethyl-3-phenylpyrazole	922.4	954.3	2	pyridines
$[C_{11}H_{12}N_2]$	141665-22-7	3(5)-ethyl-5(3)-phenylpyrazole	903.8	935.6	2	pyridines
$[C_{11}H_{12}N_2]$	10250-58-5	1,3-dimethyl-5-phenylpyrazole	924.7	956.6	2	pyridines
$[C_{11}H_{12}N_2O_2]$	73-22-3	L-tryptophan	915	948.9	−5	CH_3NH_2
$[C_{11}H_{13}N]$	4363-25-1	Benzoquinuclidine	948.8	979.8	5.6	$(CH_3)_3N$
$[C_{11}H_{14}N_2]$	13012-16-3	N,N,2,6-Tetramethyl-4-cyanoaniline	886.8	913.3	20	anilines
$[C_{11}H_{14}N_2O]$	119044-59-6	$(CH_3)_2N$-CH=N-(4-acetylphenyl)	947.3	979.8	0	Rln(1/1)
$[C_{11}H_{14}O_2]$	2282-84-0	2,4,6-$(CH_3)_3$-C_6H_2-$COOCH_3$	835.3	866.3	5	esters
$[C_{11}H_{14}O_2]$	13544-66-6	3,4,5-$(CH_3)_3$-C_6H_2-CO_2CH_3	844.6	875.5	5	esters
$[C_{11}H_{15}FSi]$	140843-92-1	4-F-C_6H_4-C($Si(CH_3)_3$)=CH_2	829.1	858.0	12	propene
$[C_{11}H_{15}N]$	54104-82-4	Pyrrolidine, 1-(4-methylphenyl)	879.4	910.2	5.6	$(CH_3)_3N$
$[C_{11}H_{15}N]$	35843-88-0	3-$(CH_3)_2NC_6H_4C(CH_3)=CH_2$	915.5	946.2	5.6	$(CH_3)_3N$
$[C_{11}H_{15}N]$	25108-56-9	4-$(CH_3)_2NC_6H_4C(CH_3)=CH_2$	938.0	964.6	20	anilines
$[C_{11}H_{15}N]$	4096-20-2	Piperidine, 1-phenyl	926.4	952.9	20	anilines
$[C_{11}H_{15}N]$	23074-42-2	Tricyclo[3.3.1.1^{3,7}]decane-1-carbonitrile	803.8	834.4	6	nitriles
$[C_{11}H_{15}NO]$	54660-04-7	Pyrrolidine, 1-(4-methoxyphenyl)	930.4	961.2	5.6	$(CH_3)_3N$
$[C_{11}H_{16}]$	700-12-9	$(CH_3)_5$-C_6H	823.5	850.7	17.6	86STO/XI
$[C_{11}H_{16}ClN_3]$	20815-38-7	$((CH_3)_2N)_2C$=N(4-ClC_6H_4)	995.5	1027.9	0	Rln(1/1)
$[C_{11}H_{16}FN_3]$	20815-37-6	$((CH_3)_2N)_2C$=N(4-FC_6H_4)	997.6	1030.0	0	Rln(1/1)
$[C_{11}H_{16}N_2]$	120235-03-2	$(CH_3)_2N$-C(4-CH_3-C_6H_4)=NCH_3	1005.5	1037.9	0	Rln(1/1)
$[C_{11}H_{16}Si]$	1923-01-9	C_6H_5-C($Si(CH_3)_3$)=CH_2	832.0	860.9	12	propene
$[C_{11}H_{17}N]$	1129-69-7	2-C_6H_{13}(c-C_5H_4N)	931.7	963.6	2	pyridines
$[C_{11}H_{17}N]$	6832-21-9	2,6-(i-C_3H_7)$_2$-pyridine	947.2	979.0	2	pyridines
$[C_{11}H_{17}N]$	613-48-9	4-$CH_3C_6H_4N(C_2H_5)_2$	931.0	962.8	2	anilines
$[C_{11}H_{17}N]$	91-67-8	3-$CH_3C_6H_4N(C_2H_5)_2$	932.2	964.1	2	anilines
$[C_{11}H_{17}NO]$	5511-18-2	1-adamantyl-$CONH_2$	880.9	912.8	2	amides
$[C_{11}H_{17}N_3]$	2556-43-6	$((CH_3)_2N)_2C$=N-C_6H_5	1006.0	1038.4	0	Rln(1/1)
$[C_{11}H_{17}N_3O_2]$	#41	N^2-(4,6-dimethylpyrimidin-2-yl)ornithine	<1007	NE	NE	not estimated
$[C_{11}H_{18}O]$	10309-50-9	4-Methylcamphor	831.4	863.3	2	unsym ketones
$[C_{11}H_{18}O]$	19066-23-0	Adamantylmethylether	831.0	860.2	11	unsym ethers
$[C_{11}H_{20}N_2]$	1132-14-5	3,5-di-t-butylpyrazole	920.8	952.7	2	pyridines
$[C_{11}H_{22}N_2O_3]$	3989-97-7	val-leu	**883.5**	NE	NE	not estimated
$[C_{11}H_{22}N_2O_3]$	13588-95-9	leu-val	**883.5**	NE	NE	not estimated

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_{11}H_{23}N_3O_3]$	22677-62-9	val-lys	**924.3**	NE	NE	not estimated
$[C_{11}H_{23}N_3O_3]$	20556-11-0	lys-val	**924.3**	NE	NE	not estimated
$[C_{11}H_{24}O_4]$	66226-75-3	$CH_3O[CH_2CH_2CH_2O]_3CH_3$	**895.1**	NE	NE	not estimated
$[C_{12}H_8]$	259-79-0	Biphenylene	819.2	848.2	11.5	Rln(4/1)
$[C_{12}H_8N_2]$	92-82-0	Phenazine	908.3	938.4	8	pyridines+Rln2
$[C_{12}H_9NO]$	5424-19-1	3-C_6H_5CO-pyridine	902.3	934.1	2	pyridines
$[C_{12}H_{10}]$	83-32-9	Acenaphthene	821.0	851.7	5.8	Rln(2/1)
$[C_{12}H_{10}]$	92-52-4	Biphenyl	782.9	813.6	5.8	Rln(2/1)
$[C_{12}H_{12}N_2O_2]$	5932-30-9	3(5)-phenyl-5(3)-ethoxycarbonylpyrazole	867.8	899.7	2	pyridines
$[C_{12}H_{14}N_2]$	20734-56-9	N,N′-Dimethyl-1,8-naphthalenediamine	930.9	960.3	10	
$[C_{12}H_{15}Cl]$	146558-43-2	α-t-butylstyrene,3-Cl	811.0	839.8	12	propene
$[C_{12}H_{15}F]$	146558-44-3	α-t-butylstyrene,3-F	809.9	838.8	12	propene
$[C_{12}H_{16}]$	5676-29-9	α-t-butylstyrene	830.3	859.2	12	propene
$[C_{12}H_{16}N_2O_6]$	362-43-6	2′,3′-O-Isopropylideneuridine	**841.7**	874.2	0	Rln(1/1)
$[C_{12}H_{16}O]$	943-27-1	4-t-C_4H_9-C_6H_4-$COCH_3$	850.6	882.5	2	unsym ketones
$[C_{12}H_{16}O_2]$	22524-51-2	2,3,5,6-$(CH_3)_4$-C_6H-$COOCH_3$	834.3	865.2	5	esters
$[C_{12}H_{16}O_2]$	26537-19-9	4-t-C_4H_9-C_6H_4-$COOCH_3$	836.2	867.1	5	esters
$[C_{12}H_{17}N]$	40832-99-3	1-H-Azepine, hexahydro-1-phenyl	925.8	956.6	5.6	$(CH_3)_3N$
$[C_{12}H_{17}NO_2]$	56066-86-5	N,N,2,6-Tetramethylaniline,4-carboxylic acid, methyl ester	913.0	945.4	0	anilines-restricted
$[C_{12}H_{18}]$	87-85-4	$(CH_3)_6$-C_6	836.0	860.6	26.4	86STO/XIA
$[C_{12}H_{18}O]$	1660-04-4	Adamantylmethylketone	833.1	864.9	2	unsym ketones
$[C_{12}H_{18}OSi]$	107099-29-6	4-CH_3O-C_6H_4-$C(Si(CH_3)_3)=CH_2$	874.0	902.9	12	propene
$[C_{12}H_{18}O_2]$	711-01-3	Tricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, methyl ester	833.1	864.1	5	esters
$[C_{12}H_{18}Si]$	120093-92-7	3-CH_3-C_6H_4-$C(Si(CH_3)_3)=CH_2$	839.4	868.3	12	propene
$[C_{12}H_{18}Si]$	17920-24-0	4-$((CH_3)_3Si)C_6H_4C(CH_3)=CH_2$	849.7	878.6	12	propene
$[C_{12}H_{18}Si]$	40595-34-4	3-$((CH_3)_3Si)C_6H_4C(CH_3)=CH_2$	849.7	878.6	12	propene
$[C_{12}H_{18}Si]$	94397-80-5	4-CH_3-C_6H_4-$C(Si(CH_3)_3)=CH_2$	848.1	877.0	12	propene
$[C_{12}H_{19}N]$	2217-07-4	$C_6H_5N(C_3H_7)_2$	931.1	963.0	2	anilines
$[C_{12}H_{19}N]$	22025-87-2	$(CH_3)_2NC_6H_4(t\text{-}C_4H_9)$	934.3	961.0	20	anilines
$[C_{12}H_{19}NO]$	3357-16-2	3-Pyrrolidino-5,5-dimethylcyclohex-2-enone	968.7	1001.2	0	Rln(1/1)
$[C_{12}H_{19}N_3]$	20815-36-5	$((CH_3)_2N)_2C=N$-(4-CH_3-C_6H_4)	1011.9	1044.3	0	Rln(1/1)
$[C_{12}H_{19}N_3O]$	20815-35-4	$((CH_3)_2N)_2C=N$-(4-CH_3O-C_6H_4)	1015.2	1047.7	0	Rln(1/1)
$[C_{12}H_{20}N_6O_7]$	3887-13-6	hexaglycine	950	NE	NE	not estimated
$[C_{12}H_{20}O]$	4789-40-6	2,5-di-t-butylfuran	863.9	894.7	5.8	Rln(2/1)
$[C_{12}H_{20}O]$	90547-83-4	4-Ethylcamphor	833.3	865.1	2	unsym ketones
$[C_{12}H_{21}N]$	6321-40-0	$(CH_2=C(CH_3)CH_2)_3N$	949.4	980.2	5.6	$(CH_3)_3N$
$[C_{12}H_{21}N]$	3717-40-6	N,N-Dimethyladamantylamine	963.0	993.9	5.6	$(CH_3)_3N$
$[C_{12}H_{21}NO]$	73495-63-3	3-Amino-tricyclo[7.3.0.0^{4,8}]dodecan-2-ol	895.6	928.0	0	Rln(1/1)
$[C_{12}H_{21}NO]$	65115-73-3	3-(N,N-Diethylamino)-5,5-dimethylcyclohex-2-enone	968.7	1001.2	0	Rln(1/1)
$[C_{12}H_{22}N_2]$	18712-47-5	3,5-di-t-butyl-4-methylpyrazole	933.8	967.5	−4	pyridines+Rln(1/2)
$[C_{12}H_{22}N_2]$	141665-18-1	1-methyl-3,5-di-t-butylpyrazole	937.1	970.8	−4	pyridines+Rln(1/2)
$[C_{12}H_{22}N_4O_5]$	926-79-4	tetra-L-alanine	944.6	NE	NE	not estimated
$[C_{12}H_{24}N_2]$	71058-67-8	1,6-Diazabicyclo[4.4.4]tetradecane	916.3	947.1	5.6	$(CH_3)_3N$
$[C_{12}H_{24}O_6]$	17455-13-9	18-crown-6	909.5	967.0	−84	84SHA/BLA
$[C_{12}H_{27}N]$	102-82-9	$(n\text{-}C_4H_9)_3N$	967.6	998.5	5.6	$(CH_3)_3N$
$[C_{12}H_{28}N_2]$	106376-59-4	Hydrazine, 1,2-dimethyl-1,2-dipentyl	946.4	977.2	5.8	Rln(2/1)
$[C_{12}H_{28}N_2]$	68970-09-2	Hydrazine, 1,2-bis(2,2-dimethylpropyl)-1,2-dimethyl	947.1	977.8	5.8	Rln(2/1)
$[C_{12}H_{30}N_3OP]$	2622-07-3	$OP(N(C_2H_5)_2)_3$	942.2	974.7	0	Rln(1/1)
$[C_{13}H_9N]$	260-94-6	Acridine	940.7	972.6	2	pyridines
$[C_{13}H_{10}]$	86-73-7	Fluorene	803.8	831.5	16	aromatics
$[C_{13}H_{10}O]$	119-61-9	$(C_6H_5)_2CO$	852.5	882.3	9	sym ketones
$[C_{13}H_{12}]$	643-93-6	3-Methylbiphenyl	795.5	828.0	0	?
$[C_{13}H_{12}]$	643-58-3	2-Methylbiphenyl	783.4	815.9	0	?
$[C_{13}H_{12}]$	101-81-5	$C_6H_5CH_2C_6H_5$	769.5	802.0	0	
$[C_{13}H_{12}]$	644-08-6	4-Methylbiphenyl	785.4	817.9	0	?
$[C_{13}H_{33}OP]$	2129-89-7	$CH_3(C_4H_9)_2PO$	**876.4**	908.9	0	Rln(1/1)
$[C_{13}H_{33}P]$	1486-28-8	$(C_4H_9)_2(CH_3)P$	939.7	972.1	0	Rln(1/1)
$[C_{13}H_{15}F_3]$	146558-45-4	α-t-butylstyrene,3-CF_3	802.2	831.1	12	propene
$[C_{13}H_{15}F_3]$	22666-67-7	α-t-butylstyrene,4-CF_3	796.5	825.3	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
$[C_{13}H_{16}N_2]$	20734-57-0	N,N,N′-Trimethyl-1,8-naphthalenediamine	951.8	984.3	0	?
$[C_{13}H_{17}ClO]$	146558-40-9	α-t-butylstyrene,4-CH_3O, 3-Cl	854.2	883.0	12	propene
$[C_{13}H_{18}]$	31006-98-1	α-t-butylstyrene,4-CH_3	845.7	874.6	12	propene
$[C_{13}H_{18}]$	146558-42-1	α-t-butylstyrene,3-CH_3	838.5	867.4	12	propene
$[C_{13}H_{18}N_2]$	84396-62-3	4-(1-adamantyl)-pyrazole	878.9	913.1	−5.8	Rln(1/2)
$[C_{13}H_{18}N_2]$	92234-54-3	1-(1-adamantyl)pyrazole	922.4	954.5	2	pyridines
$[C_{13}H_{18}O]$	22666-53-1	α-t-butylstyrene, 4-methoxy	869.1	897.9	12	propene
$[C_{13}H_{18}S]$	146558-39-6	α-t-butylstyrene,4-CH_3S	866.0	894.8	12	propene
$[C_{13}H_{21}N]$	585-48-8	2,6-(t-C_4H_9)$_2$-pyridine	951	982.9	2	pyridines
$[C_{13}H_{21}N]$	29939-31-9	2,4-(t-C_4H_9)$_2$-pyridine	952.0	983.8	2	pyridines
$[C_{13}H_{21}NO]$	13358-76-4	3-Piperidino-5,5-dimethylcyclohex-2-enone	968.3	1000.7	0	Rln(1/1)
$[C_{13}H_{21}NO]$	1502-00-7	1-adamantyl-CON$(CH_3)_2$	917.6	949.4	2	amides
$[C_{13}H_{22}N_2]$	133835-18-4	$(CH_3)_2$N-CH=N-(1-Ad)	1001.0	1033.5	0	Rln(1/1)
$[C_{13}H_{23}N]$	#177	Adamantyl-CH_2N$(CH_3)_2$	947.4	978.4	5.6	$(CH_3)_3$N
$[C_{13}H_{24}N_2]$	69340-58-5	3,3,6,9,9-pentamethyl-2,10-diazabicyclo[4.4.0]dec-1-ene	1006.9	1039.3	0	Rln(1/1)
$[C_{13}H_{24}N_2]$	141665-20-5	1,4-dimethyl-3,5-di-t-butylpyrazole	947.8	979.6	?	pyridines
$[C_{13}H_{25}N]$	75197-24-9	out-6H-1-Azabicyclo[4.4.4]tetradecane	864.5	897.0	0	Rln(3/3)
$[C_{13}H_{27}N]$	66922-18-7	2,6-Di-t-butylpiperidine	960.1	992.5	0	estimate
$[C_{14}H_{10}]$	85-01-8	Phenanthrene	795.0	825.7	5.8	Rln(2/1)
$[C_{14}H_{10}]$	120-12-7	Anthracene	846.6	877.3	5.8	Rln(2/1)
$[C_{14}H_{12}]$	530-48-3	$(C_6H_5)_2C=CH_2$	856.9	885.7	12	propene
$[C_{14}H_{12}N_2]$	75863-17-1	15,16-diazatricyclo[8.4.1.1^{3,8}]hexadeca-1,3,5,7,9,11,13-heptaene	951.4	983.8	0	?
$[C_{14}H_{14}]$	103-29-7	$C_6H_5(CH_2)_2C_6H_5$	774.1	801.8	16	toluene
$[C_{14}H_{18}]$	5325-97-3	1,2,3,4,5,6,7,8-Octahydrophenanthrene	815.5	846.2	5.8	Rln(2/1)
$[C_{14}H_{18}]$	1079-71-6	1,2,3,4,5,6,7,8-Octahydroanthracene	814.7	845.4	5.8	Rln(2/1)
$[C_{14}H_{18}N_2]$	20734-58-1	N,N,N′,N′-Tetramethyl-1,8-naphthalenediamine	995.8	1028.2	0	?
$[C_{14}H_{20}]$	146558-41-0	α-t-butylstyrene,3,5-dimethyl	845.5	874.3	12	propene
$[C_{14}H_{20}N_2O_3]$	3918-90-9	phe-val	**893.6**	NE	NE	not estimated
$[C_{14}H_{20}N_2O_3]$	3918-92-1	val-phe	**909.0**	NE	NE	not estimated
$[C_{14}H_{20}N_2O_4]$	3061-91-4	val-tyr	**909.0**	NE	NE	not estimated
$[C_{14}H_{20}N_2O_4]$	17355-09-8	tyr-val	**893.6**	NE	NE	not estimated
$[C_{14}H_{23}N]$	16245-79-7	4-(n-C_8H_{17})$C_8H_4NH_2$	862	894.5	0	86SUN/KUL
$[C_{14}H_{23}N_7O_8]$	18861-82-0	heptaglycine	980.6	NE	NE	not estimated
$[C_{14}H_{24}N_2]$	151328-46-0	$(CH_3)_2$NC(CH_3)=N(1-Ad)	1018.4	1050.8	0	Rln(1/1)
$[C_{14}H_{28}O_7]$	33089-36-0	21-crown-7	>910	NE	NE	not estimated
$[C_{14}H_{29}N]$	64326-83-6	1-Methyl-2,6-t-butylpiperidine	980.3	1011.1	5.6	$(CH_3)_3$N
$[C_{15}H_{12}]$	779-02-2	9-Methylanthracene	865.8	896.5	5.8	Rln(2/1)
$[C_{15}H_{12}]$	613-12-7	2-Methylanthracene	855.1	887.5	0	Rln(1/1)
$[C_{15}H_{12}Fe_2O_3]$	76722-37-7	$[(C_5H_5)(CO)Fe]_2(\mu\text{-}CO)(\mu\text{-}C=CH_2)$	**949.4**	981.8	0	Rln(1/1)
$[C_{15}H_{12}N_2]$	1145-01-3	3,5-diphenylpyrazole	912.7	946.3	−3.8	pyridines+Rln(1/2)
$[C_{15}H_{16}]$	34403-06-0	3-CH_3-$C_6H_4(CH_2)_2C_6H_5$	801.0	833.5	0	?
$[C_{15}H_{16}]$	1081-75-0	$C_6H_5(CH_2)_3C_6H_5$	787.6	820.1	0	
$[C_{15}H_{12}N_2]$	95935-55-0	9,5-metheno-5H,7H-pyrimido[1,6-a:3,4-a′]bisazepine	898.7	931.1	0	?
$[C_{15}H_{17}OP]$	2959-75-3	i-$C_3H_7(C_6H_5)_2$PO	**876.4**	908.9	0	Rln(1/1)
$[C_{15}H_{18}]$	189-81-9	1,4-Dimethyl-7-isopropylazulene	950.6	983.1	0	Rln(1/1)
$[C_{15}H_{24}]$	15181-11-0	1,3-di-(t-C_4H_9)-5-CH_3-C_6H_3	826.0	853.7	16	aromatics
$[C_{15}H_{27}N_5O_6]$	10183-34-3	penta-L-alanine	962	NE	NE	not estimated
$[C_{16}H_{10}]$	206-44-0	Fluoranthene	800.9	828.6	16	aromatics
$[C_{16}H_{10}]$	129-00-0	Pyrene	840.1	869.2	11.5	Rln(4/1)
$[C_{16}H_{14}N_2]$	19311-79-6	1-methyl-3,5-diphenylpyrazole	927.0	958.9	2	pyridines
$[C_{16}H_{14}N_2]$	95935-56-1	10,5-metheno-5H-bisazepino[1,2-d:2′,1′-g][1,4]diazepine,7,8-dihydro	930.1	962.6	0	?
$[C_{16}H_{16}]$	2919-20-2	(4-$CH_3C_6H_4$)$_2$C=CH_2	871.4	900.2	12	propene
$[C_{16}H_{16}N_2]$	95864-13-4	15,16-diazatricyclo[8.4.1.1^{3,8}]hexadeca-1,3,5,7,9,11,13-heptaene,15,16-dimethyl	951.9	984.4	0	?
$[C_{16}H_{18}]$	1083-56-3	$C_6H_5(CH_2)_4C_6H_5$	779.8	822.0	−33	80MAU/HUN
$[C_{16}H_{19}OP]$	56598-35-7	t-$C_4H_9(C_6H_5)_2$PO	**876.4**	908.9	0	Rln(1/1)
$[C_{16}H_{21}N_3O_3]$	24587-37-9	val-trp	**909.0**	NE	NE	not estimated
$[C_{16}H_{26}N_8O_9]$	38416-68-1	octaglycine	990.7	NE	NE	not estimated
$[C_{16}H_{27}N]$	2909-76-4	N,N-Dimethylbenzenamine,2,4-di-t-butyl	942.4	973.3	5.6	$(CH_3)_3$N

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[$C_{17}H_{20}$]	1718-50-9	$C_6H_5(CH_2)_5C_6H_5$	782.4	824.7	−33	80MAU/HUN
[$C_{17}H_{16}N_2$]	95935-57-2	11,5-metheno-5H,7H-bisazepino[1,2-a:2′,1′-d][1,5]diazocine,8,9-dihydro	942.0	974.5	0	Rln(1/1)
[$C_{18}H_{12}$]	218-01-9	Chrysene	810.1	840.9	5.8	Rln(2/1)
[$C_{18}H_{12}$]	92-24-0	Tetracene	876.5	905.5	11.5	Rln(4/1)
[$C_{18}H_{12}$]	217-59-4	Triphenylene	791.2	819.2	14.9	Rln(6/1)
[$C_{18}H_{15}As$]	603-32-7	$(C_6H_5)_3As$	**876.4**	908.9	0	Rln(3/3)
[$C_{18}H_{15}AsO$]	1153-05-5	$(C_6H_5)_3AsO$	**876.4**	906.2	9.1	Rln(3/1)
[$C_{18}H_{15}N$]	603-34-9	$(C_6H_5)_3N$	**876.4**	908.9	0	Rln(3/3)
[$C_{18}H_{15}OP$]	791-28-6	$(C_6H_5)_3PO$	**876.4**	906.2	9.1	Rln(3/1)
[$C_{18}H_{15}P$]	603-35-0	$(C_6H_5)_3P$	940.4	972.8	0	Rln(3/3)
[$C_{18}H_{15}PS$]	3878-45-3	$(C_6H_5)_3PS$	**876.4**	906.2	9.1	Rln(3/1)
[$C_{18}H_{15}Sb$]	603-36-1	$(C_6H_5)_3Sb$	**813.1**	845.5	0	Rln(3/3)
[$C_{18}H_{22}$]	1087-49-6	$C_6H_5(CH_2)_6C_6H_5$	783.8	826.1	−33	80MAU/HUN
[$C_{18}H_{20}$]	21072-42-4	*trans*-1,4-diphenylcyclohexane	771.7	804.1	0	?
[$C_{18}H_{18}N_2$]	120789-29-9	12,5-metheno-5H-bisazepino[1,2-a:2′,1′-d][1,5]diazonine,7,8,9,10-tetrahydro	940.2	972.6	0	Rln(1/1)
[$C_{18}H_{30}$]	1460-02-2	1,3,5-(t-C_4H_9)$_3$-C_6H_3	822.3	848.8	20	1,3,5-$Me_3C_6H_3$
[$C_{18}H_{32}N_6O_7$]	111652-29-0	hexa-L-alanine	981.3	NE	NE	not estimated
[$C_{18}H_{35}N_5O_6$]	153841-62-4	gly-lys-lys-gly-gly	1008.4	NE	NE	not estimated
[$C_{18}H_{35}N_5O_6$]	153841-63-5	gly-lys-gly-lys-gly	1010.8	NE	NE	not estimated
[$C_{18}H_{35}N_5O_6$]	153841-64-6	lys-gly-gly-gly-lys	1026	NE	NE	not estimated
[$C_{19}H_{20}N_2$]	123524-78-7	13,5-metheno-5H,7H-bisazepino[1,2-a:2′,1′-d][1,5]diazecine,8,9,10,11-tetrahydro	961.8	994.3	0	?
[$C_{20}H_{12}$]	198-55-0	Perylene	859.6	888.6	11.5	Rln(4/1)
[$C_{20}H_{20}$]	4493-23-6	dodecahedrane	817.5	843.8	20.6	Rln(60/5)
[$C_{20}H_{24}$]	128484-66-2	*trans*-1,4-dibenzylcyclohexane	773.3	805.7	0	?
[$C_{20}H_{22}N_2$]	123524-79-8	14,5-metheno-5H-bisazepino[1,2-a:2′,1′-d][1,5]diazacycloundecine,7,8,9,10,11,12-hexahydro	946	978.5	0	Rln(1/1)
[$C_{20}H_{32}N_{10}O$]	76960-32-2	decaglycine	1004.6	NE	NE	not estimated
[$C_{21}H_{22}$]	82400-17-7	Methyldodecahedrane	823.1	855.6	0	?
[$C_{21}H_{30}O$]	38256-01-8	(1-adamytyl)$_2$CO	862.4	894.3	2	unsym ketones
[$C_{21}H_{30}S$]	73509-04-3	(1-adamantyl)$_2$CS	882.4	912.1	9	sym ketones
[$C_{22}H_{12}$]	191-24-2	1,12-Benzoperylene	845.2	876.0	5.8	Rln(2/1)
[$C_{22}H_{14}$]	213-46-7	Picene	820.6	851.3	5.8	Rln(2/1)
[$C_{22}H_{24}$]	77387-50-9	1,16-Dimethyldodecahedrane	844.0	876.5	0	?
[$C_{24}H_{12}$]	191-07-1	Coronene	835.0	861.3	20.6	Rln(12/1)
[$C_{26}H_{54}O_8$]	3055-97-8	$C_{12}H_{25}(OC_2H_4)_7OH$	940.3	1006.7	−113.9	93LIN/ROC
[C_{60}]	99685-96-8	buchminsterfullerene	**827.5**	NE	NE	not estimated
[C_{70}]	115383-22-7	[5,6]Fullerene-C_{70}	**827.5**	NE	NE	not estimated
[CaO]	1305-78-8	CaO	1162.3	1190.6	14	89GUR/VEY
[Cl]	22537-15-1	Cl	490.1	513.6	30.1	*S*(HS)-*S*(Cl)
[ClH]	7647-01-0	HCl	530.1	556.9	19	*S*(H_2S)-*S*(HCl)
[ClLi]	7447-41-8	LiCl	800.5	827	20	linear-to-bent est.
[Co]	7440-48-4	Co	719.8	742.7	32	rot est (0.116)
[Cr]	7440-47-3	Cr	768.4	791.3	32	rot est (0.117)
[CsHO]	21351-79-1	CsOH	1092.2	1117.9	22.6	70DZI/KEB
[Cs_2O]	20281-00-9	Cs_2O	1412.2	1442.9	5.8	Rln(2/1)
[Cu]	7440-50-8	Cu	632.4	655.3	32	rot est (0.117)
[F]	14762-94-8	F	315.1	340.1	25	*S*(OH)-*S*(F)
[FH]	7664-39-3	HF	456.7	484	17.3	97EAS/SMI
[FO]	12061-70-0	OF	482.2	508.7	20	linear-to-bent est.
[F_2]	7782-41-4	F_2	305.5	332	20	linear-to-bent est.
[F_2O_2S]	2699-79-8	F_2SO_2	580.5	605.5	25	93SZU/MCM
[F_3HOSi]	91419-78-2	SiF_3OH	**611.5**	641.9	7	CH_3OH
[F_3N]	7783-54-2	NF_3	538.6	568.4	9.1	Rln(3/1)
[F_3OP]	13478-20-1	OPF_3	664.2	694.0	9.1	Rln(3/1)
[F_3P]	7783-55-3	PF_3	662.8	695.3	0	Rln(1/1)
[F_2Si]	7783-61-1	SiF_2	476.6	502.9	20.6	Rln(12/1)
[F_4S]	2551-62-4	SF_4	550.7	575.3	26.4	Rln(24/1)
[Fe]	7439-89-6	Fe	731.1	754	32	rot est (0.117)
[FeO]	1345-25-1	FeO	880.5	907	20	linear-to-bent est.

TABLE 1. Gas basicity, proton affinity and protonation entropy of *Hill sorted bases*—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[GeH_4]	7782-65-2	GeH_4	**687.1**	713.4	20.6	Rln(12/1)
[HI]	10034-85-2	HI	601.3	627.5	21	HBr
[*HKO*]	1310-58-3	KOH	1075.4	1101.8	20.4	average
[HLi]	7580-67-8	LiH	996.4	1021.7	24	88DIX/GOL
[HLiO]	1310-66-3	LiOH	972.1	1000.1	14.9	70DZI/KEB
[HNO_3]	7697-37-2	HNO_3	731.5	751.4	42	94CAC/ATT
[*HNSi*]	14515-04-9	*SiNH*	819.0	853.2	−5.8	Rln(1/2)
[HN_3]	7782-79-8	HNNN	**723.5**	756.0	0	Rln(1/1)
[HNa]	7646-69-7	NaH	1070.6	1095	27	88DIX/GOL
[*HNaO*]	1310-73-2	NaOH	1044.8	1071.8	18.2	70DZI/KEB
[HOSi]	71132-80-4:b	SiOH at O	700.1	732.6	0	?
[HOSi]	71132-80-4:a	SiOH at Si	742.8	775.3	0	Rln(1/1)
[HOSi]	97402-81-8:a	HSiO at O	777.5	810	0	Rln(1/1)
[HOSi]	97402-81-8:b	HSiO at Si	602.5	635	0	Rln(1/1)
[HOSr]	12141-14-9	SrOH	981.6	1019.4	−18	
[HO_2]	3170-83-0	HO_2•	627.5	660	0	?
[HP]	13967-14-1	PH	639.6	670.3	5.8	Rln(2/1)
[H_2]	1333-74-0	H_2	394.7	422.3	16.3	97EAS/SMI
[H_2N]	15194-15-7	NH_2	742.0	773.4	3.4	Rln(3/2)
[H_2N_2]	3618-05-1	HN=NH	772.3	803	5.8	Rln(2/1)
[$H_2N_2O_2$]	7782-94-7	H_2N-NO_2	**725.0**	757.4	0	?
[H_2O]	7732-18-5	H_2O	660.0	691	5	AUE; 97EAS/SMI
[H_2OSi]	83892-34-6	HSiOH at Si	807.5	840	0	?
[H_2OSi]	22755-01-7:a	H_2SiO at O	808.5	841	0	?
[H_2OSi]	22755-01-7:b	H_2SiO at Si	295.5	328	0	Rln(1/1)
[H_2O_2]	7722-84-1	H_2O_2	**643.8**	674.5	5.8	Rln(2/1)
[H_2O_4S]	7664-93-9	H_2SO_4	**666.9**	699.4	0	?
[H_2P]	13765-43-0	PH_2	675.7	709.2	−3.4	Rln(2/3)
[H_2S]	7783-06-4	H_2S	673.8	705	4.3	$S(PH_3)$-$S(H_2S)$
[H_2Se]	7783-07-5	H_2Se	676.4	707.8	3.8	$S(AsH_3)$-$S(H_2Se)$
[H_2Si]	13825-90-6	SiH_2	**804.1**	839.2	−9.1	Rln(2/6)
[H_2Te]	7783-09-7	H_2Te	704.5	735.9	3.8	H_2Se
[H_3N]	7664-41-7	NH_3	819.0	853.6	−6.4	97EAS/SMI
[H_3OSi]	113648-09-2:a	H_2SiOH at O	705.5	738	0	?
[H_3OSi]	113648-09-2:b	H_2SiOH at Si	556.5	589	0	?
[H_3OSi]	81429-20-1	H_3SiO at O	667.5	700	0	?
[H_3O_3P]	10294-56-1	H_3PO_3	**788.8**	821.3	0	?
[H_3P]	7803-51-2	PH_3	750.9	785	−5.6	$S(SiH_4)$-$S(PH_3)$
[H_4N_2]	302-01-2	H_2NNH_2	822.4	853.2	5.8	Rln(2/1)
[H_4OSi]	14475-38-8	H_3SiOH at O	713.9	746.4	0	Rln(1/1)
[H_4Si]	7803-62-5	SiH_4	613.4	639.7	20.6	Rln(12/1)
[H_6OSi_2]	13597-73-4	$H_3SiOSiH_3$	718.3	749	5.8	Rln(2/1)
[He]	7440-59-7	He	148.5	177.8	10.5	$S(H_2)$-$S(He)+Rln2$
[I]	14362-44-8	I	583.5	608.2	26	$S(HI)$-$S(I)$
[K_2O]	12136-45-7	K_2O	1311.8	1342.5	5.8	Rln(2/1)
[Kr]	7439-90-9	Kr	402.4	424.6	34.4	$S(HBr)$-$S(Kr)$
[La]	7439-91-0	La	991.9	1013	38	rot est (0.17)
[Li_2]	14452-59-6	Li_2	1133.1	1162	12	88DIX/GOL
[Li_2O]	12057-24-8	Li_2O	1175.3	1206	5.8	Rln(2/1)
[Lu]	7439-94-3	Lu	970.6	992	37	rot est (0.16)
[Mg]	7439-95-4	Mg	**797.3**	819.6	34	rot est (0.136)
[MgO]	1309-48-4	MgO	959.4	988	13	89GUR/VEY
[Mg_2]	29904-79-8	Mg_2	886.5	919	0	Rln(1/1)
[Mn]	7439-96-5	Mn	774.4	797.3	32	rot est (0.117)
[N]	17778-88-0	N	318.7	342.2	30	$S(CH)$-$S(N)$
[NO]	10102-43-9	NO	505.3	531.8	20	linear-to-bent est.
[NO_2]	10102-44-0	NO_2	**560.3**	591.0	5.8	Rln(2/1)
[NP]	17739-47-8	PN	**757.0**	789.4	0	?
[N_2]	7727-37-9	N_2	464.5	493.8	10.5	97EAS/SMI
[N_2O]	10024-97-2:b	N_2O at N	523.3	549.8	20	CO_2-Rln(2/1)
[N_2O]	10024-97-2:a	N_2O at O	548.7	575.2	20	CO_2-Rln(2/1)
[Na_2]	25681-79-2	Na_2	1118.2	1146.8	13	88DIX/GOL
[Na_2O]	1313-59-3	Na_2O	1345.2	1375.9	5.8	Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	ΔS_p	ΔS_p Reasons
[Ne]	7440-01-9	Ne	174.4	198.8	27	S(HF)-S(Ne)
[Ni]	7440-02-0	Ni	714.1	737	32	rot est (0.115)
[O]	17778-80-2	O	459.6	485.2	23	rot est (0.066)
[HO]	3352-57-6	OH	564.0	593.2	11	$S(NH_2)$-S(OH)
[OP]	14452-66-5	PO	649.5	682	0	Rln(1/1)
[OSi]	10097-28-6:a	SiO at O	**750.4**	777.8	17	85BOT/ROS
[OSi]	10097-28-6:b	SiO at Si	500.5	533	0	Rln(1/1)
[OSr]	1314-11-0	SrO	1180.7	1209	14	89GUR/VEY
[O_2]	7782-44-7	O_2	396.3	421	26	AUE; 84ADA/SMI
[O_2S]	7446-09-5	SO_2	643.3	672.3	11.5	AUE
[O_3]	10028-15-6	O_3	595.9	625.5	9.5	91MER/QUE
[O_3S]	7446-11-9	SO_3	**560.3**	588.3	14.9	Rln(6/1)
[O_4Os]	20816-12-0	OsO_4	**650.6**	676.9	20.6	Rln(12/1)
[P]	7723-14-0	P	604.8	626.8	35	S(HSi)-S(P)
[PS]	12281-36-6	PS	665.5	698	0	?
[P_4]	12185-10-8	P_4	714.3	742.3	14.9	Rln(12/2)
[Pd]	7440-05-3	Pd	673.4	696	33	rot est (0.13)
[Rh]	7440-16-6	Rh	745.4	768	33	rot est (0.13)
[Ru]	7440-18-8	Ru	751.4	774	33	rot est (0.13)
[S]	7704-34-9	S	640.2	664.3	28	rot est (0.104)
[SSi]	113443-18-8	SiS	**677.7**	710.2	0	Rln(1/1)
[SSi]	12504-41-5:b	SiS at Si	596.6	627	7	92BRU/GRE
[SSi]	12504-41-5:a	SiS at S	660.2	683	32.5	92BRU/GRE
[Sc]	7440-20-2	Sc	892.0	914	35	rot est (0.144)
[Si]	7440-21-3	Si	814.1	837	32	rot est (0.12)
[Ti]	7440-32-6	Ti	853.7	876	34	rot est (0.132)
[U]	7440-61-1	U	973.2	995.2	35	rot est (0.142)
[V]	7440-62-2	V	836.8	859.4	33	rot est (0.13)
[Xe]	7440-63-3	Xe	478.1	499.6	36.8	S(HI)-S(Xe)
[Y]	7440-65-5	Y	945.9	967	38	rot est (0.17)
[Zn]	7440-66-6	Zn	**586.0**	608.6	33	rot est (0.125)

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[Cs_2O]	**20281-00-9**	**Cs_2O**				**1412.2**			**1442.9**			**5.8**
84BUT/KUD		See Refs.							1442.9			
[Na_2O]	**1313-59-3**	**Na_2O**				**1345.2**			**1375.9**			**5.8**
84BUT/KUD		See Refs.							1375.9			
[K_2O]	**12136-45-7**	**K_2O**				**1311.8**			**1342.5**			**5.8**
84BUT/KUD		See Refs.							1342.5			
[BaO]	**1304-28-5**	**BaO**				**1187.6**			**1215.4**			**15.5**
81MUR		See Refs.							1215.4			
[OSr]	**1314-11-0**	**SrO**				**1180.7**			**1209**			**14**
83MUR		See Refs.							1210.7			
81MUR		See Refs.							1207.3			
[Li_2O]	**12057-24-8**	**Li_2O**				**1175.3**			**1206**			**5.8**
84BUT/KUD		See Refs.							1206			
[CaO]	**1305-78-8**	**CaO**				**1162.3**			**1190.6**			**14**
83MUR		See Refs.							1193.7			
81MUR		See Refs.							1187.4			
[Li_2]	**14452-59-6**	**Li_2**				**1133.1**			**1162**			**12**
88DIX/GOL		theory	300						1162			
[Na_2]	**25681-79-2**	**Na_2**				**1118.2**			**1146.8**			**13**
88DIX/GOL		theory	300						1146.8			
[CsHO]	**21351-79-1**	**CsOH**				**1092.2**			**1117.9**			**22.6**
72MCK/SAW		See Refs.							1110.3			42.3
70DZI/KEB		See Refs.							1117.9			22.6
[HKO]	**1310-58-3**	**KOH**				**1075.4**			**1101.8**			**20.4**
82BUR/HAY		See Refs.							1100.6			21
76DAV/KEB		See Refs.							1100.3			23.7
70DZI/KEB		See Refs.							1104.5			16.6
[HNa]	**7646-69-7**	**NaH**				**1070.6**			**1095**			**27**
88DIX/GOL		theory	300						1095			
[$C_{10}H_{16}N_4$]	**111062-21-6**	**1H-diimidazo[1,2-d:2′,1′-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro-1-methyl (MTTT)**				**>1060**			**>1091**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C{=}NH$	338	997.4	<62.2	>1060						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_9H_{14}N_4$]	**111062-19-2**	**1H-dimidazo[1,2-d:2′,1′-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro (TTT)**				**>1049**			**>1081**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	>51.2	>1049						
[HNaO]	**1310-73-2**	**NaOH**				**1044.8**			**1071.8**			**18.2**
82BUR/HAY		See Refs.							1072.1			18.2
70DZI/KEB		See Refs.							1071.5			18.2
[$C_{10}H_{19}N_3$]	**160172-95-2**	**7-isopropyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene (ITBD)**				**1039.2**			**1071.6**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	42	1039.2						
[$C_9H_{17}N_3$]	**95510-44-4**	**7-ethyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene (ETBD)**				**1035.8**			**1068.2**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	38.6	1035.8						
[$C_9H_{21}N_3$]	**151328-47-1**	**$(CH_3)_2NC(CH_3)=N-(CH_2)_3N(CH_3)_2$**				**1030.5**			**1077.5**			**−49**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	31.4	1030.5						
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	>61.1	>1016.3						
[$C_8H_{15}N_3$]	**84030-20-6**	**7-methyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene**				**1030.2**			**1062.7**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	32.7	1029.9						
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	62.8	1030.6						
[$C_9H_{21}N_3$]	**34331-58-3**	**$((CH_3)_2N)_2C=N(t\text{-}C_4H_9)$**				**1029.4**			**1061.8**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	32.2	1029.4						
[$C_{10}H_{20}N_6O_4$]	**54944-27-3**	**gly-gly-arg**				**1028.5**			**NE**			**NE**
93WU/FEN		kinetic method				1028.5						
[$C_{18}H_{35}N_7O_6$]	**153841-64-6**	**lys-gly-gly-gly-lys**				**1028**			**NE**			**NE**
93WU/FEN		kinetic method				1026						
[$C_8H_{19}N_3$]	**29166-71-0**	**$((CH_3)_2N)_2C=N(i\text{-}C_3H_7)$**				**1023.2**			**1055.6**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	26	1023.2						
[$C_7H_{13}N_3$]	**5807-14-7**	**1,5,7-triazabicyclo [4.4.0]dec-5-ene**				**1022.1**			**1054.6**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	25.5	1022.7						
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	53.8	1021.6						
[$C_7H_{17}N_3$]	**13439-88-8**	**$((CH_3)_2N)_2C=NC_2H_5$**				**1019.0**			**1051.4**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	21.8	1019.0						
[$C_{14}H_{24}N_2$]	**151328-46-0**	**$(CH_3)_2NC(CH_3)=N(1\text{-}Ad)$**				**1018.4**			**1050.8**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	50.6	1018.4						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_8H_{19}N_3$]	**151328-45-9**	**$((CH_3)_2NC(CH_3)=N(CH_2)_2N(CH_3)_2$**				**1016.1**			**1048.5**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	48.3	1016.1						
[$C_9H_{16}N_2$]	**6674-22-2**	**1,8-diazabicyclo[5,4,0]undec-7-ene**				**1015.5**			**1047.9**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	47.7	1015.5						
[$C_6H_{15}N_3$]	**13439-84-4**	**$((CH_3)_2N)_2C=NCH_3$**				**1015.2**			**1047.7**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	18	1015.2						
[$C_{12}H_{19}N_3O$]	**20815-35-4**	**$((CH_3)_2N)_2C=N\text{-}(4\text{-}CH_3O\text{-}C_6H_4)$**				**1015.2**			**1047.7**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	18	1015.2						
[$C_8H_{14}N_2$]	**19616-52-5**	**1,5-diazabicyclo[4,4,0]dec-6-ene (DBD)**				**1014.0**			**1046.4**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	16.8	1014.0						
[$C_{12}H_{19}N_3$]	**20815-36-5**	**$((CH_3)_2N)_2C=N\text{-}(4\text{-}CH_3\text{-}C_6H_4)$**				**1011.9**			**1044.3**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	14.7	1011.9						
[$C_9H_{20}N_2$]	**151328-44-8**	$(CH_3)_2N\text{-}C(C_2H_5)=N(t\text{-}C_4H_9)$				**1010.9**			**1043.3**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	43.1	1010.9						
[$C_{18}H_{35}N_7O_6$]	**153841-63-5**	**gly-lys-gly-lys-gly**				**1010.8**			**NE**			**NE**
93WU/FEN		kinetic method				1010.8						
[$C_8H_{19}N_3$]	**139033-04-8**	**$(CH_3)_2N\text{-}CH=N\text{-}(CH_2)_3N(CH_3)_2$**				**1010.6**			**1057.7**			**−49**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C=NH$	338	997.4	14.2	1013.3						
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	40.6	1010.2						
92RAC/MAR	147350-05-8	$(CH_3)_2N\text{-}C(CH_3)=N(t\text{-}C_4H_9)$	338	1005.9	2.1	1009.8						
92RAC/MAR	133835-18-4	$(CH_3)_2N\text{-}CH=N\text{-}(1\text{-}Ad)$	338	1001.0	7.9	1010.8						
92RAC/MAR	101398-58-7	$(CH_3)_2N\text{-}CH=N(CH_2)_2N(CH_3)_2$	338	996.4	10.9	1009.1						
92RAC/MAR	94793-19-8	$(CH_3)_2N\text{-}C(CH_3)=N(i\text{-}C_3H_7)$	338	999.2	9.6	1010.6						
[$C_{18}H_{35}N_7O_6$]	**153841-62-4**	**gly-lys-lys-gly-gly**				**1008.4**			**NE**			**NE**
93WU/FEN		kinetic method				1008.4						
[$C_{11}H_{18}N_4O_3$]	**#41**	**N^4-(4,6-dimethylpyrimidin-2-yl)ornithine**				**<1007**			**NE**			**NE**
93BUR/GAS	74-79-3	L-Arginine		1006.6	<0	<1007						
[$C_{13}H_{24}N_2$]	**69340-58-5**	**3,3,6,9,9-pentamethyl-2,10-diazabicyclo[4.4.0]dec-1-ene**				**1006.9**			**1039.3**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	39.1	1006.9						
[$C_6H_{14}N_4O_2$]	**74-79-3**	**L-Arginine**				**1006.6**			**1051.0**			**−40**
93LI/HAR		kinetic method										
92WU/FEN		kinetic method				1006.6						
92GOR/SPE	102-82-9	$(n\text{-}C_4H_9)_3N$	350	967.6								

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
90ISA/OMO		kinetic method-relative order										
87BOJ		kinetic method relative order										
86BOJ		kinetic method-relative order										
[$C_{11}H_{17}N_3$]	**2556-43-6**	**$((CH_3)_2N)_2C{=}N\text{-}C_6H_5$**				**1006.0**			**1038.4**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C{=}NH$	338	997.4	8.8	1006.0						
[$C_9H_{14}N_2$]	**3001-72-7**	**1,5-diazabicyclo[4.3.0]non-5-ene**				**1005.9**			**1038.3**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	38.1	1005.9						
[$C_8H_{18}N_2$]	**147350-05-8**	**$(CH_3)_2N\text{-}C(CH_3){=}N(t\text{-}C_4H_9)$**				**1005.9**			**1038.3**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	38.1	1005.9						
[$C_9H_{20}N_2$]	**151328-42-6**	**$(C_2H_5)_2N\text{-}C(CH_3){=}N(n\text{-}C_3H_7)$**				**1005.5**			**1037.9**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	37.7	1005.5						
[$C_{10}H_{22}N_2$]	**107322-35-0**	**$(CH_3)_2N\text{-}C(C_2H_5){=}N(n\text{-}C_5H_{11})$**				**1005.5**			**1037.9**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	37.7	1005.5						
[$C_{11}H_{16}N_2$]	**120235-03-2**	**$(CH_3)_2N\text{-}C(4\text{-}CH_3\text{-}C_6H_4){=}NCH_3$**				**1005.5**			**1037.9**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	37.7	1005.5						
[$C_{20}H_{32}N_{10}O$]	**76960-32-2**	**decaglycine**				**1004.6**			**NE**			**NE**
92WU/HEN2		kinetic method				1004.6						
[$C_8H_{18}N_2$]	**112752-57-5**	**$(CH_3)_2N\text{-}C(C_2H_5){=}N(i\text{-}C_3H_7)$**				**1004.6**			**1037.0**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	36.8	1004.6						
[$C_7H_{16}N_2O$]	**151328-41-5**	**$(CH_3)_2N\text{-}C(CH_3){=}N(CH_2)_2OCH_3$**				**1003.8**			**1036.2**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	36	1003.8						
[$C_9H_{20}N_2$]	**94793-24-5**	**$(CH_3)_2N\text{-}C(CH_3){=}N(n\text{-}C_5H_{11})$**				**1002.1**			**1034.5**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	34.3	1002.1						
[$C_{13}H_{22}N_2$]	**133836-18-4**	**$(CH_3)_2N\text{-}CH{=}N\text{-}(1\text{-Ad})$**				**1001.0**			**1033.5**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	33.1	1000.9						
92RAC/MAR	101398-58-7	$(CH_3)_2N\text{-}CH{=}N(CH_2)_2N(CH_3)_2$	338	996.4	7.9	1004.3						
92RAC/MAR	151328-40-4	$(CH_3)_2N\text{-}C(CH_3){=}NC_2H_5$	338	996.7	4.6	1001.3						
92RAC/MAR	94793-19-8	$(CH_3)_2N\text{-}C(CH_3){=}N(i\text{-}C_3H_7)$	338	999.2	1.7	1000.8						
92RAC/MAR	147350-05-8	$(CH_3)_2N\text{-}C(CH_3){=}N(t\text{-}C_4H_9)$	338	1005.9	−5.0	1000.8						
91DEC/GAL	80-70-6	$((CH_3)_2N)_2C{=}NH$	338	997.4	2.5	999.7						
91DEC/GAL	133835-17-3	$(CH_3)_2N\text{-}CH{=}N\text{-}(1,1\text{-dimethylpropyl})$	338	989.6	9.6	999.2						
[$C_{10}H_{14}N_2$]	**119044-57-4**	**$(CH_3)_2N\text{-}C(C_6H_5){=}NCH_3$**				**1000.9**			**1033.3**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	33.1	1000.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{10}H_{22}N_2$]	**94793-26-7**	**$(CH_3)_2N$-C(CH_3)=N(n-C_6H_{13})**				**1000.9**			**1033.3**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	33.1	1000.9						
[$C_7H_{16}N_2$]	**94793-19-8**	**$(CH_3)_2N$-C(CH_3)=N(i-C_3H_7)**				**999.2**			**1031.6**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	31.4	999.2						
[$C_7H_{16}N_2$]	**94793-20-1**	**$(CH_3)_2N$-C(CH_3)=N(n-C_3H_7)**				**997.9**			**1030.3**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	30.1	997.9						
[$C_{11}H_{16}FN_3$]	**20815-37-6**	**$((CH_3)_2N)_2C$=N(4-FC_6H_4)**				**997.6**			**1030.0**			**0**
94RAC/MAR	80-70-6	**$((CH_3)_2N)_2C$=NH**	338	997.4	0.4	997.6						
[$C_5H_{13}N_3$]	**80-70-6**	**$((CH_3)_2N)_2C$=NH**				**997.4**			**1031.6**			**−5.8**
87TAF	75-50-3	(CH_3)$_3$N	350	918.1	78.7	997.4						
86TAF/GAL	7664-41-7	NH_3	350	819	172.3	991.2						
[$C_6H_{14}N_2$]	**151328-40-4**	**$(CH_3)_2N$-C(CH_3)=NC_2H_5**				**996.7**			**1029.1**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	28.9	996.7						
[HLi]	**7580-67-8**	**LiH**				**996.4**			**1021.7**			**24**
88DIX/GOL		theory	300						1021.7			
[$C_7H_{17}N_3$]	**101398-58-7**	**$(CH_3)_2N$-CH=N(CH_2)$_2$N(CH_3)$_2$**				**996.4**			**1028.8**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	27.6	995.4						
92RAC/MAR	80-70-6	$((CH_3)_2N)_2C$=NH	338	997.4	0.4	997.6						
92RAC/MAR	133835-17-3	$(CH_3)_2N$-CH=N-(1,1-dimethylpropyl)	338	989.6	6.3	995.9						
[$C_{14}H_{18}N_2$]	**20734-58-1**	**N,N,N′,N′-Tetramethyl-1,8-naphthalenediamine**				**995.8**			**1028.2**			**0**
83TAF	87-85-4	(CH_3)$_6$-C_6	350	836.0	159.7	997.0						
78LAU/SAL	7664-41-7	NH_3	650	819	177.7	994.5						
[$C_{11}H_{16}ClN_3$]	**20815-38-7**	**$((CH_3)_2N)_2C$=N(4-ClC_6H_4)**				**995.5**			**1027.9**			**0**
94RAC/MAR	80-70-6	$((CH_3)_2N)_2C$=NH	338	997.4	−1.7	995.5						
[$C_8H_{20}N_2$]	**111-51-3**	**$(CH_3)_2N(CH_2)_4N(CH_3)_2$**				**992.7**			**1046.3**			**−71**
87TAF	75-50-3	(CH_3)$_3$N	350	918.1	70.5	992.4						
83TAF2	7664-41-7	NH_3	350	819	171.2	993.4						
79AUE/BOW	75-50-3	(CH_3)$_3$N	298	918.1	74.2	992.3						
[La]	**7439-91-0**	**La**				**991.9**			**1013**			**38**
89ELK/SUN		See Refs.							1013±9			
[$C_7H_{14}N_2$]	**151328-39-1**	**$(CH_3)_2N$-C(CH_3)=N(c-C_3H_5)**				**991.7**			**1024.1**			**0**
93DEC/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	23.9	991.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
Ylsquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_7H_{12}N_2$]	**28504-67-8**	**$(CH_3)_2N$-C(CH_3)=NCH_3**				**990.8**			**1023.2**		**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	23	990.8					
[$C_{16}H_{26}N_8O_9$]	**38416-68-1**	**octaglycine**				**990.7**			**NE**		**NE**
92WU/FEN2		kinetic method				990.7					
[$C_7H_{14}N_4$]	**673-46-1**	**N_π,N_π-dimethylhistamine**				**990.1**			**1022.0**		**2**
95HER/ABB	110-95-2	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	333	985.4	2.4	985.8					
95HER/ABB	111-51-3	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	333	992.7	−0.6	989.7					
95HER/ABB	80-70-6	$((CH_3)_2N)_2C$=NH	333	997.4	−2.4	994.8					
[$C_8N_{18}N_2$]	**133835-17-3**	**$(CH_3)_2N$-CH=N-(1,1-dimethylpropyl)**				**989.6**			**1022.0**		**0**
91DEC/GAL	3459-75-4	$(CH_3)_2N$-CH=N-(c-hexyl)	338	987.9	1.7	989.6					
91DEC/GAL	23314-06-9	$(CH_3)_2N$-CH=N(t-C_4H_9)	338	988.3	1.3	989.6					
[$C_9H_{15}N$]	**7148-07-4**	**Pyrrolidine,1-(1-cyclopenten-1-yl)-**				**988.4**			**1019.2**		**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	70.3	988.4			975.3		
[$C_7H_{16}N_2$]	**23314-06-9**	**$(CH_3)_2N$-CH=N(t-C_4H_9)**				**988.3**			**1020.8**		**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	19.9	987.7					
91DEC/GAL	110-95-2	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	338	985.4	3.3	986.6					
91DEC/GAL	80-70-6	$((CH_3)_2N)_2C$=NH	338	997.4	−7.1	990.1					
91DEC/GAL	32150-24-6	$(CH_3)_2N$-CH=N-(1-methylethyl)	338	981.0	7.9	989.0					
[$C_9H_{18}N_2$]	**3459-75-4**	**$(CH_3)_2N$-CH=N-(c-hexyl)**				**987.9**			**1020.4**		**0**
91DEC/GAL	23314-06-9	$(CH_3)_2N$-CH=N(t-C_4H_9)	338	988.3	−1.3	987.1					
91DEC/GAL	80-70-6	$((CH_3)_2N)_2C$=NH	338	997.4	−8.4	988.8					
[$C_6H_{14}N_2O$]	**134166-62-4**	**$(CH_3)_2N$-CH=N-(2-methoxyethyl)**				**986.4**			**1018.9**		**0**
92RAC/MAR	23314-06-9	$(CH_3)_2N$-CH=N(t-C_4H_9)	338	988.3	−0.4	987.9					
92RAC/MAR	111-51-3	$(CH_3)_2N(CH_2)_4N(CH_3)_2$	338	992.7	−5.0	985.0					
92RAC/MAR	80-70-6	$((CH_3)_2N)_2C$=NH	338	997.4	−10.0	987.2					
92RAC/MAR	32150-24-6	$(CH_3)_2N$-CH=N-(1-methylethyl)	338	981.0	4.6	985.6					
[$C_7H_{16}N_2$]	**85599-92-4**	**$(CH_3)_2N$-CH=N-(1-methylpropyl)**				**985.7**			**1018.1**		**0**
91DEC/GAL	85599-94-6	$(CH_3)_2N$-CH=N-(n-hexyl)	338	984.9	1.7	986.6					
91DEC/GAL	134166-62-4	$(CH_3)_2N$-CH=N-(2-methoxyethyl)	338	986.4	−1.7	984.7					
[$C_8H_{18}N_2$]	**94793-23-4**	**$(CH_3)_2N$-CH=N(n-C_5H_{11})**				**985.5**			**1018.0**		**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	16.7	984.5					
91DEC/GAL	85599-94-6	$(CH_3)_2N$-CH=N-(n-hexyl)	338	984.9	1.7	986.6					
91DEC/GAL	3717-82-6	$(CH_3)_2N$-CH=N-(n-butyl)	338	980.5	5.0	985.5					
[$C_7H_{18}N_2$]	**110-95-2**	**$(CH_3)_2N(CH_2)_4N(CH_3)_2$**				**985.4**			**1035.2**		**−58**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	64.5	985.8					

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83TAF2	7664-41-7	NH_3	350	819	165.2	986.8						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	66.9	985.0						
[$C_9H_{20}N_2$]	**85599-94-6**	**$(CH_3)_2$N-CH=N-(n-hexyl)**				**984.9**			**1017.4**			**0**
91DEC/GAL	102-82-9	$(n\text{-}C_6H_{13})_3N$	338	967.6	>12.6	>980						
91DEC/GAL	80-70-6	$((CH_3)_2N)_3$-NH	338	997.4	−12.1	985.1						
91DEC/GAL	32150-24-6	$(CH_3)_2$N-CH=N-(1-methylethyl)	338	981.0	3.8	984.8						
[$C_{10}H_{24}N_2$]	**111-18-2**	**$(CH_3)_2N(CH_2)_6N(CH_3)_2$**				**982.2**			**1035.8**			**−71**
83TAF2	7664-41-7	NH_3	350	819	161.5	983.8						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	62.4	980.5						
[$C_7H_{16}N_2$]	**67161-18-6**	**$(CH_3)_2$N-CH=N-(2-methylpropyl)**				**982.0**			**1014.5**			**0**
91DEC/GAL	32150-24-6	$(CH_3)_2$N-CH=N-(1-methylethyl)	338	981.0	0.4	981.4						
91DEC/GAL	134166-62-4	$(CH_3)_2$N-CH=N-(2-methoxyethyl)	338	986.4	−3.8	982.7						
[$C_{10}H_{14}N_2$]	**27159-75-7**	**$(CH_3)_2$N-CH=N-(phenylmethyl)**				**981.7**			**1014.1**			**0**
92RAC/MAR	32150-24-6	$(CH_3)_2$N-CH=N-(1-methylethyl)	338	981.0	0.4	981.4						
92RAC/MAR	74119-36-1	$(CH_3)_2$N-CH=N-C_2H_5	338	976.3	4.6	980.9						
92RAC/MAR	134166-62-4	$(CH_3)_2$N-CH=N-(2-methoxyethyl)	338	986.4	−3.8	982.7						
[HOSr]	**12141-14-9**	**SrOH**				**981.6**			**1019.4**			**−18**
76TAN/LIA		See Refs.							1019.4			**−18**
[$C_{18}H_{32}N_6O_7$]	**111652-29-0**	**hexa-L-alanine**				**981.3**			**NE**			**NE**
93WU/FEN		kinetic method				981.3						
[$C_6H_{14}N_2$]	**32150-24-6**	**$(CH_3)_2$N-CH=N-(1-methylethyl)**				**981.0**			**1013.5**			**0**
91DEC/GAL	109-55-7	$(CH_3)_2N(CH_2)_3NH_2$	338	975.3	8.4	981.4						
91DEC/GAL	74119-36-1	$(CH_3)_2$N-CH=N-C_2H_5	338	976.3	3.8	980.0						
91DEC/GAL	110-95-2	$(CH_3)_2N(CH_2)_3N(CH_3)_2$	338	985.4	−1.7	981.6						
[$C_{14}H_{23}N_7O_8$]	**18861-82-0**	**heptaglycine**				**980.6**			**NE**			**NE**
92WU/FEN2		See Refs.	350			980.6						
[$C_7H_{16}N_2$]	**3717-82-6**	**$(CH_3)_2$N-CH=N-(n-butyl)**				**980.5**			**1013.0**			**0**
91DEC/GAL	74119-36-1	$(CH_3)_2$N-CH=N-C_2H_5	338	976.3	5.0	981.3						
91DEC/GAL	32150-24-6	$(CH_3)_2$N-CH=N-(1-methylethyl)	338	981.0	−1.3	979.8						
[$C_{14}H_{29}N$]	**64326-83-6**	**1-Methyl-2,6-t-butylpiperidine**				**980.3**			**1011.1**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	61.8	979.9						
83TAF	87-85-4	$(CH_3)_6$-C_6	350	836.0	143.7	980.7						
[$C_{10}H_{15}N_5O_4$]	**7451-76-5**	**gly-gly-his**				**979.5**			**NE**			**NE**
93WU/FEN		kinetic method				979.5						
96CAR/CAS	926-63-6;	$(CH_3)_2(n\text{-}C_3H)N$; $(n\text{-}C_3H_7)_3N$				932-960						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
	102-69-2											
[$C_6H_{14}N_2$]	**32150-25-7**	**$(CH_3)_2N$-CH=N-(n-propyl)**				**979.2**			**1011.7**			**0**
91DEC/GAL	74119-36-1	$(CH_3)_2N$-CH=N-C_2H_5	338	976.3	2.1	978.4						
91DEC/GAL	3717-82-6	$(CH_3)_2N$-CH=N-(n-butyl)	338	980.5	−0.4	980.1						
[$C_5H_{12}N_2$]	**74119-36-1**	**$(CH_3)_2N$-CH=N-C_2H_5**				**976.3**			**1008.7**			**0**
91DEC/GAL	1122-58-3	N,N-Dimethyl-4-pyridinamine	338	971.1	1.7	973.5						
91DEC/GAL	1609-01-4	$(CH_3)_2N$-CH=N-CH_3	338	970.0	6.7	976.7						
91DEC/GAL	109-55-7	$(CH_3)_2N(CH_2)_3NH_2$	338	975.3	2.9	976.0						
[$C_5H_{14}N_2$]	**109-55-7**	**$(CH_3)_2N(CH_2)_3NH_2$**				**975.3**			**1025.0**			**−58**
83TAF2	7664-41-7	NH_3	350	819	154.7	976.3						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	56.1	974.3						
[$C_6H_{12}N_2$]	**133835-16-2**	**$(CH_3)_2N$-CH=N-(c-propyl)**				**973.8**			**1006.2**			**0**
91DEC/GAL	1609-01-4	$(CH_3)_2N$-CH=N-CH_3	338	970.0	3.3	973.4						
91DEC/GAL	74119-36-1	$(CH_3)_2N$-CH=N-C_2H_5	338	976.3	−2.1	974.2						
[$C_{10}H_{12}N_2$]	**34165-19-0**	**2,3,5-Trimethylimidazo(1,2-a)-pyridine**				**973.7**			**1005.6**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	55.4	973.7						
[I]	**7440-61-1**	**I**				**973.2**			**995.2**			**35**
77ARM/HOD		reaction onset							995.2			
[$C_6H_{13}N$]	**78733-72-9**	**$(CH_3)_2NC(CH_3)$=CHCH$_3$**				**972.9**			**1005.4**			**0**
81ELL/DIX	110-18-9;	$(CH_3)_2NCH_2CH_2CH_2NH_2$;				971-975						
	109-55-7	$(CH_3)_2NCH_2CH_2N(CH_3)_2$										
[$C_6H_{12}N$]	**60598-49-4**	**$(CH_3)_2N$-CH=N-(2-propenyl)**				**972.3**			**1004.8**			**0**
92RAC/MAR	74119-36-1	$(CH_3)_2N$-CH=N-C_2H_5	338	976.3	−2.9	973.3						
92RAC/MAR	32150-27-9	$CH_3C(N(CH_3)_2)$=NN$(CH_3)_2$	338	963.4	7.9	971.3						
[HLiO]	**1310-66-3**	**LiOH**				**972.1**			**1000.1**			**14.9**
70DZI/KEB		See Refs.							1000.1			14.9
[$C_7H_{10}N_2$]	**1122-58-3**	**N,N-Dimethyl-4-pyridinamine**				**971.1**			**997.6**			**20**
91AUE/WEB	110-86-1	pyridine	300	898.1	74.7	972.8						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	51.3	968.7						
86TAF/GAL	7664-41-7	NH_3	350	819	151.7	969.3						
83TAF2	7664-41-7	NH_3	350	819	152.4	970.1						
77ARN/CHA	110-18-9	$(CH_3)_2N(CH_2)_3N(CH_3)_2$	298	970.6	1.3	971.9						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	55.6	973.8						
[Lu]	**7439-94-3**	**Lu**				**970.6**			**992**			**37**
89ELK/SUN		See Refs.							992±15			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ref Squb	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R, T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_6H_{16}N_2$]	**110-18-9**	**$(CH_3)_2N(CH_2)_2N(CH_3)_2$**				**970.6**			**1012.8**			**−33**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	49.9	969.9						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	52.2	970.4						
75TAF	7664-41-7	NH_3	350	819	151.0	971.3						
[$C_4H_{10}N_2$]	**1609-01-4**	**$(CH_3)_2N$-CH=N-CH_3**				**970.0**			**1002.5**			**0**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	2.1	969.9						
91DEC/GAL	1122-58-3	N,N-Dimethyl-4-pyridinamine	338	971.1	−3.3	968.5						
91DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	2.1	969.9						
91DEC/GAL	109-55-7	$(CH_3)_2N(CH_2)_3NH_2$	338	975.3	−1.3	971.8						
[$C_{12}H_{19}NO$]	**3357-16-2**	**3-Pyrrolidino-5,5-dimethylcyclohex-2-enone**				**968.7**			**1001.2**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	50.3	968.7						
[$C_{13}H_{21}NO$]	**65115-73-3**	**3-(N,N-Diethylamino)-5,5-dimethylcyclohex 2-enone**				**968.7**			**1001.2**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	50.3	968.7						
[$C_9H_{10}N_2$]	**3268-61-9**	**2,7-Dimethylimidazo(1,2-a)pyridine**				**968.6**			**1000.5**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	50.3	968.6						
[$C_{13}H_{21}NO$]	**13358-76-4**	**3-Piperidino-5,5-dimethylcyclohex-2-enone**				**968.3**			**1000.7**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	49.9	968.3						
[$C_4H_8N_2$]	**1606-49-1**	**1,4,5,6-tetrahydropyrimdine**				**967.8**			**1002.0**			**−5.8**
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	−0.2	967.8						
[$C_{12}H_{27}N$]	**102-82-9**	**$(n\text{-}C_4H_9)_3N$**				**967.6**			**998.5**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	49.0	967.1						
85BOL/HOU	102-82-9	$(n\text{-}C_4H_9)_3N$	323	967.6	0	967.6						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	104.0	968.5						
[$C_9H_{10}N_2$]	**875-80-9**	**2,3-Dimethylimidazo(1,2-a)pyridine**				**966.4**			**998.2**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	48.1	966.4						
[$C_7H_{17}N$]	**6006-15-1**	**$(i\text{-}C_3H_7)N(C_2H_5)_2$**				**965.6**			**996.4**			**5.6**
77ARN/CHA	1122-58-3	N,N-Dimethyl-4-pyridinamine	298	971.1	−5.4	965.6						
[$C_9H_{24}N_3OP$]	**2327-88-0**	**$OP(CH_2N(CH_3)_2)_3$**				**965.2**			**997.7**			**0**
85BOL/HOU	102-69-2	$(n\text{-}C_3H_7)_3N$	323	960.1	4.2	964.4						
85BOL/HOU	102-82-9	$(n\text{-}C_4H_9)_3N$	323	967.6	−1.7	966.0						
[$C_9H_{10}N_2$]	**6188-30-3**	**2,5-Dimethylimidazo(1,2-a)pyridine**				**964.5**			**996.4**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	46.2	964.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YtSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_6H_{15}N$]	**7087-68-5**	**(i-C_3H_7)$_2$(C_2H_5)N**				**963.5**			**994.3**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	44.8	963.0						
83TAF2	7664-41-7	NH_3	350	819	145.5	963.9						
[$C_5H_{13}N_3$]	**32150-79-9**	**$CH_3C(N(CH_3)_2)$=NN$(CH_3)_2$**				**963.4**			**995.8**			**0**
92RAC/MAR	102-69-2	(n-C_3H_7)$_3$N	338	960.1	2.5	962.8						
92RAC/MAR	121-44-8	$(C_2H_5)_3N$	338	951	12.6	963.8						
92RAC/MAR	102-82-9	(n-C_4H_9)$_3$N	338	967.6	−4.2	963.6						
[$C_{12}H_{21}N$]	**3717-40-6**	**N,N-Dimethyladamantylamine**				**963.0**			**993.9**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	44.8	963.0						
[$C_{10}H_{13}N_5O_4$]	**961-07-9**	**Deoxyguanosine**				**962.9**			**995.4**			**0**
90GRE/LIG		kinetic method							995.4			
[$C_8H_8N_2$]	**874-39-5**	**7-Methylimidazo(1,2-a)pyridine**				**962.7**			**994.6**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	44.4	962.7						
[$C_{15}H_{27}N_5O_6$]	**10183-34-3**	**penta-L-alanine**				**962**			**NE**			**NE**
93WU/FEN		kinetic method				962						
[$C_5H_9N_3$]	**51-45-6**	**Histamine**				**961.9**			**999.8**			**−18**
93DEO/GAL	102-82-9	(n-C_4H_9)$_3$N	338	967.6	−6.5	961.9						
[$C_{19}H_{20}N_2$]	**123624-78-7**	**13,5-metheno-6H,7H-bisazepino[1,2a:2′,1′-d][1,5]diazecine,8,9,10,11-tetrahydro**				**961.8**			**994.3**			**0**
89HOU/FEN	102-82-9	(n-C_4H_9)$_3$N	313	967.6	1.3	968.9						
89HOU/FEN	102-69-2	(n-C_3H_7)$_3$N	313	960.1	1.7	961.8						
89HOU/FEN	4458-31-5	(C_2H_5)$_2$(n-C_3H_7)N	313	947.9	2.1	950.0						
[$C_7H_{15}N$]	**78733-73-0**	**$(CH_3)_2NC(C_2H_5)$=$CHCH_3$**				**961**			**991.8**			**5.6**
81ELL/DIX	121-44-8; 110-18-9	$(C_2H_5)_3N$;$(CH_3)_2NCH_2CH_2N(CH_3)_2$				951-971						
[$C_{10}H_{13}N_5O_2$]	**118-00-3**	**guanosine**				**960.9**			**993.4**			**0**
94LIG/NAP		kinetic method							993.4			
[$C_6H_{10}N_2$]	**121508-72-3**	**$(CH_3)_2$N-CH=N-(2-propynyl)**				**960.7**			**993.1**			**0**
92RAC/MAR	102-82-9	(n-C_4H_9)$_3$N	338	967.6	−7.5	960.2						
92RAC/MAR	1609-01-4	$(CH_3)_2$N-CH=N-CH_3	338	970.0	−7.9	962.1						
92RAC/MAR	32150-27-9	$CH_3C(N(CH_3)_2)$=NN$(CH_3)_2$	338	963.4	−3.3	960.0						
[$C_9H_{21}N$]	**102-69-2**	**(n-C_3H_7)$_3$N**				**960.1**			**991.0**			**5.6**
91MAU/SMI	102-82-9	(n-C_4H_9)$_3$N	300	967.6	−9.6	957.9	998.5	−12.1	986.4			
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	42.6	960.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83TAE2	7664-41-7	NH_3	350	819	143.3	961.7						
83TAE	87-85-4	$(CH_3)_6$-C_6	350	836.0	124.0	961.1						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	97.1	961.6						
75TAE	7664-41-7	NH_3	350	819	140.0	958.4						
75ARN	7664-41-7	NH_3	350	819	128.0	946.4						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	100.1	964.6						
[$C_{13}H_{27}N$]	**66922-18-7**	**2-6-Di-t-butylpiperidine**				**960.1**			**992.5**			**0**
87TAE	75-50-3	$(CH_3)_3N$	350	918.1	41.6	960.1						
83TAE	87-85-4	$(CH_3)_6$-C_6	350	836.0	121.3	958.6						
[MgO]	**1309-48-4**	**MgO**				**959.4**			**988**			**13**
81MUR		See Refs.							988			
[$C_{10}H_{13}N_5O_3$]	**958-09-8**	**Deoxyadenosine**				**959.1**			**991.5**			**0**
90GRE/LIG		kinetic method							991.5			
[$C_8H_8N_2$]	**934-37-2**	**2-Methylimidazo(1,2-a)pyridine**				**959.0**			**990.9**			**2**
87TAE	75-50-3	$(CH_3)_3N$	350	918.1	40.7	959.0						
[$C_{10}H_{20}N_4O_4$]	**10236-53-0**	**gly-gly-lys**				**958.6**			**NE**			**NE**
96CAR/CAS	926-63-6;	$(CH_3)_2$(n-C_3H_7)N;				932-985						
	110-95-2	$(CH_3)_2N(CH_2)_3N(CH_3)_2$										
[$C_{10}H_{20}N_4O_4$]	**55488-08-9**	**lys-gly-gly**				**958.6**			**NE**			**NE**
96CAR/CAS	926-63-6;	$(CH_3)_2$(n-C_3H_7)N;				932-985						
	110-95-2	$(CH_3)_2N(CH_2)_3N(CH_3)_2$										
[$C_9H_{21}N$]	**58471-09-3**	**(t-C_5H_{11})(t-C_4H_9)NH**				**958.2**			**991.4**			**−2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	40.0	958.2						
[$C_{10}H_{13}N_5O_4$]	**58-61-7**	**adenosine**				**956.8**			**989.3**			**0**
94LIG/NAP		kinetic method							989.3			
[$C_{10}H_{14}N_2$]	**56638-68-7**	**$(CH_2)_2$N-CH=N-(4-methylphenyl)**				**956.1**			**988.6**			**0**
90BOR/HOU	102-69-2	(n-$C_3H_7)_3N$	313	960.1	1.3	961.4						
90BOR/HOU	4458-31-5	(C_2H_5)$_2$(n-C_3H_7)N	313	947.9	2.9	950.9						
[$C_8H_{15}N$]	**5261-65-4**	**1-azabicyclo[2.2.2]-octane,2-methyl**				**956.1**			**986.9**			**5.6**
86HEI/HON	4458-31-5	(C_2H_5)$_2$(n-C_3H_7)N	313	947.9	3.8	951.7						
86HEI/HON	102-69-2	(n-$C_3H_7)_3N$	313	960.1	−0.4	959.7						
[$C_9H_{13}N_3O_4$]	**951-77-9**	**Deoxycytidine**				**956.0**			**988.4**			**0**
90GRE/LIG		kinetic method							988.4			
[$C_5H_{10}N_2$]	**2305-59-1**	**4,4-dimethyl-2-imidazoline**				**955.7**			**988.1**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YtSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93DEC/GAL	102-82-9	$(n\text{-}C_4H_9)_3N$	338	967.6	−12.1	955.7						
$[C_8H_{12}N_4O_3]$	**2489-13-6**	**gly-his**				**955.5**			**NE**			**NE**
96CAR/CAS	121-44-8; 102-69-2	$(C_2H_5)_3N$; $(n\text{-}C_4H_9)_3N$				951-960						
$[C_8H_{12}N_4O_3]$	**2578-58-7**	**his-gly**				**955.6**			**NE**			**NE**
96CAR/CAS	121-44-8; 102-69-2	$(C_2H_5)_3N$; $(n\text{-}C_4H_9)_3N$				951-960						
$[C_{10}H_{15}N_5O_4]$	**7758-33-0**	**gly-his-gly**				**955.5**			**NE**			**NE**
96CAR/CAS	121-44-8; 102-69-2	$(C_2H_5)_3N$; $(n\text{-}C_4H_9)_3N$				951-960						
$[C_{10}H_{20}N_4O_4]$	**45214-22-0**	**gly-lys-gly**				***955.5***			**NE**			**NE**
96CAR/CAS	121-44-8; 102-69-2	$(C_2H_5)_3N$; $(n\text{-}C_4H_9)_3N$				951-960						
$[C_8H_8N_2]$	**933-69-7**	**5-Methylimidazo(1,2-a)pyridine**				**955.4**			**987.4**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	37.1	955.4						
$[C_7H_{12}N_2]$	**45676-04-8**	**1-t-Butylimidazole**				**954.9**			**987.0**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	36.6	954.9						
$[C_7H_{14}Na_2]$	**6238-14-8**	**3-Amino-1-azabicyclo[2.2.2]octane**				**954.7**			**985.7**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	36.6	954.7						
$[C_9H_{17}NO_2]$	**#231**	**3,3-Dimethoxy-1-azabicyclo[2.2.2]octane**				**954.7**			**985.7**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_2N$	298	918.1	36.6	954.7						
$[C_8H_{19}N]$	**21981-37-3**	**$(t\text{-}C_4H_9)_2NH$**				**954.7**			**987.9**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	35.7	954.2						
83TAF2	7664-41-7	NH_3	350	819	136.4	955.2						
$[C_4H_{12}N_2]$	**110-60-1**	**1,4-butanediamine**				**954.3**			**1005.6**			**−63**
93CHE/WU		kinetic method							1004.5			65
80MAU/HAM	142-84-7	$(n\text{-}C_4H_9)_2NH$	330	929.3	22.6	953.7	962.3	42.3	1004.5	−1.9	−59.8	−61.7
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	36.1	954.3						
73AUE/WEB	107-10-8	$n\text{-}C_3H_7NH_2$	298	883.9	71.3	955.1						
$[C_9H_{19}N]$	**768-66-1**	**2,2,6,6-Tetramethyl-piperidine**				**953.9**			**987.0**			**−1.9**
84HOP/JAH	29939-31-9	2-4-$(t\text{-}C_4H_9)_2$-pyridine	298	952.0	1.7	953.6						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	36.1	954.3						
$[C_3H_9NO]$	**1184-78-7**	**$(CH_3)_3NO$**				**953.5**			**983.2**			**9.1**
80KOP/COM		See Refs.							983.2			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / Ref	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_9H_{18}N_2$]	**22766-69-4**	**1-Azabicyclo[2.2.2]octane,4-N,N-dimethylamino-**				**952.9**			**983.9**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	34.8	952.9						
[$C_{10}H_{17}NO$]	**31039-88-0**	**3-(N,N-Dimethylamino)-5,5-dimethyl-cyclohex-2-en-1-one**				**952.9**			**983.8**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	33.9	952.0						
86TAF/GAL	7664-41-7	NH_3	350	819	134.9	953.3						
[$C_8H_{17}N$]	**98-94-2**	**c-$C_6H_{11}N(CH_3)_2$**				**952.6**			**983.6**			**5.6**
86TAF/GAL	7664-41-7	NH_3	350	819	134.2	952.6						
[$C_5H_8N_2$]	**1739-84-0**	**1,2-Dimethylimidazole**				**952.6**			**984.7**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	34.3	952.6						
[$C_7H_{13}N$]	**100-75-5**	**1-azabicyclo[2.2.2]-octane**				**952.5**			**983.3**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	35.7	953.8						
86TAF/GAL	7664-41-7	NH_3	350	819	136.1	954.5						
86HEI/HON	121-44-8	$(C_2H_5)_3N$	313	951	1.3	952.3						
83TAF	87-85-4	$(CH_3)_6$-C_6	350	836.0	116.7	953.7						
80HOU/VOG		See Refs.							971.1			
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	87.4	951.9						
77STA/TAA	7664-41-7	NH_3	320	819	120.9	939.7						
75TAF	7664-41-7	NH_3	350	819	132.3	950.7						
74STA/BEA2	75-50-3	$(CH_3)_3N$	320	918.1	32.2	950.3						
[$C_6H_{15}P$]	**554-70-1**	**$(C_2H_5)_3P$**				**952.0**			**984.5**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	31.1	949.5						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	36.1	954.3						
[$C_{13}H_{21}N$]	**29939-31-9**	**2,4-(t-$C_4H_9)_2$-pyridine**				**952.0**			**983.8**			**2**
84HOP/JAH	626-23-3	(sec-$C_4H_9)_2NH$	298	947.5	3.3	950.8						
84HOP/JAH	121-44-8	$(C_2H_5)_3N$	298	951	1.7	952.7						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	34.7	952.8						
[$C_{16}H_{16}N_2$]	**95864-13-4**	**15,16-diazatricyclo[8.4.1.1^{3,8}]hexadeca-1,3,5,7,9,11,13-heptaene,15,16-dimethyl**				**951.9**			**984.4**			**0**
89HOU/FEN	121-44-8	$(C_2H_5)_3N$	313	951	0.8	951.9						
[$C_{13}H_{16}N_2$]	**20734-57-0**	**N,N,N′-Trimethyl-1,8-naphthalenediamine**				**951.8**			**984.3**			**0**
78LAU/SAL	7664-41-7	NH_3	600	819	134.7	951.8						
[$C_8H_{15}N$]	**695-88-6**	**1-azabicyclo[2.2.2]-octane, 3-methyl**				**951.7**			**982.5**			**5.6**
86HEI/HON	102-69-2	$(n\text{-}C_3H_7)_3N$	313	960.1	−5.9	954.2						
86HEI/HON	4458-31-5	$(C_2H_5)_2(n\text{-}C_3H_7)N$	313	947.9	−1.3	946.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
79AUE/BOW	75-50-3	$(CH_3)_4N$	298	918.1	36.1	954.3						
[$C_7H_{17}N$]	**57767-60-5**	**(t-C_5H_{11})$(CH_3)_2N$**				**951.5**			**982.5**			**5.6**
87TAF	75-50-3	$(CH_3)_4N$	350	918.1	33.4	951.5						
[$C_9H_{21}N$]	**3733-36-6**	**(t-C_4H_9)$C(CH_3)_2N(CH_3)_2$**				**951.4**			**982.4**			**5.6**
78SHE/GOB	7664-41-7	NH_3	320	819	132.6	951.4						
[$C_{14}H_{12}N_2$]	**75863-17-1**	**15,16-diazatricyclo[8.4.1.1^{3,8}]hexadeca-1,3,5,7,9,11,13-heptaene**				**951.4**			**983.8**			**0**
89HOU/FEN	6832-21-9	2,6-(i-C_3H_7)$_2$-pyridine	313	947.2	4.2	951.4						
[$C_9H_{12}N_2$]	**56687-95-7**	**$(CH_3)_2N$-CH=N-phenyl**				**951.3**			**983.8**			**0**
90BOR/HOU	102-69-2	(n-C_3H_7)$_3N$	313	960.1	−5.4	954.7						
90BOR/HOU	4458-31-5	(C_2H_5)$_2$(n-C_3H_7)N	313	947.9	0	947.9						
[$C_6H_{14}N_2O_2$]	**56-87-1**	**L-lysine**				**951.0**			**996**			**−42**
96CAR/CAS	142-87-7; 121-44-8	(n-C_3H_7)$_2$NH; (C_2H_5)$_3N$				929-951						
94WU/FEN		kinetic method							996			−42
93LI/HAR		kinetic method							942			
92GOR/SPE	109-89-7; 142-84-7	(C_2H_5)$_2$NH; (n-C_3H_7)$_2$NH	350			919-929						
90ISA/OMO		Kinetic method-relative order										
87TAF	75-50-3	$(CH_3)_4N$	350	918.1	21.5	942.0						
87BOJ		kinetic method-relative order										
86BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	123.1	943.9						
[$C_6H_{15}N$]	**121-44-8**	**(C_2H_5)$_3N$**				**951**			**981.8**			**5.6**
91MAU/SMI	102-82-9	(n-C_4H_9)$_3N$	602	967.6	−17.6	950.0	998.5	−22.6	975.9			
91MAU/SMI	102-69-2	(n-C_3H_7)$_3N$	300	960.1	−12.1	948.0	991.0	−12.6	978.5			
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	33.4	951.5						
86MAU/LIE	110-86-1	pyridine	600	898.1	60.3	957.4						
83TAF	7664-41-7	NH_3	350	819	134.1	952.5						
83LOC/MCI	7664-41-7	NH_3	350	819	131.8	950.2						
79MAU	107-10-8	n-$C_3H_7NH_2$	550	883.9	61.5	942.7						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	33.7	951.8						
77STA/TAA	7664-41-7	NH_3	320	819	119.2	938.0						
75TAF	7664-41-7	NH_3	350	819	130.4	948.8						
74STA/BEA2	75-50-3	$(CH_3)_3N$	320	918.1	30.5	948.7						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	88.8	953.3						
72ARN/JON	7664-41-7	NH_3	350	819	132.3	950.7						
[$C_{13}H_{21}N$]	**585-48-8**	**2,6-(t-C_4H_9)$_2$-pyridine**				**951**			**982.9**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	29.7	948.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YtSqub	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83TAF2	7664-41-7	NH_3	350	819	131.8	950.4						
83TAF	87-85-4	$(CH_3)_6$-C_6	350	836.0	111.7	948.9						
83MAU/SIE	110-86-1	pyridine	425	898.1	56.9	955.0						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	31.7	949.9						
75WOL/HAR	7664-41-7	NH_3	350	819	129.1	947.6						
75TAF	7664-41-7	NH_3	350	819	136.4	955.0						
75ARN	7664-41-7	NH_3	350	819	124.7	943.3						
[$C_5H_{17}P$]	**3405-42-3**	**$(n\text{-}C_3H_7)_2(CH_3)P$**				**950.9**			**983.5**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	32.5	950.9						
[$C_8H_{13}N$]	**#249**	**1-Azabicyclo[2.2.2]oct-2-ene, 3-methyl**				**950.8**			**981.6**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	32.7	950.8						
[$C_{15}H_{18}$]	**489-84-9**	**1,4-Dimethyl-7-isopropylazulene**				**950.6**			**983.1**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	31.1	949.5						
77WOL/ABB	87-85-4	$(CH_3)_6$-C_6	350	836.0	114.4	951.7						
[$C_{10}H_{20}N_2$]	**6130-94-5**	**1,1'-bipiperidine**				**950.4**			**981.2**			**5.8**
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	1.3	952.2						
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	9.2	948.7						
[$C_6H_9N_3O_2$]	**71-00-1**	**L-histidine**				**950.2**			**988**			**−18**
96CAR/CAS	142-84-7; 121-	$(n\text{-}C_3H_7)_2NH$; $(C_2H_5)_3N$				929-951						
94WU/FEN		kinetic method							988			−18
92GOR/SPE	110-86-1;75-	pyridine; $(t\text{-}C_4H_9)NH_2$	350			898-900						
90ISA/OMO		kinetic method-relative order										
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	29.7	949.1						
87BOJ		kinetic method-relative order										
86BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	130.4	950.0						
[$C_{10}H_{16}N_2$]	**704-01-8**	**$1,2\text{-}(N(CH_3)_2)_2C_5H_4$**				**950.2**			**982.6**			**0**
78LAU/SAL	7664-41-7	NH_3	600	819	133.1	950.1						
[$C_9H_{13}N_3O_5$]	**65-46-3**	**cytidine**				**950.0**			**982.6**			**0**
94LIG/NAP		kinetic method							982.5			
[$C_{12}H_{20}N_8O_7$]	**3887-13-6**	**hexaglycine**				**950**			**NE**			**NE**
93ZHA/ZIM	142-84-7; 111-92-2	$(n\text{-}C_3H_7)_2NH$; $(n\text{-}C_4H_9)_2NH$	300			929-935						
92WU/FEN2		kinetic method				966.6						
[$C_8H_{16}N_2$]	**14287-92-4**	**2,3-diazabicyclo[2.2.2]octane,2,3-dimethyl**				**950.0**			**980.7**			**5.8**
88NEL/RUM	108-48-5	2-6-$(CH_3)_2$-pyridine	550	931.1	18.8	949.0						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	0	951.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[CH_5N_3]	**113-00-8**	**$(NH_2)_2C{=}NH$**				**949.4**			**986.3**			**−14.9**
96AME/TOR	98-84-2	c-$C_6H_{11}(CH_3)_2$	338	952.6	−3.0	950.4						
96AME/TOR	100-76-5	1-azabicyclo[2.2.2]-octane	338	952.5	−4.9	948.4						
[$C_7N_{19}NSi$]	**23138-94-5**	**$(CH_3)_3Si(CH_2)_2N(CH_3)_2$**				**949.4**			**980.4**			**5.6**
78SHE/GOB	7664-41-7	NH_3	350	819	131.0	949.4						
[$C_8H_{21}NSi$]	**28247-29-2**	**$(CH_3)_3Si(CH_2)_3N(CH_3)_2$**				**949.4**			**980.4**			**5.6**
78SHE/GOB	7664-41-7	NH_3	350	819	131.0	949.4						
[$C_9H_{17}N$]	**673-33-6**	**c-$C_5H_{10}NCH{=}C(CH_3)_2$**				**949.4**			**978.2**			**12**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	31.2	949.4						
[$C_{12}H_{21}N$]	**6321-40-0**	**$(CH_2{=}C(CH_3)CH_2)_3N$**				**949.4**			**980.2**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	31.2	949.4						
[$C_{15}H_{12}Fe_2O_3$]	**76722-37-7**	**[$(C_5H_5)(CO)Fe]_2(\mu$-CO)(μ-C=CH_2)**				**949.4**			**981.8**			**0**
89JAC	108-18-9; 102-69-2	(i-$C_3H_7)_2NH$; (n-$C_3H_7)_3N$				939-960						
[$C_{10}H_{24}N_2$]	**6897-05-8**	**Hydrazine, 1,2-dimethyl-1,2-bis(2-methylpropyl)**				**949.0**			**979.7**			**5.8**
88NEL/RUM	935-28-4	2-6-($C_2H_5)_2$-pyridine	550	940.4	8.4	947.9						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−0.8	950.1						
[$C_8H_{16}N_2$]	**18389-95-2**	**1,1′-bipyrrolidine**				**949.0**			**979.7**			**5.8**
88NEL/RUM	935-28-4	2,6-($C_2H_5)_2$-pyridine	550	940.4	7.5	947.0						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	0	951.0						
[$C_9H_{11}BrN_2$]	**119044-60-9**	**$(CH_3)_2N$-CH=N-(4-bromophenyl)**				**948.9**			**981.3**			**0**
90BOR/HOU	4458-31-5	($C_2H_5)_2$(n-C_4H_9)N	313	947.9	1.7	946.3						
90BOR/HOU	121-44-8	$(C_2H_5)_3N$	313	951	0.4	951.5						
[$C_{11}H_{13}N$]	**4363-25-1**	**Benzoquinuclidine**				**948.8**			**979.8**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	30.2	948.3						
83TAF2	7664-41-7	NH_3	350	819	130.9	949.3						
[$C_8H_{15}N$]	**45651-41-0**	**1-azabicyclo[2,2,2]-octane,4-methyl**				**948.6**			**979.4**			**5.6**
86HEI/HON	4458-31-5	($C_2H_5)_2$(n-C_3H_7)N	313	947.9	−1.6	946.3						
86HEI/HON	121-44-8	$(C_2H_5)_3N$	313	951	0	951						
[$C_6H_{15}N$]	**918-02-5**	**$(CH_3)_2$(t-C_4H_9)N**				**948.6**			**979.6**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	29.7	947.9						
83TAF2	7664-41-7	NH_3	350	819	130.9	949.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ylcsquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_6H_{11}N_3$]	**134166-60-2**	**$(CH_3)_2N$-CH=N-CH_2CH_2CN**				**948.3**			**980.8**			**0**
92RAC/MAR	121-44-8	$(C_2H_5)_3N$	338	951	−2.5	948.7						
92RAC/MAR	98-94-2	c-$C_6H_{11}N(CH_3)_2$	338	952.6	−2.5	950.3						
92RAC/MAR	134166-59-9	$(CH_3)_2$-CH=N-CH_2CF_3	338	933.8	12.1	945.9						
[$C_8H_{16}N_2$]	**3661-15-2**	**Pyridazino[1,2-a]pyridazine,octahydro-**				**947.9**			**978.7**			**5.8**
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	7.1	946.6						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−1.7	949.3						
[$C_7H_{17}N$]	**4458-31-5**	**$(C_2H_5)_2$(n-C_3H_7)N**				**947.9**			**978.8**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	29.7	947.9						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	90.3	954.8						
[$C_5H_6N_2$]	**504-24-5**	**4-Pyridinamine**				**947.8**			**979.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	51.7	949.9						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	32.0	950.3						
84CAT/PAZ	110-86-1	pyridine	320	898.1	47.7	945.8						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	26.8	945.0						
[$C_{13}H_{24}N_2$]	**141665-20-5**	**1,4-dimethyl-3,5-di-t-butylpyrazole**				**947.8**			**979.6**			**2**
92ABB/CAB	108-18-9	$(i\text{-}C_3H_7)_2NH$	333	938.6	9.2	947.7						
92ABB/CAB	121-44-8	$(C_2H_5)_3N$	333	951	−3.3	947.9						
[$C_{10}H_{19}N$]	**31023-92-4**	**1-Azabicyclo[3,3,3]undecane(Manxine)**				**947.7**			**978.7**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	31.7	949.9						
75AUE/WEB	74-89-5	CH_3NH_2	298	864.5	81.0	945.5						
[$C_8H_{19}N$]	**626-23-3**	**(sec-C_4H_9)$_2$NH**				**947.5**			**980.7**			**−1.9**
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	83.0	947.5						
[$C_{13}H_{23}N$]	**#177**	**Adamantyl-$CH_2N(CH_3)_2$**				**947.4**			**978.4**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	29.3	947.4						
[$C_{11}H_{14}N_2O$]	**119044-59-6**	**$(CH_3)_2N$-CH=N-(4-acetylphenyl)**				**947.3**			**979.8**			**0**
90BOR/HOU	121-44-8	$(C_2H_5)_3N$	313	951	−3.8	947.3						
[$C_6H_{12}N_2$]	**5397-67-1**	**1H,5H-pyrazolo[1,20-a]pyrazole,tetrahydro**				**947.3**			**978.0**			**5.8**
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	16.3	946.5						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−2.9	948.0						
[$C_8H_{15}N$]	**35079-50-6**	**1-4-4-$(CH_3)_3$-1,2,3,4-tetrahydropyridine**				**947.3**			**979.9**			**0**
80HOU/VOG		See Refs.							979.9			
[$C_8H_{17}P$]	**#181**	**$(CH_2)_7PCH_3$**				**947.2**			**979.7**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	28.8	947.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{11}H_{17}N$]	**6832-21-9**	**2-6-(i-C_3H_7)$_2$-pyridine**				**947.2**			**979.0**			**2**
91MAU/SMI	585-48-8	2-6-(t-C_4H_9)$_2$-pyridine	357	951	−5.0	946.0						
83MAU/SIE	110-86-1	pyridine	425	898.1	50.2	948.4						
[$C_8H_{17}N$]	**27644-32-2**	**N,3,5-Trimethylpiperidine**				**947.2**			**978.1**			**5.6**
84HOP/JAH	6832-21-9	2,6-(i-C_3H_7)$_2$-pyridine	298	947.2	0	947.2						
[$C_{12}H_{28}N_2$]	**68970-09-2**	**Hydrazine, 1,2-bis(2,2-dimethylpropyl)-1,2-dimethyl**				**947.1**			**977.8**			**5.8**
88NEL/RUM	121-44-8	(C_2H_5)$_3$N	550	951	−2.1	948.9						
88NEL/RUM	935-28-4	2,6-(C_2H_5)$_2$-pyridine	550	940.4	5.9	945.3						
[$C_4H_{10}N_7$]	**110-70-3**	**CH_3NHCH_2-CH_2NHCH_3**				**946.9**			**989.2**			**−33**
90BOR/HOU	119044-59-6	(CH_3)$_2$N-CH=N-(4-acetylphenyl)	313	947.3	−0.8	946.9						
[$C_8H_{14}N$]	**22207-84-7**	**1-Azabicyclo[2.2.2]octane, 3-methylene**				**946.4**			**977.2**			**5.6**
79AUE/BOW	750-50-3	(CH_3)$_3$N	298	918.1	28.3	946.4						
[$C_{12}H_{28}N_2$]	**106376-59-4**	**Hydrazine, 1,2-dimethyl-1,2-dipentyl**				**946.4**			**977.2**			**5.8**
88NEL/RUM	108-48-5	2,6-(CH_3)$_2$-pyridine	550	931.1	15.5	945.7						
88NEL/RUM	121-44-8	(C_2H_5)$_3$N	550	951	−3.8	947.2						
[$C_5H_{14}N_2$]	**462-94-2**	**1,5-Diaminopentane**				**946.2**			**999.6**			**−70**
79AUE/BOW	75-50-3	(CH_3)$_3$N	298	918.1	26.2	944.4						
78LAU/SAL	7664-41-7	NH_3	600	819	109.6	947.7						
73YAM/KEB	75-50-3	(CH_3)$_3$N	600	918.1	4.2	945.0						
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	64.1	947.9						
[$C_6H_{16}N_2$]	**124-09-4**	**1,6-Diaminohexane**				**946.2**			**999.5**			−70
79AUE/BOW	75-50-3	(CH_3)$_3$N	298	918.1	26.4	944.5						
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	64.1	947.9						
[$C_{20}H_{22}N_2$]	**123524-79-8**	**14,5-metheno-5H-bisazepinol[1,2-a:2′,1′-d][1,5]diazacycloundecine,7,8,9,10,11,12-hexahydro**				**946**			**978.5**			**0**
89HOU/FEN		See Refs.	313			946±7						
[$C_8H_{17}N_3O_3$]	**7563-03-3**	**lys-gly**				**946.0**			**NE**			**NE**
96CAR/CAS	926-63-6; 102-69-2	(CH_3)$_2$(n-C_3H_7)N; (n-C_3H_7)$_3$N				932-960						
[$C_{10}H_{15}N_5O_4$]	**32999-80-7**	**his-gly-gly**				**946.0**			**NE**			**NE**
96CAR/CAS	926-63-6; 102-69-2	(CH_3)$_2$(n-C_3H_7)N; (n-C_3H_7)$_3$N				932-960						
[Y]	**7440-65-6**	**Y**				**945.9**			**967**			**38**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / Ye:Squib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
89ELK/SUN		See Refs.							967±6			
[$C_5H_8N_2$]	**10447-93-6**	**1-5-Dimethylimidazole**				**945.8**			**977.6**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	27.5	945.8						
[$C_7H_{14}N_2$]	**14287-89-9**	**2,3-diazabicyclo[2.2.1]heptane,2,3-dimethyl**				**945.6**			**978.0**			**0**
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−5.4	947.0						
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	12.6	944.2						
[$C_8H_{17}N_3O_4$]	**997-62-6**	**gly-lys**				**945.6**			**NE**			**NE**
96CAR/CAS	626-67-5; 121-44-8	1-Methylpiperidine; $(C_2H_5)_3N$				940-951						
[$C_{10}H_{24}N_2$]	**116149-14-5**	**Hydrazine, 1,2-dibutyl-1,2-dimethyl**				**945.2**			**976.9**			**5.8**
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	13.8	944.0						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−4.6	946.3						
[$C_6H_{15}N$]	**921-04-0**	**(sec-C_4H_9)$(CH_3)_2N$**				**945.1**			**975.9**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	27.0	945.1						
[$C_7N_{18}N_2$]	**646-19-5**	**1,7-Diaminoehptane**				**944.9**			**998.6**			**−71**
73YAM/KEB	75-50-3	$(CH_3)_3N$	600	918.1	3.8	944.9						
[$C_5H_8N_2$]	**6338-45-0**	**1,4-Dimethylimidazole**				**944.9**			**976.7**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	26.5	944.9						
[$C_{10}H_{16}N_2O_3$]	**20488-28-2**	**pro-pro**				**944.8**			**NE**			**NE**
96EWI/ZHA	108-18-9; 121-44-8	(i-$C_3H_7)_2NH$; $(C_2H_5)_3N$				939-951						
[$C_9H_{19}N$]	**16607-80-0**	**c-$C_6H_{11}CH_2N(CH_3)_2$**				**944.7**			**975.6**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	26.5	944.7						
[$C_{12}H_{22}N_4O_5$]	**926-79-4**	**tetra-L-alanine**				**944.6**			**NE**			**NE**
93WU/FEN		kinetic method				944.6						
[$C_6H_{17}NSi$]	**18182-40-6**	**$(CH_3)_3SiCH_2N(CH_3)_2$**				**943.8**			**974.5**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	25.6	943.8						
83TAF2	7664-41-7	NH_3	350	819	128.1	946.5						
78SHE/GOB	7664-41-7	NH_3	320	819	116.7	935.5						
[$C_5H_{11}N$]	**1743-55-1**	**$(CH_3)_2C{=}NC_2H_5$**				**943.5**			**976.0**			**0**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	25.4	943.5						
[$C_9H_{19}N$]	**10315-89-6**	**N-Isobutylpiperidine**				**943.5**			**974.5**			**5.6**
80HOU/VOG		See Refs.							974.5			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_7H_{10}N_2$]	**18437-57-5**	**N,N-Dimethyl-3-pyridinamine**				**943.1**			**969.6**			**20**
91AUE/WEB	110-86-1	pyridine	300	898.1	46.4	944.5						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	24.3	941.7						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	27.3	945.5						
[$C_{16}H_{27}N$]	**2909-76-4**	**N,N-Dimethylbenzenamine,2,4-di-t-butyl**				**942.4**			**973.3**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	24.3	942.4						
[$C_{12}H_{30}N_3OP$]	**2622-07-3**	**$OP(N(C_2H_5)_2)_3$**				**942.2**			**974.7**			**0**
85BOL/HOU	142-84-7	$(n\text{-}C_4H_9)_2NH$	323	929.3	9.6	938.8						
85BOL/HOU	121-44-8	$(C_2H_5)_3N$	323	951	−3.8	947.4						
85BOL/HOU	616-39-7	$(CH_3)(C_2H_5)_2N$	323	940.0	0.4	940.5						
[$C_{17}H_{16}N_2$]	**95935-57-2**	**11,5-metheno-5H,7H-bisazepino[1,2-a:2′,1′-d][1,5]diazocine,8,9-dihydro**				**942.0**			**974.5**			**0**
89HOU/FEN	110-96-3	$(i\text{-}C_4H_9)_2NH$	313	925.1	0.8	925.9						
89HOU/FEN	626-67-5	1-Methylpiperidine	313	940.1	2.9	943.1						
89HOU/FEN	935-28-4	2,6-$(C_2H_5)_2$-pyridine	313	940.4	0.4	940.9						
[$C_8H_{19}N$]	**18675-04-8**	**$(CH_3)_3C(CH_2)_2N(CH_3)_2$**				**942.0**			**973.0**			**5.6**
78SHE/GOB	7664-41-7	NH_3	350	819	123.6	942.0						
[$C_7H_{10}N_2$]	**5683-33-0**	**N,N-Dimethyl-2-pyridinamine**				**941.6**			**968.2**			**20**
91AUE/WEB	110-86-1	pyridine	300	898.1	43.0	941.1						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	23.9	942.0						
[$C_9H_{15}N$]	**102-70-5**	**$[CH_2{=}CHCH_2]_3N$**				**941.3**			**972.3**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	22.0	940.1						
83TAF2	7664-41-7	NH_3	350	819	123.6	942.0						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	24.4	942.5						
75TAF	7664-41-7	NH_3	350	819	120.8	939.2						
75ARN	7664-41-7	NH_3	350	819	110.5	928.9						
[$C_8H_{20}N_2$]	**3337-88-4**	**Hydrazine, 1,2-dimethyl-1,2-dipropyl**				**941.2**			**971.9**			**5.8**
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	10.9	941.1						
88NEL/RUM	121-44-8	$(C_2H_5)_3N$	550	951	−9.6	941.3						
[$C_{13}H_9N$]	**260-94-6**	**Acridine**				**940.7**			**972.6**			**2**
79MAU	107-10-8	$n\text{-}C_3H_7NH_2$	550	883.9	58.6	940.7						
[$C_9H_{13}N$]	**935-28-4**	**2,6-$(C_2H_5)_2$-pyridine**				**940.4**			**972.3**			**2**
91MAU/SMI	6832-21-9	2,6-$(i\text{-}C_3H_7)_2$-pyridine	525	947.2	−7.1	940.1						
83MAU/SIE	110-86-1	pyridine	425	898.1	42.7	940.8						
[$C_{18}H_{15}P$]	**603-35-0**	**$(C_6H_5)_3P$**				**940.4**			**972.8**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
86TRA/MUN	108-18-9; 121-44-8	$(i\text{-}C_3H_7)_2NH$; $(C_2H_5)_3N$				939-951						
82IKU/KEB	594-09-2	$(CH_3)_3P$	320	926.3	13.4	939.7						
$[C_{26}H_{54}O_8]$	**3055-97-8**	**$(C_{12}H_{25}(OC_2H_4)_7OH$**				**940.3**			**1006.7**			**−113.9**
93LIN/ROC	121-69-7	$C_6H_5N(CH_3)_2$	298	909.2	31.4	940.3	941.1	71.5	1012.6	2	−133.9	−131.9
$[C_7H_6N_2]$	**274-76-0**	**Imidazo(1,2-a)pyridine**				**940.3**			**972.1**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	22.0	940.3						
$[C_{18}H_{18}N_2]$	**120789-29-9**	**12-5-metheno-5H-bisazepino[1,2-a:2′,1′-d][1,5]diazonine,7,8,9,10-tetrahydro**				**940.2**			**972.6**			**0**
89HOU/FEN	110-96-3	$(i\text{-}C_3H_9)_2NH$	313	925.1	0.4	925.5						
89HOU/FEN	120-94-5	N-Methylpyrrolidine	313	934.8	5.4	940.3						
89HOU/FEN	935-28-4	2-6-$(C_2H_5)_2$-pyridine	313	940.4	−0.4	940.0						
$[C_9H_{18}N_2]$	**283-58-9**	**1,5-Diazabicyclo[3.3.3]undecane**				**940.1**			**971.1**			**5.6**
81ALD/ARR	7664-41-7	NH_3	320	819	121.3	940.1						
$[C_6H_{13}N]$	**626-67-5**	**1-Methylpiperidine**				**940.1**			**971.1**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	21.1	939.2						
83TAF2	7664-41-7	NH_3	350	819	122.6	941.0						
76AUE/WEB	75-50-3	$(CH_3)_3N$	298	918.1	22.0	940.1						
75ARN	7664-41-7	NH_3	350	819	114.6	933.0						
$[C_5H_{14}N]$	**616-39-7**	**$(CH_3)(C_2Hs5)_2N$**				**940.0**			**971.0**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	21.5	939.6						
83TAF2	7664-41-7	NH_3	350	819	123.1	941.5						
75TAF	7664-41-7	NH_3	350	819	120.4	938.8						
75ARN	7664-41-7	NH_3	350	819	110.0	928.4						
$[C_3H_{10}N_2]$	**109-76-2**	**1,3-Diaminopropane**				**940.0**			**987.0**			**−49**
80MAU/HAM	142-84-7	$(n\text{-}C_3H_7)_2NH$	600	929.3	−2.8	940.6	962.3	24.3	986.5	−1.9	−45.2	−47.1
80MAU/HAM	75-50-3	$(CH_3)_3N$	600	918.1	4.2	938.7	948.9	37.7	986.6	5.6	−55.6	−50
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	21.5	939.6						
73YAM/KEB	75-50-3	$(CH_3)_3N$	600	918.1	4.2	938.7	948.9	54.4	1003.3	5.6	−86.2	−80.6
73AUE/WEB	107-10-8	$n\text{-}C_3H_7NH_2$	298	883.9	58.6	942.4						
$[C_{13}H_{13}P]$	**1486-28-8**	**$(C_5H_5)(CH_3)P$**				**939.7**			**972.1**			**0**
82IKU/KEB	594-09-2	$(CH_3)_3P$	320	926.3	13.4	939.7						
$[C_5H_{13}N]$	**996-35-0**	**$(CH_3)_2(i\text{-}C_3H_7)N$**				**939.6**			**970.6**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	21.5	939.6						
83TAF2	7664-41-7	NH_3	350	819	123.1	941.5						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	75.1	939.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_7H_{17}N$]	**10076-31-0**	**$(CH_3)_2$(neo-C_5H_{11})N**				**939.5**			**970.5**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$)	350	918.1	20.6	938.7						
83TAF2	7664-41-7	NH_3	350	819	121.7	940.1						
78SHE/GOB	7664-41-7	NH_3	350	819	121.3	939.7						
[$C_8H_{21}NSi$]	**66365-05-7**	**$(CH_3)_2$(t-C_4H_9)SiN(CH_3)$_2$**				**938.8**			**969.8**			**5.6**
78SHE/GOB	7664-41-7	NH_3	350	819	120.4	938.8						
[$C_8H_{15}N$]	**108-18-9**	**(i-C_3H_7)$_2$NH**				**938.6**			**971.9**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	20.1	938.6						
83TAF2	7664-41-7	NH_3	350	819	120.8	939.6						
83LOC/MCI	7664-41-7	NH_3	350	819	120.8	939.6						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	73.3	937.8						
75ARN	7664-41-7	NH_3	350	819	106.7	925.5						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	79.1	943.6						
[$C_7H_{13}N$]	**13929-94-7**	**1-Azabicyclo[2.2.2]oct-2-ene**				**938.6**			**969.4**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	20.5	938.6						
[$C_6H_{15}N$]	**927-62-8**	**$(CH_3)_2$(n-C_4H_9)N**				**938.2**			**969.2**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	20.1	938.3						
[$C_2H_6N_2$]	**143-37-3**	**$CH_3C(=NH)NH_2$**				**938.2**			**970.7**			**0**
96GON/MO	142-84-7	(n-C_4H_9)$_2$NH	338	929.3	8.0	937.2						
96GON/MO	120-94-5	N-Methylpyrrolidine	338	934.8	3.4	938.4						
96GON/MO	108-18-9	(i-C_3H_7)$_2$NH	338	938.6	0.6	939.2						
96GON/MO	103-83-3	$C_6H_5CH_2N(CH_3)_2$	338	937.4	0.4	938.1						
[$C_7H_{18}N_2$]	**52598-10-4**	**(n-C_4H_9)(CH_3)NN(CH_3)$_2$**				**938.1**			**970.5**			**0**
84MAU/NEL	6415-12-9	$(CH_3)_2NN(CH_3)_2$	600	917.9	18.4	938.1						
[$C_7H_{14}N_2$]	**6523-20-1**	**2-Methyl-1,2-diazabicyclo[2.2.2]-octane**				**938.1**			**968.9**			**5.6**
84MAU/NEL	6415-12-9	$(CH_3)_2NN(CH_3)_2$	600	917.9	20.1	938.1						
[$C_{11}H_{15}N$]	**25108-56-9**	**4-$(CH_3)_2NC_6H_4C(CH_3)=CH_2$**				**938.0**			**946.6**			**20**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	20.6	938.0						
[$C_6H_{15}N$]	**7230-24-9**	**$(CH_3)_2$(i-C_4H_9)N**				**937.8**			**968.7**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	19.7	937.8						
[$C_9H_{13}N$]	**103-83-3**	**$C_6H_5CH_2N(CH_3)_2$**				**937.4**			**968.4**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	20.1	938.3						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	18.5	936.6						
[$C_{12}H_{22}N_2$]	**141665-18-1**	**1-methyl-3,5-di-t-butylpyrazole**				**937.1**			**970.8**			**−4**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSqmb	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
92ABB/CAB	594-39-8	t-$C_4H_{11}NH_2$	333	903.6	5.7	909.2						
92ABB/CAB	142-84-7	(n-C_3H_7)$_2$NH	333	929.3	6.9	936.3						
92ABB/CAB	108-18-9	(i-C_3H_7)$_2$NH	333	938.6	−1.0	937.7						
92ABB/CAB	616-39-7	$(CH_3)(C_2H_5)_2N$	333	940.0	−2.9	937.4						
[$C_8H_{11}P$]	**672-66-2**	**$C_6H_5P(CH_3)_2$**				**936.8**			**969.2**			**0**
82IKU/KEB	594-09-2	$(CH_3)_3P$	320	926.3	10.5	936.8						
[$C_6H_{13}P$]	**39763-50-3**	**$(CH_2)_5PCH_3$**				**936.7**			**969.4**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	18.3	936.7						
[$C_7H_{12}FN$]	**#321**	**3-Fluoro-1-azabicyclo[3.2.1]octane**				**936.7**			**967.5**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	18.6	936.7						
[$C_6H_{13}NO$]	**53687-79-9**	**c-$C_5H_{10}N(2\text{-}OCH_3)$**				**936.7**			**969.9**			**−2**
79AUE/BET	75-50-3	$(CH_3)_3N$	298	918.1	18.6	936.7						
[$C_7H_{18}N_2$]	**60678-73-1**	**(t-C_4H_9)$(CH_3)NN(CH_3)_2$**				**936.4**			**968.8**			**0**
84MAU/NEL	108-48-5	2,6-$(CH_3)_2$-pyridine	600	931.1	4.6	936.4						
[$C_7H_{16}N_2$]	**49840-68-8**	**1H-1,2-diazepine,hexahydro-1,2-dimethyl**				**936.1**			**966.8**			**5.8**
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	5.4	935.6						
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	−2.9	936.6						
[$C_3H_{15}NSi$]	**18135-05-2**	**$(CH_3)_3SiN(CH_3)_2$**				**936**			**966.8**			**5.6**
83HEN/FRE	109-89-7; 121-44-8	$(C_2H_5)_2NH$;$(C_2H_5)_3N$				919-951						
[$C_6H_{14}N_2$]	**26163-37-1**	**Pyridazine, hexahydro-1,2,-dimethyl**				**935.4**			**966.1**			**5.6**
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	−1.7	937.9						
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	7.1	937.4						
84MAU/NEL	613-48-9	4-$CH_3C_6H_4N(C_2H_5)_2$	600	931.0	0.8	930.7						
84MAU/NEL	108-48-5	2,6-$(CH_3)_2$-pyridine	600	931.1	5.4	935.5						
[$C_8H_{19}N$]	**111-92-2**	**$(n\text{-}C_4H_9)_3NH$**				**935.3**			**968.6**			**−1.9**
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	70.8	935.3						
75ARN	7664-41-7	NH_3	350	819	102.9	921.7						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	71.3	935.8						
[$C_8H_{20}N_2$]	**4267-00-9**	**$(C_2H_5)_2NN(C_2H_5)_2$**				**935.3**			**964.3**			**11.6**
84MAU/NEL	613-48-9	4-$CH_3C_6H_4N(C_2H_5)_2$	600	931.0	4.2	932.3						
84MAU/NEL	589-93-5	2,5-$(CH_3)_2$-pyridine	600	926.9	14.2	938.3						
[$C_8H_8N_2$]	**1632-83-3**	**1-methylbenzimidazole**				**935.2**			**967.0**			**2**
88CAT/CLA	108-18-9	(i-C_3H_7)$_2$NH	~300	938.6	−2.9	935.7						
88CAT/CLA	598-56-1	$(CH_3)_2(C_2H_5)N$	~300	929.1	5.4	934.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	16.9	935.2						
[$C_5H_{11}N$]	**120-94-5**	**N-Methylpyrrolidine**				**934.8**			**965.6**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	16.0	934.1						
78TAA/WOL	110-86-1	pyridine	350	898.1	34.7	932.7						
76AUE/WEB	75-50-3	$(CH_3)_3N$	298	918.1	17.1	935.2						
75TAF	7664-41-7	NH_3	350	819	117.6	936.0						
75ARN	7664-41-7	NH_3	350	819	107.5	925.9						
73TAF/TAA	110-86-1	pyridine	350	898.1	38.0	935.9						
[$C_9H_{11}N$]	**36556-06-6**	**Isoquinoline,5,6,7,8-tetrahydro-**				**934.7**			**966.6**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	16.6	934.7						
[$C_8N_{17}N$]	**1003-84-5**	**1,4,4-Trimethylpiperidine**				**934.7**			**966.7**			**5.6**
80HOU/VOG		See Refs.							965.7			
[$C_6H_{12}N_2$]	**280-57-9**	**1,4-Diazabicyclo[2.2.2]octane**				**934.6**			**963.4**			**12**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	17.1	935.2						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	73.2	937.7						
75ARN	7664-41-7	NH_3	350	819	105.0	923.1						
74STA/BEA2	75-50-3	$(CH_3)_3N$	320	918.1	15.9	933.9						
[$C_5H_{11}N$]	**6163-56-0**	**$CH_3CH{=}CHN(CH_3)_2$**				**934.5**			**967.0**			**0**
81ELL/DIX	616-47-7; 102-70-5	1H-methylimidazole; $(CH_2{=}CHCH_2)_3N$				928-941						
[$C_6H_{13}N$]	**6906-32-7**	**$(CH_3)_2C{=}CHN(CH_3)_2$**				**934.5**			**967.0**			**0**
81ELL/DIX	616-47-7; 108-18-9	1H-methylimidazole; $(i\text{-}C_3H_7)_2NH$				928-939						
[$C_{12}H_{19}N$]	**22025-87-2**	**$(CH_3)_2NC_6H_4(t\text{-}C_4H_9)$**				**934.3**			**961.0**			**20**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	16.9	934.3						
83TAF2	7664-41-7	NH_3	350	819	118.5	936.2						
[$C_6H_{16}N_2$]	**60678-65-1**	**$(n\text{-}C_3H_7)(CH_3)NN(CH_3)_2$**				**934.3**			**966.8**			**0**
84MAU/NEL	6415-12-9	$(CH_3)_2NN(CH_3)_2$	600	917.9	14.6	934.3						
[$C_7H_{14}ClN$]	**49665-74-9**	**$c\text{-}C_5H_9N,2\text{-}CH_2Cl,1\text{-}CH_3$**				**934.2**			**965.0**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	16.1	934.2						
[$C_9H_{11}N$]	**10500-57-9**	**Quinoline,5,6,7,8-tetrahydro-**				**934.1**			**966.0**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	16	934.1						
[$C_{12}H_{22}N_2$]	**18712-47-6**	**3,5-di-t-butyl-4-methylpyrazole**				**933.8**			**967.5**			**−4**
92ABB/CAB	142-84-7	$(n\text{-}C_3H_7)_2NH$	333	929.3	4.4	933.7						
92ABB/CAB	108-18-9	$(i\text{-}C_3H_7)_2NH$	333	938.6	−4.7	934.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
92ABB/CAB	108-48-5	2,6-$(CH_3)_2$-pyridine	333	931.1	2.4	933.7						
[$C_5H_9F_3N$]	**134166-59-9**	**$(CH_3)_2$N-CH=N-CH_2CF_3**				**933.8**			**966.2**			**0**
92RAC/MAR	142-84-7	(n-$C_3H_7)_2$NH	338	929.3	3.8	933.0						
92RAC/MAR	120-94-5	N-Methylpyrrolidine	338	934.8	−0.4	934.6						
92RAC/MAR	139033-03-7	$(CH_3)_2$N-CH=N-OCH_3	338	915.8	>14	>930						
[CH_2O]	**19710-56-6**	**HCOH (hydroxymethylene)**				**933.4**			**965.9**			**0**
82PAU/BEH2	**19961-27-4;** 626-67-5	**(C_2H_5)(i-C_3H_7)NH; N-methylpiperidine**				927-940						
[$C_6H_{16}N_2$]	**23337-93-1**	**Hydrazine, 1,2-diethyl-1,2-dimethyl**				**933.0**			**963.7**			**5.8**
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	2.1	932.3						
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	−5.9	933.6						
[$C_{10}H_{14}N_2$]	**54-11-5**	**3-(2-(N-methylpyrrolidinyl))pyridine**				**932.6**			**963.4**			**5.6**
91BER/DEC	142-84-7	(n-$C_3H_7)_2$NH	338	929.3	3.1	932.1						
91BER/DEC	120-94-5	N-Methylpyrrolidine	338	934.8	−1.6	933.2						
[$C_{11}H_{17}N$]	**91-67-8**	**3-$CH_3C_6H_4N(C_2H_5)_2$**				**932.2**			**964.1**			**2**
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	23.0	932.2						
[$C_4H_{11}NO$]	**13325-10-5**	**$NH_2(CH_2)_4OH$**				**932.1**			**984.5**			**−67**
80MAU/HAM	110-86-1	pyridine	330	898.1	31.8	932.0	930	54	984	2	−67	−65
[$C_5H_{13}N$]	**926-63-6**	**$(CH_3)_2$(n-C_3H_7)N**				**931.9**			**962.8**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	13.7	931.9						
80HOU/VOG		See Refs.							959.4			
[$C_7H_{12}BrN$]	**#364**	**3-Bromo-1-azabicyclo[2.2.2]octane**				931.8			**962.6**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	13.7	931.8						
[$C_{11}H_{17}N$]	**1129-69-7**	**2-C_6H_{13}(c-C_5H_4N)**				**931.7**			**963.6**			**2**
83MAU/SIE	110-86-1	pyridine	425	898.1	33.5	931.6						
[C_7H_9N]	**108-48-5**	**2,6-$(CH_3)_2$-pyridine**				**931.1**			**963.0**			**2**
92ABB/CAB	142-84-7	(n-$C_3H_7)_2$NH	333	929.3	2.1	931.2						
91AUE/WEB	110-86-1	pyridine	300	898.1	32.7	930.8						
91MAU/SMI	585-48-8	2,6-(t-$C_4H_9)_2$-pyridine	480	951	−20.1	930.9						
83MAU/SIE	110-86-1	pyridine	425	898.1	32.6	930.8						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	13.7	931.8						
75ARN	7664-41-7	NH_3	350	819	101.7	920.3						
[$C_{12}H_{19}N$]	**2217-07-4**	**$C_6H_5N(C_3H_7)_2$**				**931.1**			**963.0**			**2**
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	21.8	931.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] Ye8quib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	$\Delta\dot{S}_p$(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_9H_{17}N_2$]	**494-97-3**	**3-(2-pyrrolidinyl)pyridine**				**931.0**			**964.0**			**−2**
91BER/DEC	123-75-1	Pyrrolidine	338	915.3	14.1	929.4						
91BER/DEC	120-94-5	N-Methylpyrrolidine	338	934.8	−2.5	932.6						
[$C_{11}H_{17}N$]	**613-48-9**	**4-$CH_3C_6H_4N(C_2H_5)_2$**				**931.0**			**962.8**			**2**
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	21.8	931.0						
[$C_{12}H_{14}N_2$]	**20734-56-9**	**N,N′-Dimethyl-1,8-naphthalenediamine**				**930.9**			**960.3**			**10**
78LAU/SAL	7664-41-7	NH_3	600	819	116.7	930.8						
[C_7H_9N]	**108-47-4**	**2,4-$(CH_3)_2$-pyridine**				**930.8**			**962.9**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	32.7	930.8						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	12.7	930.8						
[C_8H_9N]	**533-35-7**	**3,4-Cyclopentenopyridine**				**930.5**			**962.4**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	12.2	930.4						
[$C_{11}H_{15}NO$]	**54660-04-7**	**Pyrrolidine, 1-(4-methoxyphenyl)**				**930.4**			**961.2**			**5.6**
88CAU/CER		See Refs.				930.4						
[$C_{16}H_{14}N_2$]	**95936-56-1**	**10,5-metheno-5H-bisazepino[1,2-d:2′,1′-g][1,4]diazepine,7,8-dihydro**				**930.1**			**962.6**			**0**
89HOU/FEN	108-48-5	2,6-$(CH_3)_2$-pyridine	313	931.1	−1.7	929.5						
89HOU/FEN	142-84-7	$(n\text{-}C_4H_7)_2NH$	313	929.3	1.7	930.9						
[$C_9H_{13}N$]	**5944-41-2**	**2-(t-C_4H_9)-pyridine**				**929.8**			**961.7**			**2**
91MAU/SMI	585-48-8	2,6-(t-C_4H_9)$_2$-pyridine	397	951	−17.2	933.8						
91MAU/SMI	6832-21-9	2,6-(i-C_4H_7)$_2$-pyridine	485	947.2	−19.2	927.9						
83MAU/SIE	110-86-1	pyridine	425	898.1	31.0	929.1						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	10.3	928.4						
[C_6H_7NO]	**620-08-6**	**4-(CH_3O)-pyridine**				**929.8**			**961.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	31.2	929.4						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	12.4	930.7						
81TAA/SUM	7664-41-7	NH_3	320	819	103.8	922.6						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	11.2	929.4						
75TAF	7664-41-7	NH_3	350	819	110.7	929.3						
75ARN	7664-41-7	NH_3	350	819	101.3	919.8						
72TAA/HEN	110-86-1	pyridine	320	898.1	36.4	934.5						
[$C_4H_6N_2$]	**693-98-1**	**2-Methylimidazole**				**929.6**			**963.4**			**−4**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	11.0	929.6						
[$C_6H_{16}N_3OP$]	**7778-06-5**	**c-$OP(N(CH_3)_2)N(CH_3)CH_2CH_2N(CH_3)$**				**929.3**			**961.7**			**0**
85BOL/HOU	496-15-1	2,3-Dihydroindole	323	926.3	0.4	926.8						
85BOL/HOU	598-56-1	$(CH_3)_2(C_2H_5)N$	323	929.1	2.5	931.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSqmb	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_6H_{15}N$]	**142-84-7**	**(n-C_3H_7)$_2$NH**				**929.3**			**962.3**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	9.6	928.1						
83TAF	7664-41-7	NH_3	350	819	111.2	930.0						
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	40.2	923.3						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	13.2	931.3						
75TAF	7664-41-7	NH_3	350	819	111.2	930.0						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	67.3	931.8						
[$C_4H_{11}N$]	**598-56-1**	**$(CH_3)_2(C_2H_5)N$**				**929.1**			**960.1**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	10.5	928.7						
83TAF2	7664-41-7	NH_3	350	819	112.1	930.5						
76AUE/WEB	75-50-3	$(CH_3)_3N$	298	918.1	11.2	929.4						
75TAF	7664-41-7	NH_3	350	819	109.4	927.8						
75ARN	7664-41-7	NH_3	350	819	100.0	918.4						
[$C_6H_{18}N_3OP$]	**680-31-9**	**$OP(N(CH_3)_2)_3$**				**928.7**			**958.6**			**9.1**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	10.1	928.0						
84BOE/HOU	142-84-7	(n-C_3H_7)$_2$NH	~323	929.3	0.4	929.4						
[$C_5H_{12}N_2$]	**38704-89-1**	**Pyrazolidine, 1,2-dimethyl**				**928.6**			**959.3**			**5.8**
88NEL/RUM	935-28-4	2,6-$(C_2H_5)_2$-pyridine	550	940.4	−11.7	927.8						
88NEL/RUM	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	−0.8	929.4						
[$C_6H_{12}N_2$]	**99-98-9**	**4-$H_2NC_6H_4N(CH_3)_2$**				**928.4**			**956.0**			**20**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	11.0	928.4						
[$C_8H_{14}N_4O_5$]	**637-84-3**	**tetraglycine**				**928.2**			**973.8**			**−44**
93ZHA/ZHM	109-06-8; 109-89-7	2-CH_3-C_5H_4N; $(C_2H_5)_2NH$	300			917-919						
93WU/LEB	127-19-5; 107-10-8	$CH_3CON(CH_3)_2$; n-$C_3H_7NH_2$	300			877-884						
93CHE/WU		kinetic method							973.8			**−44**
92WU/FEN2		kinetic method				924.8						
[$C_4H_8O_2$]	**922-69-0**	**$CH_2=C(OCH_3)_2$**				**928.1**			**957.0**			**12**
89OSA/DEL	142-84-7	(n-C_3H_7)$_2$NH	313	929.3	−1.3	927.8						
89OSA/DEL	110-89-4	Piperidine	313	921	6.3	927.1						
89OSA/DEL	598-56-1	$(CH_3)_2(C_2H_5)N$	313	929.1	0.4	929.4						
[$C_{10}H_{15}N$]	**91-66-7**	**$C_6H_5N(C_2H_5)_2$**				**927.9**			**959.8**			**2**
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	325	909.2	17.6	926.8						
73YAM/KEB	7664-41-7	NH_3	600	819	112.5	929.0						
[$C_4H_6N_2$]	**616-47-7**	**1-methylimidazole**				**927.7**			**959.6**			**2**
88CAT/CLA	111-49-9	Hexahydroazepine	~300	923.5	3.3	926.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
88CAU/CLA	598-56-1	$(CH_3)_2(C_2H_5)N$	~300	929.1	~2.5	926.6						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	8.2	926.5						
86MAU/LIE	121-44-8	$(CH_3CH_2)_3N$	600	951	−23.0	929.1						
86MAU/LIE	108-99-6	3-(CH_3)-pyridine	600	911.6	19.7	931.3						
83TAF2	7664-41-7	NH_3	350	819	114.9	933.4						
81ELL/DIX	142-84-7; 108-18-9	$(C_3H_7)_2NH$; (i-$C_3H_7)_2NH$				929-939						
[$C_5H_5N_5O$]	**73-40-5**	**Guanine**				**927.6**			**959.5**			**2**
90GRE/LIG		kinetic method							959.5			
75WIL/MCC	124-40-3; 75-50-3	$(CH_3)_2NH$; $(CH_3)_3N$				896-918						
[C_7H_9N]	**583-61-9**	**2,3-$(CH_3)_2$-pyridine**				**927.0**			**958.9**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	28.3	926.5						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	9.3	927.4						
[$C_{16}H_{14}N_2$]	**19311-79-6**	**1-methyl-3,5-diphenylpyrazole**				**927.0**			**958.9**			**2**
92ABB/CAB	3978-81-2	4-(t-C_4H_9)-pyridine	333	925.8	2.2	928.0						
92ABB/CAB	142-84-7	(n-$C_3H_7)_2NH$	333	929.3	−3.1	926.0						
[C_7H_9N]	**589-93-5**	**2,5-$(CH_3)_2$-pyridine**				**926.9**			**958.8**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	28.3	926.5						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	9.3	927.4						
[$C_5H_{11}N$]	**2155-94-4**	**CH_2=$CHCH_2N(CH_3)_2$**				**926.8**			**957.8**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	8.7	926.8						
83TAF2	7664-41-7	NH_3	350	819	108.9	927.3						
[$C_5H_{13}N$]	**19961-27-4**	**(C_2H_5)(i-C_3H_7)NH**				**926.7**			**960.0**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	8.2	926.7						
83TAF2	7664-41-7	NH_3	350	819	108.9	927.7						
[$C_{10}H_{19}N_3O_4$]	**1187-50-4**	**leu-gly-gly**				**926.7**			**NE**			**NE**
93WU/FEN		kinetic method				926.7						
[C_7H_9NO]	**23579-92-2**	**2-(CH_3OCH_2)-pyridine**				**926.4**			**958.3**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	8.3	926.4						
[$C_{11}H_{15}N$]	**4096-20-2**	**Piperidine, 1-phenyl**				**926.4**			**952.9**			**20**
88CAU/CER		See Refs.				926.7						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	8.7	926.1						
83TAF2	7664-41-7	NH_3	350	819	109.4	927.1						
[C_8H_9N]	**496-15-1**	**2,3-Dihydroindole**				**926.3**			**957.1**			**5.6**
85BOL/HOU	496-15-1	2,3-Dihydroindole	323	926.3	0	926.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[C_3H_9P]	**594-09-2**	**$(CH_3)_3P$**				**926.3**			**958.8**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	7.8	926.2						
82IKU/KEB	594-09-2	$(CH_3)_3P$	320	926.3	0	926.3						
75TAF	7664-41-7	NH_3	350	819	107.1	925.8						
74STA/BEA	75-50-3	$(CH_3)_3N$	320	918.1	6.7	924.9						
[$C_9H_{12}N_2O$]	**6331-71-1**	**4-NH_2-$C_6H_4CON(CH_3)_2$**				**925.9**			**956.9**			**5**
94GRU/CAL	110-89-4; 108-47-4	piperidine; 2,4-$(CH_3)_2$-pyridine				921-931						
[$C_9H_{13}N$]	**3978-81-2**	**4-(t-C_4H_9)-pyridine**				**925.8**			**957.7**			**2**
92ABB/CAB	142-84-7	$(n\text{-}C_3H_7)_2NH$	333	929.3	−4.6	924.5						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	8.8	926.9						
[$C_{12}H_{17}N$]	**40832-99-3**	**1-H-Azepine, hexahydro-1-phenyl**				**925.8**			**956.6**			**5.6**
88CAU/CER		See Refs.				925.8						
[C_8H_9N]	**533-37-9**	**2,3-Cyclopentenopyridine**				**925.6**			**957.5**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	7.3	925.5						
[C_7H_7N]	**56911-27-4**	**3,4-Cyclobutenopyridine**				**925.6**			**957.5**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	7.3	925.5						
[C_7H_9N]	**583-58-4**	**3,4-$(CH_3)_2$-pyridine**				**925.5**			**957.3**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	27.3	925.5						
[C_5H_9NO]	**5264-35-7**	**c-C_4H_6N(2-OCH_3)**				**925.5**			**957.9**			**0**
79AUE/BEI	75-50-3	$(CH_3)_3N$	298	918.1	7.3	925.5						
[$C_8H_{13}N$]	**609-72-3**	**N,N,2-trimethylaniline**				**925.3**			**951.8**			**20**
94BOH/DEC	110-89-4	Piperidine	338	921	4.3	924.5						
94BOH/DEC	109-06-8	2-(CH_3)-pyridine	338	917.3	8.9	925.5						
94BOH/DEC	142-84-7	$(n\text{-}C_3H_7)_2NH$	338	929.3	−2.5	925.9						
[$C_7H_{12}N_2O_3$]	**2578-57-6**	**pro-gly**				**925.1**			**NE**			**NE**
96EWI/ZHA	110-89-4; 142-84-7	Piperidine; $(n\text{-}C_3H_7)_2NH$				921-929						
[$C_9H_{15}N_3O_4$]	**7561-25-3**	**pro-gly-gly**				**925.1**			**NE**			**NE**
96EWI/ZHA	110-89-4; 142-84-7	Piperidine; $(n\text{-}C_3H_7)_2NH$				921-929						
[$C_8H_{19}N$]	**110-96-3**	**$(i\text{-}C_4H_9)_2NH$**				**925.1**			**958.1**			**−1.9**
75ARN	7664-41-7	NH_3	350	819	105.4	924.2						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	61.5	926.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_{11}H_{12}N_2$]	**10250-58-5**	**1,3-dimethyl-5-phenylpyrazole**				**924.7**			**956.6**			**2**
92ABB/CAB	3978-81-2	4-(t-C_4H_9)-pyridine	333	925.8	−0.4	925.4						
92ABB/CAB	536-75-4	4-(C_5H_5)-pyridine	333	919.2	4.9	924.1						
[$C_8H_{11}N$]	**75981-47-4**	**2-(i-C_3H_7)-pyridine**				**924.6**			**956.4**			**2**
83MAU/SIE	110-86-1	pyridine	425	898.1	26.4	924.5						
[$C_9H_{21}OP$]	**17513-58-5**	**(i-C_3H_7)$_3$PO**				**924.5**			**954.4**			**9.1**
85BOL/HOU	496-15-1	2,3-Dihydroindole	323	926.3	−1.3	925.0						
85BOL/HOU	142-84-7	(n-C_3H_7)$_2$NH	323	929.3	−5.0	924.0						
[C_4H_9N]	**5763-87-1**	**$(CH_3)_2NCH{=}CH_2$**				**924.4**			**956.8**			**0**
81ELL/DIX	110-89-4; 616-42-7	piperidine; 1-methylimidazole				921-928						
[$C_{11}H_{24}N_2O_3$]	**20556-11-0**	**lys-val**				**924.3**			**NE**			**NE**
93GOR/AMS	109-89-7; 142-84-7	(C_2H_5)$_3$NH; (C_4H_7)$_2$NH	350			919-929						
[$C_{11}H_{24}N_2O_3$]	**22677-62-9**	**val-lys**				**924.3**			**NE**			**NE**
93GOR/AMS	109-89-7; 142-84-7	(C_2H_5)$_3$NH; (C_4H_7)$_2$N	350			919-929						
[$C_{10}H_{15}N$]	**4913-13-7**	**3,5-$(CH_3)_2C_6H_3N(CH_3)_2$**				**924.3**			**956.1**			**2**
85LIA/JAC	121-69-7	$C_6H_5(CH_3)_2$	320	909.2	15.1	924.3						
[$C_9H_{17}N_3O_4$]	**5874-90-8**	**tri-L-alanine**				**924.1**			**NE**			**NE**
93WU/FEN		kinetic method				924.1						
[$C_8H_{11}N$]	**622-39-9**	**2-(C_3H_7)-pyridine**				**923.8**			**955.7**			**2**
89HOU/FEN	95935-56-1	10,5-metheno-5H-bisazepino[1,2-d:2′,1′-g][1,4]diazepine,7,8-dihydro	313	930.1	−6.3	923.8						
[$C_8H_{11}N$]	**696-30-0**	**4-(i-C_3H_7)-C_5H_4N**				**923.8**			**956.7**			**2**
92ABB/CAB	10250-58-5	1,3-dimethyl-5-phenylpyrazole	333	924.7	−0.9	923.8						
[$C_6H_{13}N$]	**111-49-9**	**Hexahydroazepine**				**923.5**			**956.7**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	5.0	923.5						
[C_7H_9N]	**591-22-0**	**3,5-$(CH_3)_3$-pyridine**				**923.5**			**955.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	25.4	923.5						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	58.6	923.1						
[$C_7H_{12}ClN$]	**42332-45-6**	**3-Chloro-1-azabicyclo[2.2.2]octane**				**923.5**			**954.3**			**5.6**
86HEI/HON	110-89-4	Piperidine	313	921	1.3	922.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSqnb	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
86HEI/HON	496-15-1	2,3-Dihydroindole	313	926.3	−2.5	923.8						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	6.3	924.5						
[C_6H_7NS]	**22581-72-2**	**4-(CH_3S)-pyridine**				**923.3**			**955.2**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	24.9	923.0						
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	5.0	923.3						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	5.8	923.9						
[$C_{10}H_{15}N$]	**769-06-2**	**N,N,2,6-Tetramethylaniline**				**923.2**			**954.1**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	5.0	923.2						
[$C_6H_{13}N$]	**1611-12-7**	**n-C_3H_7CH=NC_2H_5**				**923.0**			**955.5**			**0**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	4.9	923.0						
[$C_5H_6N_2$]	**462-08-8**	**3-Pyridinamine**				**922.6**			**954.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	24.4	922.6						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	4.4	900.9						
[$C_9H_{13}NO$]	**701-56-4**	**4-$CH_3OC_6H_4N(CH_3)_2$**				**922.4**			**949.1**			**20**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	5.0	922.4						
[$C_{14}H_{18}N_2$]	**92234-54-3**	**1-(1-adamantyl)pyrazole**				**922.4**			**954.5**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	4.1	922.4						
[$C_{11}H_{12}N_2$]	**10250-60-9**	**1,5-dimethyl-3-phenylpyrazole**				**922.4**			**954.3**			**2**
92ABB/CAB	696-30-0	4-(i-C_3H_7)-C_5H_4N	333	923.8	−0.5	923.3						
92ABB/CAB	536-75-4	4-(C_2H_5)-pyridine	333	919.2	2.3	921.6						
[C_7H_7N]	**56911-25-2**	**2,3-Cyclobutenopyridine**				**922.0**			**953.9**			**2**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	3.9	922.0						
[$C_{10}H_{19}N_3O_4$]	**2576-67-2**	**gly-leu-gly**				**921.8**			**NE**			**NE**
93WU/TEN		kinetic method				921.8						
[C_9H_7N]	**91-22-5**	**Quinoline**				**921.4**			**953.2**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	26.4	924.5						
81MCL/CAM	583-58-4	3,4-dimethylpyridine:kinetic method	425					−1.7	944.7			
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	36.0	918.2						
[C_3H_8Si]	**4112-23-6**	**$(CH_3)_2Si$=CH_2**				**921.0**			**947.5**			**20**
90ALL/MCM	110-89-4; 108-18-9	piperidine; (i-$C_3H_7)_2NH$				921-939						
82PHI/HEH	7664-41-7	NH_3	350	819	102.5	920.2						
79PHI/POL	110-89-4; 19961-27-4	piperidine; (C_2H_5)(i-C_4H_7)NH	320			921-927						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M- Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{10}H_{17}N_5O_6$]	**7093-67-6**	**pentaglycine**				**921**			**NE**			**NE**
93ZELAZZIM	109-06-8; 109-89-7	2-CH_3-C_5H_4N; $(C_2H_5)_2NH$	300			917-919						
93WU/LEB	78-81-9; 13952-84-6	i-$C_4H_9NH_2$; s-$C_4H_9NH_2$	300			891-896						
92WU/HEN2		See Refs.				947.4						
[$C_{10}H_{18}N_2O_5$]	**3062-07-5**	**val-glu**				**921**			**NE**			**NE**
93GOR/AMS	75-50-3; 109-89-7	$(CH_3)_3N$; $(C_2H_5)_2NH$	350			918-919						
[$C_5H_{11}N$]	**110-89-4**	**Piperidine**				**921**			**954.0**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	1.4	919.9						
83TAF	7664-41-7	NH_3	350	819	102.1	920.8						
78LAU/SAL	7664-41-7	NH_3	600	819	96.7	914.3						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	56.1	920.6						
75TAF	7664-41-7	NH_3	350	819	102.1	920.8						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	58.1	922.6						
75ARN	7664-41-7	NH_3	350	819	93.3	912.1						
73YAM/KEB	7664-41-7	NH_3	600	819	102.5	920.2						
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	40.5	924.4						
71BOW/AUE	75-50-3	$(CH_3)_3N$	298	918.1	4.9	923.0						
[$C_4H_6N_2$]	**822-36-6**	**4-Methylimidazole**				**920.9**			**952.8**			**2**
87TAF	7664-41-7	NH_3	350	819	105.3	923.8						
86MAU/LIE	110-86-1	pyridine	600	898.1	19.9	918.0						
[$C_{11}H_{20}N_2$]	**1132-14-5**	**3,5-di-t-butylpyrazole**				**920.8**			**952.7**			**2**
92ABB/CAB	696-30-0	4-(i-C_3H_7)-C_5H_4N	333	923.8	−2.5	921.3						
92ABB/CAB	536-75-4	4 (C_2H_5)-pyridine	333	919.2	1.1	920.3						
[C_7H_9N]	**100-71-0**	**2-(C_2H_5)-pyridine**				**920.6**			**952.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	22.0	920.1						
83MAU/SIE	110-86-1	pyridine	425	898.1	22.2	920.3						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	2.9	921.1						
[$C_7H_6N_2$]	**51-17-2**	**Benzimidazole**				**920.5**			**953.8**			**−3**
84FLA/MAQ		kinetic method				916						
83CAT/ELG		kinetic method				925						
[$C_4H_{11}NO_2$]	**111-42-2**	**$(HOCH_2CH_2)_2NH$**				**920**			**953.0**			**−2**
86SUN/KUL		See Refs.	300			920			954			**0**
[$C_7H_{12}ClN$]	**96943-88-3**	**1-azabicyclo[2.2.2]-octane, 2-chloro**				**920.0**			**950.8**			**5.6**
86HEI/HON	496-15-1	2,3-Dihydroindole	313	926.3	−5.9	920.4						
86HEI/HON	110-89-4	Piperidine	313	921	−1.3	919.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_9H_7N]	**119-65-3**	**Isoquinoline**				**919.9**			**951.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	25.9	924.0						
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	33.5	915.7						
[$C_5H_{14}N_2$]	**51-80-9**	**$(CH_3)_2NCH_2N(CH_3)_2$**				**919.8**			**952.2**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	1.4	919.8						
[$C_{10}H_{11}N_3$]	**119044-58-5**	**$(CH_3)_2N$-CH=N-(4-cyanophenyl)**				**919.8**			**952.2**			**0**
90BOR/HOU	109-89-7	$(C_2H_5)_2NH$	313	919.4	−0.4	919.0						
90BOR/HOU	109-06-8	2-(CH_3)-pyridine	313	917.3	3.3	920.6						
90BOR/HOU	110-89-4	Piperidine	313	921	−0.8	920.1						
90BOR/HOU	591-22-0	3,5-$(CH_3)_2$-pyridine	313	923.5	−4.2	919.4						
[$C_4H_{11}N$]	**109-89-7**	**$(C_2H_5)_2NH$**				**919.4**			**952.4**			**−1.9**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	0.9	919.4						
87BIS/RUH		appearance							965±15			
83TAF	7664-41-7	NH_3	350	819	100.7	919.5						
79MAU	107-10-8	n-$C_4H_9NH_2$	550	883.9	31.8	914.9						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	54.7	919.2						
75TAF	7664-41-7	NH_3	350	819	98.8	917.6						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	57.1	921.6						
75ARN	7664-41-7	NH_3	350	819	90.4	909.1						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	58.6	923.1						
72ARN/JON	7664-41-7	NH_3	350	819	100.7	919.5						
[$C_4H_{11}N$]	**4747-21-1**	**$CH_3NH(i\text{-}C_3H_7)$**				**919.4**			**952.4**			**−2**
90BOR/HOU	119044-58-5	$(CH_3)_2N$-CH=N-(4-cyanophenyl)	313	919.8	−0.4	919.4						
[C_7H_9N]	**536-75-4**	**4(C_2H_5)-pyridine**				**919.2**			**951.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	20.5	918.6						
76AUE/WEB2	75-50-3	$(CH_3)_3N$	298	918.1	1.5	919.6						
[$C_8H_{14}N_2$]	**13618-34-3**	**3,5-diethyl-4-methylpyrazole**				**919.2**			**952.8**			**−4**
92ABB/CAB	536-75-4	4-(C_2H_5)-pyridine	333	919.2	0.6	920.0						
92ABB/CAB	108-89-4	4-(CH_3)-pyridine	333	915.3	3.2	918.7						
[$C_6H_{13}O_3P$]	**7735-82-2**	**cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane**				**919.1**			**951.6**			**0**
80HOD/HOU	110-89-4	Piperidine	320	921	−0.8	920.1						
80HOD/HOU	108-89-4	4-(CH_3)-pyridine	320	915.3	2.5	917.9						
[$C_5H_{15}N_2OP$]	**2511-17-3**	**$OP(N(CH_3)_2)_2(CH_3)$**				**918.9**			**951.3**			**0**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	0.5	918.9						
84BOL/HOU	75-50-3	$(CH_3)_3N$	~323	918.1	0.8	919.1						

TABLE 2. *Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued*

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{10}H_{18}N_2O_3$]	**20488-27-1**	**val-pro**				**918.8**			**NE**			**NE**
93GOR/AMS	75-50-3; 109-89-7	$(CH_3)_3N$; $(C_2H_5)_2NH$	350			918-919						
[$C_7H_{12}ClN$]	**5960-95-2**	**1-azabicyclo[2.2.2]-octane, 4-chloro**				**918.6**			**949.4**			**5.6**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	0.5	918.6						
86HEI/HON	75-50-3	$(CH_3)_3N$	313	918.1	0.4	918.5						
86HEI/HON	109-89-7	$(C_2H_5)_2NH$	313	919.4	−0.4	918.9						
[$C_9H_{21}OP$]	**1496-94-2**	**$OP(n\text{-}C_3H_7)_3$**				**918.4**			**948.2**			**9.1**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	0.5	918.4						
84BOL/HOU	75-50-3	$(CH_3)_3N$	323	918.1	0.4	918.5						
[C_3H_9N]	**75-50-3**	**$(CH_3)_3N$**				**918.1**			**948.9**			**5.6**
97EAS/SMI		theory	298									5.6
95SMI/RAD		theory	298						951.6			
91MAU/SIE	124-40-3	$(CH_3)_2NH$	600	896.5	23.4	917.6	929.5	20.5	950.0	−2	5.0	3.0
91MAU/SIE	110-86-1	pyridine	600	898.1	20.1	917.1	930	22.2	952.2	2	−3.8	−1.8
87TAF	7664-41-7	NH_3	350	819	100.7	919.1						
83TAF2	7664-41-7	NH_3	350	819	100.2	918.6						
83TAF	7664-41-7	NH_3	350	819	100.7	919.1						
83LOC/MCI	7664-41-7	NH_3	350	819	100.7	919.1						
80MAU/HAM	110-86-1	pyridine	330	898.1	18.4	916.4						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	52.7	917.2						
75TAF	7664-41-7	NH_3	350	819	97.9	916.3						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	52.2	916.7						
75ARN	7664-41-7	NH_3	350	819	89.5	907.9						
74STA/BEA2	75-50-3	$(CH_3)_3N$	320	918.1	0	918.1						
74STA/BEA	75-50-3	$(CH_3)_3N$	320	918.1	0	918.1						
72HEN/TAA	7664-41-7	NH_3	350	819	99.8	918.2						
72BRI/YAM	7664-41-7	NH_3	600	819	97.5	912.9						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	56.1	920.6						
72ARN/JON	7664-41-7	NH_3	350	819	99.8	918.2						
71BOW/AUE	75-50-3	$(CH_3)_3N$	298	918.1	0	918.1						
[$C_9H_{13}N$]	**99-97-8**	**$4\text{-}CH_3C_6H_4N(CH_3)_2$**				**918.1**			**950.0**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	−0.5	917.9						
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	9.2	918.4						
[$C_{10}H_{19}N_3O_4$]	**14857-82-0**	**gly-gly-leu**				**918.1**			**NE**			**NE**
93WU/FEN		kinetic method				918.1						
[$C_4H_5N_3O$]	**71-30-7**	**Cytosine**				**918**			**949.9**			**2**
90GRE/LIG		kinetic method							953.1			
79MAU	109-89-7	$(C_2H_5)_2NH$	535	919.4	−6.3	912.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
75WIL/MCC	124-40-3; 75-50-3	$(CH_3)_2NH$; $(CH_3)_3N$				896-918						
[$C_4H_{12}N_2$]	**6415-12-9**	**$(CH_3)_2NN(CH_3)_2$**				**917.9**			**948.7**			**5.8**
84MAU/NEL	108-48-5	2,6-$(CH_3)_2$-pyridine	600	931.1	−142	915.8						
84MAU/NEL	108-99-6	3-(CH_3)-pyridine	600	911.6	9.2	919.7						
84MAU/NEL	108-48-5	2,6-$(CH_3)_2$-pyridine	550	931.1	−11.7	918.5						
[$C_7H_{13}N_3O_4$]	**3146-40-5**	**ala-gly-gly**				**917.8**			**NE**			**NE**
93WU/FEN		kinetic method				917.8						
[$C_9H_{11}N_3O_2$]	**74739-51-8**	**$(CH_3)_2N$-CH=N-(4-nitrophenyl)**				**917.8**			**950.2**			**0**
90BOR/HOU	123-75-1	Pyrrolidine	313	915.3	0.8	916.1						
90BOR/HOU	109-06-8	2-(CH_3)-pyridine	313	917.3	2.1	919.4						
[$C_4H_7N_3$]	**1192-21-8**	**1-methyl-5-aminopyrazole**				**917.6**			**949.5**			**2**
92ABB/CAB	108-99-6	3-(CH_3)-pyridine	333	911.6	5.8	917.4						
92ABB/CAB	536-75-4	4-(C_5H_4)-pyridine	333	919.2	−1.3	917.9						
[$C_{13}H_{21}NO$]	**1502-00-7**	**1-adamantyl-CON$(CH_3)_2$**				**917.6**			**949.4**			**2**
97HOM/HER	594-39-8	t-$C_4H_{11}NH_2$	333	903.6	9.8	913.1						
97HOM/HER	108-99-6	3-(CH_3)-pyridine	333	911.6	5.9	917.5						
97HOM/HER	108-89-4	4-(CH_3)-pyridine	333	915.3	2.3	917.7						
[$C_6H_{10}N_2$]	**1072-91-9**	**1,3,5-Trimethylpyrazole**				**917.4**			**949.3**			**2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	−0.9	917.4						
[C_6H_6N]	**2348-49-4**	**C_6H_5NH radical**				**917.4**			**949.8**			**0**
82MAU	108-89-4; 109-89-7	4-CH_3-pyridine; $(C_2H_5)_2NH$				915-919						
[$C_{10}H_{13}NO_2$]	**7291-00-1**	**4-CH_3O-$C_6H_4CON(CH_3)_2$**				**917.4**			**948.3**			**5**
94GRU/CAL	108-89-4; 109-89-7	4-CH_3-pyridine; $(C_2H_5)_2NH$				915-919						
[$C_{10}H_{12}NS$]	**74362-50-8**	**4-$CH_3SC_6H_4C(CH_3)=CH_2$**				**917.4**			**946.2**			**12**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	−0.5	917.4						
[C_3H_9NO]	**156-87-6**	**$NH_2(CH_2)_3OH$**				**917.3**			**962.5**			**−43**
80MAU/HAM	75-50-3	$(CH_3)_3N$	330	918.1	−1.7	917.9	948.9	14.6	963.6	5.6	−49	−43.4
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	18.1	914.5						
[C_6H_7N]	**109-06-8**	**2-(CH_3)-pyridine**				**917.3**			**949.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	16.1	914.3						
87TAF	7664-41-7	NH_3	350	819	107.1	925.7						
83TAF2	7664-41-7	NH_3	350	819	107.1	925.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83MAU/SIE	110-86-1	pyridine	425	898.1	17.2	915.3						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	17.6	914.0						
[$C_8H_{12}F_3N$]	**#363**	**1-Azabicyclo[2.2.2]octane,4-trifluoromethyl-**				**916.8**			**947.6**			**5.6**
87TAF	7664-41-7	NH_3	350	819	98.4	916.8						
[$C_6H_{11}N_3O_4$]	**556-33-2**	**triglycine**				**916.8**			**966.8**			**−59**
98ZHA/ZIM	75-31-0; 110-86-1	$(i\text{-}C_3H_7)NH_2$; C_5H_5N	300			889-898						
93WU/LEB	127-19-5; 107-10-8	$CH_3CON(CH_3)_2$; $n\text{-}C_3H_7NH_2$	300			877-884						
93CHE/WU		kinetic method							966.8			−59
92WU/HEN2		kinetic method				908.8						
[$C_7H_{10}ClN$]	**#449**	**3-Chloro-1-azabicyclo[2.2.2]oct-2-ene**				**916.7**			**947.5**			**5.6**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	−1.5	916.7						
[$C_9H_{12}N_2O_6$]	**58-96-8**	**Uridine**				**916.6**			**947.6**			**5**
94LIG/NAP		kinetic method							946.7			
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_5H_{12}N_2S$]	**2782-91-4**	**SC[$N(CH_3)_2$]$_2$**				**916.6**			**947.6**			**5**
93ABB/MO	330-73-4	4-(C_2H_5)-pyridine	333	919.2	2.1	917.0						
93ABB/MO	108-89-4	4-(CH_3) pyridine	333	915.3	1.1	916.3						
[$C_{10}H_{17}NO$]	**52305-49-4**	**tricyclo[4.4.0.0^{3,8}]decan-4-ol-5-amino, stereoisomer**				**916.6**			**949.0**			**0**
83HOU/RUF	108-89-4	4-(CH_3)-pyridine	1300	915.3	1.3	916.6						
[$C_{10}H_{17}N$]	**768-94-5**	**Tricyclo[3.3.1.1^{3,7}]decane-1-amine**				**916.3**			**948.8**			**0**
89BRO/COO	536-75-4	4-(C_2H_5)-pyridine	300	919.2	−2.1	916.5						
87TAF	7664-41-7	NH_3	350	819	97.0	915.7						
[$C_6H_{11}N$]	**124-02-7**	**$(CH_2{=}CHCH_2)_2NH$**				**916.3**			**949.3**			**−2**
87TAF	7664-41-7	NH_3	350	819	97.5	916.3						
83TAF2	7664-41-7	NH_3	350	819	97.5	916.3						
[$C_{12}H_{24}N_2$]	**71058-67-8**	**1,6-Diazabicyclo[4.4.4]tetradecane**				**916.3**			**947.1**			**5.6**
81ALD/ARR	7664-41-7	NH_3	320	819	97.5	916.2						
[$C_8H_{15}NO$]	**17997-65-8**	**cis-3-Aminobicyclo[2.2.2]octan-2-ol**				**916.2**			**948.6**			**0**
83HOU/RUF	108-89-4	4-(CH_3)-pyridine	1300	915.3	0.8	916.2						
[$C_6H_{10}N_2$]	**5519-42-6**	**3,4,5-Trimethylpyrazole**				**916.0**			**949.3**			**−3**
87TAF	7664-41-7	NH_3	350	819	97.0	915.8						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ylide	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_8H_{13}NO$]	**873-95-0**	**3-Amino-5,5-dimethylcyclohex-2-enone**				**915.9**			**946.9**			**5**
87TAF	7664-41-7	NH_3	350	819	97.5	915.9						
[C_3H_2]	**16166-40-5**	**cyclopropenylidene**				**915.9**			**951.1**			**−9.1**
95CHY/SQU	7664-41-7	NH_3					853.6	97.5	951.1			
[$C_{10}H_{14}N_2O_5$]	**50-89-5**	**Thymidine**				**915.9**			**948.3**			**0**
90GRE/LIG		kinetic method							948.3			
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_4H_{10}N_2O$]	**139033-03-7**	**$(CH_3)_2N$-CH=N-OCH_3**				**915.8**			**948.3**			**0**
92RAC/MAR	123-75-1	Pyrrolidine	338	915.3	0	915.2						
92RAC/MAR	109-89-7	$(C_2H_5)_2NH$	338	919.4	−2.9	916.4						
[$C_6H_{15}NO$]	**4048-33-3**	**$NH_2(CH_2)_6OH$**				**915.7**			**969.0**			**−70**
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	−2.4	915.7						
[$C_9H_{13}N$]	**121-72-2**	**3-$CH_3C_6H_4N(CH_3)_2$**				**915.7**			**942.1**			**20**
87TAF	7664-41-7	NH_3	350	819	97.9	915.6						
77POL/DEV	62-53-3	$C_6H_5NH_2$	350	850.6	65.4	915.1						
[$C_5H_9N_3$]	**134166-58-8**	**$(CH_3)_2N$-CH−N-CH_2CN**				**915.5**			**948.0**			**0**
92RAC/MAR	123-75-1	Pyrrolidine	338	915.3	0	915.2						
92RAC/MAR	139033-03-7	$(CH_3)_2N$-CH=N-OCH_3	338	915.8	0	915.8						
[C_7H_9N]	**536-78-7**	**3-(C_2H_5)-pyridine**				**915.5**			**947.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	17.1	915.2						
89BRO/COO	768-94-5	Tricyclo[3.3.1.1^{3,7}]decane-1-amine	300	916.3	−0.4	916.5						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	18.5	915.0						
[$C_9H_{15}N_3O_4$]	**14379-76-1**	**gly-gly-pro**				**915.5**			**NE**			**NE**
96EWI/ZHA	108-99-6; 109-89-7	3-(CH_3)-pyridine; $(C_2H_5)_2NH$				912-919						
[$C_9H_{15}N_3O_4$]	**2441-63-6**	**gly-pro-gly**				**915.5**			**NE**			**NE**
96EWI/ZHA	108-99-6; 109-89-7	3-(CH_3)-pyridine; $(C_2H_5)_2NH$				912-919						
[$C_{11}H_{15}N$]	**35843-88-0**	**3-$(CH_3)_2NC_6H_4C(CH_3)=CH_2$**				**915.5**			**946.2**			**5.6**
87TAF	7664-41-7	NH_3	350	819	97.0	915.4						
[C_6H_7N]	**108-89-4**	**4-(CH_3)-pyridine**				**915.3**			**947.2**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	16.1	914.2						
87TAF	7664-41-7	NH_3	350	819	96.6	915.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ref/Squib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83TAF	7664-41-7	NH_3	350	819	96.6	915.1						
78TAF	7664-41-7	NH_3	350	819	97.9	916.5						
75ARN	7664-41-7	NH_3	350	819	97.9	916.5						
72TAA/HEN	110-86-1	pyridine	320	898.1	22.6	920.7						
[$C_5H_6N_2$]	**504-29-0**	**2-Pyridinamine**				**915.3**			**947.2**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	16.6	914.7						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	−2.4	915.7						
[C_4H_9N]	**123-75-1**	**Pyrrolidine**				**915.3**			**948.3**			**−2**
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	−3.2	915.3						
83TAF	7664-41-7	NH_3	350	819	97.5	916.3						
81TAA/SUM	7664-41-7	NH_3	320	819	89.1	908.0						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	50.8	915.3						
75TAF	7664-41-7	NH_3	350	819	97.9	916.7						
75ARN	7664-41-7	NH_3	350	819	89.5	908.3						
71BOW/AUE	75-50-3	$(CH_3)_3N$	298	918.1	−1.3	916.9						
[$C_{10}H_{13}N$]	**4096-21-3**	**N-Phenylpyrrolidine**				**915.1**			**941.6**			**20**
88CAU/CER		See Refs.				912.8						
87TAF	7664-41-7	NH_3	350	819	97.0	914.7						
83TAF2	7664-41-7	NH_3	350	819	97.5	915.2						
[$C_4H_{14}N_3OP$]	**3732-86-3**	**$OP(NH_2)(N(CH_3)_2)_2$**				**915.0**			**947.5**			**0**
88BOL/HOU	109-06-8	2-(CH_3)-pyridine	323	917.3	−1.7	915.6						
85BOL/HOU	109-89-7	$(C_2H_5)_2NH$	323	919.4	−5.0	914.4						
[$C_5H_{13}N_2OP$]	**16606-18-1**	**c-P(O)CH_3N(CH_3)CH_2CH_2N(CH_3)**				**915.0**			**947.5**			**0**
85BOL/HOU	108-89-4	4-(CH_3)-pyridine	323	915.3	−1.7	913.7						
85BOL/HOU	109-06-8	2-(CH_3)-pyridine	323	917.3	−0.8	916.5						
[$C_{11}H_{12}N_2O_2$]	**73-22-3**	**L-tryptophan**				**915**			**948.9**			**−5**
93LI/HAR		kinetic method							931			
92GOR/SPE	75-64-9; 75-50-3	(t-C_4H_9)NH_2; $(CH_3)_3N$	350			900-918						
90ISA/OMO		kinetic method-relative order										
87TAF	75-50-3	$(CH_3)_3N$	350	918.1	0	918.7						
87BOJ		kinetic method-relative order										
86BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	100.7	919.6						
[$C_7H_{13}N_3O_4$]	**19729-30-7**	**gly-gly-ala**				**914.8**			**NE**			**NE**
93WU/FEN		kinetic method				914.8						
[$C_4H_{10}N_2$]	**110-85-0**	**Piperazine**				**914.7**			**943.7**			**11.5**
73AUE/WEB	107-10-8	n-$C_4H_9NH_2$	298	883.9	30.8	914.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ylid/Squib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{10}H_{19}NO$]	**29910-43-8**	**2-Naphthalenol, 3-aminodecahydro-(2, 3β, 4α, 8$\alpha\beta$)**				**914.5**			**947.0**			**0**
83HOU/RUF	108-99-6	3-(CH_3)-pyridine	300	911.6	2.9	914.5						
[$C_{10}H_{17}NO$]	**33540-02-2**	**tricyclo[4.4.0.0^{3,8}]decan-4-ol-5-amino, stereoisomer**				**914.5**			**947.0**			**0**
83HOU/RUF	108-99-6	3-(CH_3)-pyridine	300	911.6	2.9	914.5						
[$C_8H_{14}N_2$]	**96440-80-1**	**3(5)-methyl-5(3)-t-butylpyrazole**				**914.3**			**946.2**			**2**
92ABB/CAB	536-75-4	4-(C_2H_5)-pyridine	333	919.2	−4.9	914.3						
[$C_6H_{13}O_3P$]	**41821-91-4**	**trans-2-Methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane**				**914.1**			**946.6**			**0**
80HOD/HOU	109-06-8	2-(CH_3)-pyridine	320	917.3	−5.9	911.5						
80HOD/HOU	109-89-7	$(C_2H_5)_2NH$	320	919.4	−6.3	913.1						
80HOD/HOU	108-99-6	3-(CH_3)-pyridine	320	911.6	6.3	917.9						
[$C_9H_{12}N_2O$]	**33322-60-0**	**3-NH_2-$C_6H_4CON(CH_3)_2$**				**913.5**			**944.4**			**5**
94GRU/CAL	108-99-6; 108-89-4	3-(CH_3)-pyridine; 4-(CH_3)-pyridine				912-915						
[$C_{12}H_{17}NO_2$]	**56066-86-5**	**N,N-2,6-Tetramethylaniline,4-carboxylic acid, methyl ester**				**913.0**			**945.4**			**0**
87TAF	7664-41-7	NH_3	350	819	94.3	913.0						
[$C_{15}H_{12}N_2$]	**1145-01-3**	**3,5-diphenylpyrazole**				**912.7**			**946.3**			**−3.8**
92ABB/CAB	594-39-8	t-$C_5H_{11}NH_2$	333	903.6	6.2	909.7						
92ABB/CAB	108-89-4	4-(CH_3)-pyridine	333	915.3	−0.5	915.0						
92ABB/CAB	108-99-6	3-(CH_3)-pyridine	333	911.6	1.6	913.4						
[$C_2H_8N_2$]	**107-15-3**	**1,2-Diaminoethane**				**912.5**			**951.6**			**−22.1**
80MAU/HAM	142-84-7	$(n\text{-}C_3H_7)_2NH$	600	929.3	−22.2	913.2	962.3	−12.1	950.2	−1.9	−16.7	−18.6
80MAU/HAM	124-40-3	$(CH_3)_2NH$	600	896.5	7.5	910.0	929.5	22.2	951.7	−2	−24.3	−26.3
80MAU/HAM	110-86-1	pyridine	600	898.1	5.9	911.2	930	20.9	950.9	2	−25.1	−23.1
80MAU/HAM	109-89-7	$(C_2H_5)_2NH$	600	919.4	−12.1	913.4	952.4	−0.8	951.6	−1.9	−18.8	−20.7
73YAM/KEB	124-40-3	$(CH_3)_2NH$	600	896.5	8.4	910.9	929.5	40.2	969.7	−2	−53.1	−55.1
73AUE/WEB	107-10-8	n-$C_4H_7NH_2$	298	883.9	31.7	915.6						
[$C_8H_{14}N_2$]	**141665-16-9**	**1-methyl-3-t-butylpyrazole**				**912.5**			**944.4**			**2**
92ABB/CAB	108-89-4	4-(CH_3)-pyridine	333	915.3	−2.8	912.5						
92ABB/CAB	108-99-6	3-(CH_3)-pyridine	333	911.6	1.0	912.6						
[$C_5H_5N_5$]	**73-24-5**	**Adenine**				**912.5**			**942.8**			**7**
90GRE/LIG		kinetic method							948.1			
79MAU	109-89-7	$(C_2H_5)_2NH$	570	919.4	−7.1	909.9	952.4	−10.9	941.5	−1.9	6.7	4.8

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
79MAU	110-86-1	pyridine	570	898.1	10.5	907.3	930	6.7	936.7	2	6.7	8.7
75WIL/MCC	124-40-3; 75-	$(CH_3)_2NH$; $(CH_3)_3N$				896-918						
[$C_9H_{13}N$]	**613-97-8**	**$C_6H_5N(CH_3)(C_2H_5)$**				**912.4**			**939.0**			**20**
78LAU/SAL	7664-41-7	NH_3	600	819	101.3	912.3						
73YAM/KEB	7664-41-7	NH_3	600	819	101.3	912.3						
[C_7H_7N]	**100-43-6**	**4-Vinylpyridine**				**912.3**			**944.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	13.7	911.8						
79AUE/BOW	75-50-3	$(CH_3)_3N$	298	918.1	-5.4	912.8						
[$C_6H_{18}N_3PS$]	**3732-82-9**	**$SP(N(CH_3)_2)_3$**				**912.2**			**942.0**			**9.1**
88WEB/HOU	108-89-4	4-(CH_3)-pyridine	313	915.3	-1.0	914.2						
88WEB/HOU	108-99-6	3-(CH_3)-pyridine	313	911.6	-1.3	910.2						
[$C_{10}H_{10}N_2$]	**479-27-6**	**1,8-Diaminonaphthalene**				**912.1**			**944.5**			**0**
78LAU/SAL	110-89-4	Piperidine	600	921	8.4	912.1						
[C_6H_7N]	**108-99-6**	**3-(CH_3)-pyridine**				**911.6**			**943.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	11.7	909.9						
87TAF	7664-41-7	NH_3	350	819	92.9	911.5						
86TAF/ANV	108-99-6	3-(CH_3)-pyridine	350	911.6	0	911.6						
86MAU/LIE	110-86-1	pyridine	600	898.1	17.6	915.8						
83TAF2	7664-41-7	NH_3	350	819	94.3	912.9						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	13.2	909.6						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	45.4	909.9						
[C_3H_8Pb]	**82065-01-8**	**$(CH_3)_2Pb{=}CH_2$**				**911.5**			**938.0**			**20**
82PIE/HEH	7664-41-7	NH_3	350	819	93.8	911.5						
[C_6H_7NO]	**7295-76-3**	**3-(CH_3O)-pyridine**				**910.9**			**942.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	10.3	908.4						
87TAF	7664-41-7	NH_3	350	819	94.7	913.3						
83TAF2	7664-41-7	NH_3	350	819	95.6	914.2						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	11.7	908.2						
[C_9H_7NO]	**1613-37-2**	**Quinoline-1-oxide**				**910.8**			**943.3**			**0**
79MAU	107-10-8	n-$C_3H_7NH_2$	526	883.9	28.0	910.8						
[$C_{10}H_{14}FN$]	**14994-35-5**	**N,N,2,6-Tetramethylaniline,4-fluoro**				**910.7**			**943.2**			**0**
87TAF	7664-41-7	NH_3	350	819	92.0	910.7						
[$C_8H_{18}O_5$]	**112-60-7**	**$HO[CH_2CH_2O]_4H$**				**>910**			**NE**			**NE**
92LIO/BRO	17455-13-9	18-crown-6		909.5	>0	>910			See Refs.			
[$C_{14}H_{28}O_7$]	**33089-36-0**	**21-crown-7**				**>910**			**NE**			**NE**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
92LIO/BRO	17455-13-9	18-crown-6		909.5	>0	>910			See Refs.			
[$C_{10}H_{22}O_6$]	**4792-15-8**	**HO[CH_2CH_2O]$_5$H**				**>910**			**NF**			**NF**
92LIO/BRO	17455-13-9	18-crown-6		909.5	>0	>910			See Refs.			
[$C_9H_8N_2$]	**4838-00-0**	**2-Methyl-2H-indazole**				**909.6**			**941.4**			**2**
88CAT/CLA	7295-76-3	3-(CH_3O)-pyridine	~300	910.9	−1.3	909.6						
88CAT/CLA	75-64-9	t-$C_4H_9NH_2$	~300	899.9	10.5	910.3						
88CAT/CLA	594-39-8	t-$C_5H_{11}NH_2$	~300	903.6	4.2	907.8						
87TAF	7664-41-7	NH_3	350	819	92.0	910.6						
84FLA/MAQ		kinetic method				903.7						
[C_5H_9N]	**7223-38-3**	**HCCCH$_2$N(CH_3)$_2$**				**909.5**			**940.3**			**5.6**
87TAF	7664-41-7	NH_3	350	819	91.1	909.5						
[$C_{12}H_{24}O_6$]	**17455-13-9**	**18-crown-6**				**909.5**			**967.0**			**−84**
98LIO/BRO		kinetic method										
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	37.2	907.2	884.6	82.4	967.0	2	−86	−84
83MAU	110-86-1	pyridine	600	898.1	11.3	912.6						
83MAU	289-80-5	Pyridazine	600	877.1	3.8	908.4						
[C_4H_9N]	**1190-79-0**	**CH_3CH=NC_2H_5**				**909.4**			**941.9**			**0**
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	44.9	909.4						
[C_3H_7N]	**4427-28-5**	**CH_2=C(CH_3)NH_2**				**909.3**			**941.8**			**0**
81ELL/DIX		See Refs.							941.8			
[$C_3H_4N_2$]	**288-32-4**	**Imidazole**				**909.2**			**942.8**			**−3.8**
88CAT/CLA	594-39-8	t-$C_5H_{11}NH_2$	~300	903.6	3.8	907.3						
88CAT/CLA	108-99-6	3-(CH_3)-pyridine	~300	911.6	−2.5	909.1						
88CAT/CLA	1628-89-3	2-(CH_3O)-pyridine	~300	902.8	7.5	910.3						
87TAF	7664-41-7	NH_3	350	819	91.5	910.4						
86TAF/ANV	1628-89-3	2-(CH_3O)-pyridine	350	902.8	7.5	910.6						
86TAF/ANV	108-99-6	3-(CH_3)-pyridine	350	911.6	−2.5	909.4						
86TAF/ANV	594-39-8	t-$C_5H_{11}NH_2$	350	903.6	3.8	907.2						
86MAU/LIE	110-86-1	pyridine	600	898.1	3.1	903.0						
84FLA/MAQ		kinetic method										
[$C_8H_{11}N$]	**121-69-7**	**$C_6H_5N(CH_3)_2$**				**909.2**			**941.1**			**2**
87TAF	7664-41-7	NH_3	350	819	90.6	909.2						
85LIA/JAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	0	909.2						
83TAF	7664-41-7	NH_3	350	819	91.1	909.6						
83LOC/MCI	7664-41-7	NH_3	350	819	90.6	909.2						
78LAU/SAL	7664-41-7	NH_3	600	819	90.8	907.3						
77POL/DEV	62-53-3	$C_6H_5NH_2$	350	850.6	57.2	907.8						
75TAF	7664-41-7	NH_3	350	819	91.1	909.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
73YAM/KEB	7664-41-7	NH_3	600	819	90.8	907.3						
[C_3H_9N]	**624-78-2**	**$(CH_3)(C_2H_5)NH$**				**909.2**			**942.2**			**−2**
87TAF	7664-41-7	NH_3	350	819	90.6	909.4						
83TAF2	7664-41-7	NH_3	350	819	90.6	909.4						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	44.4	908.9						
75TAF	7664-41-7	NH_3	350	819	87.4	906.2						
75ARN	7664-41-7	NH_3	350	819	87.4	906.2						
[$C_{10}H_{18}N_2O_3$]	**52899-09-9**	**pro-val**				**909.0**			**NE**			**NE**
93GOR/AMS	75-64-9; 75-50-3	$(t\text{-}C_4H_9)NH_2$; $(CH_3)_3N$	350			900-918						
[$C_{14}H_{20}N_2O_3$]	**3918-92-1**	**val-phe**				**909.0**			**NE**			**NE**
93GOR/AMS	75-64-9; 75-50-3	$(t\text{-}C_4H_9)NH_2$; $(CH_3)_3N$	350			900-918						
[$C_{10}H_{20}N_2O_3$]	**14486-09-0**	**val-met**				**909.0**			**NE**			**NE**
93GOR/AMS	75-64-9; 75-50-3	$(t\text{-}C_4H_9)NH_2$; $(CH_3)_3N$	350			900-918						
[$C_{14}H_{20}N_2O_4$]	**3061-91-4**	**val-tyr**				**909.0**			**NE**			**NE**
93GOR/AMS	75-64-9; 75-50-3	$(t\text{-}C_4H_9)NH_2$; $(CH_3)_3N$	350			900-918						
[$C_{16}H_{21}N_3O_3$]	**24587-37-9**	**val-trp**				**909.0**			**NE**			**NE**
93GOR/AMS	75-64-9; 75-50-3	$(t\text{-}C_4H_9)NH_2$; $(CH_3)_3N$	350			900-918						
[$C_{10}H_{14}N_2O$]	**59-26-7**	**N,N-diethylnicotinamide**				**909.0**			**940.9**			**2**
91BER/DEC	121-69-7	$C_6H_5N(CH_3)_2$	338	909.2	0	909.2						
91BER/DEC	75-64-9	$t\text{-}C_4H_9NH_2$	338	899.9	7.5	907.1						
91BER/DEC	108-89-4	4-(CH_3)-pyridine	338	915.3	−5.0	910.3						
91BER/DEC	110-86-1	pyridine	338	898.1	11.3	909.4						
[C_3H_7N]	**503-29-7**	**Azetidine**				**908.6**			**943.4**			**−7.8**
92ABB/CAN	108-89-4	4-(CH_3)-pyridine	333	915.3	6.2	909.5						
92ABB/CAN	594-39-8	$t\text{-}C_5H_{11}NH_2$	333	903.6	3.4	907.1						
92ABB/CAN	108-99-6	3-(CH_3)-pyridine	333	911.6	−1.5	910.5						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	43.0	907.4						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	44.4	908.9						
71BOW/AUE	75-50-3	$(CH_3)_3N$	298	918.1	−10.3	907.9						
[$C_7H_6N_2$]	**271-63-6**	**7-Azaindole**				**908.3**			**940.2**			**2**
87TAF	7664-41-7	NH_3	350	819	89.7	908.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[$C_{12}H_8N_2$]	**92-82-0**	**Phenazine**				**908.3**			**938.4**			**8**
79MAU	107-10-8	n-$C_3H_7NH_2$	514	883.9	27.2	908.3						
[$C_{11}H_9N$]	**939-23-1**	**4-phenyl-pyridine**				**907.8**			**939.7**			**2**
97SHE/STE		See Refs.							939.7±2.1			
[$C_7H_8O_2$]	**1004-36-0**	**2,6-Dimethyl-4-pyrone**				**907.3**			**941.5**			**−5.8**
87TAF	7664-41-7	NH_3	350	819	88.3	907.3						
[$C_8H_{14}N_2$]	**141665-17-0**	**1-methyl-5-t-butylpyrazole**				**907.3**			**939.2**			**2**
92ABB/CAB	594-39-8	t-$C_4H_{11}NH_2$	333	903.6	2.6	905.9						
92ABB/CAB	694-31-5	1,5-Dimethylpyrazole	333	902.8	6.0	908.8						
[$C_6H_6N_4$]	**2004-03-7**	**6-Methylpurine**				**907.3**			**939.2**			**2**
75WIL/MCC	124-40-3; 75-50-3	$(CH_3)_2NH$; $(CH_3)_3N$				896-918						
[$C_{10}H_{10}Ni$]	**1271-28-9**	**Ni(C_5H_5)$_2$**				**907.3**			**935.7**			**13.4**
81STE/BEA	7664-41-7	NH_3	320	819	79.9	898.5						
76COR/BEA	109-89-7	$(C_2H_5)_2NH$	320	919.4	−6.7	912.4						
76COR/BEA	75-50-3	$(CH_3)_3N$	320	918.1	−7.1	910.9						
[$C_6H_{15}OP$]	**597-50-2**	**$(C_2H_5)_3PO$**				**906.8**			**936.6**			**9.1**
85BOL/HOU	108-99-5	3-(CH_3)-pyridine	323	911.6	−5.4	906.0						
85BOL/HOU	624-78-2	$(CH_3)(C_2H_5)NH$	323	909.2	−1.3	907.7						
[$C_{10}H_{12}ClN$]	**4280-30-2**	**Pyrrolidine, 1-(4-chlorophenyl)**				**906.6**			**937.4**			**5.6**
88CAU/CER		See Refs.				906.6						
[$C_{10}H_{13}NO$]	**2124-31-4**	**4-[$(CH_3)_2N$]-C_6H_4-$COCH_3$**				**906.3**			**932.8**			**20**
87TAF	7664-41-7	NH_3	350	819	90.6	908.3						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	75.7	904.2						
[C_6H_7NS]	**18438-38-5**	**2-(CH_3S)-pyridine**				**906.0**			**937.8**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	7.8	906.0						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	41.5	906.0						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	9.3	905.7						
[$C_6H_{12}N_2O_3$]	**1948-31-8**	**di-L-alanine**				**905.6**			**NE**			**NE**
93WU/FEN		kinetic method				905.6						
[$C_7H_{12}N_2O_3$]	**704-15-4**	**gly-pro**				**905.6**			**NE**			**NE**
96EWI/ZHA	108-91-8; 108-99-6	c-$C_6H_{11}NH_2$; 3-(CH_3)-pyridine				900-912						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_4H_7N_3$]	**1904-31-0**	**1-methyl-3-aminopyrazole**				**905.6**			**937.4**			**2**
92ABB/CAB	108-99-6	3-(CH_3)-pyridine	333	911.6	−4.6	907.0						
92ABB/CAB	594-39-8	t-$C_5H_{11}NH_2$	333	903.6	0.7	904.0						
[$C_7H_{11}NO$]	**3731-38-2**	**1-Azabicyclo[2.2.2]octan-3-one**				**905.2**			**936.0**			**5.6**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	8.8	905.2						
[CH_2Fe]	**95260-85-4**	**$FeCH_2$**				**905.2**			**937.7**			**0**
89JAC/GOR	110-86-1; 100-43-6	pyridine; 4-vinylpyridine				898-912						
[CH_2Co]	**116492-58-1**	**$CoCH_2$**				**905.2**			**937.7**			**0**
89JAC/GOR	110-86-1; 100-43-6	pyridine; 4-vinylpyridine				898-912						
[$C_7H_{11}F_2N$]	**#524**	**3,3-Difluoro-1-azabicyclo[2.2.2]octane**				**904.8**			**935.6**			**5.6**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	8.3	904.8						
[C_6H_7NS]	**18794-33-7**	**3-(CH_3S)-pyridine**				**904.7**			**936.5**			**2**
87TAF	7664-41-7	NH_3	350	819	86.0	904.6						
[$C_8H_{12}N_2$]	**51627-76-0**	**1-azabicyclo[2.2.2]-octane, 3-cyano**				**904.6**			**935.4**			**5.6**
86HEI/HON	594-39-8	t-$C_5H_{11}NH_2$	313	903.6	−0.4	903.0						
86HEI/HON	624-78-2	$(CH_3)(C_2H_5)NH$	313	909.2	−2.9	906.2						
[$C_8H_6N_2$]	**253-66-7**	**Cinnoline**				**904.4**			**936.3**			**2**
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	22.2	904.4						
[$C_6H_{18}N_3PSe$]	**7422-73-3**	**$SeP(N(CH_3)_2)_3$**				**904.3**			**934.1**			**9.1**
88WEB/HOU	594-39-8	t-$C_5H_{11}NH_2$	313	903.6	0.4	903.8						
88WEB/HOU	108-91-8	c-$C_6H_{11}NH_2$	313	899.6	5.4	904.8						
[C_3H_7N]	**1072-44-2**	**N-Methylaziridine**				**904.1**			**934.8**			**5.6**
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	39.5	904.1						
[$C_{11}H_{12}N_2$]	**141665-22-7**	**3(5)-ethyl-5(3)-phenylpyrazole**				**903.8**			**935.6**			**2**
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	5.8	905.4						
92ABB/CAB	110-86-1	pyridine	333	898.1	6.0	904.1						
92ABB/CAB	594-39-8	t-$C_5H_{11}NH_2$	333	903.6	−1.5	901.8						
[$C_{10}H_{13}NO_2$]	**16518-64-2**	**3-$(CH_3)_2NC_6H_4COOCH_3$**				**903.8**			**930.2**			**20**
87TAF	7664-41-7	NH_3	350	819	86.0	903.7						
[$C_5H_{13}N$]	**594-39-8**	**t-$C_5H_{11}NH_2$**				**903.6**			**837.8**			**−6**
87TAF	7664-41-7	NH_3	350	819	87.9	906.8						
86TAF/ANV	7664-41-7	NH_3	350	819	80.3	899.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	40.0	904.5						
[$C_9H_{11}N$]	**1962-08-9**	**4-$H_2NC_6H_4C(CH_3)=CH_2$**				**903.3**			**929.8**			**20**
87TAF	7664-41-7	NH_3	350	819	85.6	903.3						
[$C_4H_{12}NOP$]	**50663-05-3**	**OP(N(CH_3)$_2$)(CH_3)$_2$**				**903.0**			**935.5**			**0**
87TAF	7664-41-7	NH_3	350	819	84.7	903.3						
84BOL/HOU	75-64-9	t-$C_4H_9NH_2$	~323	899.9	2.9	902.7						
[$C_{10}H_{14}BrN$]	**50638-54-5**	**N,N,2,6-Tetramethylaniline,4-bromo-**				**902.9**			**935.4**			**0**
87TAF	7664-41-7	NH_3	350	819	84.2	902.9						
[C_6H_7NO]	**1628-89-3**	**2-(CH_3O)-pyridine**				**902.8**			**934.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	4.4	902.5						
87TAF	7664-41-7	NH_3	350	819	83.3	901.9						
86TAF/ANV	7664-41-7	NH_3	350	819	76.1	894.7						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	38.1	902.6						
76COO/KAT	7664-41-7	NH_3	350	819	86.0	904.6						
76AUE/WEB2	124-40-3	$(CH_3)_2NH$	298	896.5	5.9	902.3						
[C_6H_7NO]	**1003-73-2**	**3-methyl-pyridine-1-oxide**				**902.8**			**935.2**			**0**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	9.6	902.8						
[$C_5H_8N_2$]	**694-31-5**	**1,5-Dimethylpyrazole**				**902.8**			**934.3**			**3**
87TAF	7664-41-7	NH_3	350	819	84.2	902.7						
[$C_9H_{11}N$]	**3334-89-2**	**Azetidine, 1-phenyl**				**902.4**			**933.2**			**5.6**
88CAU/CER		See Refs.				902.4						
[$C_8H_{12}N_2$]	**26458-78-6**	**1-azabicyclo[2.2.2]-octane,4-cyano**				**902.3**			**933.1**			**5.6**
87TAF	7664-41-7	NH_3	350	819	84.7	903.1						
86HEI/HON	624-78-2	$(CH_3)(C_2H_5)NH$	313	909.2	−5.9	903.2						
86HEI/HON	594-39-8	t-$C_5H_{11}NH_2$	313	903.6	−2.6	900.5						
86HEI/HON	50663-05-3	OP(N(CH_3)$_2$)(CH_3)$_2$	313	903.0	−0.4	902.5						
[$C_5H_8N_2$]	**694-48-4**	**1,3-Dimethylpyrazole**				**902.3**			**933.9**			**3**
87TAF	7664-41-7	NH_3	350	819	83.7	902.3						
[$C_8H_{11}N$]	**64-04-0**	**$C_6H_5CH_2CH_2NH_2$**				**902.3**			**936.2**			**−5**
87TAF	7664-41-7	NH_3	350	819	83.3	902.2						
[$C_{12}H_9NO$]	**5424-19-1**	**3-C_6H_5CO-pyridine**				**902.3**			**934.1**			**2**
91BER/DEC	13952-84-6	sec-$C_4H_9NH_2$	338	895.7	6.9	902.3						
91BER/DEC	110-86-1	pyridine	338	898.1	4.1	902.2						
91BER/DEC	108-91-8	c-$C_6H_{11}NH_2$	338	899.6	3.0	902.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_4H_8S_2$]	**51102-74-0**	**CH_2=C(SCH_3)$_2$**				**902.2**			**931.1**			**12**
89OSA/DEL	108-91-8	c-$C_6H_{11}NH_2$	313	899.6	0.8	900.2						
89OSA/DEL	108-99-6	3-(CH_3)-pyridine	313	911.6	−6.3	905.2						
89OSA/DEL	75-64-9	t-$C_4H_9NH_2$	313	899.9	1.7	901.3						
[C_8H_7N]	**120-72-9**	**Indole**				**901.9**			**933.4**			**3**
87TAF	7664-41-7	NH_3	350	819	83.3	901.8						
[$C_9H_{11}NO$]	**611-74-5**	**$C_6H_5CON(CH_3)_2$**				**901.8**			**932.7**			**5**
94GRU/CAL	103-69-5; 108-45-2	$C_6H_5NHC_2H_5$; 1,3-$(NH_2)_2$-C_6H_4				893-899						
87TAF	7664-41-7	NH_3	350	819	83.3	901.7						
[$C_8H_{12}N_2O_2$]	**5744-51-4**	**1,5-dimethyl-3-ethoxycarbonylpyrazole**				**901.5**			**933.4**			**2**
92ABB/CAB	694-31-5	1,5-Dimethylpyrazole	333	902.8	−1.4	901.4						
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	2.1	901.7						
[$C_5H_{11}NO_2S$]	**63-68-3**	**L-Methionine**				**901.5**			**935.4**			**−5**
93LI/HAR		kinetic method-See Refs.							920.5			−1.3
92GOR/SPE	110-86-1; 75-64-9	pyridine; (t-C_4H_9)NH_2	350			898-900						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	82.4	901.3						
87ROI		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	82.4	901.3						
[$C_{10}H_{13}NO$]	**18992-80-8**	**3-$(CH_3)_2NC_6H_4COCH_3$**				**901.5**			**928.0**			**20**
87TAF	7664-41-7	NH_3	350	819	83.7	901.4						
[$C_7H_{13}N$]	**31002-73-0**	**Bicyclo[2.2.1]heptan-2-amine,endo**				**901.3**			**935.3**			**−5**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	4.9	901.3						
[$C_7H_{13}N$]	**7242-92-4**	**Bicyclo[2.2.1]heptan-2-amine,exo**				**901.3**			**935.3**			**−5**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	4.9	901.3						
[$C_{10}H_{10}N_2$]	**3463-26-1**	**1-methyl-3-phenylpyrazole**				**900.8**			**932.6**			**2**
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	1.9	901.5						
92ABB/CAB	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	6.3	900.0						
[C_3S]	**109545-35-9**	**C_3S**				**900.5**			**933**			**0**
92MAC/SUD		theory	298						933			
[$C_{10}H_{10}N_2$]	**3463-27-2**	**1-methyl-5-phenylpyrazole**				**900.5**			**932.4**			**2**
92ABB/CAB	594-39-8	t-$C_5H_{11}NH_2$	333	903.6	−3.5	899.8						
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	1.5	901.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[$C_{10}H_{10}N_2$]	**3347-62-4**	**3(5)-methyl-5(3)-phenylpyrazole**				**900.2**			**932.1**			**2**
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	0.7	900.3						
92ABB/CAB	694-31-5	1,5-Dimethylpyrazole	333	902.8	−2.7	900.1						
[$C_5H_8N_2$]	**67-51-6**	**3,5-dimethylpyrazole**				**900.1**			**933.5**			**−3**
92ABB/CAB	110-86-1	pyridine	333	898.1	1.8	900.1						
92ABB/CAB	594-39-8	t-$C_5H_{11}NH_2$	333	903.6	−5.9	897.6						
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	0.3	900.1						
87TAF	7664-41-7	NH_3	350	819	83.7	902.6						
[$C_5H_{10}N_2O_3$]	**56-85-9**	**L-Glutamine**				**900**			**937.8**			**−18**
93LI/HAR		kinetic method							938			
92GOR/SPE	110-86-1; 75-64-9	pyridne; (t-C_4H_9)NH_2	350			898-900						
90ISA/OMO		kinetic method-relative order										
87TAF	7644-41-7	NH_3	350	819	68.6	888.2						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	68.6	888.2						
[$C_3H_9O_3P$]	**121-45-9**	**$P(OCH_3)_3$**				**899.9**			**929.7**			**9.1**
80HOD/MCD	108-91-8	c-$C_6H_{11}NH_2$	300	899.6	0.4	900.0						
80HOD/MCD	110-86-1	pyridine	300	898.1	1.7	899.8						
[$C_4H_{11}N$]	**75-64-9**	**t-$C_4H_9NH_2$**				**899.9**			**934.1**			**−6**
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	111.7	895.1	802.1	131.8	933.9	20	−33.5	−13.5
91MAU/SIE	75-31-0	i-$C_3H_7NH_2$	600	889.0	15.1	903.4	923.8	10.0	933.9	−8	8.4	0.4
91MAU/SIE	110-86-1	pyridine	600	898.1	−0.4	900.1	930	5.4	935.4	2	−9.2	−7.2
91MAU/SIE	75-04-7	$C_2H_5NH_2$	600	878	27.2	905.5	912.0	25.9	937.9	−5.1	2.1	−3.0
87TAF	7664-41-7	NH_3	350	819	81.5	900.4						
83TAF	7664-41-7	NH_3	350	819	81.5	900.4						
83LOC/MCI	7664-41-7	NH_3	350	819	81.5	900.4						
80MAU	7664-41-7	NH_3	550	819	70.7	889.6						
79MAU	107-10-8	n-$C_3H_7NH_2$	514	883.9	13.8	897.9						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	35.1	899.6						
75TAF	7664-41-7	NH_3	350	819	78.3	897.2						
75ARN	7664-41-7	NH_3	350	819	78.3	897.2						
72HEN/TAA	7664-41-7	NH_3	350	819	80.5	899.5						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	34.2	898.7						
72ARN/JON	7664-41-7	NH_3	350	819	80.5	899.5						
[$C_{10}H_{20}O_5$]	**33100-27-5**	**15-Crown-5**				**899.7**			**943.8**			**−39**
92LIO/BRO		kinetic method										
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	33.9	894.8	884.6	54.0	938.5	2	−41	−39
83MAU	289-80-5	Pyridazine	600	877.1	7.5	898.7						
83MAU	110-86-1	pyridine	600	898.1	−7.9	902.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M -- Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_6H_{13}N$]	**108-91-8**	**c-$C_6H_{11}NH_2$**				**899.6**			**934.4**			**−8**
89TOM/ABB	7664-41-7	NH_3	298	819	75.7	894.7						
87TAF	7664-41-7	NH_3	350	819	80.1	899.2						
83TAF	7664-41-7	NH_3	350	819	80.1	899.2						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	35.1	899.6						
75TAF	7664-41-7	NH_3	350	819	80.1	899.2						
75ARN	7664-41-7	NH_3	350	819	80.1	899.2						
73YAM/KEB	7664-41-7	NH_3	600	819	81.6	901.1						
[$C_5H_{12}N_2O$]	**632-22-4**	**[$(CH_3)_2N]_2C{=}O$**				**899.6**			**930.6**			**5**
87TAF	7664-41-7	NH_3	350	819	81.0	899.4						
86TAF/GAL	7664-41-7	NH_3	350	819	81.1	899.6						
[$C_6H_{11}NO$]	**23135-18-4**	**2-propenamide,N,N-dimethyl-**				**899.4**			**930.3**			**5**
90WOL/GRU	110-86-1	pyridine	320	898.1	0.8	898.9						
90WOL/GRU	75-64-9	t-$C_4H_9NH_2$	320	899.9	0.2	899.9						
[$C_8H_{15}NO$]	**40335-14-6**	**trans-3-Aminobicyclo[2.2.2]octan-2-ol**				**899.2**			**933.1**			**−5**
83HOU/RUF	108-91-8	c-$C_6H_{11}NH_2$	1300	899.6	0.4	899.2						
[$C_{10}H_{14}ClN$]	**2873-89-4**	**4-$ClC_6H_4N(C_2H_5)_2$**				**899.2**			**931.0**			**2**
85LEA/IAC	121-69-7	$C_6H_5N(CH_3)_2$	320	909.2	10.0	899.2						
[$C_6H_8N_2$]	**108-45-2**	**1,3-$C_6H_4(NH_2)_2$**				**899.2**			**929.9**			**5.8**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	51.0	900.5						
78LAU/SAL	7664-41-7	NH_3	600	819	82.4	897.8						
[$C_{10}H_{20}N_2O_4$]	**14486-13-6**	**met-val**				**899.0**			**NE**			**NE**
93GOR/AMS	110-86-1; 75-64-9	C_5H_5N; (t-C_4H_9)NH_2	350			898-900						
[$C_3H_4N_2S$]	**96-50-4**	**2-Aminothiazole**				**898.7**			**930.6**			**2**
87TAF	7664-41-7	NH_3	350	819	80.1	898.7						
[C_4H_5NS]	**3581-87-1**	**2-Methylthiazole**				**898.7**			**930.6**			**2**
87TAF	7664-41-7	NH_3	350	819	80.1	898.6						
[$C_7H_7N_3$]	**13351-73-0**	**1-methylbenzotriazole**				**898.7**			**931.2**			**0**
89TOM/ABB	108-91-8	c-$C_6H_{11}NH_2$	298	899.6	0.8	900.5						
89TOM/ABB	110-86-1	pyridine	298	898.1	−1.3	896.9						
[$C_{15}H_{12}N_2$]	**95935-55-0**	**9,5-metheno-5H,7H-pyrimidol[1,6-a:3,4-a']bisazepine**				**898.7**			**931.1**			**0**
89HOU/FEN	110-86-1	pyridine	313	898.1	0.4	898.6						
[$C_9H_{11}NO$]	**100-10-7**	**4-$CHOC_6H_4N(CH_3)_2$**				**898.3**			**924.8**			**20**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSqub	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R, T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	80.5	898.2						
[$C_8H_{10}FN$]	**403-46-3**	**4-$FC_6H_4N(CH_3)_2$**				**898.3**			**924.8**			**20**
87TAF	7664-41-7	NH_3	350	819	80.5	898.2						
[C_7H_5N]	**2510-22-7**	**4-ethynyl-pyridine**				**898.2**			**930.1**			**2**
97SHE/STE		See Refs.							930.1±4.6			
[C_3H_7N]	**38697-07-3**	**$(CH_3)_2C{=}NH$**				**898.2**			**932.3**			**−5.8**
81ELL/DIX	124-40-3; 75-64-9	$(CH_3)_2NH$; (t-C_4H_9)NH_2				896-900						
[$C_6H_{14}OSi$]	**1833-53-0**	**$CH_2{=}(CH_3)OSi(CH_3)_3$**				**898.2**			**930.6**			**0**
82HEN/WEI	124-40-3; 75-64-9	$(CH_3)_2NH$; t-$C_4H_9NH_2$				896-900						
[$C_9H_{12}O_3$]	**621-23-8**	**1,3,5-$C_6H_3(OCH_3)_3$**				**898.2**			**926.7**			**13**
87TAF	7664-41-7	NH_3	350	819	80.1	898.1						
83TAF2	7664-41-7	NH_3	350	819	80.1	898.1						
[C_5H_5N]	**110-86-1**	**pyridine**				**898.1**			**930**			**2**
97EAS/SMI		theory	298									2.2
95SMI/RAD		theory	298						929.8			
95CHY/SQU	7664-41-7	NH_3	298				853.6	78.7	932.3			
91MAU/SIE	75-31-0	i-$C_3H_7NH_2$	600	889.0	10.9	896.9	923.8	5.9	929.7	−8	7.5	−0.5
91MAU/SIE	75-04-7	$C_2H_5NH_2$	600	878	23.8	899.7	912.0	15.9	927.9	−5.1	13.0	7.9
87TAF	7664-41-7	NH_3	350	819	80.5	899.1						
86TAF/GAL	7664-41-7	NH_3	350	819	80.5	899.1						
86MAU/LIE	110-86-1	pyridine	600	898.1	0	898.1						
85TAF	7664-41-7	NH_3	350	819	81.0	899.6						
83MAU/SIE	110-86-1	pyridine	425	898.1	0	898.1						
83MAU	110-86-1	pyridine	600	898.1	0	898.1						
80MAU/HAM	110-86-1	pyridine	600	898.1	0	898.1						
80MAU	7664-41-7	NH_3	550	819	72.4	889.3						
79MAU	107-10-8	n-$C_3H_7NH_2$	520	883.9	12.6	894.9						
78LAU/SAL	7664-41-7	NH_3	600	819	73.6	890.1						
77COO/KRU		relative order-See Refs.										
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	33.7	898.2						
75TAF	7664-41-7	NH_3	350	819	77.8	896.4						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	31.2	895.7						
75ARN	7664-41-7	NH_3	350	819	77.8	896.4						
72BRI/YAM	7664-41-7	NH_3	600	819	77.8	894.3						
[$C_{10}H_{22}O_5$]	**143-24-8**	**$CH_3O[CH_2CH_2O]_4CH_3$**				**897.8**			**953.8**			**−79**
92LIO/BRO		kinetic method										
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	28.9	897.8	884.6	69.0	953.6	2	−81	−79

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_6H_{18}N_3P$]	**1608-26-0**	**$P(N(CH_3)_2)_3$**				**897.7**			**930.1**			**0**
85BOL/HOU	124-40-3	$(CH_3)_2NH$	323	896.5	1.3	897.7						
[C_5H_5NO]	**109-00-2**	**3-(OH)-pyridine**				**897.7**			**929.5**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−0.5	897.7						
[$C_7H_{12}N_2$]	**52096-24-9**	**n-Butylpyrazole**				**897.3**			**928.8**			**3**
87TAF	7664-41-7	NH_3	350	819	78.7	897.2						
[$C_7H_8N_2O$]	**2835-68-9**	**4-NH_2-$C_6H_4CONH_2$**				**896.9**			**927.9**			**5**
94GRU/CAL	13952-84-6; 110-86-1	2-butylamine; C_5H_5N				896-898						
[$C_9H_{10}FNO$]	**33322-64-4**	**3-F-$C_6H_4CON(CH_3)_2$**				**896.9**			**927.9**			**5**
94GRU/CAL	13952-84-6; 110-86-1	2-butylamine; C_5H_5N				896-898						
[$C_9H_{10}FNO$]	**24167-56-4**	**4-F-$C_6H_4CON(CH_3)_2$**				**896.9**			**927.9**			**5**
94GRU/CAL	13952-84-6; 110-86-1	2-butylamine; C_5H_5N				896-898						
[$C_9H_{10}ClNO$]	**24167-52-0**	**3-Cl-$C_6H_4CON(CH_3)_2$**				**896.9**			**927.9**			**5**
94GRU/CAL	13952-84-6; 110-86-1	2-butylamine; C_5H_5N				896-898						
[$C_9H_{10}ClNO$]	**14062-80-7**	**4-Cl-$C_6H_4CON(CH_3)_2$**				**896.9**			**927.9**			**5**
94GRU/CAL	13952-84-6; 110-86-1	2-butylamine; C_5H_5N				896-898						
[C_2H_7NO]	**141-43-5**	**$NH_2(CH_2)_2OH$**				**896.8**			**930.3**			**−3.3**
80MAU/HAM	124-40-3	$(CH_3)_2NH$	600	896.5	0	896.8	929.5	0.8	930.3	−2	−1.3	−3.3
[$C_5H_8N_2$]	**1072-68-0**	**1,4-Dimethylpyrazole**				**896.8**			**928.4**			**3**
87TAF	7664-41-7	NH_3	350	819	78.3	896.8						
[$C_8H_{17}NO$]	**26153-90-2**	**neo-$C_5H_{11}CON(CH_3)_2$**				**896.7**			**927.7**			**5**
87TAF	7664-41-7	NH_3	350	819	78.3	896.7						
[$C_{10}H_{23}N$]	**2016-57-1**	**n-($C_{10}H_{21}$)NH_2**				**896.5**			**930.4**			**−5**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	0	896.5						
[C_2H_7N]	**124-40-3**	**$(CH_3)_2NH$**				**896.5**			**929.5**			**−2**
97EAS/SMI		theory	298									−1.9
93SZU/MCM	75-64-9	t-$C_4H_9NH_2$	600	899.9	−3.3	895.3	934.1	−3.8	930.4	−6	0.8	−5.2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
93SMI/RAD		theory	298						931.7			
93SMI/RAD		theory	0						925.9			
93SMI/RAD		theory	600						936.4			
91MAU/SIE	110-86-1	pyridine	600	898.1	−4.2	895.2	930	0.8	930.8	2	−7.5	−5.5
91MAU/SIE	75-31-0	i-$C_3H_7NH_2$	600	889.0	7.9	895.1	923.8	5.0	928.8	−8	5.0	−3.0
87TAF	7664-41-7	NH_3	350	819	78.3	897.0						
87BIS/RUH		appearance						955±15				
83TAF	7664-41-7	NH_3	350	819	78.3	897.0						
83LOC/MCI	7664-41-7	NH_3	350	819	76.9	895.7						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	32.2	896.7						
75TAF	7664-41-7	NH_3	350	819	76.9	895.7						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	31.7	896.2						
75ARN	7664-41-7	NH_3	350	819	76.9	895.7						
72HEN/TAA	7664-41-7	NH_3	350	819	76.9	895.7						
72BRI/YAM	7664-41-7	NH_3	600	819	76.6	894.2						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	33.3	897.7						
72ARN/ION	7664-41-7	NH_3	350	819	76.9	895.7						
[$C_8H_{10}ClN$]	**698-69-1**	**4-Cl$C_6H_4N(CH_3)_2$**				**896.4**			**922.9**			**20**
87TAF	7664-41-7	NH_3	350	819	78.7	896.4						
[$C_{10}H_{13}NO_2$]	**7290-99-5**	**3-CH_3O-$C_6H_4CON(CH_3)_2$**				**896.0**			**927.0**			**5**
94GRU/CAL	103-69-5; 108-45-2	$C_6H_5NHC_2H_5$; 1,3-$(NH_2)_2$-C_6H_4				893-899						
[$C_{10}H_{13}NO$]	**6935-65-5**	**3-CH_3-$C_6H_4CON(CH_3)_2$**				**896.0**			**927.0**			**5**
94GRU/CAL	103-69-5; 108-45-2	$C_6H_5NHC_2H_5$; 1,3-$(NH_2)_2$-C_6H_4				893-899						
[$C_{10}H_{13}NO$]	**14062-78-3**	**4-CH_3-$C_6H_4CON(CH_3)_2$**				**896.0**			**927.0**			**5**
94GRU/CAL	103-69-5; 108-45-2	$C_6H_5NHC_2H_5$; 1,3-$(NH_2)_2$-C_6H_4				893-899						
[$C_{10}H_8$]	**275-51-4**	**azulene**				**896**			**925.2**			**11**
91MAU/SIE	110-86-1	pyridine	600	898.1	1.3	896.7	930	−4.2	925.8	2	9.2	11.2
91MAU/SIE	121-69-7	$C_6H_5N(CH_3)_2$	600	909.2	−8.4	898.1	941.1	−18.0	923.1	2	16.3	18.3
91MAU/SIE	75-31-0	i-$C_3H_7NH_2$	600	889.0	10.0	893.3	923.8	0.4	924.2	−8	15.9	7.9
87TAF	7664-41-7	NH_3	350	819	108.5	926.6						
83TAF2	7664-41-7	NH_3	350	819	108.5	926.6						
80MAU	110-86-1	pyridine	550	898.1	0	895.9						
77WOL/ABB	87-85-4	$(CH_3)_6$-C_6	350	836.0	82.8	919.6						
75WOL/HAR	7664-41-7	NH_3	350	819	103.3	921.5						
[$C_{10}H_{17}NO$]	**33701-54-1**	**5-amino-tricyclo[4.4.0.0^{3,8}]decan-4-ol**				**896.0**			**928.4**			**0**
83HOU/RUF	110-86-1	pyridine	300	898.1	−2.1	896.1						
83HOU/RUF	108-91-8	c-$C_6H_{11}NH_2$	300	899.6	−3.8	895.8						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_7H_{15}N$]	**3218-02-8**	**c-$C_6H_{11}CH_2NH_2$**				**895.8**			**926.6**			**5.6**
87TAF	7664-41-7	NH_3	350	819	77.3	895.7						
[$C_4H_{11}N$]	**13952-84-6**	**sec-$C_4H_9NH_2$**				**895.7**			**929.7**			**−5**
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	31.2	895.7						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	29.3	893.8						
[C_8H_9N]	**696-18-4**	**Aziridine, 1-phenyl**				**895.7**			**926.5**			**5.6**
88CAU/CER		see Refs.				895.7						
[$C_8H_{12}N_2$]	**90196-91-1**	**1-azabicyclo[2.2.2]-octane, 2-cyano**				**895.6**			**926.4**			**5.6**
86HEI/HON	110-86-1	pyridine	313	898.1	−2.5	895.6						
86HEI/HON	108-91-8	c-$C_6H_{11}NH_2$	313	899.6	−3.8	895.6						
[$C_{12}H_{21}NO$]	**73495-63-3**	**3-Amino-tricyclo[7.3.0.0^{4,8}]dodecan-2-ol**				**895.6**			**928.0**			**0**
83HOU/RUF	110-86-1	pyridine	300	898.1	−2.1	896.1						
83HOU/RUF	108-91-8	c-$C_6H_{11}NH_2$	300	899.6	−3.8	895.8						
83HOU/RUF	13952-84-6	sec-$C_4H_9NH_2$	300	895.7	0.8	894.9						
[$C_5H_8N_2$]	**2820-37-3**	**3(5),4-dimethylpyrazole**				**895.4**			**927.3**			**2**
92ABB/CAB	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	2.2	895.9						
92ABB/CAB	110-86-1	pyridine	333	898.1	−3.3	894.9						
[$C_7H_{15}NO$]	**24331-71-3**	**t-$C_4H_9CON(CH_3)_2$**				**895.2**			**927.1**			**2**
97HOM/HER	110-86-1	pyridine	333	898.1	−2.4	895.8						
97HOM/HER	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	1.0	894.7						
[$C_{11}H_{24}O_4$]	**66226-75-3**	**$CH_3O[CH_2CH_2CH_2O]_3CH_3$**				**895.1**			**NE**			**NE**
92LIO/BRO	294-93-9; 33100-27-5	12-crown-4; 15-Crown-5				891-900						
[$C_3H_8N_2S$]	**534-13-4**	**SC(NHCH$_3$)$_2$**				**895.1**			**926.0**			**5**
93ABB/MO	75-64-9	t-$C_4H_9NH_2$	333	899.9	−3.0	896.5						
93ABB/MO	110-58-7	n-$C_5H_{11}NH_2$	333	889.5	4.4	893.6						
[$C_8H_{19}N$]	**111-86-4**	**n-(C_8H_{17})NH_2**				**895.0**			**928.9**			**−5**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	−1.5	895.0						
[C_6H_7NO]	**694-85-9**	**1-Methyl-2-pyridinone**				**894.8**			**925.8**			**5**
87TAF	7664-41-7	NH_3	350	819	76.4	894.9						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	31.7	896.2						
76COO/KAT	110-86-1	pyridine	350	898.1	−4.6	893.4						
[$C_7H_7NO_2$]	**2459-09-8**	**Pyridine-4-carboxylic acid, methyl ester**				**894.7**			**926.6**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−0.5	897.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	73.2	891.8						
[$C_2H_8N_2$]	**57-14-7**	**$(CH_3)_2NNH_2$**				**894.7**			**927.1**			**0**
87TAF	7664-41-7	NH_3	350	819	77.3	896.0						
84MAU/NEL	110-86-1	pyridine	600	898.1	−5.4	893.3						
83TAF2	7664-41-7	NH_3	350	819	76.9	895.6						
75TAF	7664-41-7	NH_3	350	819	74.1	892.8						
75ARN	7664-41-7	NH_3	350	819	74.1	892.8						
[C_3H_9NO]	**109-85-3**	**$CH_3OCH_2CH_2NH_2$**				**894.6**			**928.6**			**−5.1**
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	10.7	894.6						
[$C_6H_{11}NO$]	**4030-18-6**	**Acetylpyrrolidine**				**894.4**			**925.4**			**5**
87TAF	7664-41-7	NH_3	350	819	76.0	894.4						
[$C_6H_{13}NO$]	**685-91-6**	**$CH_3CON(C_2H_5)_2$**				**894.4**			**925.4**			**5**
87TAF	7664-41-7	NH_3	350	819	76.0	894.4						
[C_9H_9N]	**6921-29-5**	**$(HCCCH_2)_3N$**				**894.4**			**925.2**			**5.6**
87TAF	7664-41-7	NH_3	350	819	76.0	894.4						
83TAF2	7664-41-7	NH_3	350	819	76.0	894.4						
75TAF	7664-41-7	NH_3	350	819	73.2	891.6						
75ARN	7664-41-7	NH_3	350	819	73.2	891.6						
[C_4H_9NS]	**631-67-4**	**$CH_3C(S)N(CH_3)_2$**				**894.4**			**925.3**			**5**
93ABB/MO	110-86-1	pyridine	333	898.1	−2.0	896.1						
93ABB/MO	6921-29-5	$(HCCCH_2)_3N$	333	894.4	0.9	895.3						
93ABB/MO	110-58-7	n-$C_5H_{11}NH_2$	333	889.5	2.5	891.7						
[$C_{10}H_{13}NO_2$]	**1202-25-1**	**4-$(CH_3)_2NC_6H_4COOCH_3$**				**894.1**			**920.6**			**20**
87TAF	7664-41-7	NH_3	350	819	76.4	894.1						
[$C_9H_{13}NO$]	**15799-79-8**	**3-Methoxy-N,N-dimethylbenzenamine**				**894.1**			**920.6**			**20**
87TAF	7664-41-7	NH_3	350	819	76.4	894.1						
[C_7H_6O]	**502-87-4**	**4-Methylene-2,5-cyclohexadiene-1-one**				**894.0**			**923.8**			**9**
77DIT/NIB	7664-41-7	NH_3	~300	819	75	894			See Refs.			
[$C_5H_{13}N$]	**5813-64-9**	**neo-$C_5H_{11}NH_2$**				**894.0**			**928.3**			**−6**
87TAF	7664-41-7	NH_3	350	819	74.6	893.6						
83TAF2	7664-41-7	NH_3	350	819	73.7	892.7						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	29.8	894.3						
[$C_7H_8N_4$]	**27258-04-4**	**Di(1-pyrazolyl)methane**				**893.9**			**924.7**			**5.8**
87TAF	7664-41-7	NH_3	350	819	75.5	893.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_7H_7NO_2$]	**93-60-7**	**methylnicotinate**				**893.8**			**925.6**			**2**
91BER/DEC	107-10-8	n-$C_3H_7NH_2$	338	883.9	9.8	893.5						
91BER/DEC	110-86-1	pyridine	338	898.1	−4.9	893.3						
91BER/DEC	110-91-8	Morpholine	338	891.2	1.0	892.1						
91AUE/WEB	110-86-1	pyridine	300	898.1	0.5	897.7						
87TAF	7664-41-7	NH_3	350	819	73.7	892.3						
[$C_{14}H_{20}N_2O_4$]	**17355-09-8**	**tyr-val**				**893.6**			**NE**			**NE**
93GOR/AMS	75-31-0; 110-86-1	(i-C_3H_7)NH_2; C_5H_5N	350			889-898						
[$C_{14}H_{20}N_2O_4$]	**3918-90-9**	**phe-val**				**893.6**			**NE**			**NE**
93GOR/AMS	75-31-0; 110-86-1	(i-C_3H_7)NH_2; C_5H_5N	350			889-898						
[$C_6H_{15}N$]	**111-26-2**	**n-$C_6H_{13}NH_2$**				**893.5**			**927.5**			**−5**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	−2.9	893.5						
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	4.9	888.8						
[$C_8H_{12}N_2O_2$]	**5744-40-1**	**1,3-dimethyl-5-ethoxycarbonylpyrazole**				**893.1**			**924.9**			**2**
92ABB/CAB	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	0.2	893.9						
92ABB/CAB	109-73-9	n-$C_4H_9NH_2$	333	886.6	4.8	891.1						
92ABB/CAB	75-64-9	t-$C_4H_9NH_2$	333	899.9	−5.5	894.1						
[$C_8H_{11}N$]	**103-69-5**	**$C_6H_5NHC_2H_5$**				**892.9**			**924.8**			**2**
81MCL/CAM	13952-84-6	sec-$C_4H_9NH_2$	425				929.7	−4.6	925.1			
81MCL/CAM	111-26-2	n-$C_6H_{13}NH_2$	425				927.5	−2.9	924.5			
78LAU/SAL	7664-41-7	NH_3	600	819	77.0	893.5						
73YAM/KEB	7664-41-7	NH_3	600	819	77.0	893.5						
[C_5H_5NO]	**694-59-7**	**pyridine-1-oxide**				**892.9**			**923.6**			**5.8**
92MIS/TER	7664-41-7	NH_3	343	819	72.4	890.9						
79MAU	107-10-8	n-$C_3H_7NH_2$	550	883.9	13.4	894.6						
[$C_4H_9O_3P$]	**31131-06-9**	**2-Methoxy-1,3,2-dioxa-phosphorinane**				**892.8**			**925.3**			**0**
80HOD/HOU	110-86-1	pyridine	320	898.1	5.4	892.7						
[$C_4H_8Se_2$]	**99030-02-1**	**CH_2=C($SeCH_3$)$_2$**				**892.6**			**921.5**			**12**
89OSA/DEL	110-58-7; 13952-84-6	n-$C_5H_{11}NH_2$, $CH_3CH(NH_2)C_2H_5$	313			890-896						
[$C_6H_{11}NO$]	**931-20-4**	**c-C_5H_8N(2-O)1-CH_3**				**892.6**			**924.4**			**2**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	−3.9	892.6						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	28.3	892.8						
76COO/KAT	7664-41-7	NH_3	350	819	71.4	890.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_8H_{18}O_4$]	**112-49-2**	**$CH_3O[CH_2CH_2O]_3CH_3$**				**892.4**			**946.6**			**−73**
92LIO/BRO		kinetic method-relative order only										
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	20.9	888.6	884.6	56.1	940.6	2	−71	−69
83MAU	289-80-5	Pyridazine	600	877.1	−6.3	895.1	907.2	38.1	945.3	7.8	−74	−66.2
83MAU	372-47-4	3-F-pyridine	600	870.1	0.4	893.0	902.0	51.0	953.0	2	−85	−83
[C_3H_7N]	**75-55-8**	**2-Methylaziridine**				**892.1**			**925.1**			**−2**
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	−4.4	892.1						
[$C_9H_{11}NO_3$]	**60-18-4**	**L-tyrosine**				892.1			**926**			**−5**
93LI/HAR		kinetic method							926			−3.7
92GOR/SPE	75-31-0; 110-86-1	$(i\text{-}C_3H_7)NH_2$; pyridine	350			889-898						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	86.5	905.4						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	86.5	905.4						
[$C_6H_{10}F_3N$]	**657-36-3**	**4-Trifluoromethylpiperidine**				**892.0**			**925.1**			**−2**
87TAF	7664-41-7	NH_3	350	819	73.2	892						
[Sc]	**7440-20-2**	**Sc**				**892.0**			**914**			**35**
89ELK/SUN		See Refs.							914±9			
84TOL/BEA		See Refs.							907.5			
[$C_6H_{13}NO$]	**21678-37-5**	**$i\text{-}C_3H_7CON(CH_3)_2$**				**891.8**			**923.7**			**2**
97HOM/HER	107-10-8	$n\text{-}C_3H_7NH_2$	333	883.9	7.8	891.4						
97HOM/HER	5813-64-9	$neo\text{-}C_5H_{11}NH_2$	333	894.0	−1.5	892.2						
[C_5H_9NO]	**872-50-4**	**1-Methyl-2-pyrrolidinone**				**891.6**			**923.5**			**2**
87TAF	7664-41-7	NH_3	350	819	71.8	890.4						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	28.3	892.8						
[$C_4H_8N_2O_3$]	**70-47-3**	**L-Asparagine**				**891.5**			**929**			**−17**
93LI/HAR		kinetic method-See Refs.							929			−17
92GOR/SPE	75-31-0; 110-86-1	$(i\text{-}C_3H_7)NH_2$; pyridine	350			889-898						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	75.1	894.6						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	75.1	894.6						
[$C_3H_6N_2S$]	**96-45-7**	**2-imidazolinethione**				**891.2**			**921.9**			**5.8**
93ABB/MO	75-64-9	$t\text{-}C_4H_9NH_2$	333	899.9	−7.2	892.3						
93ABB/MO	110-58-7	$n\text{-}C_5H_{11}NH_2$	333	889.5	−0.1	889.1						
93ABB/MO	107-10-8	$n\text{-}C_3H_7NH_2$	333	883.9	8.7	892.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_4H_9NO]	**110-91-8**	**Morpholine**				**891.2**			**924.3**			**−2**
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	7.3	891.2						
[C_7H_6O]	**539-80-0**	**2,4,6-Cycloheptatriene-1-one**				**891.0**			**920.8**			**9**
83CAS/FRE	107-10-8; 110-86-1	$C_4H_7NH_2$; pyridine				884-898						
77DEI/NIB	7664-41-7	NH_3	300	819	92	911						
[$C_7H_{12}N_2$]	**15802-80-9**	**3(5)-t-burtylpyrazole**				**891.0**			**922.8**			**2**
92ABB/CAB	109-73-9	n-$C_4H_9NH_2$	333	886.6	4.1	890.4						
92ABB/CAB	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	−2.1	891.6						
[$C_4H_{11}N$]	**78-81-9**	**i-$C_4H_9NH_2$**				**890.8**			**924.8**			**−5**
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	26.4	890.8						
75ARN	7664-41-7	NH_3	350	819	78.3	897.2						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	23.4	887.9						
[$C_6H_{13}NO$]	**760-79-2**	**n-$C_3H_7CON(CH_3)_2$**				**890.8**			**921.7**			**5**
87TAF	7664-41-7	NH_3	350	819	72.3	890.7						
[$C_8H_{16}O_4$]	**294-93-9**	**12-crown-4**				**890.5**			**927.2**			**−14**
92LIO/BRO		kinetic method										
83HLA/BLA	372-48-5	2-F-pyridine	500	852.7	31.4	887.3	884.6	45.6	930.2	2	−29	−27
83MAU	110-86-1	pyridine	600	898.1	−11.5	891.4	930	−5.0	925.0	2	−11	−9
83MAU	289-80-5	Pyridazine	600	877.1	6.0	889.7	907.2	13.8	921.0	7.8	−13	−5.2
[$C_8H_8N_2$]	**13436-48-1**	**1-methylindazole**				**890.5**			**922.4**			**2**
88CAT/CLA	657-36-3	4-Trifluormethylpiperidine	~300	892.0	−1.3	890.8						
88CAT/CLA	1628-89-3	2-(CH_3O)-pyridine	~300	902.8	−10.5	892.3						
88CAT/CLA	109-73-9	n-$C_4H_9NH_2$	~300	886.6	3.3	890.0						
87TAF	7664-41-7	NH_3	350	819	71.4	890.0						
84FLA/MAQ		kinetic method				~891.2						
[C_7H_9N]	**100-61-8**	**$C_6H_5NHCH_3$**				**890.1**			**916.6**			**20**
78LAU/SAL	7664-41-7	NH_3		819	63.2	890.1						
72BRI/YAM	7664-41-7	NH_3		819	63.2	890.1						
[$C_9H_{14}O_2$]	**4683-45-8**	**3-Methoxy-5,5-dimehtylcyclohex-2-enone**				**890.1**			**922.6**			**0**
87TAF	7664-41-7	NH_3	350	819	71.4	890.1						
[$C_3H_5N_3$]	**1820-80-0**	**3(5)-aminopyrazole**				**889.6**			**921.5**			**2**
92ABB/CAB	5813-64-9	neo-$C_5H_{11}NH_2$	333	894.0	−3.4	890.4						
92ABB/CAB	109-73-9	n-$C_4H_9NH_2$	333	886.6	2.6	888.9						
[$C_5H_{13}N$]	**110-58-7**	**n-$C_5H_{11}NH_2$**				**889.5**			**923.5**			**−5**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	3.3	887.2						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	27.3	891.8						
77COO/KRU		relative order-See Refs.										
[C_4H_9NO]	**1187-58-2**	**$C_2H_5CONHCH_3$**				**889.4**			**920.4**			**5**
87TAF	7664-41-7	NH_3	350	819	70.9	889.4						
[C_6H_6ClN]	**3678-62-4**	**2-Cl-4-(CH_3)-pyridine**				**889.4**			**921.2**			**2**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	24.9	889.4						
[$C_7H_{17}N$]	**111-68-2**	**n-$C_7H_{15}NH_2$**				**889.3**			**923.2**			**−5**
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	5.4	889.3						
[C_3H_9N]	**75-31-0**	**i-$C_3H_7NH_2$**				**889.0**			**923.8**			**−8**
91MAU/SIE	75-04-7	$C_2H_5NH_2$	600	878	13.0	891.8	912.0	12.1	924.1	−5.1	1.7	−3.4
91MAU/SIE	288-47-1	thiazole	600	872.1			904	28.0	932.0			
91MAU/SIE	372-47-4	3-F-pyridine	600	870.1	18.0	891.1	902.0	25.9	927.9	2	−13.4	−11.4
87TAF	7664-41-7	NH_3	350	819	70.5	889.6						
86MAU/LIE	110-86-1	pyridine	600	898.1	−14.4	886.7						
83TAF	7664-41-7	NH_3	350	819	70.5	889.6						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	25.9	890.4						
75TAF	7664-41-7	NH_3	350	819	70.5	889.6						
72HEN/TAA	7664-41-7	NH_3	350	819	70.5	889.6						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	23.9	888.4						
72ARN/JON	7664-41-7	NH_3	350	819	70.5	889.6						
[$C_9H_{11}NO_2$]	**63-91-2**	**L-phenylalanine**				**888.9**			**922.9**			**−5**
93LI/HAR		kinetic method							915			
92GOR/SPE	75-31-0; 110-86-1	(i-C_3H_7)NH_2; pyridine	350			889-898						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	76.4	895.4						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	76.4	895.4						
79MAU/HUN	109-73-9	n-$C_4H_9NH_2$	570	886.6	−3.8	882.1						
79MAU/HUN	62-53-3	$C_6H_5NH_2$	500	850.6	25.9	877.9						
[$C_3H_7NO_2$]	**107-97-1**	**Sarcosine**				**888.7**			**921.2**			**0**
87TAF	7664-41-7	NH_3	350	819	70.0	888.7						
83LOC/MCI	7664-41-7	NH_3	350	819	70.0	888.7						
[$C_4H_9NO_3$]	**72-19-5**	**L-threonine**				**888.5**			**922.5**			**−5**
93LI/HAR		kinetic method							911			
92GOR/SPE	110-86-1; 75-64-9	pyridine; (t-C_4H_9)NH_2	350			898-900						
90ISA/OMO		kinetic method-relative order										

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	69.6	888.5						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	69.6	888.5						
[$C_5H_4N_4$]	**120-73-0**	**Purine**				**888.2**			**920.1**			**2**
79MAU	107-10-8	n-$C_3H_7NH_2$	515	883.9	5.9	888.2						
75WIL/MCC	74-89-5; 124-40-3	CH_3NH_2; $(CH_3)_2NH$				864-896						
[$C_6H_{11}NO_3$]	**26629-33-4**	**$CH_3CONHCH(CH_3)COOCH_3$**				**888.0**			**938.6**			**−61**
83MAU	372-47-4	3-F-pyridine	600	870.1	0.8	889.8	902.0	40.2	942.1	2	−65.7	−63.7
83MAU	372-48-5	2-F-pyridine	600	852.7	14.6	886.2	884.6	51.5	936.0	2	−61.5	59.5
[$C_9H_{10}F_3NS$]	**#585**	**3-$(SCF_3)C_6H_4N(CH_3)_2$**				**887.7**			**914.2**			**20**
87TAF	7664-41-7	NH_3	350	819	70.0	887.7						
[C_4H_3NO]	**145355-49-3**	**CH_3NCCCO**				**887.5**			**920**			**0**
91FLA/HAV		theory							920			
[C_6H_9N]	**625-84-3**	**2,5-Dimethylpyrrole**				**887.1**			**918.7**			**3**
86MAU/LIE	110-86-1	pyridine	600	898.1	−10.5	887.4						
86MAU/LIE	372-47-4	3-F-pyridine	600	870.1	16.7	886.5						
[C_3H_8FN]	**462-41-9**	**$FCH_2CH_2CH_2NH_2$**				**886.9**			**920.9**			**−5**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	22.5	886.9						
[$C_{11}H_{14}N_2$]	**13012-16-3**	**N,N,2,6-Tetramethyl-4-cyanoaniline**				**886.8**			**913.3**			20
87TAF	7664-41-7	NH_3	350	819	69.1	886.8						
[$C_4H_{11}N$]	**109-73-9**	**n-$C_4H_9NH_2$**				**886.6**			**921.5**			−8
87TAF	7664-41-7	NH_3	350	819	66.8	885.9						
83TAF	7664-41-7	NH_3	350	819	66.8	885.9						
83LOC/MCI	7664-41-7	NH_3	350	819	67.7	886.8						
79MAU	107-10-8	n-$C_3H_7NH_2$	515	883.9	2.1	886.6						
77COO/KRU		relative order-See Refs.										
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	23.9	888.4						
75TAF	7664-41-7	NH_3	350	819	66.4	885.4						
75ARN	7664-41-7	NH_3	350	819	66.4	885.4						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	22.0	886.5						
[Mg_2]	**29904-79-8**	**Mg_2**				**886.5**			**919**			0
77PO/POR		See Refs.							919±30			
[$C_6H_{12}N_2O_4$]	**6620-95-7**	**ser-ser**				**886.4**			**NE**			NE

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94MCK/BEL	107-10-8; 75-31-0	n-$C_3H_7NH_2$; i-$C_3H_7NH_2$				884-889						
[$C_5H_{10}N_2O_4$]	**7361-43-5**	**ser-gly**				**886.4**			**NE**			NE
94MCK/BEL	107-10-8; 75-31-0	n-$C_3H_7NH_2$; i-$C_3H_7NH_2$				884-889						
[$C_6H_6N_2O$]	**98-92-0**	**nicotinamide**				**886.4**			**918.3**			2
91BER/DEC	78-81-9	i-$C_4H_9NH_2$	338	890.8	−0.8	889.8						
91BER/DEC	127-19-5	Dimethylacetamide	338	877.0	5.8	883.0						
[$C_5H_{10}N_2O$]	**80-73-9**	**1,3,-Dimethyl-2-imidazolidinone**				**886.0**			**918.4**			0
87TAF	7664-41-7	NH_3	350	819	67.3	886.0						
[$C_{10}H_{14}N_2O_2$]	**24558-36-9**	**N,N,2,6-Tetramethyl-4-nitroaniline**				**886.0**			**918.4**			0
87TAF	7664-41-7	NH_3	350	819	67.3	886.0						
[$C_5H_9NO_2$]	**147-85-3**	**L-proline**				**886.0**			**920.5**			−7
96EWI/ZHA	110-86-1; 108-91-8	pyridine; c-$C_6H_{11}NH_2$				898-900						
93LI/HAR		kinetic method-See Refs.							920.5			−7
92GOR/SPE	75-64-9; 75-50-3	(t-C_4H_9)NH_2; $(CH_3)_3N$	350			900-918						
90ISA/OMO		kinetic method-relative order										
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	92.0	911.0						
79MAU/HUN	75-64-9	t-$C_4H_9NH_2$	570	899.9	−0.4	899.7						
79MAU/HUN	109-73-9	n-$C_4H_9NH_2$	570	886.6	10.5	896.8						
73YAM/KEB	7664-41-7	NH_3	600	819	46.0	865.2						
[C_5H_4BrN]	**1120-87-2**	**4-Br-pyridine**				**886.0**			**917.8**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−12.2	885.9						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	21.5	886.0						
[$C_6H_{10}O_3$]	**22157-30-8**	**$CH_3C(OCH_3)$=$CHCOOCH_3$**				**885.8**			**916.8**			**5**
92MOR/MAR	109-73-9	n-$C_4H_9NH_2$	338	886.6	−1.2	885.0						
92MOR/MAR	107-10-8	n-$C_3H_7NH_2$	338	883.9	3.1	886.7						
[C_6H_6ClNO]	**17228-63-6**	**6-Chloro-1-methyl-2(1H)pyridinone**				**885.6**			**918.5**			**−1.9**
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	21.0	885.5						
[$C_8H_{12}O$]	**10599-58-3**	**2,3,4,5-tetramethylfuran**				**884.8**			**915.5**			**5.8**
85HOU/ROL	107-10-8	n-$C_3H_7NH_2$	313	883.9	0.4	884.2						
85HOU/ROL	109-73-9	n-$C_4H_9NH_2$	313	886.6	−1.7	884.8						
85HOU/ROL	75-31-0	i-$C_3H_7NH_2$	313	889.0	−3.3	885.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_7H_7NO]	**350-03-8**	**3-(CH_3CO)-pyridine**				**884.3**			**916.2**			**2**
91BER/DEC	109-73-9	n-$C_4H_9NH_2$	338	886.6	1.0	887.2						
91BER/DEC	127-19-5	Dimethylacetamide	338	877.0	6.8	883.9						
87TAF	7664-41-7	NH_3	350	819	63.2	881.7						
83TAF2	7664-41-7	NH_3	350	819	63.2	881.7						
[C_5H_4ClN]	**626-61-9**	**4-Cl-pyridine**				**884.2**			**916.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−12.7	885.5						
87TAF	7664-41-7	NH_3	350	819	65.0	883.6						
83TAF	7664-41-7	NH_3	350	819	65.9	884.5						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	21.0	885.5						
75TAF	7664-41-7	NH_3	350	819	64.5	883.1						
75ARN	7664-41-7	NH_3	350	819	64.5	883.1						
[C_3H_9N]	**107-10-8**	**n-$C_3H_7NH_2$**				**883.9**			**917.8**			**−5**
87TAF	7664-41-7	NH_3	350	819	64.5	883.5						
83TAF	7664-41-7	NH_3	350	819	64.5	883.5						
83LOC/MCI	7664-41-7	NH_3	350	819	65.9	884.8						
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	0	883.9						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	21.5	886.0						
75TAF	7664-41-7	NH_3	350	819	63.6	882.5						
75ARN	7664-41-7	NH_3	350	819	63.6	882.5						
73AUE/WEB	107-10-8	n-$C_3H_7NH_2$	298	883.9	0	883.9						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	19.0	883.5						
[C_4H_9N]	**2878-14-0**	**CH_2=C(CH_3)CH_2NH_2**				**883.6**			**917.5**			**−5**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	19.0	883.5						
[$C_{11}H_{22}N_2O_3$]	**3989-97-7**	**val-leu**				**883.6**			**NE**			**NE**
93GOR/AMS	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
[$C_{11}H_{22}N_2O_3$]	**13588-95-9**	**leu-val**				**883.5**			**NE**			**NE**
93GOR/AMS	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
[$C_8H_{16}N_2O_3$]	**27493-61-4**	**val-ala**				**883.5**			**NE**			**NE**
93GOR/AMS	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
[$C_6H_{13}NO_2$]	**73-32-5**	**L-isoleucine**				**883.6**			**917.4**			**−5**
93LI/HAR		kinetic method							912			
92GOR/SPE	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	71.4	890.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	71.4	890.3						
[$C_{10}H_{20}N_2O_3$]	**3918-94-3**	**val-val**				**883.5**			**NE**			**NE**
93GOR/AMS	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
[C_7H_7NO]	**1122-54-9**	**1-(4-Pyridinyl)-ethanone**				**882.9**			**914.7**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	14.6	883.5						
87TAF	7664-41-7	NH_3	350	819	63.2	881.7						
83TAF2	7664-41-7	NH_3	350	819	64.1	882.6						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	19.0	883.5						
[$C_{21}H_{30}S$]	**73509-04-03**	**(1-adamantyl)$_2$CS**				**882.4**			**912.1**			**9**
93ABB/MO	107-10-8	n-$C_3H_7NH_2$	333	883.9	−1.1	882.3						
93ABB/MO	107-11-9	H_2C=$CHCH_2NH_2$	333	875.5	7.4	882.4						
[$C_9H_8N_2$]	**2458-26-6**	**3(5)-phenylpyrazole**				**882.3**			**914.2**			**2**
92ABB/CAB	109-73-9	n-$C_4H_9NH_2$	333	886.6	−4.1	882.2						
92ABB/CAB	107-10-8	n-$C_3H_7NH_2$	333	883.9	−1.3	882.4						
[$C_2H_6N_2O$]	**598-41-4**	**$H_2NCH_2CONH_2$ (glycinamide)**				**882.3**			**NE**			**NE**
96KIN/RID	75-04-7; 109-73-9	$C_2H_5NH_2$; n-$C_4H_9NH_2$				878-887						
[$C_4H_{11}NO$]	**3710-84-7**	**$(C_2H_5)_2NOH$**				**882.2**			**914.7**			**0**
83BAR/BAS	107-10-8	n-$C_3H_7NH_2$	300	883.9	−1.7	882.2						
[$C_{10}H_{12}O$]	**1712-69-2**	**4-$CH_3OC_6H_4C(CH_3)$=CH_2**				**882.2**			**911.1**			**12**
87TAF	7664-41-7	NH_3	350	819	64.1	882.1						
83TAF2	7664-41-7	NH_3	350	819	64.1	882.1						
[$C_4H_8Cl_3N$]	**36726-94-0**	**$CCl_3CH_2N(CH_3)_2$**				**882.0**			**912.8**			**5.6**
87TAF	7664-41-7	NH_3	350	819	63.6	882.0						
[C_8H_7N]	**14235-81-5**	**4-H_2N-C_6H_4-CCH**				**882.0**			**912.7**			**5.8**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	80.8	882.0						
[$C_4H_8N_2O_3$]	**556-50-3**	**diglycine**				**882**			**NE**			**NE**
93ZHA/ZIM	107-11-9; 100-46-9	$CH_2CHCH_2NH_2$; $C_6H_5CH_2NH_2$	300			876-879						
93WU/LEB	107-11-9; 127-19-5	CH_2=$CHCH_2NH_2$; $CH_3CON(CH_3)_2$	300			876-877						
92WU/FEN2		kinetic method				890						
	593-67-9; 75-04-7	CH_3=$CHNH_2$; $C_2H_5NH_2$				866-878						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_9H_{10}F_3N$]	**329-00-0**	**3-$CF_3C_6H_4N(CH_3)_2$**				**881.8**			**908.3**			**20**
87TAF	7664-41-7	NH_3	350	819	64.1	881.7						
[$C_{10}H_{14}N_2O_4$]	**100852-80-0**	**1-methyl-3,5-diethoxycarbonylpyrazole**				**881.5**			**913.4**			**2**
92ABB/CAB	1122-54-9	1-(4-Pyridinyl) ethanone	333	882.9	−0.8	882.1						
92ABB/CAB	289-80-5	Pyridazine	333	877.1	3.9	881.2						
[C_5H_4FN]	**694-52-0**	**4-F-pyridine**				**881.2**			**913.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−15.6	882.5						
87TAF	7664-41-7	NH_3	350	819	61.3	879.9						
81TAA/SUM	7664-41-7	NH_3	320	819	56.9	875.7						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	16.6	881.1						
75TAF	7664-41-7	NH_3	350	819	62.2	880.8						
[C_7H_9NO]	**536-90-3**	**3-$CH_3OC_6H_4NH_2$**				**881.1**			**913.0**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	30.5	881.1						
[$C_5H_{10}N_2O_4$]	**687-63-8**	**gly-ser**				**880.9**			**NE**			**NE**
94MCK/BEL	75-04-7; 107-10-8	$C_2H_5NH_2$; n-$C_3H_7NH_2$				878-884						
[$C_{11}H_{17}NO$]	**5511-18-2**	**1-adamantyl-$CONH_2$**				**880.9**			**912.8**			**2**
97HOM/HER	289-80-5	Pyridazine	333	877.1	3.8	881.2						
97HOM/HER	107-10-8	n-$C_3H_7NH_2$	333	883.9	−2.9	880.8						
[$C_3H_7NO_3$]	**56-45-1**	**L-Serine**				**880.7**			**914.6**			**−5**
93LI/HAR		kinetic method							904			
92GOR/SPE	74-89-5; 372-47-4	CH_3NH_2; 3-F-pyridine	350			864-870						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	61.3	880.3						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	61.3	880.3						
	108-44-1; 372-47-4	3-CH_3-aniline; 3-F-pyridine				864-870						
[$C_6H_{13}NO_2$]	**61-90-5**	**L-leucine**				**880.6**			**914.6**			**−5**
93LI/HAR		kinetic method							909			
92GOR/SPE	75-04-7; 75-31-0	$C_2H_5NH_2$; (i-C_3H_7)NH_2	350			878-889						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	67.3	886.2						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	67.3	886.2						
79MAU/HUN	109-73-9	n-$C_4H_9NH_2$	570	886.6	−4.6	881.2						
79MAU/HUN	75-04-7	$C_2H_5NH_2$	520	878	−0.4	877.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ref/Squib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
79MAU/HUN	62-53-3	$C_6H_5NH_2$	500	850.6	25.1	877.1						
[$C_7H_7NO_2$]	**14188-94-4**	**1-(3-pyridinyl-1-oxide)ethanone**				**880.6**			**913.1**			**0**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	−12.6	880.6						
[$C_6H_{11}NO$]	**6976-91-6**	**2-propenamide, N,N,2-trimethyl-**				**880.6**			**911.5**			**5**
90WOL/GRU	100-46-9	$C_6H_5CH_2NH_2$	320	879.4	1.4	880.6						
[$C_6H_{14}O_2$]	**13179-96-9**	**$CH_3O(CH_2)_4OCH_3$**				**880.6**			**931.5**			**−62**
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	15.1	880.6	884.6	46.4	931.0	2	−64	−62
[FeO]	**1345-25-1**	**FeO**				**880.5**			**907**			**20**
84CAS/FRE	107-10-8; 110-86-1	n-$C_3H_7NH_2$; pyridine				884-898						
80MUR		See Refs.							907			
[$C_5H_4N_4O$]	**68-94-0**	**Hypoxanthine**				**880.5**			**912.3**			**2**
75WIL/MCC	74-89-5; 124-40-3	CH_3NH_2; $(CH_3)_2NH$				864-896						
[$C_4H_4N_2S_2$]	**2001-93-6**	**Dithiouracil**				**880.5**			**911.4**			**5**
75WIL/MCC	74-89-5; 124-40-3	CH_3NH_2; $(CH_3)_2NH$				864-896						
[$C_4H_6N_2$]	**930-36-9**	**1-methylpyrazole**				**880.1**			**912.0**			**2**
88CAT/CLA	109-73-9	n-$C_4H_9NH_2$	300	886.6	−6.3	880.4						
88CAT/CLA	75-04-7	$C_2H_5NH_2$	300	878	2.9	880.9						
87TAF	7664-41-7	NH_3	350	819	60.4	879.0						
[$C_5H_{11}NOS$]	**#638**	**$C_2H_5OC(S)N(CH_3)_2$**				**880.0**			**911.0**			*5*
93ABB/MO	107-10-8	n-$C_3H_7NH_2$	333	883.9	−3.4	880.1						
93ABB/MO	289-80-5	Pyridazine	333	877.1	2.9	880.1						
[C_3H_9OP]	**676-96-0**	**$OP(CH_3)_3$**				**880.0**			**909.7**			**9.1**
87TAF	7664-41-7	NH_3	350	819	60.9	879.1						
84BOL/HOU	107-10-8	n-$C_3H_7NH_2$	~323	883.9	−2.5	881.1						
84BOL/HOU	75-04-7	$C_2H_5NH_2$	~323	878	2.1	879.8						
[C_3H_5N]	**18295-52-8**	**vinylimine**				**879.7**			**912.1**			**0**
95BOU/SAL	107-11-9; 107-10-8	CH_2=$CHNH_2$; n-$C_3H_7NH_2$				876-884						
[$C_6H_{15}O_4P$]	**78-40-0**	**$OP(OC_2H_5)_3$**				**879.6**			**909.3**			**9.1**
87TAF	7664-41-7	NH_3	350	819	60.9	879.1						
84BOL/HOU	75-04-7	$C_2H_5NH_2$	~323	878	0.4	878.1						
84BOL/HOU	107-10-8	n-$C_3H_7NH_2$	~323	883.9	−2.1	881.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
80HOD/MCD	75-04-7; 621-23-8	$C_2H_5NH_2$; 1,3,5-$(CH_3O)_3C_6H_3$	300			878-898						
[$C_7H_{16}O_2$]	**111-89-7**	**$CH_3O(CH_2)_5OCH_3$**				**879.5**			**931.3**			**−6.5**
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	13.4	879.5	884.6	46.4	931.0	2	−67	−65
[C_7H_7N]	**16118-22-2**	**$C_6H_5CH{=}NH$**				**879.4**			**911.9**			**0**
90PEE/ING	765-30-0; 75-31-0	c-$C_3H_5NH_2$; (i-C_3H_7)NH_2				870-889						
[$C_{11}H_{15}N$]	**54104-82-4**	**Pyrrolidine, 1-(4-methylphenyl)**				**879.4**			**910.2**			**5.6**
88CAU/CER		See Refs.				879.4						
[C_7H_9N]	**100-46-9**	**$C_6H_5CH_2NH_2$**				**879.4**			**913.3**			**−5**
87TAF	7664-41-7	NH_3	350	819	60.4	879.3						
83TAF2	7664-41-7	NH_3	350	819	60.4	879.3						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	27.3	891.8						
[$C_6H_{10}N_2$]	**4395-98-6**	**4-Cyanopiperidine**				**879.2**			**912.3**			**−2**
87TAF	7664-41-7	NH_3	350	819	60.4	879.2						
[$C_5H_9NO_4$]	**56-86-0**	**L-GlutamicAcid**				**879.1**			**913.0**			**−5**
92GOR/SPE	75-50-3; 109-89-7	$(CH_3)_3N$; $(C_2H_5)_2NH$	350			918-919						
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	59.9	878.9						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	59.9	878.9						
[$C_{13}H_{18}N_2$]	**84396-62-3**	**4-(1-adamanthyl)-pyrazole**				**878.9**			**913.1**			**−5.8**
94NOT/HER	289-80-5	Pyridazine	333	877.1	1.2	878.7						
94NOT/HER	107-11-9	$H_2C{=}CHCH_2NH_2$	333	875.5	3.3	878.8						
94NOT/HER	107-10-8	n-$C_3H_7NH_2$	333	883.9	−5.0	878.9						
[C_7H_7NO]	**556-18-3**	**4-$NH_2C_6H_4CHO$**				**878.6**			**910.4**			**2**
87TAF	7664-41-7	NH_3	350	819	59.9	878.5						
[C_5H_4BrN]	**626-55-1**	**3-Br-pyridine**				**878.2**			**910.0**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	20.0	878.1						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	13.7	878.2						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	13.7	878.2						
[C_6H_6ClNO]	**17228-64-7**	**2-Cl-6-(CH_3O)-pyridine**				**878.0**			**909.9**			**2**
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	11.7	878.0						
[C_2H_7N]	**75-04-7**	**$C_2H_5NH_2$**				**878**			**912.0**			**−5.1**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
97EAS/SMI		theory	298									−5.1
95SMI/RAD		theory	298						914			
94DEC/EXN	765-30-0	c-$C_3H_5NH_2$	338	869.9	5.9	875.7						
91MAU/SIE	372-47-4	3-F-pyridine	600	870.1	5.9	878.1	902.0	10.0	912.0	2	−6.7	−4.7
87TAF	7664-41-7	NH_3	350	819	57.7	876.6						
87BIS/RUH		Appearance							940±15			
86TAF/ANV	7664-41-7	NH_3	350	819	52.7	871.7						
86TAF/ANV	75-04-7	$C_2H_5NH_2$	350	878	0	878						
83TAF	7664-41-7	NH_3	350	819	58.1	877.1						
83LOC/MCI	7664-41-7	NH_3	350	819	58.1	877.1						
80MAU	7664-41-7	NH_3	550	819	50.2	868.9						
79MAU	75-04-7	$C_2H_5NH_2$	535	878	0	878						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	14.6	879.1						
75TAF	7664-41-7	NH_3	350	819	58.1	877.1						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	13.2	877.7						
75ARN	7664-41-7	NH_3	350	819	58.1	877.1						
74STA/BEA	75-04-7	$C_2H_5NH_2$	320	878	0	878						
72HEN/TAA	7664-41-7	NH_3	350	819	58.6	877.5						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	13.2	877.7						
72ARN/JON	7664-41-7	NH_3	350	819	58.6	877.5						
[C_3H_7P]	**676-59-5**	**$(CH_3)_2PH$**				**877.9**			**912.0**			**−5.8**
87TAF	7664-41-7	NH_3	350	819	59.0	878.0						
74STA/BEA	7664-41-7	NH_3	320	819	54.0	873.0						
[C_5H_8O]	**1487-15-6**	**5-Methyl-2,3-dihydrofuran**				**877.9**			**910.3**			**0**
86BOU/DJA	75-04-7	$C_2H_5NH_2$	313	878	−2.1	875.8						
86BOU/DJA	626-55-1	3-Br-pyridine	313	878.2	1.7	879.9						
[$C_4H_4N_2$]	**289-80-5**	**Pyridazine**				**877.1**			**907.2**			**7.8**
87TAF	7664-41-7	NH_3	350	819	58.1	876.4						
86TAF/ANV	75-04-7	$C_2H_5NH_2$	350	878	0	877.4						
83TAF2	7664-41-7	NH_3	350	819	62.2	880.5						
79MAU	107-10-8	n-$C_3H_7NH_2$	535	883.9	−3.3	877.5						
[C_4H_9NO]	**127-19-5**	**Dimethylacetamide**				**877.0**			**908.0**			**5**
87TAF	7664-41-7	NH_3	350	819	58.6	877.0						
86TAF/GAL	7664-41-7	NH_3	350	819	58.7	877.1						
83TAF	7664-41-7	NH_3	350	819	58.6	877.0						
75TAF	7664-41-7	NH_3	350	819	61.3	879.8						
[C_8H_9NO]	**99-92-3**	**4-NH_2-C_6H_4-$COCH_3$**				**877.0**			**908.8**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	47.7	877.0						
[C_6H_7N]	**6921-28-4**	**$(HCCCH_2)_2NH$**				**876.9**			**910.0**			**−2**
87TAF	7664-41-7	NH_3	350	819	58.1	876.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
83TAF2	7664-41-7	NH_3	350	819	58.1	876.9						
[$C_{10}H_{10}Ru$]	**1287-13-4**	**$(C_5H_5)_2Ru$**				**876.8**			**899.1**			**34**
81STE/BEA	7664-41-7	NH_3	320	819	58.6	876.8						
[$C_9H_{10}F_3N$]	**329-17-9**	**4-$CF_3C_6H_4N(CH_3)_2$**				**876.8**			**903.2**			**20**
87TAF	7664-41-7	NH_3	350	819	59.0	876.7						
[$C_5H_{11}NO_2$]	**72-18-4**	**L-valine**				**876.7**			**910.6**			**−5**
93LI/HAR		kinetic method							907.2			
92GOR/SPE	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
90ISA/OMO		kinetic method-relative order										
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	62.2	881.2						
79MAU/HUN	109-73-9	n-$C_4H_9NH_2$	520	886.6	−8.4	877.6						
79MAU/HUN	75-04-7	$C_2H_5NH_2$	520	878	−1.7	876.3						
79MAU/HUN	62-53-3	$C_6H_5NH_2$	520	850.6	22.6	874.7						
[$C_{18}H_{12}$]	**92-24-0**	**Tetracene**				**876.5**			**905.5**			**11.5**
80MAU	7664-41-7	NH_3	550	819	61.9	876.4						
[$C_{18}H_{15}As$]	**603-32-7**	**$(C_6H_5)_3As$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{18}H_{15}AsO$]	**1153-05-5**	**$(C_6H_5)_3AsO$**				**876.4**			**906.2**			**9.1**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{18}H_{15}N$]	**603-34-9**	**$(C_6H_5)_3N$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{18}H_{15}PS$]	**3878-45-3**	**$(C_6H_5)_3PS$**				**876.4**			**906.2**			**9.1**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{18}H_{15}OP$]	**791-28-6**	**$(C_6H_5)_3PO$**				**876.4**			**906.2**			**9.1**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{13}H_{13}OP$]	**2129-89-7**	**$CH_3(C_6H_5)_2PO$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_8H_{11}OP$]	**10311-08-7**	**$(CH_3)_2(C_6H_5)PO$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{16}H_{19}OP$]	**56598-35-7**	**t-$C_4H_9(C_6H_5)_2PO$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{15}H_{17}OP$]	**2959-75-3**	**i-$C_3H_7(C_6H_5)_2PO$**				**876.4**			**908.9**			**0**
86TRA/MUN	109-09-1; 107-10-8	2-Cl-pyridine; n-$C_3H_7NH_2$				869-884						
[$C_{10}H_{10}F_3NO$]	**90238-10-1**	**3-CF_3-$C_6H_4CON(CH_3)_2$**				**876.2**			**907.1**			**5**
94GRU/CAL	109-04-6; 100-46-9	2-Br-pyridine; $C_6H_5CH_2NH_2$				873-879						
[C_6H_6ClN]	**18368-63-3**	**2-Cl-6-(CH_3)-pyridine**				**876.2**			**908.0**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−22.0	876.2						
79AUE/BOW	124-40-3	$(CH_3)_2NH$	298	896.5	−6.3	890.1						
[C_8H_{12}]	**822-93-5**	**$(c\text{-}C_3H_5)_2C{=}CH_2$**				**875.8**			**904.7**			**12**
87TAF	7664-41-7	NH_3	350	819	57.7	875.7						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	18.6	883.0						
77WOL/ABB	87-85-4	$(CH_3)_6$-C_6	350	836.0	39.8	876.5						
[C_3H_7N]	**107-11-9**	**$H_2C{=}CHCH_2NH_2$**				**875.5**			**909.5**			**−5.1**
87TAF	7664-41-7	NH_3	350	819	56.7	875.7						
83TAF2	7664-41-7	NH_3	350	819	56.3	875.2						
80AUE/WEB	151-564	Aziridine	298	872.5	2.7	875.2						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	11.7	876.2						
75ARN	7664-41-7	NH_3	350	819	54.9	873.9						
[C_3H_7NS]	**758-16-7**	**$(CH_3)_2NC(=S)H$**				**875.5**			**906.4**			**5**
94DEC/EXN	75-04-7	$C_2H_5NH_2$	338	878	−2.8	874.8						
94DEC/EXN	288-47-1	thiazole	338	872.1	4.9	876.9						
94DEC/EXN	74-89-5	CH_3NH_2	338	864.5	11.4	875.4						
94DEC/EXN	765-30-0	c-$C_3H_5NH_2$	338	869.9	5.4	874.8						
93ABB/MO	107-11-9	$H_2C{=}CHCH_2NH_2$	333	875.5	0.1	875.3						
93ABB/MO	289-80-5	Pyridazine	333	877.1	−1.6	875.6						
[$C_{10}H_9N$]	**134-32-7**	**1-Napththalenamine**				**875.1**			**907.0**			**2**
78LAU/SAL	7664-41-7	NH_3	600	819	58.6	875.1						
[$C_4H_7NO_4$]	**56-84-8**	**L-aspartic acid**				**875**			**908.9**			**−5**
92GOR/SPE	74-89-5; 372-47-4	CH_3NH_2; 3-F-pyridine	350			864-870						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
90ISA/OMO		kinetic method										
87TAF	7664-41-7	NH_3	350	819	60.9	879.8						
87BOJ		kinetic method										
83LOC/MCI	7664-41-7	NH_3	350	819	60.9	879.8						
[$C_7H_{10}S$]	**38381-24-7**	**(c-C_3H_5)$_2$CS**				**874.5**			**904.3**			**9**
93ABB/MO	107-11-9	H_2C=CHCH$_2$NH$_2$	333	875.5	−0.6	874.4						
93ABB/MO	1453-58-3	3(5)-methylpyrazole	333	874.2	0.0	874.0						
93ABB/MO	7554-65-6	4-methylpyrazole	333	873.4	1.6	874.6						
[$C_8H_{10}F_5NS$]	**#678**	**3-(CH$_3$)$_2$NC$_6$H$_4$SF$_5$**				**874.5**			**901.0**			**20**
87TAF	7664-41-7	NH_3	350	819	56.7	874.4						
[$C_{10}H_{16}$]	**16609-28-2**	**1,5,5-Trimethyl-3-methylenecyclohexene**				**874.2**			**904.9**			**6**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	9.8	874.2						
[$C_4H_6N_2$]	**1453-58-3**	**3(5)-methylpyrazole**				**874.2**			**906.0**			**2**
92ABB/CAB	289-80-5	Pyridazine	333	877.1	−3.0	874.3						
92ABB/CAB	765-30-0	c-$C_3H_5NH_2$	333	869.9	3.3	872.9						
87TAF	7664-41-7	NH_3	350	819	56.7	875.3						
[$C_7H_{14}N_2O_3$]	**686-43-1**	**val-gly**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_8H_{16}N_2O_4$]	**13588-94-8**	**val-ser**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_7H_{14}N_2O_3$]	**1963-21-9**	**gly-val**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_8H_{16}N_2O_3$]	**3303-15-5**	**ala-val**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_9H_{16}N_2O_5$]	**13433-04-0**	**asp-val**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_9H_{16}N_2O_5$]	**20556-16-5**	**val-asp**				**874.1**			**NE**			**NE**
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
[$C_6H_8N_2$]	**106-50-3**	**1,4-C$_6$H$_4$(NH$_2$)$_2$**				**874.0**			**905.9**			**2**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSqnb	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
HLAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	23.4	874.0						
[$C_3H_5N_3$]	**28466-26-4**	**4-NH_2-pyrazole**				**874.0**			**907.6**			**−3.8**
94NOT/HER	289-80-5	Pyridazine	333	877.1	−2.6	874.9						
94NOT/HER	107-11-9	H_2C=$CHCH_2NH_2$	333	875.5	−1.7	873.8						
94NOT/HER	7554-65-6	4-methylpyrazole	333	873.4	−0.4	873.1						
[$C_{12}H_{18}OSi$]	**107099-29-6**	**4-CH_3O-C_6H_4-C(Si(CH_3)$_3$)=CH_2**				**874.0**			**902.9**			**12**
92MIS/ARI2	109-09-1	2-Cl-pyridine	308	869	4.6	873.5						
92MIS/ARI2	127-19-5	Dimethylacetamide	308	877.0	−2.5	874.5						
[$C_8H_6N_2$]	**91-19-0**	**Quinoxaline**				**873.7**			**903.8**			**8**
79MAU	75-04-7	$C_2H_5NH_2$	535	878	−1.3	873.7						
[$C_{10}H_{10}F_3NO$]	**25771-21-5**	**4-CF_3-C_6H_4CON(CH_3)$_2$**				**873.5**			**904.5**			**5**
94GRU/CAL	109-04-6; 106-50-3	2-Br-pyridine; 1,4-$(NH_2)_2$-C_6H_4				873-874						
[C_8H_8]	**502-86-3**	**1,4-C_6H_4(=CH_2)$_2$**				**873.5**			**900.6**			**18**
81POL/RAI	109-09-1; 75-04-7	2-Cl-pyridine; $C_2H_5NH_2$	350			869-878						
[$C_3H_8N_2O$]	**96-31-1**	**OC($NHCH_3$)$_2$**				**873.5**			**903.3**			**9**
93ABB/MO	107-11-9	H_2C=$CHCH_2NH_2$	333	875.5	−1.3	873.7						
93ABB/MO	765-30-0	c-$C_3H_5NH_2$	333	869.9	3.9	873.2						
[$C_4H_6N_2$]	**7554-65-6**	**4-methylpyrazole**				**873.4**			**906.8**			**−3**
92ABB/CAB	765-30-0	c-$C_3H_5NH_2$	333	869.9	2.5	872.2						
92ABB/CAB	289-80-5	Pyridazine	333	877.1	−3.6	873.9						
87TAF	7664-41-7	NH_3	350	819	55.4	874.2						
[C_5H_9NO]	**2680-03-7**	**2-propenamide, N,N-dimethyl**				**873.4**			**904.3**			**5**
90WOL/GRU	100-46-9	$C_6H_5CH_2NH_2$	320	879.4	−5.8	873.4						
[C_7H_9NO]	**90-04-0**	**2-$CH_3OC_6H_4NH_2$**				**873.3**			**905.2**			**2**
78LAU/SAL	74-89-5	CH_3NH_2	600	864.5	7.1	868.9						
73YAM/KEB	62-53-3	$C_6H_5NH_2$	600	850.6	27.2	877.8						
[C_5H_4BrN]	**109-04-6**	**2-Br-pyridine**				**873.0**			**904.8**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−23.4	874.7						
83TAF2	7664-41-7	NH_3	350	819	52.6	871.2						
79AUE/BET	74-89-5	CH_3NH_2	298	864.5	10.3	874.8						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	10.3	874.7						
75TAF	7664-41-7	NH_3	350	819	49.4	868.0						
75ARN	7664-41-7	NH_3	350	819	49.4	868.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSqub	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_5H_5NO]	**872-85-5**	**4-Pyridinecarboxaldehyde**				**872.8**			**904.6**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−25.4	872.8						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	8.3	872.8						
[C_2H_5N]	**151-56-4**	**Aziridine**				**872.5**			**905.5**			**−2**
83TAF2	7664-41-7	NH_3	350	819	53.1	871.9						
80AUE/WEB	75-04-7	$C_2H_5NH_2$	298	878	−5.6	872.4						
80AUE/WEB	765-30-0	c-$C_3H_5NH_2$	298	869.9	−4.4	865.5						
80AUE/WEB	626-60-8	3-Cl-pyridine	298	871.5	−1.0	870.6						
80AUE/WEB	372-47-4	3-F-pyridine	298	870.1	2.4	872.6						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	9.3	873.8						
73TAF	7664-41-7	NH_3	350	819	54.5	873.2						
75AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	8.3	872.8						
75ARN	7664-41-7	NH_3	350	819	54.5	873.2						
[$C_8H_{10}F_5NS$]	**#696**	**4-$SF_5C_6H_4N(CH_3)_2$**				**872.2**			**898.7**			**20**
87TAF	7664-41-7	NH_3	350	819	54.5	872.1						
[C_3H_3NS]	**288-47-1**	**thiazole**				**872.1**			**904**			**2**
94DEC/EXN	765-30-0	c-$C_3H_5NH_2$	338	869.9	0	869.5						
91MAU/SIE	74-89-5	CH_3NH_2	600	864.5			899.0	6.3	905.3			
91MAU/SIE	372-48-5	2-F-pyridine	600	852.7			884.6	18.8	903.4			
87TAF	7664-41-7	NH_3	350	819	47.1	865.7						
86MAU/LIE	110-86-1	pyridine	600	898.1	−31.7	866.5						
[$C_4H_8F_3N$]	**819-06-7**	**$CF_3CH_2N(CH_3)_2$**				**871.9**			**902.7**			**5.6**
87TAF	7664-41-7	NH_3	350	819	53.5	871.9						
83TAF	7664-41-7	NH_3	350	819	54.0	872.4						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	6.8	871.3						
[$C_9H_8N_2$]	**10199-68-5**	**4-(C_6H_5)-pyrazole**				**871.8**			**906.0**			**−5.8**
94NOT/HER	765-30-0	c-$C_3H_5NH_2$	333	869.9	1.5	871.3						
94NOT/HER	107-11-9	$H_2C{=}CHCH_2NH_2$	333	870.5	−5.1	872.4						
[C_8H_8]	**32796-95-5**	**1,2-$C_6H_4(=CH_2)_2$**				**871.7**			**898.8**			**18**
81POL/KAI	626-60-8; 819-06-7	3-Cl-pyridine; $CF_3CH_2N(CH_3)_2$	350			872-872						
[C_5H_4ClN]	**626-60-8**	**3-Cl-pyridine**				**871.5**			**903.4**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−22.9	875.2						
87TAF	7664-41-7	NH_3	350	819	52.6	871.2						
86TAF/ANV	626-60-8	3-Cl-pyridine	350	871.5	0	871.5						
83LOC/MCI	7664-41-7	NH_3	350	819	52.6	871.2						
80MAU	7664-41-7	NH_3	550	819	48.1	865.0						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	10.7	875.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
75TAF	7664-41-7	NH_3	350	819	52.6	871.2						
[$C_{16}H_{16}$]	**2919-20-2**	**(4-$CH_3C_6H_4)_2C{=}CH_2$**				**871.4**			**900.2**			**12**
87TAF	7664-41-7	NH_3	350	819	53.1	871.2						
77WOL/ABB	87-85-4	$(CH_3)_6$-C_6	350	836.0	34.8	871.5						
[$C_4H_{10}N_2$]	**4901-75-1**	**c-C(CH_3)(C_2H_5)NHNH**				**871.3**			**903.8**			0
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	6.8	871.3						
[$C_5H_{14}O_3$]	**111-96-6**	**$CH_3(OCH_2CH_2)_2OCH_3$**				**870.9**			**918.8**			**−52**
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	6.5	869.8	884.6	33.1	917.6	2	−54	−52
83MAU	289-80-5	Pyridazine	600	877.1	−23.5	871.5	907.2	5.9	913.1	7.8	−49	−41.2
83MAU	372-47-4	3-F-pyridine	600	870.1	−15.6	870.8	902.0	23.8	925.8	2	−66	−64
83MAU	372-48-5	2-F-pyridine	600	852.7	2.4	871.3	884.6	35.6	920.1	2	−55	−53
[$C_7H_{10}N_2O_2$]	**4027-57-0**	**3(5)-methyl-5(3)-ethoxycarbonylpyrazole**				**870.8**			**902.6**			**2**
92ABB/CAB	1453-58-3	3(5)-methylpyrazole	333	874.2	−4.0	870.2						
92ABB/CAB	7554-65-6	4-methylpyrazole	333	873.4	−2.2	871.1						
92ABB/CAB	107-10-8	n-$C_4H_7NH_2$	333	883.9	−13.0	870.7						
[$C_{10}H_{10}O_2$]	**90843-31-5**	**1-(2,3-dihydro-5-benzofuranyl)-ethanone**				**870.7**			**902.6**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	41.4	870.7						
[C_7H_9NS]	**1783-81-9**	**3-$CH_3SC_6H_4NH_2$**				**870.3**			**902.1**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	19.7	870.3						
[$C_8H_{10}N_2O_2$]	**100-23-2**	**N,N-Dimethyl-4-nitroaniline**				**870.2**			**896.7**			**20**
87TAF	7664-41-7	NH_3	350	819	51.3	868.9						
84ROL/HOU	626-60-8	3-Cl-pyridine	320	871.5	−1.3	869.9						
84ROL/HOU	109-04-6	2-Br-pyridine	320	873.0	−0.8	871.8						
[C_5H_4FN]	**372-47-4**	**3-F-pyridine**				**870.1**			**902.0**			**2**
91MAU/SIE	116-11-0	$CH_2{=}C(CH_3)OCH_3$	600	866.1			894.9	8.4	903.3	12	−10.5	1.5
91MAU/SIE	74-89-5	CH_3NH_2	600	864.5	12.1	873.9	899.0	4.6	903.6	−7	12.6	5.6
91MAU/SIE	288-47-1	thiazole	600	872.1			904	1.7	905.7			
91AUE/WEB	110-86-1	pyridine	300	898.1	−27.3	870.8						
87TAF	7664-41-7	NH_3	350	819	49.0	867.5						
86MAU/LIE	110-86-1	pyridine	600	898.1	−27.7	870.4						
83TAF2	7664-41-7	NH_3	350	819	48.5	867.1						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	6.3	870.8						
[$C_9H_{10}N_2O_3$]	**7291-02-3**	**3-NO_2-$C_6H_4CON(CH_3)_2$**				**869.9**			**900.9**			**5**
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_3OH; 2-Bry-pyridine				867-873						
[$C_9H_{10}N_2O_3$]	**7291-01-2**	**4-NO_2-$C_6H_4CON(CH_3)_2$**				**869.9**			**900.9**			***5***

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_4OH; 2-Br-pyridine				867-873						
[C_8H_9NO]	**619-55-6**	**4-CH_3-$C_6H_4CONH_2$**				**869.9**			**900.9**			**5**
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_4OH; 2-Br-pyridine				867-873						
[$C_8H_9NO_2$]	**5813-86-5**	**3-CH_3O-$C_6H_4CONH_2$**				**869.9**			**900.9**			**5**
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_4OH; 2-Br-pyridine				867-873						
[C_8H_9NO]	**618-47-3**	**3-CH_3-$C_6H_4CONH_2$**				**869.9**			**900.9**			**5**
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_4OH; 2-Br-pyridine				867-873						
[$C_7H_8N_2O$]	**3544-24-9**	**3-NH_2-$C_6H_4CONH_2$**				**869.9**			**900.9**			**5**
94GRU/CAL	95-55-6; 109-04-6	2-NH_2-C_6H_4OH; 2-Br-pyridine				867-873						
[C_3H_7N]	**765-30-0**	**c-$C_3H_5NH_2$**				**869.9**			**904.7**			**−7.9**
94DEC/EXN	74-89-5	CH_3NH_2	338	864.5	5.8	870.3						
87TAF	7664-41-7	NH_3	350	819	51.3	870.3						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	4.4	868.9						
[$C_7H_{11}N$]	**87-62-7**	**2,6-dimethylaniline**				**869.8**			**901.7**			**2**
94BOH/DEC	765-30-0	c-$C_3H_5NH_2$	338	869.9	1.1	870.6						
94BOH/DEC	95-53-4	2-methylaniline	338	859.1	10	869.1						
[C_5H_4ClNO]	**1851-22-5**	**3-chloro-pyridine-1-oxide**				**869.7**			**902.2**			**0**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	−23.4	869.7						
[$C_4H_8F_3N$]	**819-46-6**	**$CF_3(CH_2)_3NH_2$**				**869.6**			**903.5**			**−5**
87TAF	7664-41-7	NH_3	350	819	49.9	868.8						
83TAF2	7664-41-7	NH_3	350	819	49.9	868.8						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	5.9	870.3						
75TAF	7664-41-7	NH_3	350	819	49.0	867.9						
75ARN	7664-41-7	NH_3	350	819	49.0	867.9						
[$C_8H_9NO_2$]	**3424-93-9**	**4-CH_3O-$C_6H_4CONH_2$**				**869.4**			**900.3**			**5**
94GRU/CAL	95-54-5; 109-04-6	1,2-$C_6H_4(NH_2)_2$; 2-Br-pyridine				866-873						
[$C_3H_7NO_2S$]	**52-90-4**	**L-Cysteine**				**869.3**			**903.2**			**−5**
93LI/HAR		kinetic method							898			
92GOR/SPE	109-97-7; 372-48-5	pyrrole; 2-F-pyridine	350			844-853						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / Ys Squib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGD(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
90ISA/OMO		kinetic method-relative order										
87TAF	7664-41-7	NH_3	350	819	49.9	868.8						
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH_3	350	819	49.9	868.8						
[$C_{13}H_{18}O$]	**22666-53-1**	**α-t-butylstyrene, 4-methoxy**				**869.1**			**897.9**			**12**
92NAK/NOM	127-19-5	Dimethylacetamide	343	877.0	−5.9	870.9						
92NAK/NOM	109-09-1	2-Cl-pyridine	343	869	0	868.6						
92NAK/NOM	626-60-8	3-Cl-pyridine	343	871.5	−3.3	867.8						
[$C_{10}H_{14}N_2O_2S$]	**28809-04-3**	**S-(2-(4-pyridyl)ethyl)cysteine**				**>869**			**NE**			**NE**
93BUR/GAS	52-90-4	L-Cysteine		869.3		See Refs.						
[C_5H_4ClN]	**109-09-1**	**2-Cl-pyridine**				**869**			**900.9**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−27.3	870.8						
87TAF	7664-41-7	NH_3	350	819	50.3	868.9						
83TAF2	7664-41-7	NH_3	350	819	50.3	868.9						
80MAU	7664-41-7	NH_3	550	819	46.0	862.9						
79MAU	75-04-7	$C_2H_5NH_2$	546	878	−4.2	872.1						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	6.3	870.8						
75TAF	7664-41-7	NH_3	350	819	49.4	868.0						
75ARN	7664-41-7	NH_3	350	819	49.4	868.0						
[$C_7H_7NO_2$]	**118-92-3**	**2-NH_2-benzoic acid**				**869.0**			**901.5**			**0**
95TAN/ISB	108-44-1; 106-50-3	3-$CH_3C_6H_4NH_2$; 1,4-$C_6H_4(NH_2)_2$				864-874						
[C_4H_9NOS]	**16703-45-0**	**$CH_3OC(S)N(CH_3)_2$**				**869.0**			**900.0**			**5**
93ABB/MO	765-30-0	c-$C_3H_5NH_2$	333	869.9	−1.0	868.4						
93ABB/MO	107-47-1	(t-$C_4H_9)_2S$	333	864.0	5.4	869.6						
[$C_7H_6N_2$]	**271-44-3**	**1H-Indazole**				**868.9**			**900.8**			**2**
88CAT/CLA	3796-24-5	4-(CF_3)-pyridine	~300	862.0	7.5	869.6						
88CAT/CLA	109-09-1	2-Cl-pyridine	~300	869	−0.8	868.2						
87TAF	7664-41-7	NH_3	350	819	50.3	868.9						
84FLA/MAQ		kinetic method										
[C_7H_9NO]	**104-94-9**	**4-$CH_3OC_6H_4NH_2$**				**868.5**			**900.3**			**2**
87TAF	7664-41-7	NH_3	350	819	49.9	868.5						
81TAA/SUM	7664-41-7	NH_3	320	819	45.6	864.4						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	3.9	868.4						
77SUM/POL	7664-41-7	NH_3	350	819	49.9	868.5						
[$C_9H_{10}N_2$]	**38803-30-4**	**3-$(CH_3)_2NC_6H_4CN$**				**868.1**			**894.6**			**20**
87TAF	7664-41-7	NH_3	350	819	50.3	868.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_{12}H_{12}N_2O_2$]	**5932-30-9**	**3(5)-phenyl-5(3)-ethoxycarbonylpyrazole**				**867.8**			**899.7**			**2**
92ABB/CAB	765-30-0	c-$C_3H_5NH_2$	333	869.9	−1.4	868.1						
92ABB/CAB	107-47-1	$(t\text{-}C_4H_9)_2S$	333	864.0	2.9	867.2						
[$C_3H_7NO_2$]	**56-41-7**	**L-alanine**				**867.7**			**901.6**			**−5**
93LI/HAR		kinetic method							897			
92GOR/SPE	372-47-4; 75-04-7	3-F-pyridine; $C_2H_5NH_2$	350			870-878						
90ISA/OMO		kinetic method relative order										
87TAF	7664-41-7	NH_3	350	819	50.3	869.3						
87BOJ		kinetic method-relative order										
83LOC/MCI	7654-41-7	NH_3	350	819	50.3	869.3						
79MAU/HUN	62-53-3	$C_6H_5NH_2$	500	850.6	25.9	877.9	882.5	17.6	900.0	2	9.2	11.2
79MAU/HUN	74-89-5	CH_3NH_2	520	864.5	0.4	864.5						
[C_5H_4FNO]	**695-37-4**	**3-fluoro-pyridine-1-oxide**				**867.6**			**900.1**			**0**
92MIS/TER	694-56-7	pyridine-1-oxide	343	892.9	−25.5	867.6						
[$C_8H_{10}N_2O_2$]	**619-31-8**	**3-$(NO_2)C_6H_4N(CH_3)_2$**				**867.6**			**894.1**			**20**
87TAF	7664-41-7	NH_3	350	819	49.9	867.6						
[C_3H_8Sn]	**82065-00-7**	**$(CH_3)_2Sn{=}CH_2$**				**867.1**			**893.6**			**20**
82PIE/HEH	7664-41-7	NH_3	350	819	49.4	867.1						
[C_4H_9NO]	**625-50-3**	**Acetamide, N-ethyl-**				**867.0**			**898.0**			**5**
92DEC/EXN	765-30-0	c-$C_3H_5NH_2$	338	869.9	−2.6	866.8						
92DEC/EXN	74-89-5	CH_3NH_2	338	864.5	3.2	867.3						
[C_6H_7NO]	**95-55-6**	**2-$(OH)C_6H_4NH_2$**				**866.9**			**898.9**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	16.3	866.9						
[C_6H_7NO]	**591-27-6**	**3-$(OH)C_6H_4NH_2$**				**866.9**			**898.8**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	16.3	866.9						
[$C_6H_9O_3P$]	**281-33-4**	**2,8,9-Trioxa-1-phosphadamantane**				**866.8**			**899.3**			**0**
80HOD/HOU	107-47-1	$(t\text{-}C_4H_9)_2S$	320	864.0	0.4	864.6						
80HOD/HOU	109-09-1	2-Cl-pyridine	320	869	−0.4	868.6						
[C_2H_5N]	**593-67-9**	**$CH_2{=}CHNH_2$**				**866.5**			**898.9**			**0**
81ELL/DIX	108-44-1; 109-09-1	3-CH_3-aniline; 2-Cl-pyridine				864-869						
[CH_6N_2]	**60-34-4**	**CH_3NHNH_2**				**866.4**			**898.8**			**0**
80AUE/WEB	151-56-4	Aziridine	298	872.5	−7.2	865.3						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	2.9	867.4						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_8H_{11}N$]	**587-02-0**	**3-$C_2H_5C_6H_4NH_2$**				**866.1**			**897.9**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	15.5	866.1						
[C_4H_8O]	**116-11-0**	**CH_2=$C(CH_3)OCH_3$**				**866.1**			**894.9**			**12**
91MAU/SIE	372-48-5	2-F-pyridine	600	852.7	16.3	866.0	884.6	10.0	894.6	2	11.3	13.3
91MAU/SIE	74-89-5	CH_3NH_2	600	864.5			899.0	−6.7	892.3	−7	23.8	16.8
91MAU/SIE	75-04-7	$C_2H_5NH_2$	600	878			912.0	−23.0	889.0	−5.1	31.0	25.9
88MAQ/JOR	372-47-4	3-F-pyridine	300	870.1	−4.6	865.5						
[$C_{13}H_{18}S$]	**146558-39-6**	**α-t-butylstyrene,4-CH_3S**				**866.0**			**894.8**			**12**
92NAK/NOM	512-56-1	$OP(OCH_3)_3$	343	860.8	5.4	866.1						
92NAK/NOM	106-49-0	4-$CH_3C_6H_4NH_2$	343	864.8	2.9	867.3						
92NAK/NOM	109-09-1	2-Cl-pyridine	343	869	−4.2	864.4						
[C_6H_{10}]	**3664-56-0**	**1,3,3-Trimethylcyclopropene**				**865.9**			**895.4**			**10**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	1.5	865.9						
[$C_{15}H_{12}$]	**779-02-2**	**9-Methylanthracene**				**865.8**			**896.5**			**5.8**
80MAU	109-09-1	2-Cl-pyridine	588	869	−3.8	864.1						
80MAU	626-60-8	3-Cl-pyridine	608	871.5	−2.9	867.4						
[$C_6H_8N_2$]	**95-54-5**	**1,2-$C_6H_4(NH_2)_2$**				**865.8**			**896.5**			**5.8**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	16.3	865.8						
[$C_5H_{11}NO_2$]	**687-48-9**	**$(CH_3)_2NCOOC_2H_5$**				**865.6**			**896.6**			**5**
83TAF2	7664-41-7	NH_3	350	819	47.1	865.6						
[$C_7H_8N_2O_2$]	**100-15-2**	**N-Methyl-4-nitroaniline**				**865.1**			**891.6**			**20**
84ROL/HOU	372-47-4	3-F-pyridine	320	870.1	−4.6	865.1						
[C_3H_9As]	**593-88-4**	**$(CH_3)_3As$**				**864.9**			**897.3**			**0**
75HOD/BEA	74-89-5	CH_3NH_2	320	864.5	0.4	864.8						
[C_7H_9N]	**106-49-0**	**4-$CH_3C_6H_4NH_2$**				**864.8**			**896.7**			**2**
87TAF	7664-41-7	NH_3	350	819	46.2	864.8						
81TAA/SUM	7664-41-7	NH_3	320	819	42.3	861.1						
77SUM/POL	7664-41-7	NH_3	350	819	46.2	864.8						
75ARN	7664-41-7	NH_3	350	819	49.0	867.5						
[$C_{13}H_{25}N$]	**75197-24-9**	**out-6H-1-Azabicyclo[4,4,4]tetradecane**				**864.5**			**897.0**			**0**
81ALD/ARR	7664-41-7	NH_3	320	819	45.6	864.5						
[CH_5N]	**74-89-5**	**CH_3NH_2**				**864.5**			**899.0**			**−7**
97EAS/SMI		theory	298									−6.6
93SZU/MCM	124-40-3	$(CH_3)_3NH$	600	896.5	−33.5	864.5	929.5	−29.7	899.8	−2	−5.9	−7.9
93SMI/RAD		theory	0						895			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ref(M)	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	298						901			
93SMI/RAD		theory	600						906			
91MAU/SIE	372-48-5	2-F-pyridine	600	852.7	6.7	862.1	884.6	16.3	900.9	2	−16.3	−14.3
87TAF	7664-41-7	NH_3	350	819	44.8	863.9						
87BIS/RUH		Appearance							930±15			
83TAF	7664-41-7	NH_3	350	819	44.8	863.9						
83LOC/MCI	7664-41-7	NH_3	350	819	44.8	863.9						
79LOC/HUN	62-53-3	$C_6H_5NH_2$	382	850.6	11.1	862.4						
78LAU/SAL	7664-41-7	NH_3	600	819	41.8	861.0						
76AUE/WEB	74-89-5	CH_3NH_2	298	864.5	0	864.5						
75TAF	7664-41-7	NH_3	350	819	44.8	863.9						
75HOD/BEA	74-89-5	CH_3NH_2	320	864.5	0	864.5						
75AUE/WEB	74-89-5	CH_3NH_2	298	864.5	0	864.5						
72HEN/TAA	7664-41-7	NH_3	350	819	46.2	865.3						
72BRI/YAM	7664-41-7	NH_3	600	819	45.2	864.4						
72AUE/WEB	74-89-5	CH_3NH_2	298	864.5	0	864.5						
72ARN/JON	7664-41-7	NH_3	350	819	46.2	865.3						
[$C_5H_8N_2$]	**35520-41-3**	**trans-dimethylamino acrylonitrile**				**864.3**			**896.8**			**0**
93BER/HEL	107-47-1	$(t\text{-}C_4H_9)_2S$	~338	864.0	0	864.4						
93BER/HEL	78-59-1	isophorone	~338	861.6	2.5	864.2						
[$C_8H_{18}S$]	**107-47-1**	**$(t\text{-}C_4H_9)_2S$**				**864.0**			**893.8**			**9**
87TAF	7664-41-7	NH_3	350	819	45.8	864.0						
86TAF/ANV	107-47-1	$(t\text{-}C_4H_9)_2S$	350	864.0	0	864.0						
83TAF2	7664-41-7	NH_3	350	819	45.3	863.5						
[C_7H_7O]	**88170-17-6**	**4-OH-benzyl**				**864**			**896.5**			**0**
94HOK/YAN		kinetic method				864						
[C_7H_9N]	**108-44-1**	**$3\text{-}CH_3C_6H_4NH_2$**				**864.0**			**896.8**			**2**
87TAF	7664-41-7	NH_3	350	819	45.8	864.3						
83LOC/MCI	7664-41-7	NH_3	350	819	45.8	864.3						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	12.6	863.1						
77SUM/POL	7664-41-7	NH_3	350	819	46.2	864.8						
77POL/DEV	62-53-3	$C_6H_5NH_2$	350	850.6	13.7	864.3						
77COO/KRU		relative order- See Refs.										
75TAF	7664-41-7	NH_3	350	819	46.2	864.8						
[$C_{12}H_{20}O$]	**4789-40-6**	**2,5-di-t-butylfuran**				**863.9**			**894.7**			**5.8**
85HOU/ROL	74-89-5	CH_3NH_2	313	864.5	−0.4	863.9						
[CH_4N_2S]	**62-56-6**	**$SC(NH_2)_2$**				**863.9**			**893.7**			**9**
93ABB/MO	765-30-0	$c\text{-}C_3H_5NH_2$	333	869.9	−4.8	864.5						
93ABB/MO	107-47-1	$(t\text{-}C_4H_9)_2S$	333	864.0	−1.1	862.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_9H_{10}O_2$]	**100-06-1**	**4-CH_3O-C_6H_4-$COCH_3$**				**863.7**			**895.6**			**2**
87TAF	7664-41-7	NH_3	350	819	45.3	863.9						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	33.9	863.2						
[$C_4H_5N_3O_2$]	**3034-42-2**	**1-Methyl-5-nitroimidazole**				**863.5**			**895.3**			**2**
87TAF	7664-41-7	NH_3	350	819	44.8	863.4						
[$C_3H_7O_3P$]	**3741-36-4**	**2-Methoxy-1,3,2-dioxaphospholane**				**862.7**			**896.1**			**0**
80HOD/HOU	107-47-1	(t-C_4H_9)$_2$S	320	864.0	0.4	864.6						
80HOD/HOU	109-09-1	2-Cl-pyridine	320	869	−8.4	860.7						
[$C_9H_{10}N_2$]	**1197-19-9**	**1,4-$(CH_3)_2NC_6H_4CN$**				**862.6**			**889.1**			**20**
87TAF	7664-41-7	NH_3	350	819	44.8	862.5						
[$C_{21}H_{30}O$]	**38256-01-8**	**(1-adamytyl)$_2$CO**				**862.4**			**894.3**			**2**
93ABB/MO	107-47-1	(t-C_4H_9)$_2$S	333	864.0	−2.1	862.2						
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	10.0	862.7						
[$C_2H_7O_3P$]	**868-85-9**	**$(CH_3O)_2PHO$**				**862.4**			**894.8**			**0**
82PIE/HEH2	512-56-1; 108-44-1	$(CH_3O)_3PO$; 3-$CH_3C_6H_4NH_2$				861-864						
[C_6H_8O]	**3710-43-8**	**2,4-dimethylfuran**				**862.3**			**894.7**			**0**
85HOU/ROL	74-89-5	CH_3NH_2	313	864.5	−2.1	862.3						
[$C_6H_4F_3N$]	**3796-24-5**	**4-(CF_3)-pyridine**				**862.0**			**893.9**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−35.6	862.5						
87TAF	7664-41-7	NH_3	350	819	43.0	861.6						
86TAF/ANV	3796-24-5	4-(CF_3)-pyridine	350	862.0	0	862.0						
83TAF	7664-41-7	NH_3	350	819	43.0	861.6						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	−2.4	862.0						
75TAF	7664-41-7	NH_3	350	819	42.6	861.1						
75ARN	7664-41-7	NH_3	350	819	42.6	861.1						
72TAA/HEN	110-86-1	pyridine	320	898.1	−49.0	849.2						
[$C_{14}H_{23}N$]	**16245-79-7**	**4-(n-C_8H_{17})$C_6H_4NH_2$**				**862**			**894.5**			**0**
86SUN/KUL		See Refs.	300			862			895.4			
[$C_9H_{14}O$]	**78-59-1**	**Isophorone**				**861.6**			**893.5**			**2**
87TAF	7664-41-7	NH_3	350	819	43.0	861.6						
[C_7H_7NO]	**55-21-0**	**$C_6H_5CONH_2$**				**861.2**			**892.1**			**5**
94GRU/CAL	68-12-2; 95-54-5	$HCON(CH_3)_2$; 1,2-$(NH_2)_2$-C_6H_4				857-866						
[$C_5H_9NO_3$]	**1117-77-7**	**$CH_3CONHCH_2COOCH_3$**				**861**			**892.0**			**5**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
83MAU		See Refs.				861						
[$C_3H_9O_4P$]	**512-56-1**	**$OP(OCH_3)_3$**				**860.8**			**890.6**			**9.1**
87TAF	7664-41-7	NH_3	350	819	42.6	860.8						
86TAF/ANV	512-56-1	$OP(OCH_3)_3$	350	860.8	0	860.8						
82PIE/HEH						845.2						
80HOD/MCD	62-53-3	$C_6H_5NH_2$	300	850.6	5.9	856.5						
[$C_6H_4F_3N$]	**3796-23-4**	**3-(CF_3)-pyridine**				**860.7**			**892.5**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−37.1	861.0						
87TAF	7664-41-7	NH_3	350	819	41.6	860.2						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−3.4	861.1						
75TAF	7664-41-7	NH_3	350	819	42.1	860.7						
75ARN	7664-41-7	NH_3	350	819	42.1	860.7						
[$C_3H_4N_2$]	**288-13-1**	**Pyrazole**				**860.5**			**894.1**			**−3.8**
88CAT/CLA	107-47-1	$(t\text{-}C_4H_9)_2S$	300	864.0	−4.2	859.8						
88CAT/CLA	78-59-1	Isophorone	300	861.6	−0.8	860.8						
88CAT/CLA	3796-24-5	4-(CF_3)-pyridine	300	862.0	−0.8	861.2						
87TAF	7664-41-7	NH_3	350	819	41.6	860.5						
86TAF/ANV	3796-24-5	4-(CF_3)-pyridine	350	862.0	−0.8	861.5						
86TAF/ANV	107-47-1	$(t\text{-}C_4H_9)_2S$	350	864.0	−4.2	860.5						
86TAF/ANV	512-56-1	$OP(OCH_3)_3$	350	860.8	−2.5	859.0						
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	52.2	859.5						
84FLA/MAQ		kinetic method										
[CTe]	**12012-15-6**	**CTe at C**				**860.4**			**892**			**3**
85JAS/STE		theory							892			
[$C_8H_{18}O$]	**6163-66-2**	**$(t\text{-}C_4H_9)_2O$**				**860.0**			**887.4**			**17**
87TAF	7664-41-7	NH_3	350	819	42.1	859.9						
[C_7H_5NO]	**273-53-0**	**benzoxazole**				**859.8**			**891.6**			**2**
88MAQ/JOR	116-11-0	$CH_2=C(CH_3)OCH_3$	~300	866.1	−6.3	859.8						
[C_4H_8S]	**7594-44-7**	**$CH_2=C(CH_3)\text{-}SCH_3$**				**859.7**			**888.6**			**12**
89OSA/DEL	372-48-5	2-F-pyridine	313	852.7	4.2	856.8						
89OSA/DEL	116-11-0	$CH_2=C(CH_3)OCH_3$	313	866.1	−3.8	862.3						
89OSA/DEL	4789-40-6	2,5-di-t-butylfuran	313	863.9	−4.2	859.7						
[$C_{20}H_{12}$]	**198-55-0**	**Perylene**				**859.6**			**888.6**			**11.5**
80MAU	109-09-1	2-Cl-pyridine	520	869	−5.9	861.1						
80MAU	62-53-3	$C_6H_5NH_2$	525	850.6	9.6	858.1						
[C_7H_9N]	**95-53-4**	**2-methylaniline**				**859.1**			**890.9**			**2**
94BOH/DEC	2450-71-7	$HCCCH_2NH_2$	338	853.5	6	859.2						

J. Phys. Chem. Ref. Data, Vol. 27, No. 3, 1998

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
94BOH/DEC	1121-37-5	$(c\text{-}C_3H_5)_2CO$	338	850.6	8.1	859.0						
[$C_5H_{12}O_2$]	**17081-21-9**	**$CH_3O(CH_2)_3OCH_3$**				**858.6**			**897.2**			**−20.6**
83MAU	372-47-4	3-F-pyridine	600	870.1	−20.9	856.0	902.0	−3.3	898.6	2	−29.3	−27.3
83MAU	372-48-5	2-F-pyridine	600	852.7	1.3	860.8	884.6	15.1	899.6	2	−23	−21
83MAU	544-40-1	$(n\text{-}C_4H_9)_2S$	600	842.1	8.2	859.1	871.8	21.8	893.6	9	−22.6	−13.6
[$C_{10}H_9F_6N$]	**34060-81-6**	**$3,5\text{-}(CF_3)_2C_6H_3N(CH_3)_2$**				**858.4**			**884.9**			**20**
87TAF	7664-41-7	NH_3	350	819	40.7	858.4						
[C_2H_6FN]	**406-34-8**	**$CH_2FCH_2NH_2$**				**858.0**			**892.0**			**−5**
87TAF	7664-41-7	NH_3	350	819	39.4	858.3						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−8.3	856.2						
75TAF	7664-41-7	NH_3	350	819	39.8	858.7						
75ARN	7664-41-7	NH_3	350	819	39.8	858.7						
[$C_4H_9NO_2$]	**105-40-8**	**$CH_3NHCOOC_2H_5$**				**857.8**			**888.8**			**5**
87TAF	7664-41-7	NH_3	350	819	39.4	857.8						
[C_7H_{12}]	**1000-86-8**	**$(CH_3)_2C{=}CHC(CH_3){=}CH_2$**				**857.6**			**886.5**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	38.6	857.6						
[C_3H_7NO]	**79-16-3**	**Acetamide, N-methyl**				**857.6**			**888.5**			**5**
92DEC/EXN	765-30-0	$c\text{-}C_3H_5NH_2$	338	869.9	−9.2	860.2						
92DEC/EXN	74-89-5	CH_3NH_2	338	864.5	−2.7	861.4						
92DEC/EXN	372-48-5	2-F-pyridine	338	852.7	5.4	858.0						
92ABB/CAN	2450-71-7	$HCCCH_2NH_2$	333	853.5	0.2	853.3						
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	2.3	854.9						
[$C_4H_7N_2$]	**39687-97-3**	**N′-cyano-N,N-dimethyl formamidine**				**857.3**			**889.7**			0
93BER/HEL	16584-00-2	2-methyl-2H-benzotriazole	338	855.9	−2.1	853.6						
93BER/HEL	78-59-1	Isophorone	338	861.6	−3.3	858.4						
93BER/HEL	107-47-1	$(t\text{-}C_4H_9)_2S$	338	864.0	−4.6	859.8						
[$C_5H_{11}NO$]	**754-10-9**	**$t\text{-}C_4H_9CONH_2$**				**857.2**			**889.0**			?
97HOM/HER	687-48-9	$(CH_3)_2NCOOC_2H_5$	333	865.6	3.1	868.8						
97HOM/HER	2450-71-7	$HCCCH_2NH_2$	333	853.5	3.3	856.5						
97HOM/HER	107-47-1	$(t\text{-}C_4H_9)_2S$	333	864.0	−6.5	857.8						
[$C_{14}H_{12}$]	**530-48-3**	**$(C_6H_5)_2C{=}CH_2$**				**856.9**			**885.7**			12
87TAF	7664-41-7	NH_3	350	819	38.0	856.1						
79AUE/BOW	7664-41-7	NH_3	298	819	38.6	857.6						
77WOL/ABB	87-85-4	$(CH_3)_6\text{-}C_6$	350	836.0	18.8	855.5						
75WOF/HAR	7664-41-7	NH_3	350	819	38.9	857.0						
75TAF	7664-41-7	NH_3	350	819	37.5	855.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M- Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_6H_8]	**15082-13-0**	**1-Methyl-3-methylenecyclobutene**				**856.9**			**891.0**			−5.8
79AUE/BOW	7664-41-7	NH_3	298	819	37.1	856.9						
[C_3H_7NO]	**68-12-2**	**$(CH_3)_2NCHO$**				**856.6**			**887.5**			5
92ABB/CAB	372-48-5	2-F-pyridine	333	852.7	2.9	855.5						
87TAF	7664-41-7	NH_3	350	819	36.6	855.0						
79LOC/HUN	62-53-3	$C_6H_5NH_2$	382	850.6	4.0	854.3						
79AUE/BOW	79-89-5	CH_3NH_2	298	864.5	−5.4	859.1						
75TAF	7664-41-7	NH_3	350	819	36.6	855.0						
[$C_9H_{10}OS$]	**1778-09-2**	**4-CH_3S-C_6H_4-$COCH_3$**				**856.3**			**888.2**			2
87TAF	7664-41-7	NH_3	350	819	37.5	856.1						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	27.2	856.5						
[C_4H_7NO]	**23350-58-5**	**2-butenamide**				**856.1**			**887.1**			5
90WOL/GRU	68-12-2	$(CH_3)_2NCHO$	320	856.6	0.4	857.0						
90WOL/GRU	119-61-9	$(C_6H_5)_2CO$	320	852.5	2.7	855.3						
[C_5H_9N]	**19540-05-7**	**1-Azabicyclo[1,1,0]butane**				**856.1**			**886.9**			**5.6**
79AUE/BOW	7664-41-7	NH_3	298	819	37.1	856.1						
75AUE/WEB2	75-07-0	CH_3CHO	298	736.5	100.4	836.9						
[$C_7H_7N_3$]	**16584-00-2**	**2-methyl-2H-benzotriazole**				**855.9**			**890.1**			**−5.8**
89TOM/ABB	68-12-2	$(CH_3)_2NCHO$	298	856.6	−0.4	856.1						
89TOM/ABB	288-13-1	Pyrazole	298	860.5	−5.0	855.5						
[$C_2H_3N_3$]	**288-88-0**	**1,2,4-Triazole**				**855.9**			**886.0**			**8**
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	52.2	855.9						
[$C_4H_4N_2$]	**289-95-2**	**Pyrimidine**				**855.7**			**885.8**			**7.8**
87TAF	7664-41-7	NH_3	350	819	36.6	854.9						
86TAF/ANV	100-48-1	4-Pyridinecarbonitrile	350	848.8	5.9	854.3						
83TAF2	7664-41-7	NH_3	350	819	36.6	854.9						
79MAU	75-04-7	$C_2H_5NH_2$	510	878	−17.6	857.7						
[C_9H_8O]	**768-60-5**	**4-CH_3O-C_6H_4-CCH**				**855.7**			**886.4**			**5.8**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	54.4	855.7						
85MAR/MOD	7664-41-7	NH_3	300	819	24.7	843.7						
[$C_6H_4F_3N$]	**368-48-9**	**2-(CF_3)-pyridine**				**855.2**			**887.1**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−43.0	855.2						
87TAF	7664-41-7	NH_3	350	819	36.6	855.2						
75TAF	7664-41-7	NH_3	350	819	36.6	855.2						
[$C_{15}H_{12}$]	**613-12-7**	**2-Methylanthracene**				**855.1**			**887.5**			**0**
80MAU	62-53-3	$C_6H_5NH_2$	544	850.6	0.4	851.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
80MAU	109-09-1	2-Cl-pyridine	544	869	−10.9	858.6						
[$C_4H_{10}O_2$]	**110-63-4**	**$HO(CH_2)_4OH$**				**854.9**			**915.6**			**−95**
95CHE/STO	98-86-2	$C_6H_5COCH_3$	600	829.3	−5.5	852.9	861.1	51.5	912.6	2	−95.0	−93.0
95CHE/STO	534-22-5	2-methylfuran	600	833.5	−5.1	856.9	865.9	55.6	921.6	0	−101.3	−101.3
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−37.6	826.9						
[C_2H_5N]	**#804**	**$•CH_2CH_2NH_2$**				**854.5**			**887**			**0**
89HOL/LOS			298						887			
[$C_{13}H_{17}ClO$]	**146558-40-9**	**α-t-butylstyrene, 4-CH_3O, 3-Cl**				**854.2**			**883.0**			**12**
92NAK/NOM	62-53-3	$C_6H_5NH_2$	343	850.6	3.3	853.5						
92NAK/NOM	372-48-5	2-F-pyridine	343	852.7	2.5	854.8						
[C_9H_8S]	**56041-85-1**	**4-CH_3S-C_6H_4-CCH**				**854.1**			**886.6**			**0**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	52.7	854.1						
[CH_9O_3PS]	**152-18-1**	**$SP(OCH_3)_3$**				**853.9**			**883.6**			**9.1**
80HOD/MCD	123-11-5	4-$CH_3OC_6H_4CHO$	300	849.3	4.6	853.9						
[Ti]	**7440-32-6**	**Ti**				**853.7**			**876**			**34**
88ELK/ARM		See Refs.							876±11			
[$C_4H_8N_2$]	**926-64-7**	**$NCCH_2N(CH_3)_2$**				**853.7**			**884.5**			**5.6**
87TAF	7664-41-7	NH_3	350	819	35.2	853.6						
83TAF2	7664-41-7	NH_3	350	819	35.2	853.6						
75ARN	7664-41-7	NH_3	350	819	35.2	853.6						
[C_2H_6OS]	**67-68-5**	**$(CH_3)_2SO$**				**863.7**			**884.4**			**5.8**
87TAF	7664-41-7	NH_3	350	819	35.2	853.6						
83TAF	7664-41-7	NH_3	350	819	35.2	853.6						
79LAU	7664-41-7	NH_3	650	819	38.5	853.3						
77MCA	67-56-1; 64-17-5	CH_3OH; C_2H_5OH				725-746						
75TAF	7664-41-7	NH_3	350	819	35.2	853.6						
[C_3H_5N]	**2450-71-7**	**$HCCCH_2NH_2$**				**853.5**			**887.4**			**-5**
92ABB/CAB	372-48-5	2-F-pyridine	333	852.7	2.5	855.5						
87TAF	7664-41-7	NH_3	350	819	33.9	852.8						
83TAF2	7664-41-7	NH_3	350	819	33.9	852.8						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−12.7	851.8						
[$C_3H_5F_3N$]	**460-39-9**	**$CF_3CH_2CH_2NH_2$**				**853.2**			**887.2**			**5**
87TAF	7664-41-7	NH_3	350	819	33.9	852.8						
83TAF2	7664-41-7	NH_3	350	819	33.9	852.8						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−11.2	853.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
75TAF	7664-41-7	NH_3	350	819	32.9	851.9						
75ARN	7664-41-7	NH_3	350	819	32.9	851.9						
[$C_5H_{10}O_2$]	**5057-98-7**	**cis-1,2-cyclopentanediol**				**853.1**			**885.6**			**0**
89MEY/BUR	7664-41-7	NH_3					853.6	32	885.6			
[C_7H_7O]	**155174-22-4**	**3-OH-benzyl**				**853**			**885.5**			**0**
94HOK/YAN		kinetic method				853						
[$C_8H_9NO_2$]	**619-45-4**	**4-NH_2-C_6H_4-$COOCH_3$**				**853.0**			**883.9**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	33.5	853.0						
[$C_{10}H_{12}$]	**1195-32-0**	**4-$CH_3C_6H_4C(CH_3)CH_2$**				**852.9**			**881.8**			**12**
89GAL/SPE						849.4						
87TAF	7664-41-7	NH_3	350	819	34.8	852.9						
87TAF	7664-41-7	NH_3	350	819	34.8	852.9						
[C_2H_5NS]	**62-55-5**	**CH_3CSNH_2**				**852.8**			**884.6**			**2**
94DEC/EXN	2450-71-7	$HCCCH_2NH_2$	338	853.5	−1.8	851.4						
94DEC/EXN	74-89-5	CH_3NH_2	338	864.5	−9.3	854.8						
93ABB/MO	74-89-5	CH_3NH_2	333	864.5	−10.4	853.8						
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	−1.7	851.0						
[C_5H_4FN]	**372-48-5**	**2-F-pyridine**				**852.7**			**884.6**			**2**
91MAU/SIE	109-97-7	pyrrole	600	843.8	10.5	854.5	875.4	8.8	884.2	2.8	2.5	5.3
91MAU/SIE	288-42-6	oxazole	600	844.5	9.2	853.7	876.4	8.8	885.2	2	−0.4	1.6
91MAU/SIE	107-25-5	CH_2=CH-OCH_3	600	830.3	19.2	852.6	859.2	29.7	888.9	12	−17.2	−3.2
91MAU/SIE	62-53-3	$C_6H_5NH_2$	600	850.6	4.6	855.2	882.5	2.1	884.5	2	3.8	5.8
91AUE/WEB	110-86-1	pyridine	300	898.1	−46.9	851.3						
87TAF	7664-41-7	NH_3	350	819	33.9	852.4						
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	44.2	849.7						
83TAF	7664-41-7	NH_3	350	819	33.9	852.4						
83LOC/MCI	7664-41-7	NH_3	350	819	33.4	852.0						
79LOC/HUN	62-53-3	$C_6H_5NH_2$	382	850.6	1.5	852.1						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	−8.3	856.2						
75TAF	7664-41-7	NH_3	350	819	32.9	851.5						
75ARN	7664-41-7	NH_3	350	819	32.9	851.5						
[C_2H_5N]	**20729-41-3**	**CH_3CH=NH**				**852.6**			**885.1**			**0**
81ELL/DIX	108-42-9; 109-09-1	3-$CH_3C_6H_4NH_2$; 2-ClC_5H_4N				836-869						
79ELL/EAD	108-42-9; 109-09-1	3-$CH_3C_6H_4NH_2$; 2-ClC_5H_4N				836-869						
[$C_{13}H_{10}O$]	**119-61-9**	**$(C_6H_5)_2CO$**				**852.5**			**882.3**			**9**
87TAF	7664-41-7	NH_3	350	819	33.9	852.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GD(R)	ΔGD(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
85VAN/LEA		See Refs.										
83TAF	7664-41-7	NH_3	350	819	34.3	852.6						
[$C_2H_5NO_2$]	**56-40-6**	**glycine**				**852.2**			**886.5**			**−6**
94MCK/BEL	109-97-7; 62-53-3	pyrrole; $C_6H_5NH_2$				844-851						
93ZHA/ZIM	109-97-7; 62-53-3	pyrrole; $C_6H_5NH_2$	300			844-851						
93WU/LEB	62-53-3; 68-12-2	$C_6H_5NH_2$; $HCON(CH_3)_2$	300			851-857						
93LI/HAR		kinetic method							884.6			
92GOR/SPE	98-86-2; 109-97-7	acetophenone; pyrrole	350			829-844						
90ISA/OMO		kinetic method										
87TAF	7664-41-7	NH_3	350	819	37.5	856.5						
87BOJ		kinetic method										
83LOC/MCI	7664-41-7	NH_3	350	819	37.5	856.5						
79MAU/HUN	100-70-9	2-Pyridinecarbonitrile	570	841	7.9	851.1						
79MAU/HUN	62-53-3	$C_6H_5NH_2$	500	850.6	0	852.2	882.5	0	882.5	2	0	2
79LOC/HUN	62-53-3	$C_6H_5NH_2$	382	850.6	5.0	856.3						
[C_2H_5N]	**1761-67-7**	**CH_2=NCH_3**				**852.1**			**884.6**			**0**
90PEE/ING	62-53-3; 67-68-5	$C_6H_5NH_2$; $(CH_3)_2SO$				851-854						
[$C_{10}H_{16}S$]	**7519-74-6**	**thiocamphor**				**852.0**			**883.9**			**2**
93ABB/MO	7541-16-4	$(CH_3)_2NCOOCH_3$	333	847.3	2.5	849.9						
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	−3.5	849.2						
93ABB/MO	290-37-9	Pyrazine	333	847.0	4.3	851.5						
93ABB/MO	1121-37-5	$(c\text{-}C_4H_5)_2CO$	333	850.6	6.0	856.8						
[$C_9H_{18}S$]	**54396-69-9**	**$(t\text{-}C_4H_9)_2CS$**				**852.0**			**881.8**			**9**
93ABB/MO	2450-71-7	$HCCCH_2NH_2$	333	853.5	−2.4	850.6						
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	−0.4	852.1						
93ABB/MO	290-37-9	Pyrazine	333	847.0	6.4	853.4						
[C_7H_7O]	**3174-48-9**	**4-Me-phenoxy**				**852**			**884.5**			**0**
94HOK/YAN		kinetic method				852						
[$C_9H_9ClO_2$]	**37612-52-5**	**3-Cl-4-CH_3O-C_6H_3-$COCH_3$**				**851.9**			**883.7**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	22.6	851.9						
[$C_8H_8O_2$]	**99-93-4**	**4-HO-C_6H_4-$COCH_3$**				**851.9**			**883.7**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	22.6	851.9						
[$C_6H_{10}O_2$]	**110-13-4**	**$CH_3COCH_2CH_2COCH_3$**				**851.8**			**892.0**			**−26**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87BOU/HOP	372-48-5	2-F-pyridine	313	852.7	−3.8	849.3						
87BOU/HOP	100-48-1	4-Pyridinecarbonitrile	313	848.8	2.9	852.0						
83MAU	372-48-5	2-F-pyridine	600	852.7	−10.5	850.7	884.6	10.9	895.5	2	−35.6	−33.6
83MAU	109-97-7	pyrrole	600	843.8	2.3	854.7	875.4	16.3	891.7	2.8	−23.4	−20.6
[$C_7H_5O_2Rh$]	**12192-97-1**	**$(C_5H_5)Rh(CO)_2$**				**851.8**			**882.5**			**5.8**
81STE/BEA	7664-41-7	NH_3	320	819	33	851.8						
[C_4H_9N]	**4923-79-9**	**Azetidine, N-methyl-**				**851.7**			**882.5**			**5.6**
92ABB/CAN	2450-71-7	$HCCCH_2NH_2$	333	853.5	−0.2	852.9						
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	−2.3	850.3						
[C_6H_5]	**2396-01-2**	**phenyl radical**				**851.5**			**884**			**0**
88LIA/BAR									884			
87KIN/BUR	7732-18-5	H_2O		660.0			691	163	854			
87KIN/BUR	67-56-1	CH_3OH		724.5			754.3	118	872.3			
87KIN/BUR	7664-41-7	NH_3		819			853.6	21	874.6			
[C_4H_7NO]	**2679-13-2**	**N-methyl-2-azetidinone**				**851.3**			**882.2**			**5**
92ABB/CAN	290-37-9	Pyrazine	333	847.0	4.9	851.9						
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	−2.0	850.6						
[$C_{10}H_{12}O$]	**3637-01-2**	**$3,4\text{-}(CH_3)_2C_6H_3\text{-}COCH_3$**				**851.0**			**882.8**			**2**
93KUK/STR	122-00-9	$4\text{-}CH_3\text{-}C_6H_4\text{-}COCH_3$	320	843.6	6	849.6						
92MIS/KAN	98-86-2	$C_6H_5COCH_3$	308	829.3	23.0	852.3						
[$C_{10}H_{12}O$]	**89-74-7**	**$2,4\text{-}(CH_3)_2C_6H_3\text{-}COCH_3$**				**850.8**			**882.6**			**2**
93KUK/STR	122-00-9	$4\text{-}CH_3\text{-}C_6H_4\text{-}COCH_3$	320	843.6	7	850.6						
[$C_{12}H_{16}O$]	**943-27-1**	**$4\text{-}t\text{-}C_4H_9\text{-}C_6H_4\text{-}COCH_3$**				**850.6**			**882.5**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	21.3	850.6						
[$C_{10}H_{12}S$]	**#838**	**$3\text{-}(CH_3S)C_6H_4C(CH_3)=CH_2$**				**850.6**			**879.6**			**12**
87TAF	7664-41-7	NH_3	350	819	32.5	850.6						
[$C_7H_{10}O$]	**1121-37-5**	**$(c\text{-}C_3H_5)_2CO$**				**850.6**			**880.4**			**9**
87TAF	7664-41-7	NH_3	350	819	32.9	851.2						
83TAF	87-85-4	$(CH_3)_6\text{-}C_6$	350	836.0	13.3	850.1						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	41.0	823.1						
[C_6H_7N]	**62-53-3**	**$C_6H_5NH_2$**				**850.6**			**882.5**			**2**
91MAU/SIE	765-43-5	$c\text{-}C_3H_5COCH_3$	600	823	24.3	847.3	854.9	19.7	874.5	2	7.9	9.9
87TAF	7664-41-7	NH_3	350	819	31.6	850.2						
83TAF	7664-41-7	NH_3	350	819	31.6	850.2						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	0	850.6						
80MAU	7664-41-7	NH_3	550	819	24.3	841.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
79MAU/HUN	62-53-3	$C_6H_5NH_2$	500	850.6	0	850.6						
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−21.8	854.5						
79LOC/HUN	62-53-3	$C_6H_5NH_2$	382	850.6	0	850.6						
78LAU/SAL	7664-41-7	NH_3	600	819	28.9	845.3						
77POL/DEV	62-53-3	$C_6H_5NH_2$	350	850.6	0	850.6						
77COO/KRU		relative order-See Refs.										
76LAU/KEB	71-43-2	C_6H_6	600	725.4	107.1	839.4						
75TAF	7664-41-7	NH_3	350	819	32.9	851.5						
75ARN	7664-41-7	NH_3	350	819	32.9	851.5						
72BRI/YAM	7664-41-7	NH_3	600	819	37.2	853.7						
[C_4H_8Sc]	**114659-08-4**	**CH_2=C(CH_3)-ScCH_3**				**850.5**			**879.4**			**12**
89OSA/DEL	372-48-5	2-F-pyridine	313	852.7	−2.1	850.5						
[$C_5H_9O_3P$]	**1449-91-8**	**4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane**				**850.3**			**882.8**			**0**
80HOD/HOU	430-67-1; 107-47-1	$CF_2HCH_2NH_2$; $(t\text{-}C_4H_9)_2S$	320			837-864						
[$C_5H_6N_2O_2$]	**65-71-4**	**Thymine**				**850.0**			**880.9**			**5**
90GRE/LIG		kinetic method							880.9			
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−27.6	847.9						
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_9H_{18}NO$]	**2564-83-2**	**2,2,6,6-tetramethyl-1-piperidinyloxy radical**				**849.8**			**882.3**			**0**
95CHE/KAS	290-37-9; 372-48-5	Pyrazine(1,4-Diazine); 2-F-pyridine				847-853						
[$C_6H_{12}O_2$]	**823-18-7**	**cis-1,3-cyclohexandiol**				**849.7**			**882.2**			**0**
85GUE/HOU	110-63-4	$HO(CH_2)_4OH$	323	854.9	−3	849.7						
[$C_9H_{12}N_2O_4$]	**37687-24-4**	**3,5-diethoxycarbonylpyrazole**				**849.7**			**881.6**			**2**
92ABB/CAB	2450-71-7	$HCCCH_2NH_2$	333	853.5	−4.5	848.7						
92ABB/CAB	372-48-5	2-F-pyridine	333	852.7	−2.1	850.6						
[$C_{12}H_{18}Si$]	**17920-24-0**	**4-((CH_3)$_3$Si)$C_6H_4C(CH_3)$=CH_2**				**849.7**			**878.6**			**12**
87TAF	7664-41-7	NH_3	350	819	31.6	849.7						
[$C_{12}H_{18}Si$]	**40595-34-4**	**3-((CH_3)$_3$Si)$C_6H_4C(CH_3)$=CH_2**				**849.7**			**878.6**			**12**
87TAF	7664-41-7	NH_3	350	819	31.6	849.7						
[$C_6H_8O_2$]	**504-02-9**	**c-hexane-1,3-dione**				**849.4**			**881.2**			**2**
87BHOU/HOP	372-48-5	2-F-pyridine	313	852.7	−2.1	850.6						
87BOU/HOP	928-55-2	C_2H_5OCH=$CHCH_3$	313	847.7	1.3	849.1						
87BOU/HOP	141-79-7	$(CH_3)_2C$−CH(C=O)CH_3	313	846.9	1.3	848.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M-- Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
83MAU	372-48-5	2-F-pyridine	600	852.7	7.5	860.3						
83MAU	109-97-7	pyrrole	600	843.8	14.2	858.3						
[C_4H_7NO]	**79-39-0**	**2-propenamide, 2-methyl-**				**849.4**			**880.4**			**5**
90WOL/GRU	62-53-3	$C_6N_5NH_2$	320	850.6	−1.3	849.2						
90WOL/GRU	122-00-9	4-CH_3-C_6H_4-$COCH_3$	320	843.6	5.9	849.5						
[$C_8H_8O_2$]	**123-11-5**	**4-$CH_3OC_6H_4CHO$**				**849.3**			**881.1**			**2**
87TAF	7664-41-7	NH_3	350	819	30.7	849.2						
87TAF2	7664-41-7	NH_3	350	819	45.3	863.9						
[$C_6H_4N_2$]	**100-48-1**	**4-Pyridinecarbonitrile**				**848.8**			**880.6**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−49.3	848.8						
87TAF	7664-41-7	NH_3	350	819	29.7	848.3						
86TAF/ANV	100-48-1	4-Pyridinecarbonitrile	350	848.8	0	848.8						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	−14.2	850.3						
75TAF	7664-41-7	NH_3	350	819	29.7	848.3						
75ARN	7664-41-7	NH_3	350	819	29.7	848.3						
[C_9H_8ClOS]	**32467-66-6**	**3-Cl-4-CH_3S-C_6H_3-$COCH_3$**				**848.6**			**880.4**			**2**
92MIS/KAN	98-86-2	$C_6H_5COCH_3$	308	829.3	18.8	848.1						
[$C_{12}H_{18}Si$]	**94397-80-5**	**4-CH_3-C_6H_4-$C(Si(CH_3)_3)=CH_2$**				**848.1**			**877.0**			**12**
92MIS/ARI2	100-70-9	2-Pyridinecarbonitrile	308	841	7.9	848.9						
92MIS/ARI2	100-48-1	4-Pyridinecarbonitrile	308	848.8	−0.8	847.8						
92MIS/ARI2	100-54-9	3-Pyridinecarbonitrile	308	845.1	2.5	847.5						
[$C_3H_7NO_2$]	**5806-90-6**	**Acetamide, N-methoxy**				**848.0**			**879.0**			**5**
92DEC/EXN	109-97-7	pyrrole	338	843.8	4.0	847.7						
92DEC/EXN	68-12-2	$(CH_3)_2NCHO$	338	856.6	−7.7	848.9						
[$C_3H_6F_3N$]	**2730-67-8**	**$CF_3CH_2NHCH_3$**				**848.0**			**881.1**			**−2**
87TAF	7664-41-7	NH_3	350	819	28.8	847.6						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−16.1	848.4						
75TAF	7664-41-7	NH_3	350	819	28.8	847.6						
[$C_5H_{10}O$]	**4696-26-8**	**trans-$CH_3CH=CH$-OC_2H_5**				**848.0**			**876.9**			**12**
89OSA/DEL	114659-08-4	$CH_2=C(CH_3)$-$SeCH_3$	313	850.5	−2.5	848.0						
[$C_5H_{10}O$]	**928-55-2**	**$C_2H_5OCH=CHCH_3$**				**847.7**			**876.6**			**12**
86BOU/DJA	141-79-7	$(CH_3)_2C=CH(C=O)CH_3$	313	846.9	!	847.7						
[C_3O]	**11127-17-6**	**CCCO**				**847.7**			**880.2**			**0**
93MAC/SUD		theory	298						880.2			
89BOT		theory	298						885±5			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_2H_3N_3$]	**288-36-8**	**1,2,3-triazole**				**847.4**			**879.3**			**2**
88CAT/CLA	372-48-5	2-F-pyridine	~300	852.7	−6.7	846.0						
88CAT/CLA	68-12-2	$(CH_3)_2NCHO$	~300	856.6	−7.1	849.5						
88CAT/CLA	100-54-9	3-Pyridinecarbonitrile	~300	845.1	1.7	846.8						
[C_4H_9NO]	**6281-94-3**	**n-C_3H_7NHCHO**				**847.4**			**878.4**			**5**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−17.1	847.4						
[$C_4H_9NO_2$]	**7541-16-4**	**$(CH_3)_2NCOOCH_3$**				**847.3**			**878.3**			**5**
87TAF	7664-41-7	NH_3	350	819	28.8	847.3						
[$C_6H_4N_2O$]	**14906-64-0**	**3-cyano-pyridine-1-oxide**				**847.1**			**879.6**			**0**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	−46.0	847.1						
[$C_4H_4N_2$]	**290-37-9**	**Pyrazine**				**847.0**			**877.1**			**7.8**
86TAF	7664-41-7	NH_3	350	819	25.9	844.2						
83TAF2	7664-41-7	NH_3	350	819	27.9	846.2						
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−25.1	849.7						
[$C_6H_{10}O$]	**141-79-7**	**$(CH_3)_2C{=}CH(C{=}O)CH_3$**				**846.9**			**878.7**			**2**
88BOU/DJA	100-48-1	4-Pyridinecarbonitrile	313	848.8	−1.7	847.1						
88BOU/DJA	372-48-5	2-F-pyridine	313	852.7	−6.3	846.4						
86KAM/YOU	108-20-3	$(i\text{-}C_3H_7)_2O$	333	828.1	8.6	837.2						
[C_6H_6IN]	**626-01-7**	**3-I-$C_6H_4NH_2$**				**846.8**			**878.7**			**2**
81LAU/NIS	62-53-3	$C_5H_5NH_2$	600	850.6	−3.8	846.8						
[C_4H_9NO]	**563-83-7**	**i-$C_3H_7CONH_2$**				**846.7**			**878.6**			**2**
97HOM/HER	100-48-1	4-Pyridinecarbonitrile	333	848.8	1.5	850.2						
97HOM/HER	100-70-9	2-Pyridinecarbonitrile	333	841	−1.1	839.9						
97HOM/HER	2450-71-7	$HCCCH_2NH_2$	333	853.5	−3.2	850.0						
97HOM/HER	678-48-9	$(CH_3)_2NCOOC_2H_5$	333	865.6	−3.4	862.3						
[$C_6H_{14}S$]	**625-80-9**	**$(i\text{-}C_3H_7)_2S$**				**846.6**			**876.4**			**9**
87TAF	7664-41-7	NH_3	350	819	28.4	846.6						
83TAF2	7664-41-7	NH_3	350	819	28.4	846.6						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−18.1	846.4						
[$C_{14}H_{10}$]	**120-12-7**	**Anthracene**				**846.6**			**877.3**			**5.8**
85VAN/LEA		See Refs.										
80MAU	151-18-8	$H_2N(CH_2)_2CN$	482	832.5	1.3	831.8						
80MAU	62-53-3	$C_6H_5NH_2$	482	850.6	−3.3	846.6						
[$C_6H_8N_2O_2$]	**37622-90-5**	**4-(C_2H_5COO)-pyrazole**				**846.5**			**880.7**			**−5.8**
94NOT/HER	2450-71-7	$HCCCH_2NH_2$	333	853.5	−7.5	846.0						
94NOT/HER	372-48-5	2-F-pyridine	333	852.7	−6.3	846.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSqnib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
94NOT/HER	544-40-1	$(n\text{-}C_3H_7)_2S$	333	842.1	3.8	846.3						
[C_7H_6FNO]	**824-76-9**	**4-F-$C_6H_4CONH_2$**				**846.3**			**877.2**			**5**
94GRU/CAL	106-47-8; 62-53-3	4-Cl-$C_6H_4NH_2$; $C_6H_5NH_2$				842-851						
[C_7H_6ClNO]	**619-56-7**	**4-Cl-$C_6H_4CONH_2$**				**846.3**			**877.2**			**5**
94GRU/CAL	106-47-8; 62-53-3	4-Cl-$C_6H_4NH_2$; $C_6H_5NH_2$				842-851						
[C_7H_6ClNO]	**618-48-4**	**3-Cl-$C_6H_4CONH_2$**				**846.3**			**877.2**			**5**
94GRU/CAL	106-47-8; 62-53-3	4-Cl-$C_6H_4NH_2$; $C_6H_5NH_2$				842-851						
[C_7H_6FNO]	**455-37-8**	**3-F-$C_6H_4CONH_2$**				**846.3**			**877.2**			**5**
94GRU/CAL	106-47-8; 62-53-3	4-Cl-$C_6H_4NH_2$; $C_6H_5NH_2$				842-851						
[$C_6H_{10}N_2$]	**1530-87-6**	**Piperidine, 1-carbonitrile-**				**846.1**			**876.7**			**6**
93BER/HEL	544-40-1	$(n\text{-}C_3H_9)_2S$	~338	842.1	2.1	844.3						
93BER/HEL	290-37-9	Pyrazine	~338	847.0	0.8	847.9						
[C_7H_7O]	**155174-21-3**	**2-OH-benzyl**				**846**			**878.5**			**0**
94HOK/YAN		kinetic method				846						
[$C_{13}H_{18}$]	**31006-98-1**	**α-t-butylstyrene,4-CH_3**				**845.7**			**874.6**			**12**
92NAK/NOM	100-48-1	4-Pyridinecarbonitrile	343	848.8	−2.1	846.2						
92NAK/NOM	100-54-9	3-Pyridinecarbonitrile	343	845.1	0.8	845.5						
[$C_2H_5N_5$]	**871-31-8**	**CH_3CH_2NNN**				**845.5**			**878**			**0**
89ATT/CAC		See Refs.	358						878±21			
[$C_{14}H_{20}$]	**146558-41-0**	**α-t-butylstyrene,3,5-dimethyl**				**845.5**			**874.3**			**12**
92NAK/NOM	100-54-9	3-Pyridinecarbonitrile	343	845.1	1.3	845.9						
92NAK/NOM	123-54-6	$CH_3COCH_2COCH_3$	343	836.8	9.6	845.3						
[$C_3H_7NO_2$]	**13115-24-7**	**Acetamide, N-hydroxy-N-methyl**				**845.3**			**876.2**			**5**
92DEC/EXN	289-95-2	Pyrimidine	338	855.7	−10.1	845.6						
92DEC/EXN	109-97-7	pyrrole	338	843.8	1.3	845.1						
[C_3H_7NO]	**79-05-0**	**$C_2H_5CONH_2$**				**845.3**			**876.2**			**5**
97HOM/HER	111-47-7	$(n\text{-}C_4H_9)_2S$	333	834.9	6.7	841.7						
97HOM/HER	1121-37-5	$(c\text{-}C_5H_9)_2CO$	333	850.6	0.9	851.7						
97HOM/HER	290-37-9	Pyrazine	333	847.0	−3.7	843.4						
97HOM/HER	625-80-9	$(i\text{-}C_3H_7)_2S$	333	846.6	−1.0	845.8						
97HOM/HER	372-48-5	2-F-pyridine	333	852.7	−9.0	843.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{22}H_{12}$]	**191-24-2**	**1,12-Benzoperylene**				**845.2**			**876.0**			**5.8**
80MAU	62-53-3	$C_6H_5NH_2$	508	850.6	0	849.8						
80MAU	7664-41-7	NH_3	550	819	24.7	840.6						
[$C_6H_4N_2$]	**100-54-9**	**3-Pyridinecarbonitrile**				**845.1**			**877.0**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−52.7	845.4						
87TAF	7664-41-7	NH_3	350	819	26.1	844.7						
83TAF2	7664-41-7	NH_3	350	819	25.6	844.2						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	−19.5	845.0						
75TAF	7664-41-7	NH_3	350	819	27.0	845.6						
75ARN	7664-41-7	NH_3	350	819	27.0	845.6						
[C_7H_7O]	**41115-75-7**	**3-Me-phenoxy**				**845**			**877.5**			**0**
94HOK/YAN		kinetic method				845						
[$C_{11}H_{14}O_2$]	**13544-66-6**	**3,4,5-$(CH_3)_3$-C_6H_2-CO_2CH_3**				**844.6**			**875.5**			**5**
96DEC/EXN	62-53-3	$C_6H_5NH_2$	338	850.6	−5	845.5						
96DEC/EXN	23617-71-2	2,4-$(CH_3)_2$-C_6H_3-$COOCH_3$	338	837.2	7.3	844.5						
96DEC/EXN	111-47-7	$(n\text{-}C_3H_7)_2S$	338	834.9	8.6	843.7						
[C_3H_3NO]	**288-42-6**	**oxazole**				**844.5**			**876.4**			**2**
91MAU/SIE	62-53-3	$C_6H_5NH_2$	600	850.6	−3.8	846.8	882.5	−9.2	873.2	2	9.2	11.2
91MAU/SIE	372-48-5	2-F-pyridine	600	852.7	−9.2	843.5	884.6	−8.8	875.8	2	0.4	2.4
91MAU/SIE	765-43-5	c-$C_3H_5COCH_3$	600	823	19.7	842.7	854.9	17.6	872.4	2	3.3	5.3
91MAU/SIE	109-97-7	pyrrole	600	843.8	3.3	847.4	875.4	0.4	875.8	2.8	4.2	7.0
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	36.4	841.9						
[$C_{10}H_{12}O$]	**5379-15-8**	**3,5-(CH_3)=C_6H_3-$COCH_3$**				**844.2**			**876.0**			**2**
93KUK/STR	122-00-9	4-CH_3-C_6H_4-$COCH_3$	320	843.6	−1	842.6						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	15.9	845.2						
[$C_{22}H_{24}$]	**77387-50-9**	**1,16-Dimethyldodecahedrane**				**844.0**			**876.5**			**0**
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	31.4	844.0						
[C_4H_5N]	**109-97-7**	**pyrrole**				**843.8**			**875.4**			**2.8**
97EAS/SMI		theory	298									2.8
93SZU/MCM	7664-41-7	NH_3	600	819	29.7	845.6	853.6	23.8	877.4	−6.4	9.6	3.2
93SZU/MCM	74-89-5	CH_3NH_2	600	864.5	−15.9	845.6	899.0	−25.9	873.1	−7	16.3	9.3
91MAU/SIE	7664-41-7	NH_3	600	819	28.5	844.7	853.6	20.9	874.5	6.4	12.6	6.2
91MAU/SIE	765-43-5	c-$C_3H_5COCH_3$	600	823	15.9	838.7	854.9	20.9	875.8	2	−7.9	−5.9
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	35.1	840.4						
81HOU/SCH	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−26.8	849.2						
79LAU	7664-41-7	NH_3	650	819	25.4	841.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
79AUE/BOW	7664-41-7	NH_3	298	819	25.4	844.4					
73YAM/KEB	7664-41-7	NH_3	600	819	29.9	846.2					
[C_7H_8S]	**100-68-5**	**$C_6H_5SCH_3$**				**843.7**			**872.6**		**12**
87TAF	7664-41-7	NH_3	350	819	25.6	843.7					
[$C_{10}H_{12}O$]	**25108-57-0**	**3-$CH_3OC_6H_4C(CH_3)=CH_2$**				**843.7**			**872.6**		**12**
87TAF	7664-41-7	NH_3	350	819	25.6	843.7					
[$C_9H_{10}O$]	**122-00-9**	**4-CH_3-C_6H_4-$COCH_3$**				**843.6**			**875.5**		**2**
87TAF	7664-41-7	NH_3	350	819	25.2	843.7					
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	16.3	845.6					
81BRO/ABB	7664-41-7	NH_3	320	819	22.2	841.0					
[$C_6H_4N_2O$]	**14906-59-3**	**4-cyano-pyridine-1-oxide**				**842.7**			**873.4**		**5.8**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	−50.2	842.7					
[$C_{10}H_{12}O$]	**2142-71-4**	**2,3-$(CH_3)=C_6H_3$-$COCH_3$**				**842.7**			**874.6**		**2**
93KUK/STR	122-00-9	4-CH_3-C_6H_4-$COCH_3$	320	843.6	−1	842.6					
[C_4H_{10}]	**4663-22-3**	**c-$C_3H_5C(CH_3)=CH_2$**				**842.7**			**871.6**		**12**
87TAF	7664-41-7	NH_3	350	819	25.2	843.2					
83TAF2	7664-41-7	NH_3	350	819	25.6	843.7					
79AUE/BOW	7664-41-7	NH_3	298	819	22.0	841.0					
[$C_5H_4N_2O_2$]	**1122-61-8**	**4-(NO_2)-pyridine**				**842.5**			**874.3**		**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−56.1	842.0					
87TAF	7664-41-7	NH_3	350	819	22.9	841.5					
83TAF2	7664-41-7	NH_3	350	819	22.9	841.5					
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−19.5	845.0					
75TAF	7664-41-7	NH_3	350	819	23.8	842.4					
75ARN	7664-41-7	NH_3	350	819	23.8	842.4					
72TAA/HEN	110-86-1	pyridine	320	898.1	−75.7	822.4					
[$C_{10}H_{12}$]	**26444-18-8**	**3-$CH_3C_6H_4C(CH_3)=CH_2$**				**842.4**			**871.3**		**12**
87TAF	7664-41-7	NH_3	350	819	24.3	842.3					
[$C_8H_{18}S$]	**544-40-1**	**$(n\text{-}C_4H_9)_2S$**				**842.1**			**871.8**		**9**
87TAF	7664-41-7	NH_3	350	819	23.8	842.0					
[C_7H_7O]	**3174-49-0**	**2-Me-phenoxy**				**842**			**874.5**		**0**
94HOK/YAN		kinetic method				842					
[C_6H_6ClN]	**106-47-8**	**4-$ClC_6H_4NH_2$**				**842.0**			**873.8**		**2**
87TAF	7664-41-7	NH_3	350	819	23.3	841.9					
83TAF2	7664-41-7	NH_3	350	819	23.3	841.9					

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YtSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
77SUM/POL	7664-41-7	NH_3	350	819	24.7	843.3						
75TAF	7664-41-7	NH_3	350	819	24.7	843.3						
75ARN	7664-41-7	NH_3	350	819	24.7	843.3						
[$C_{12}H_{16}N_2O_6$]	**362-43-6**	**2′,3′-O-isopropylideneuridine**				**841.7**			**874.2**			**0**
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_9H_{14}N_2O_6$]	**5627-05-4**	**5,6-Dihydrouridine**				**841.7**			**874.2**			**0**
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_5H_3ClN_4$]	**87-42-3**	**6-Chloropurine**				**841.7**			**873.6**			**2**
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_4H_4N_2O$]	**557-01-7**	**2(1H)-Pyrimidinone**				**841.7**			**872.7**			**5**
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_4H_4N_2O_2$]	**66-22-8**	**Uracil**				**841.7**			**872.7**			**5**
75WIL/MCC	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_{10}H_{12}O$]	**2142-73-6**	**2,5-$(CH_3)_2C_6H_3$-$COCH_3$**				**841.6**			**873.5**			**2**
93KUK/STR	122-00-9	4-CH_3-C_6H_4-$COCH_3$	320	843.6	−2	841.6						
[$C_7H_{16}O$]	**17348-59-3**	**(i-C_3H_7)O(t-C_4H_9)**				**841.5**			**870.7**			**11**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−22.9	841.5						
[C_6H_6BrN]	**591-19-5**	**3-Br$C_6H_4NH_2$**				**841.4**			**873.2**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−9.2	841.4						
[$C_{10}H_{10}Fe$]	**102-54-5**	**$(C_5H_5)_2Fe$**				**841.3**			**863.6**			**34**
89MAU	372-48-5	2-F-pyridine	600	852.7	0.4	843.5	884.6	−15.1	869.5	2	25.9	27.9
89MAU	109-97-7	pyrrole	600	843.8	5.0	839.5	875.4	−9.2	866.2	2.8	23.4	26.2
88IKO/SUN	98-86-2	$C_6H_5COCH_3$	500	829.3	19.2	842.1	861.1	−2.5	858.6	2	43.5	45.5
88IKO/SUN	626-60-8	3-Cl-pyridine	500	871.5	−25.1	840.0	903.4	−36.0	867.4	2	35	37
88IKO/SUN	68-12-2	$(CH_3)_2NCHO$	500	856.6	−7.1	843.7						
88IKO/SUN	109-97-7	pyrrole	500	843.8	7.9	845.5						34.2
75FOS/BEA2	4143-41-3; 74-89-5	(E)-$CH_3N{=}NCH_3$; CH_3NH_2				834-864						
[C_8H_{14}]	**72014-90-5**	**$(CH_3)_2C{=}C(CH_3)C(CH_3){=}CH_2$**				**841.0**			**869.9**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	22.0	841.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M– Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_4H_{10}O_3$]	**3068-00-6**	**$HOCH_2CH(OH)CH_2CH_2OH$**				**841**			**905.9**			**−109**
86SUN/KUL		See Refs.	300			841			904			
[$C_6H_4N_2$]	**100-70-9**	**2-Pyridinecarbonitrile**				**841**			**872.9**			**2**
91AUE/WEB	110-86-1	pyridine	300	898.1	−56.1	842.0						
87TAF	7664-41-7	NH_3	350	819	20.1	838.7						
83TAF2	7664-41-7	NH_3	320	819	18.0	836.8						
79MAU/HUN	62-53-3	$C_6H_5NH_2$	350	850.6	−8.7	841.9						
76AUE/WEB2	74-89-5	CH_3NH_2	298	864.5	−22.5	842.0						
[C_2S]	**12602-41-4**	**C_2S**				**840.7**			**869.9**			**12**
92MAC/SUD		theory	298						869.6			
[C_4H_8O]	**109-92-2**	**$C_2H_5OCH{=}CH_2$**				**840.4**			**870.1**			**9.5**
94KOP/ANV	541-10-1	$(n\text{-}C_4H_9)_2S$	373	842.1	−0.4	841.6						
94KOP/ANV	111-47-7	$(n\text{-}C_3H_7)_2S$	373	834.9	3.3	838.3						
91MAU/SHI	288-42-6	oxazole	600	844.5	−0.4	841.8	876.4	−4.6	871.8	2	7.5	9.5
91MAU/SHI	372-48-5	2-F-pyridine	600	852.7	−10.5	840.0	884.6	−15.1	869.5	2	7.1	9.1
86BOT/DJA	622-97-9	$4\text{-}CH_3\text{-}C_6H_4\text{-}CH{=}CH_2$	313	832.8	0	832.9						
[$C_{16}H_{10}$]	**129-00-0**	**Pyrene**				**840.1**			**869.2**			**11.5**
85VAN/LEA		See Refs.										
80MAU	151-18-8	$H_2N(CH_2)_2CN$	549	832.5	9.6	838.0						
80MAU	62-53-3	$C_6H_5NH_2$	514	850.6	−6.3	842.3						
[ClHCl]	**2108-20-5**	**ClHCl**				**839.9**			**874.1**			**−5.8**
85LIA/KAR	98-86-2; 62-53-3	$CH_3COC_6H_5$; $C_6H_5NH_2$				829-851						
[C_3H_5NO]	**79-06-1**	**2-propenamide**				**839.8**			**870.7**			**5**
90WOL/GRU	122-00-9	$4\text{-}CH_3\text{-}C_6H_4\text{-}COCH_3$	320	843.6	−3.4	840.2						
90WOL/GRU	98-83-9	$C_6H_5\text{-}C(CH_3){=}CH_2$	320	835.3	3.9	839.3						
[C_6H_6FN]	**371-40-4**	**$4\text{-}F\text{-}C_6H_4NH_2$**				**839.7**			**871.5**			**2**
87TAF	7664-41-7	NH_3	350	819	21.1	839.6						
81TAA/SUM	7664-41-7	NH_3	320	819	19.2	838.1						
75TAF	7664-41-7	NH_3	350	819	22.9	841.5						
75ARN	7664-41-7	NH_3	350	819	22.9	841.5						
[$C_9H_{10}O_3$]	**121-98-2**	**$4\text{-}CH_3O\text{-}C_6H_4\text{-}COOCH_3$**				**839.6**			**870.6**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	20.1	839.6						
[C_9H_7ClO]	**120136-29-0**	**$3\text{-}Cl\text{-}4\text{-}CH_3O\text{-}C_6H_3\text{-}CCH$**				**839.5**			**871.9**			**0**
92MIS/ARI	536-74-3	$C_6H_5\text{-}CCH$	323	801.3	38.1	839.5						
[C_9H_7FO]	**120136-28-9**	**$3\text{-}F\text{-}4\text{-}CH_3O\text{-}C_6H_3\text{-}CCH$**				**839.5**			**871.9**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

{Formula} YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	38.1	839.5						
[$C_{12}H_{18}Si$]	**120093-92-7**	**3-CH_3-C_6H_4-C(Si(CH_3)$_3$)=CH_2**				**839.4**			**868.3**			**12**
92MIS/ARI2	123-54-6	$CH_3COCH_2COCH_3$	308	836.8	2.5	839.1						
92MIS/ARI2	108-20-3	(i-C_3H_7)$_2$O	308	828.1	10.0	838.2						
92MIS/ARI2	100-70-9	2-Pyridinecarbonitrile	308	841	0	840.9						
[$C_9H_{10}O_2$]	**586-37-8**	**3-CH_3O-C_6H_4-$COCH_3$**				**839.3**			**871.2**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	10.0	839.3						
[$C_{10}H_{12}$]	**1124-20-5**	**Benzene, 1-methyl-3-(1-methylethenyl)-**				**838.7**			**867.6**			**12**
89GAL/SPI		See Refs.				838.7						
[$C_8H_{18}O$]	**6863-58-7**	**(sec-C_4H_9)$_2$O**				**838.5**			**865.9**			**17**
82MAU	111-43-3	(n-C_3H_7)$_2$O	335	810.5	28.0	838.5						
[$C_{13}H_{18}$]	**146558-42-1**	***α*-t-butylstyrene,3-CH_3**				**838.5**			**867.4**			**12**
92NAK/NOM	123-54-6	$CH_3COCH_2COCH_3$	343	836.8	3.8	839.5						
92NAK/NOM	108-20-3	(i-C_3H_7)$_2$O	343	828.1	9.2	837.6						
[C_5H_9N]	**7188-38-7**	**t-C_4H_9NC**				**838.3**			**870.7**			**0.1**
86MAU/KAR	62-53-3	$C_6H_5NH_2$	335	850.6	−9.2	841.5						
86MAU/KAR	109-97-7	pyrrole	335	843.8	−3.8	840.1						
86MAU/KAR	108-20-3	(i-C_3H_7)$_2$O	335	828.1	4.6	833.3						
[C_6H_8O]	**20843-07-6**	**3,4-dimethylfuran**				**838.3**			**869.0**			**5.8**
85HOU/ROL	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	1.7	838.3						
[$C_8H_{12}O$]	**4694-17-1**	**5,5-Dimethylcyclohex-2-ene-1-one**				**837.9**			**869.8**			**2**
87TAF	7664-41-7	NH_3	350	819	19.2	837.8						
86TAF/GAL	7664-41-7	NH_3	350	819	19.4	837.9						
[$C_{10}H_{12}O_2$]	**38404-42-1**	**3,4-(CH_3)$_3$-C_6H_3-CO_2CH_3**				**837.5**			**868.5**			**5**
96DEC/EXN	111-47-7	(n-C_3H_7)$_2$S	338	834.9	1.4	836.5						
96DEC/EXN	123-54-6	$CH_3COCH_2COCH_3$	338	836.8	2.4	838.5						
96DEC/EXN	108-20-3	(i-C_3H_7)$_2$O	338	828.1	9	837.6						
[$C_5H_4N_2O_3$]	**1124-33-0**	**4-(NO_2)-pyridine-1-oxide**				**837.3**			**868.0**			**5.8**
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	−55.6	837.3						
[$C_{10}H_{12}O_2$]	**23617-71-2**	**2,4-(CH_3)$_2$-C_6H_3-$COOCH_3$**				**837.2**			**868.2**			**5**
93DEC/ERT	108-20-3	(i-C_3H_7)$_2$O	338	828.1	9.3	837.9						
93DEC/ERT	111-47-1	(n-C_3H_7)$_2$S	338	834.9	1.5	836.6						
[$C_5H_8O_2$]	**123-54-6**	**$CH_3COCH_2COCH_3$**				**836.8**			**873.5**			−14
93DEC/ERT	89-71-4	2-CH_3-$C_6H_4COOCH_3$	338	827.3	7	835.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	16.9	836.3						
83TAF2	7664-41-7	NH_3	350	819	18.5	837.9						
83MAU	111-47-7	$(n\text{-}C_3H_7)_2S$	600	834.9	−2.5	839.3	864.7	5.0	869.7	9	−12.6	−3.6
83MAU	109-97-7	pyrrole	600	843.8	−10.7	838.1	875.4	−0.4	875.0	2.8	−17.2	−14.4
83CAS/KIM	111-43-3	$(N\text{-}C_3H_7)_2O$	323	810.5	23.8	835.1						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−27.3	837.1						
[V]	**7440-62-2**	**V**				**836.8**			**859.4**			**33**
85ELK/ARM									859±6			
[$C_2H_5F_2N$]	**430-67-1**	**$CF_2HCH_2NH_2$**				**836.6**			**870.5**			**−5.1**
86TAF	7664-41-7	NH_3	320	819	17.2	836.1						
83TAF2	7664-41-7	NH_3	350	819	18.3	837.2						
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−27.8	836.7						
75TAF	7664-41-7	NH_3	350	819	19.2	838.2						
75ARN	7664-41-7	NH_3	350	819	19.2	838.2						
[$C_9H_{10}O$]	**585-74-0**	**3-CH_3-C_6H_4-$COCH_3$**				**836.4**			**868.2**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	7.1	836.4						
[$C_4H_7O_3P$]	**280-45-5**	**2,6,7-Trioxa-1-phosphabicyclo[2.2.2.]octane**				**836.4**			**868.8**			**0**
80HOD/HOU	87-85-4	$(CH_3)_6$-C_6	320	836.0	0	836.5						
80HOD/HOU	123-54-6	$CH_3COCH_2COCH_3$	320	836.8	0	836.6						
[C_6H_8ClN]	**108-42-9**	**3-Cl-$C_6H_4NH_2$**				**836.3**			**868.1**			**2**
87TAF	7664-41-7	NH_3	350	819	18.8	837.3						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−13.0	837.6						
79LAU	7664-41-7	NH_3	650	819	17.7	833.7						
77SUM/POL	7664-41-7	NH_3	350	819	18.3	835.9						
75ARN	7664-41-7	NH_3	350	819	20.6	839.2						
[C_5H_8O]	**34314-83-5**	**4-Methyl-2,3-dihydrofuran**				**836.2**			**868.6**			**0**
86BOU/DJA	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	−0.5	836.2						
[$C_{12}H_{16}O_2$]	**26537-19-9**	**4-t-C_4H_9-C_6H_4-$COOCH_3$**				**836.2**			**867.1**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	17.2	836.7						
[C_9H_7ClS]	**120136-30-3**	**3-Cl-4-CH_3S-C_6H_3-CCH**				**836.1**			**868.6**			**0**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	34.7	836.1						
[$C_8H_{11}ClO$]	**17530-69-7**	**3-Chloro-5,5-dimethylcyclohexen-2-one**				**836.0**			**867.9**			**2**
87TAF	7664-41-7	NH_3	350	819	17.4	836.0						
[$C_{12}H_{18}$]	**87-85-4**	**$(CH_3)_6$-C_6**				**836.0**			**860.6**			**26.4**
87TAF	7664-41-7	NH_3	350	819	19.7	837.0						
86STO/LI	527-53-7	1,2,3,5-$(CH_3)_4$-C_6H_2	300	816.5	19.2	835.8	845.6	14.6	860.2	11.4	16.1	27.5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
86STO/LI	700-12-9	$(CH_3)_5$-C_6H	300	823.5	11.3	834.8	850.7	8.8	859.5	17.6	7.7	25.3
83TAF	7664-41-7	NH_3	350	819	19.2	836.6						
77WOL/ABB	630-08-0	CO	350			836.8						
76WOL/DEV	71-43-2	C_6H_6	320	725.4	105.0	830.4						
75WOL/HAR	7664-41-7	NH_3	350	819	22.0	839.3						
[C_6H_{10}]	**1118-58-7**	**$CH_3CH{=}CHC(CH_3){=}CH_2$**				**836**			**864.9**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	17.1	836.1						
[$C_8H_6F_3NO$]	**1801-10-1**	**3-CF_3-$C_6H_4CONH_2$**				**836.0**			**866.9**			**5**
94GRU/CAL	108-20-3; 109-97-7	$(i\text{-}C_3H_7)_2O$; pyrrole				828-844						
[C_7H_5N]	**931-54-4**	**C_6H_5NC**				**836.0**			**868.4**			**0**
86MAU/KAR	108-20-3; 109-97-7	$(i\text{-}C_3H_7)_2O$; pyrrole	335			828-844						
[$C_9H_{10}O$]	**93-55-0**	**$C_6H_5COC_2H_5$**				**835.6**			**867.4**			**2**
87TAF	7664-41-7	NH_3	350	819	16.9	835.5						
[C_6H_6FN]	**372-19-0**	**3-F-$C_6H_4NH_2$**				**836.6**			**867.3**			**2**
87TAF	7664-41-7	NH_3	350	819	16.0	834.6						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−13.4	837.2						
77SUM/POL	7664-41-7	NH_3	350	819	16.0	834.6						
[C_9H_{10}]	**98-83-9**	**C_6H_5-$C(CH_3){=}CH_2$**				**835.3**			**864.2**			**12**
87TAF	7664-41-7	NH_3	350	819	16.0	834.1						
86SAN/BAL	108-20-3	$(i\text{-}C_3H_7)_2O$	428	828.1	8.4	837.1						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	28.9	840.0						
78TAF/WOL	7664-41-7	NH_3	320	819	15.1	833.7						
77WOL/ABB	87-85-4	$(CH_3)_6$-C_6	350	836.0	−4.6	832.2						
75WOL/HAR	7664-41-7	NH_3	350	819	16.5	834.6						
75TAF	7664-41-7	NH_3	350	819	16.5	834.6						
[$C_{11}H_{14}O_3$]	**2282-84-0**	**2,4,6-$(CH_3)_3$-C_6H_2-$COOCH_3$**				**836.3**			**866.3**			*5*
93DEC/ERT	111-47-7	$(n\text{-}C_3H_7)_2S$	338	834.9	−0.2	834.9						
93DEC/ERT	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	7.1	835.7						
[C_6H_8O]	**625-86-5**	**2,5-dimethylfuran**				**835.2**			**865.9**			**5.8**
86MAU		See Refs.	600			843.5						
85HOU/ROL	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	1.3	837.9						
83MAU	109-97-7	pyrrole	600	843.8	−10.0	832.9						
[$C_{24}H_{12}$]	**191-07-1**	**Coronene**				**835.0**			**861.3**			**20.6**
80MAU	151-18-8	$H_2N(CH_2)_2CN$	548	832.5	4.6	830.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
80MAU	62-53-3	$C_6H_5NH_2$	547	850.6	−6.7	839.3						
[$C_6H_{14}S$]	**111-47-7**	**(n-C_3H_7)$_2$S**				**834.9**			**864.7**			**9**
96DEC/EXN	62-53-3	$C_6H_5NH_2$	338	850.6	−13.8	836.5						
86TAF	7664-41-7	NH_3	320	819	14.6	833.3						
83TAF2	7664-41-7	NH_3	350	819	14.2	832.4						
[$C_3H_3ClN_2$]	**15965-31-8**	**4-Cl-pyrazole**				**834.9**			**868.5**			**−3.8**
94NOT/HER	123-54-6	$CH_3COCH_2COCH_3$	333	836.8	−1.6	834.9						
94NOT/HER	544-40-1	(n-C_4H_9)$_2$S	333	842.1	−7.2	835.3						
[$C_2H_6B_4$]	**20693-67-8**	**1,6-$C_2B_4H_6$**				**834.8**			**863.8**			**11.5**
80DIX	7664-41-7; 62-53-3	NH_3; $C_6H_5NH_2$				819-851						
[$C_9H_{10}OS$]	**1441-99-2**	**3-CH_3S-C_6H_4-$COCH_3$**				**834.7**			**866.6**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	5.4	834.7						
[$C_6H_{10}O$]	**1567-72-2**	**3-methyl-3-penten-2-one(Z)**				**834.5**			**866.4**			**2**
88BOU/DJA	110-87-2	2H-Pyran, 3, 4-dihydro-	313	833.4	0.4	833.7						
88BOU/DJA	625-86-5	2,5-dimethylfuran	313	835.2	−2.1	833.2						
88BOU/DJA	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	0	836.6						
[C_4H_6O]	**1191-99-7**	**2,5-Dihydrofuran**				**834.4**			**866.9**			**0**
86BOU/DJA	622-97-9	4-CH_3-C_6H_3-CH=CH_2	313	832.8	−0.4	832.6						
86BOU/DJA	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	−0.4	836.3						
[$C_2H_6N_2$]	**4143-41-3**	**(E)-CH_3N=NCH_3**				**834.4**			**865.1**			**5.8**
92GAR/RUT		theory							883			
74FOS/WIL	430-67-1	$CF_2HCH_2NH_2$	320	836.6	−2.1	834.3						
72FOS/BEA	7664-41-7; 74-89-5	NH_3; CH_3NH_2				819-864						
[$C_{12}H_{16}O_2$]	**22524-51-2**	**2,3,5,6-(CH_3)$_4$-C_6H-$COOCH_3$**				**834.3**			**865.2**			**5**
93DEC/ERT	108-20-3	(i-C_3H_7)$_2$O	338	828.1	5.5	834.1						
93DEC/ERT	98-86-2	$C_6H_5COCH_3$	338	829.3	5.3	834.5						
[$C_6H_6N_2O_2$]	**100-01-6**	**4-Nitroaniline**				**834.2**			**866.0**			**2**
84ROL/HOU	108-20-3	(i-C_3H_7)$_2$O	320	828.1	4.6	833.0						
84ROL/HOU	123-54-6	$CH_3COCH_2COCH_3$	320	836.8	−1.3	835.3						
[$C_6H_{10}O$]	**4376-23-2**	**3-hexen-2-one(E)**				**833.8**			**865.6**			**2**
88BOU/DJA	20843-07-6	3,4-dimethylfuran	313	838.3	−4.6	833.7						
88BOU/DJA	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	−2.1	834.5						
88BOU/DJA	625-86-5	2,5-dimethylfuran	313	835.2	−4.6	830.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{10}H_{12}O_2$]	**13730-55-7**	**2,5-(CH_3)2-C_6H_3-$COOCH_3$**				**833.7**			**864.7**			**5**
93DEC/ERT	93-58-3	$C_6H_5CO_2CH_3$	338	819.5	5.6	825.1						
93DEC/ERT	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	5.7	834.3						
93DEC/ERT	111-47-7	$(n\text{-}C_3H_7)_2S$	338	834.9	−1.9	833.2						
[C_9H_9F]	**350-40-3**	**4-$FC_6H_4C(CH_3)=CH_2$**				**833.7**			**862.6**			**12**
87TAF	7664-41-7	NH_3	350	819	15.6	833.6						
87TAF2	7664-41-7	NH_3	350	819	15.6	833.6						
[C_8H_8]	**277-10-1**	**Cubane**				**833.6**			**859.9**			**20.6**
86SAN/BAL	98-83-9	C_6H_5-$C(CH_3)=CH_2$	428	835.3	−2.9	831.3						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	25.9	836.0						
[C_5H_6O]	**534-22-5**	**2-methylfuran**				**833.5**			**865.9**			**0**
86MAU/LIE	109-97-7	pyrrole	600	843.8	−7.5	837.1						
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	28.9	835.0						
85HOU/ROL	108-20-3	$(i\text{-}C_3H_7)_2O$	313	828.1	0	828.4						
[C_5H_8O]	**110-87-2**	**2H-Pyran, 3, 4-dihydro-**				**833.4**			**865.8**			**0**
86BOU/HAN	20843-07-6	3,4-dimethylfuran	313	838.3	−3.8	834.6						
86BOU/HAN	108-20-3	$(i\text{-}C_3H_7)_2O$	313	828.1	4.2	832.6						
[$C_{10}H_{12}O_2$]	**25081-39-4**	**3,5-$(CH_3)_2$-C_6H_3-$COOCH_3$**				**833.4**			**864.3**			**5**
96DEC/EXN	111-47-7	$(n\text{-}C_3H_7)_2S$	338	834.9	−2.2	832.9						
96DEC/EXN	123-54-6	$CH_3COCH_2COCH_3$	338	835.8	−1.2	834.9						
96DEC/EXN	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	5.4	834.0						
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	12.1	831.6						
[$C_9H_{10}O_2S$]	**3795-79-7**	**4-CH_3S-C_6H_4-$COOCH_3$**				**833.3**			**864.3**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	13.8	833.3						
[$C_7H_{14}S$]	**7133-37-1**	**c-$C_6H_{11}SCH_3$**				**833.3**			**864.5**			**4**
87TAF	7664-41-7	NH_3	350	819	14.6	833.1						
[$C_{12}H_{20}O$]	**90547-83-4**	**4-Ethylcamphor**				**833.3**			**865.1**			**2**
87TAF	7664-41-7	NH_3	350	819	14.6	833.2						
[$C_4H_7F_2NO$]	**667-50-5**	**$CF_2HCON(CH_3)_2$**				**833.1**			**864.1**			**5**
87TAF	7664-41-7	NH_3	350	819	14.6	833.1						
82PIE/HEH2									867			
[$C_{12}H_{18}O_2$]	**711-01-3**	**Tricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, methyl ester**				**833.1**			**864.1**			**5**
87TAF	7664-41-7	NH_3	350	819	14.6	833.1						
[$C_{12}H_{18}O$]	**1660-04-4**	**Adamantylmethylketone**				**833.1**			**864.9**			**2**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
97HOM/HER	98-86-2	$C_6H_5COCH_3$	333	829.3	6.9	836.1						
97HOM/HER	108-20-3	$(i\text{-}C_3H_7)_2O$	333	828.1	4.7	833.4						
97HOM/HER	111-47-7	$(n\text{-}C_3H_7)_2S$	333	834.9	−2.0	833.2						
97HOM/HER	123-54-6	$CH_3COCH_2COCH_3$	333	836.8	−3.6	832.6						
87TAF	7664-41-7	NH_3	350	819	11.4	830.0						
[C_9H_{10}]	**622-97-9**	**4-CH_3-C_6H_4-$CH{=}CH_2$**				**832.8**			**861.7**			**12**
89GAL/SPE						831.8						
84HAR/HOU	7664-41-7	NH_3	323	819	14.2	832.8						
[$C_{10}H_{12}O_2$]	**15012-36-9**	**2,3-$(CH_3)_2$-C_6H_3-$COOCH_3$**				**832.7**			**863.6**			**5**
93DEC/ERT	89-71-4	2-CH_3-$C_6H_4COOCH_3$	338	827.3	6.3	833.6						
93DEC/ERT	98-86-2	$C_6H_5COCH_3$	338	829.3	3.2	832.4						
93DEC/ERT	111-47-7	$(n\text{-}C_3H_7)_2S$	338	834.9	−3.6	831.5						
93DEC/ERT	123-54-6	$CH_3COCH_2COCH_3$	338	836.8	−2.3	833.8						
93DEC/ERT	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	3.5	832.1						
[C_2H_5NO]	**60-35-5**	**CH_3CONH_2**				**832.6**			**863.6**			**5**
73YAM/KEB	7664-41-7	NH_3	320	819	13.8	832.6						
[C_5H_8O]	**625-33-2**	**$CH_3CH{=}CHC(=O)CH_3$**				**832.5**			**864.3**			**2**
84BOU/HOP	108-20-3	$(i\text{-}C_3H_7)_2O$	323	828.1	4.2	832.7						
84BOU/HOP	123-54-6	$CH_3COCH_2COCH_3$	323	836.8	−4.2	832.3						
[$C_8H_8O_3$]	**99-76-3**	**4-HO-C_6H_4-$COOCH_3$**				**832.5**			**863.4**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	13.0	832.5						
[$C_3H_6N_2$]	**151-18-8**	**$H_2N(CH_2)_2CN$**				**832.5**			**866.4**			**−5**
87TAF	7664-41-7	NH_3	350	819	11.9	830.8						
83TAF2	7664-41-7	NH_3	350	819	11.9	830.8						
80MAU	7664-41-7	NH_3	550	819	10.0	828.7						
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−40.2	837.8						
75ARN	7664-41-7	NH_3	350	819	14.6	833.6						
[$C_7H_7NO_2$]	**150-13-0**	**4-NH_2-benzoic acid**				**832.3**			**864.7**			**0**
95TAN/ISB	98-86-2; 98-83-9	$C_6H_5COCH_3$; C_6H_5-$C(CH_3){=}CH_2$				829-835						
[$C_7H_7NO_2$]	**99-05-8**	**3-NH_2-benzoic acid**				**832.3**			**864.7**			**0**
95TAN/ISB	98-86-2; 98-83-9	$C_6H_5COCH_3$; C_6H_5-$C(CH_3){=}CH_2$				829-835						
[$C_{11}H_{16}Si$]	**1923-01-9**	**C_6H_5-$C(Si(CH_3)_3){=}CH_2$**				**832.0**			**860.9**			**12**
92MIS/AR12	123-54-6	$CH_3COCH_2COCH_3$	308	836.8	−3.8	832.9						
92MIS/AR12	108-20-3	$(i\text{-}C_3H_7)_2O$	308	828.1	2.9	831.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_8H_6F_3NO$]	**1891-90-3**	**4-CF_3-$C_6H_4CONH_2$**				**831.8**			**862.8**			**5**
94GRU/CAL	108-20-3; 372-19-0	(i-C_3H_7)$_2$O; 3-F-$C_6H_4NH_2$				828-835						
[$C_8H_8O_2$]	**121-71-1**	**3-HO-C_6H_4-$COCH_3$**				**831.8**			**863.6**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	2.5	831.8						
[C_8H_{12}]	**497-35-8**	**2-Methylenebicyclo[2.2.1]heptane**				**831.8**			**860.7**			**12**
79AUE/BOW	74-89-5	CH_3NH_2	298	864.5	−32.7	831.8						
[C_4H_8OS]	**926-67-0**	**$CH_3C(S)OC_2H_5$**				**831.8**			**863.6**			**2**
93ABB/MO	123-54-6	$CH_3COCH_2COCH_3$	333	836.8	5.6	830.8						
93ABB/MO	108-20-3	(i-C_3H_7)$_2$O	333	828.1	4.0	832.6						
93ABB/MO	352-93-2	(C_2H_5)$_2$S	333	827.0	5.2	832.4						
[$C_3H_6S_2$]	**2168-84-5**	**$CH_3C(=S)SCH_3$**				**831.5**			**860.7**			**11**
83CAS/KIM	111-43-3	(n-C_3H_7)$_2$O	323	810.5	20.9	831.5						
[$C_9H_{18}O$]	**815-24-7**	**(t-C_4H_9)$_2$CO**				**831.5**			**861.3**			**9**
87TAF	7664-41-7	NH_3	350	819	13.3	831.5						
82PIE/HEH2									864			
[$C_{11}H_{18}O$]	**10309-50-9**	**4-Methylcamphor**				**831.4**			**863.3**			**2**
87TAF	7664-41-7	NH_3	350	819	12.8	831.4						
[$C_4H_9NO_2$]	**540-80-7**	**t-C_4H_9ONO**				**831.4**			**863.9**			**0**
78FAR/MCM	7664-41-7; 109-97-7	NH_3; pyrrole				819-844						
[$C_{11}H_{18}O$]	**19066-23-0**	**Adamantylmethylether**				**831.0**			**860.2**			**11**
87TAF	7664-41-7	NH_3	350	819	12.8	830.9						
[$C_3H_6OS_2$]	**19708-81-7**	**$CH_3OC(S)SCH_3$**				**830.8**			**862.6**			**2**
93ABB/MO	123-54-6	$CH_3COCH_2COCH_3$	333	836.8	−5.7	830.7						
93ABB/MO	108-20-3	(i-C_3H_7)$_2$O	333	828.1	2.2	830.9						
[$C_7H_{14}S$]	**6572-99-2**	**Heptamethylenesulfide**				**830.7**			**860.5**			**9**
87TAF	7664-41-7	NH_3	350	819	12.4	830.6						
[$C_3H_6N_2$]	**5616-32-0**	**CH_3NHCH_2CN**				**830.7**			**863.8**			**−2**
87TAF	7664-41-7	NH_3	350	819	11.9	830.7						
83TAF2	7664-41-7	NH_3	350	819	11.9	830.7						
[$C_9H_{10}O_2$]	**99-75-2**	**4-CH_3-C_6H_4-$COOCH_3$**				**830.6**			**861.6**			**5**
96DEC/EXN	123-54-6	$CH_3COCH_2COCH_3$	338	836.8	−4.1	832.0						
96DEC/EXN	108-20-3	(i-C_3H_7)$_2$O	338	828.1	2.2	830.8						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
96DEC/EXN	565-80-0	$(i\text{-}C_3H_7)_2CO$	338	820.5	9.7	830.4						
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	9.6	829.1						
[C_3H_6O]	**107-25-5**	**CH_2=CH-OCH_3**				**830.3**			**859.2**			**12**
95SMI/RAD		theory	298						849.2			
91MAU/SIE	753-90-2	$CF_3CH_2NH_2$	600	812.9	23.8	831.6	846.8	13.0	859.8	−5	18.4	13.4
91MAU/SIE	7664-41-7	NH_3	600	819			853.6	0.8	854.4			
89OSA/DEL	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	−5.9	830.6						
89OSA/DEL	108-20-3	$(i\text{-}C_3H_7)_2O$	313	828.1	0.4	828.6						
[$C_{12}H_{16}$]	**5676-29-9**	***α*-t-butylstyrene**				**830.3**			**859.2**			**12**
92NAK/NOM	123-54-6	$CH_3COCH_2COCH_3$	343	836.8	−4.6	831.1						
92NAK/NOM	108-20-3	$(i\text{-}C_3H_7)_2O$	343	828.1	1.3	829.6						
92NAK/NOM	765-43-5	$c\text{-}C_5H_5COCH_3$	343	823	7.5	830.1						
[$C_3H_3FN_2$]	**35277-02-2**	**4-fluoropyrazole**				**829.4**			**863.0**			**−4**
92ABB/CAB	123-54-6	$CH_3COCH_2COCH_3$	333	836.8	−6.9	829.6						
92ABB/CAB	108-20-3	$(i\text{-}C_3H_7)_2O$	333	828.1	0.7	829.5						
[C_3H_6S]	**1822-74-8**	**CH_2=CH-SCH_3**				**829.3**			**858.2**			**12**
89OSA/DEL	123-54-6	$CH_3COCH_2COCH_3$	313	836.8	−5.4	831.1						
89OSA/DEL	107-25-5	CH_2=CH-OCH_3	313	830.3	−1.3	829.0						
89OOSA/DEL	108-20-3	$(i\text{-}C_3H_7)_2O$	313	828.1	−0.4	827.8						
[C_8H_8O]	**98-86-2**	**$C_6H_5COCH_3$**				**829.3**			**861.1**			**2**
91MAU/SIE	7664-41-7	NH_3	600	819	12.1	828.6	853.6	8.8	862.4	−6.4	4.6	−1.8
91MAU/SIE	95-13-6	indene	600	819.6	8.4	830.7	848.8	10.9	859.7	11	−4.2	6.8
91MAU/SIE	100-42-5	$C_6H_5CHCH_2$	600	809.2	20.5	831.3	839.5	23.0	862.5	7.4	−4.2	3.2
87TAF	7664-41-7	NH_3	350	819	7.8	826.4						
86TAF/GAL	7664-41-7	NH_3	350	819	8.0	826.5						
85VAN/LEA		See Refs.										
83TAF	7664-41-7	NH_3	350	819	7.8	826.4						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	19.7	830.9						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	37.2	819.5						
79LAU	7664-41-7	NH_3	650	819	9.1	825.1						
[$C_{11}H_{15}FSi$]	**140843-92-1**	**4-F-C_6H_4-C(Si$(CH_3)_3$)=CH_2**				**829.1**			**858.0**			**12**
92MIS/AR12	108-20-3	$(i\text{-}C_3H_7)_2O$	308	828.1	1.3	829.4						
92MIS/AR12	565-80-0	$(i\text{-}C_3H_7)_2CO$	308	820.5	8.4	828.8						
[$C_{10}H_{12}$]	**7399-49-7**	**Benzene, 1-methyl-2-(1-methylethenyl)-**				**828.9**			**857.8**			**12**
89GAL/SPE						828.9						
[$C_{10}H_{14}O_3$]	**#997**	**3-Acetyl-5,5-dimethylcyclohexen-2-one**				**828.8**			**861.2**			**0**
87TAF	7664-41-7	NH_3	350	819	10.1	828.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[CCl_2]	**1605-72-7**	**CCl_2**				**828.5**			**861**			**0**
91PAU/SQU		threshold value	298						861			
85LIA/KAR	107-12-0;	C_2H_5CN; n-C_3H_7CN				763-768						
	109-74-0											
78AUS/LIA2	60-29-7	$(C_2H_5)_2O$		801		<801						
[C_3HNO]	**145798-71-6**	**HNCCCO**				**828.5**			**861**			**0**
94FLA/HAV		theory							861			
[$C_6H_{14}O$]	**108-20-3**	**(i-C_3H_7)$_2$O**				**828.1**			**855.5**			**17**
87TAF	7664-41-7	NH_3	350	819	9.2	827.0						
86SAN/BAL	565-80-0	(i-C_3H_7)$_2$CO	428	820.5	8.8	828.3						
86SAN/BAL	693-65-2	(n-C_5H_{11})$_2$O	428	825.3	4.2	829.5						
86SAN/BAL	111-43-3	(n-C_3H_7)$_2$O	428	810.5	20.5	831.0						
83CAS/KIM	111-43-3	(n-C_3H_7)$_2$O	323	810.5	16.3	826.8						
82MAU	111-43-3	(n-C_3H_7)$_2$O	335	810.5	16.3	826.8						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	40.6	822.6						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	45.6	821.3						
79AUE/BOW	7664-41-7	NH_3	298	819	11.2	830.2						
[C_{60}]	**99685-96-8**	**buchminsterfullerene**				**827.5**			**NE**			**NE**
91MCE/CAL	7664-41-7;	NH_3; 1,2,3,4,5,6-(CH$_3$)$_6$-C_6				819-836						
	87-85-4											
[C_{70}]	**115383-22-7**	**[5,6]Fullerene-C_{70}**				**827.5**			**NE**			**NE**
91MCE/CAL	7664-41-7;	NH_3; 1,2,3,4,5,6-(CH$_3$)$_6$-C_6				819-836						
	87-85-4											
[$C_9H_9ClO_3$]	**37908-98-8**	**3-Cl-4-CH_3O-C_6H_3-$COOCH_3$**				**827.5**			**858.4**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	7.9	827.5						
[$C_{10}H_{16}O$]	**76-22-2**	**Camphor**				**827.3**			**859.2**			**2**
87TAF	7664-41-7	NH_3	350	819	8.7	827.3						
[$C_9H_8CrO_3$]	**41311-89-1**	**(C_5H_5)Cr(CO)$_3$$CH_3$**				**827.3**			**859.8**			**0**
81STE/BEA	7664-41-7	NH_3	320	819	8.4	827.3						
[$C_9H_{10}O_2$]	**89-71-4**	**2-CH_3-$C_5H_4$$COOCH_3$**				**827.3**			**858.3**			**5**
93DEC/ERT	93-58-3	$C_6H_5CO_2CH_3$	338	819.5	9.4	828.9						
93DEC/ERT	98-86-2	$C_6H_5COCH_3$	338	829.3	−2.6	826.6						
93DEC/ERT	565-80-0	(i-C_3H_7)$_2$CO	338	820.5	5.8	826.5						
93DEC/ERT	108-20-3	(i-C_3H_7)$_2$O	338	828.1	−1.3	827.3						
[C_9H_8O]	**4265-25-2**	**2-methylbenzofuran**				**827.2**			**859.6**			**0**
88BOU/DJA	107-86-8	3-methyl-2-butenal	313	825.0	2.1	827.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_6H_5O]	**2122-46-5**	**C_6H_5O radical**				**827**			**857.7**			**5.8**
94HOK/YAN		kinetic method				827						
80DEF/MCI	625-54-7; 352-93-2	(i-C_3H_7)OC_2H_5; $(C_2H_5)_2S$				814-827						
[$C_4H_{10}S$]	**352-93-2**	**$(C_2H_5)_2S$**				**827.0**			**856.7**			**9**
87TAF	7664-41-7	NH_3	350	819	7.3	825.6						
83TAF2	7664-41-7	NH_3	350	819	7.3	825.6						
79AUE/BOW	7664-41-7	NH_3	298	819	9.3	828.3						
[$C_6H_{14}O$]	**637-92-3**	**C_2H_5O(t-C_4H_9)**				**826.9**			**856.0**			**11**
87TAF	7664-41-7	NH_3	350	819	8.7	826.8						
83TAF2	7664-41-7	NH_3	350	819	8.7	826.8						
[C_4H_6]	**3100-04-7**	**1-Methylcyclopropene**				**826.9**			**856.0**			**11**
79AUE/BOW	7664-41-7	NH_3	298	819	7.8	826.8						
[C_5H_{10}]	**16906-27-7**	**1-ethenyl-1-methylcyclopropane**				**826.9**			**856.7**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	7.8	826.8						
[$C_9H_{10}O_2$]	**99-36-5**	**3-CH_3-C_6H_4-$COOCH_3$**				**826.8**			**857.7**			**5**
96DEC/EXN	123-54-6	$CH_3COCH_2COCH_3$	338	836.8	−7.7	828.4						
96DEC/EXN	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	−1.7	826.9						
96DEC/EXN	565-80-0	$(i\text{-}C_3H_7)_2CO$	338	820.5	5.8	826.5						
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	5.9	825.4						
[C_8H_7FO]	**403-42-9**	**4-F-C_6H_4-$COCH_3$**				**826.8**			**858.6**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−2.5	826.8						
[CH_2N_2]	**334-88-3**	**CH_2NN**				**826.7**			**858.9**			**1**
94HOR/GLA		theory							883			
94GLU/SZU		theory	298						883.7			
84BEA/EYE		See Refs.							841-866			
72FOS/BEA	7664-41-7; 4143-41-3	NH_3; (E)-$CH_3N{=}NCH_3$				819-834						
[C_5H_6S]	**554-14-3**	**2-Methylthiophene**				**826.5**			**859.0**			**0**
86MAU		See Refs.	600									
83MAU	765-43-5	c-$C_3H_5COCH_3$	600	823	2.9	826.5						
[C_9H_{10}]	**611-15-4**	**Benzene, 1-ethenyl-2-methyl**				**826.3**			**855.2**			**12**
89GAL/SPE						826.3						
[$C_5H_{10}S$]	**1613-51-0**	**Tetrahydrothiopyran**				**826.0**			**855.8**			**9**
87TAF	7664-41-7	NH_3	350	819	7.8	826.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YtSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{15}H_{24}$]	**15181-11-0**	**1,3-di-(t-C_4H_9)-5-CH_3-C_6H_3**				**826.0**			**853.7**			**16**
91BUK/GRU	7664-41-7	NH_3	300	819	7	826						
[$C_3H_8O_2$]	**504-63-2**	**HO(CH_2)$_3$OH**				**825.9**			**876.2**			**−60**
95CHE/STO	108-67-8	1,3,5-(CH_3)$_3$-C_6H_3	600	808.6	−6.3	825.1	836.2	42.7	878.9	16.2	−81.6	−65.4
95CHE/STO	100-42-5	$C_6H_5CHCH_2$	600	809.2	−3.9	825.5	839.5	34.7	874.2	7.4	−64.4	−57.0
95CHE/STO	98-86-2	$C_6H_5COCH_3$	600	829.3	−20.9	827.0	861.1	18.0	879.1	2	−64.9	−62.9
[$C_9H_{10}O_3$]	**5368-81-0**	**3-CH_3O-C_6H_4-$COOCH_3$**				**825.8**			**856.7**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	6.3	825.8						
[C_9H_9Cl]	**1712-70-5**	**4-$ClC_6H_4C(CH_3)$=CH_2**				**825.4**			**854.3**			**12**
87TAF	7664-41-7	NH_3	350	819	7.3	825.4						
83TAF2	7664-41-7	NH_3	350	819	7.3	825.4						
[$C_9H_9ClO_2S$]	**105442-23-7**	**3-Cl-4-CH_3S-C_6H_3-$COOCH_3$**				**825.4**			**856.3**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	5.9	825.4						
[$C_{10}H_{22}O$]	**693-65-2**	**(n-C_5H_{11})$_2$O**				**825.3**			**852.7**			**17**
86SAN/BAL	93-58-3	$C_6H_5CO_2CH_3$	428	819.5	6.3	824.2						
86SAN/BAL	565-80-0	(i-C_3H_7)$_2$CO	428	820.5	4.2	823.7						
86SAN/BAL	111-43-3	(n-C_3H_7)$_2$O	428	810.5	16.3	826.8						
79AUE/BOW	7664-41-7	NH_3	298	819	7.3	826.3						
[$C_{10}H_{12}O$]	**2142-76-9**	**2,6-(CH_3)$_2$$C_6H_3$-$COCH_3$**				**825.2**			**857.0**			**2**
93KUK/STR	98-86-2	$C_6H_5COCH_3$	320	829.3	−4	825.3						
[$C_7H_6F_3N$]	**98-16-8**	**3-$CF_3C_6H_4NH_2$**				**825.1**			**856.9**			**2**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−25.5	825.1						
[C_5H_8O]	**107-86-8**	**2-methyl-2-butenal**				**825.0**			**856.9**			**2**
88BOU/DJA	502-49-8	cyclooctanone	313	819.6	2.5	822.2						
88BOU/DJA	693-65-2	(n-C_5H_{11})$_2$O	313	825.3	2.1	827.6						
[$C_8H_{16}O$]	**5857-36-3**	**i-C_3H_7CO(t-C_4H_9)**				**825.0**			**856.9**			**2**
87TAF	7664-41-7	NH_3	350	819	6.4	825.0						
[C_8H_7ClO]	**99-91-2**	**4-Cl-C_6H_4-$COCH_3$**				**824.8**			**856.6**			**2**
87TAF	7664-41-7	NH_3	350	819	4.6	823.2						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−2.9	826.4						
[$C_{10}H_{12}O_2$]	**14920-81-1**	**2,6-(CH_3)$_2$-C_6H_3-$COOCH_3$**				**824.3**			**855.3**			**5**
93DEC/ERT	93-58-3	$C_6H_5CO_2CH_3$	338	819.5	−0.8	818.7						
93DEC/ERT	565-80-0	(i-C_3H_7)$_2$CO	338	820.5	4.8	825.5						
93DEC/ERT	108-20-3	(i-C_3H_7)$_2$O	338	828.1	−1.7	826.9						
93DEC/ERT	89-71-4	2-CH_3-$C_6H_4COOCH_3$	338	827.3	−1	826.3						

J. Phys. Chem. Ref. Data, Vol. 27, No. 3, 1998

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
Ys Squib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_4H_7N]	**627-36-1**	**i-C_3H_7NC**				**824.3**			**856.8**			**0**
86MAU/KAR	565-80-0;	$(i\text{-}C_3H_7)_2CO$; $(i\text{-}C_3H_7)_2O$	335			821-828						
	108-20-3											
[C_6H_5NO]	**586-96-9**	**Nitrosobenzene**				**823.6**			**854.3**			**5.8**
80REE/FRE	7664-41-7;	NH_3; $(i\text{-}C_3H_7)_2O$				819-828						
	108-20-3											
[$C_{11}H_{16}$]	**700-12-9**	**$(CH_3)_5$-C_6H**				**823.5**			**850.7**			**17.6**
86STO/LI	108-67-8	1,3,5-$(CH_3)_3$-C_6H_3	300	808.6	15.1	823.7	836.2	14.8	851.0	16.2	1.1	17.3
86STO/LI	527-53-7	1,2,3,5-$(CH_3)_4$-C_6H_2	300	816.5	6.8	823.3	845.6	5.2	850.7	11.4	5.3	16.7
[C_6H_{10}]	**4549-74-0**	**$CH_3CH{=}C(CH_3)CH{=}CH_2$**				**823.4**			**852.3**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	4.4	823.4						
[$C_7H_6N_2O_4$]	**645-09-0**	**3-NO_2-$C_6H_4CONH_2$**				**823.2**			**854.2**			**5**
94GRU/CAL	142-96-1;	$(n\text{-}C_3H_9)_2O$; $(i\text{-}C_3H_7)_2O$				818-828						
	108-20-3											
[$C_{21}H_{22}$]	**82400-17-7**	**Methyldodecahedrane**				**823.1**			**855.6**			**0**
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	10.5	823.1						
[$C_2H_5NO_2$]	**546-88-3**	**Acetamide,N-hydroxy**				**823.0**			**854.0**			**5**
92DEC/EXN	108-20-3	$(i\text{-}C_3H_7)_2O$	338	828.1	−4.6	824.0						
92DEC/EXN	110-01-0	c-C_4H_8S	338	819.3	2.3	821.8						
[C_5H_8O]	**765-43-5**	**c-$C_3H_5COCH_3$**				**823**			**854.9**			**2**
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	40.2	821.2	802.1	52.3	854.4	20	−20.1	−0.1
91MAU/SIE	753-90-2	$CF_3CH_2NH_2$	600	812.9	11.7	822.5	846.8	7.9	854.8	−5	5.9	0.9
91MAU/SIE	7664-41-7	NH_3	600	819			853.6	3.8	857.4			
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	21.8	827.3						
83TAF	7664-41-7	NH_3	350	819	3.2	821.8						
[$C_9H_{16}O$]	**3350-30-9**	**c-Nonanone**				**822.8**			**852.6**			**9**
87TAF	7664-41-7	NH_3	350	819	4.6	822.8						
[C_9H_8]	**766-97-2**	**4-CH_3-C_6H_4-CCH**				**822.5**			**853.2**			**5.8**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	23.0	824.3						
85MAR/MOD	7664-41-7	NH_3	~300	819	1.7	820.7						
[H_4N_2]	**302-01-2**	**H_2NNH_2**				**822.4**			**853.2**			**5.8**
84MAU/NEL	111-43-3	$(n\text{-}C_3H_7)_2O$	600	810.5	8.8	822.6						
84MAU/NEL	765-43-5	c-$C_3H_5COCH_3$	600	823	−0.4	821.4						
84MAU/NEL	109-97-7	pyrrole	600	843.8	−19.7	823.2						
75ARN	7664-41-7	NH_3	350	819	18.3	836.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[$C_9H_{10}O_2S$]	**90721-40-7**	**3-CH_3S-C_6H_4-$COOCH_3$**				**822.4**			**853.4**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	2.9	822.4						
[$C_{18}H_{30}$]	**1460-02-2**	**1,3,5-(t-C_4H_9)$_3$-C_6H_3**				**822.3**			**848.8**			**20**
91BUK/GRU	123-39-7	$HCONHCH_3$	300	820.3	2	822.3						
[$C_{10}H_{10}O_2$]	**6781-42-6**	**3-CH_3CO-C_6H_4-$COCH_3$**				**822.3**			**852.0**			**9**
94DEC/EXN2	111-43-3	(n-C_3H_7)$_2O$	338	810.5	9.6	820.4						
94DEC/EXN2	142-96-1	(n-C_4H_9)$_2O$	338	818.3	4.3	822.9						
94DEC/EXN2	98-86-2	$C_6H_5COCH_3$	338	829.3	−5.5	823.5						
[C_3H_8Ge]	**82064-99-1**	**$(CH_3)_2Ge=CH_2$**				**822.2**			**851.1**			**12**
82PIE/HEH	7664-41-7	NH_3	350	819	4.1	822.2						
[C_3H_6Se]	**76573-19-8**	**$CH_2=CH$-$SeCH_3$**				**822.0**			**850.9**			**12**
89OSA/DEL	108-20-3	(i-C_3H_7)$_2O$	313	828.1	−4.6	823.6						
89OSA/DEL	502-49-8	cyclooctanone	313	819.6	0.4	820.0						
[C_6H_4FO]	**2145-21-3**	**4-F-phenoxy**				**822**			**854.5**			**0**
94HOK/YAN		kinetic method				822						
[$C_9H_{18}O$]	**502-56-7**	**(n-C_4H_9)$_2CO$**				**821.9**			**853.7**			**2**
87TAF	7664-41-7	NH_3	350	819	3.2	821.8						
[C_3H_5NO]	**930-21-2**	**2-Azetidinone**				**821.7**			**852.6**			**5**
92ABB/CAN	565-80-0	(i-C_3H_7)$_2CO$	333	820.5	−0.9	819.7						
92ABB/CAN	352-93-2	(C_2H_5)$_2S$	333	827.0	−3.7	823.4						
92ABB/CAN	76-22-2	Camphor	333	827.3	−5.0	822.2						
[C_5H_6O]	**930-27-8**	**3-methylfuran**				**821.5**			**854.0**			**0**
85HOU/ROL	142-96-1	(n-C_4H_9)$_2O$	313	818.3	0.8	819.3						
85HOU/ROL	693-65-2	(n-C_5H_{11})$_2O$	313	825.3	−2.1	823.4						
[$C_3H_6N_2$]	**1467-79-4**	**$(CH_3)_2NCN$**				**821.4**			**852.1**			**6**
87TAF	7664-41-7	NH_3	350	819	7.3	825.7						
86MAR/TOP	74-90-8	HCN	300	681.6	136.4	818.0						
86MAR/TOP	78-82-0	i-C_3H_7CN	300	772.8	48.1	821.0						
[$C_{10}H_{10}O_3$]	**13031-43-1**	**4-CH_3COO-C_6H_4-$COCH_3$**				**821.3**			**853.2**			**2**
87TAF	7664-41-7	NH_3	350	819	2.3	820.9						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−7.5	821.7						
[$C_{10}H_{10}O_2$]	**1009-61-6**	**4-CH_3CO-C_6H_4-$COCH_3$**				**821.0**			**850.8**			**9**
94DEC/EXN2	142-96-1	(n-C_4H_9)$_2O$	338	818.3	2.3	820.9						
94DEC/EXN2	98-86-2	$C_6H_5COCH_3$	338	829.3	−7.5	821.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94DEC/EXN2	2868-37-3	c-$C_3H_5COOCH_3$	338	811.2	6.8	817.8						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−5.0	824.0						
[$C_{12}H_{10}$]	**83-32-9**	**Acenaphthene**				**821.0**			**851.7**			**5.8**
80MAU	7664-41-7	NH_3	550	819	5.0	821.0						
[$C_{22}H_{14}$]	**213-46-7**	**Picene**				**820.6**			**851.3**			**5.8**
80MAU	7664-41-7	NH_3	550	819	4.6	820.6						
[C_9H_{10}]	**100-80-1**	**3-CH_3-C_6H_4-CH=CH_2**				**820.6**			**849.4**			**12**
89GAL/SPE						820.5						
[$C_7H_{14}O$]	**565-80-0**	**(i-C_3H_7)$_2$CO**				**820.5**			**850.3**			**9**
87TAF	7664-41-7	NH_3	350	819	1.8	820.1						
86SAN/BAL	93-58-3	$C_6H_5CO_2CH_3$	428	819.5	1.7	820.7						
86SAN/BAL	142-96-1	(n-C_4H_9)$_2$O	428	818.3	2.1	821.4						
86SAN/BAL	111-43-3	(n-C_3H_7)$_2$O	428	810.5	12.1	823.6						
83TAF	87-85-4	$(CH_3)_6$-C_6	350	836.0	−17.8	819.0						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	33.9	816.0						
[$C_5H_8O_2$]	**623-43-8**	**CH_3CH=CHCOOCH$_3$**				**820.4**			**851.3**			**5**
90WOL/GRU	110-71-4	$CH_3OCH_2CH_2OCH_3$	320	820.2	0.6	820.4						
[C_7H_8]	**121-46-0**	**Bicyclo[2.2.1]hepta-2.5-diene**				**820.3**			**849.3**			**11.5**
86HOU/SCH	7664-41-7	NH_3	323	819	1.7	820.3						
[C_2H_5NO]	**123-39-7**	**HCONHCH$_3$**				**820.3**			**851.3**			**5**
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	38.1	820.3						
[$C_4H_{10}O_2$]	**110-71-4**	**$CH_3OCH_2CH_2OCH_3$**				**820.2**			**858.0**			**−18**
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	−33.9	822.8	884.6	−23.4	861.2	2	−21	−19
83MAU	624-89-5	$CH_3SC_2H_5$	600	815.3	−1.5	820.4	846.5	7.5	854.0	4	−15	−11
83MAU	111-43-3	(n-C_3H_7)$_2$O	600	810.5	−3.3	817.7	837.9	9.2	847.1	17	−21	−4
[$C_3H_8O_3$]	**56-81-5**	**$HOCH_2CH(OH)CH_2OH$**				**820**			**874.8**			**−75**
86SUN/KUL		See Refs.	300			820			874			
[C_9H_8O]	**104 87 0**	**4-$(CH_3)C_6H_4CHO$**				**820.0**			**851.8**			**2**
87TAF	7664-41-7	NH_3	350	819	1.4	820.0						
83TAF2	7664-41-7	NH_3	350	819	1.4	820.0						
[$C_{10}H_7CrO_3$]	**32984-97-7**	**($C_6H_5CH_2$)Cr(CO)$_3$**				**819.9**			**852.4**			**0**
81STE/BEA	7664-41-7	NH_3	320	819	1	819.9						
[$C_{10}H_{10}$]	**6366-06-9**	**3,6-$(CH_3)_2$-C_6H_3-CCH**				**819.7**			**850.4**			**5.8**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	18.4	819.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSqnb	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_9H_8]	**95-13-6**	**indene**				**819.6**			**848.8**			**11**
91MAU/SIE	96-22-0	$(C_2H_5)_2CO$	600	807	14.2	820.6	836.8	11.3	848.1	9	5.0	14.0
91MAU/SIE	100-42-5	$C_6H_5CHCH_2$	600	809.2	12.1	820.3	839.5	15.1	854.5	7.4	−5.0	2.4
89KAF/MAU	100-42-5	$C_6H_5CHCH_2$	570	809.2	11	819.2	839.5	15.1	854.6	7.4	−5	2.4
89KAF/MAU	96-22-0	$(C_2H_5)_2CO$	570	807	12.7	819.2	836.8	11.3	848.1	9	5	14
89KAF/MAU	98-86-2	$C_6H_5COCH_3$	570	829.3	−7.8	819.0	861.1	−10.8	850.3	2	3.8	5.8
[$C_8H_{14}O$]	**502-49-8**	**cyclooctanone**				**819.6**			**849.4**			**9**
84BOU/HOU	502-42-1	cycloheptanone	300	815.9	3.8	819.6						
[C_3HN_3]	**290-87-9**	**1,3,5-Triazine**				**819.6**			**848.8**			**11**
79MAU	75-04-7	$C_2H_5NH_2$	550	878	54.4	819.6						
[$C_8H_8O_2$]	**93-58-3**	**$C_6H_5CO_2CH_3$**				**819.5**			**850.5**			**5**
93DEC/ERT	108-20-3	$(n\text{-}C_3H_7)_2O$	338	828.1	−9.5	819.1						
93DEC/ERT	98-86-2	$C_6H_5COCH_3$	338	829.3	−9	820.2						
93DEC/ERT	565-80-0	$(i\text{-}C_3H_7)_2CO$	338	820.5	−1.9	818.8						
87TAF	7664-41-7	NH_3	350	819	−2.7	815.7						
86SAN/BAL	142-96-1	$(n\text{-}C_4H_9)_2O$	428	818.3	0.8	820.6						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	10.5	822.5						
86SAN/BAL	598-98-1	$t\text{-}C_4H_9COOCH_3$	428	814.2	5.4	819.7						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	29.7	811.9						
[$C_6H_{10}F_3NO$]	**400-59-9**	**$CF_3CONH(n\text{-}C_4H_9)$**				**819.4**			**850.3**			**5**
87TAF	7664-41-7	NH_3	350	819	0.9	819.3						
83TAF2	7664-41-7	NH_3	350	819	0.9	819.3						
[C_4H_8S]	**110-01-0**	**$c\text{-}C_4H_9S$**				**819.3**			**849.1**			**9**
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	5.9	817.1						
87TAF	7664-41-7	NH_3	350	819	2.3	820.5						
83CAS/KIM	111-43-3	$(n\text{-}C_3H_7)_2O$	323	810.5	9.6	820.3						
[$C_{12}H_8$]	**259-79-0**	**Biphenylene**				**819.2**			**848.2**			**11.5**
80MAU	7664-41-7	NH_3	550	819	4.6	819.1						
[$C_8H_8O_3$]	**19438-10-9**	**3-HO-C_6H_4-$COOCH_3$**				**819.1**			**850.0**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−0.8	818.7						
[HNSi]	**14515-04-9**	**SiNH**				**819.0**			**853.2**			**−5.8**
88WLO/ROD	7664-41-7	NH_3	295	819	0	819.0						
[H_3N]	**7664-41-7**	**NH_3**				**819**			**853.6**			**−6.4**
97EAS/SMI		theory	298									−6.4
96MAR/LEE		theory	298						853.1			
93SMI/RAD		theory	298						853.6			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	600						858.8			
93SMI/RAD		theory	0						847.4			
93DEL		theory	298						852.3			
87TAF	7664-41-7	NH_3	350	819	0	819						
87POP/CER		theory	298									
86TAF/GAL	7664-41-7	NH_3	300	819	0	819						
84JEN/MOR		See Refs.	298						857.7			
83TAF2	7664-41-7	NH_3	350	819	0	819						
83TAF	7664-41-7	NH_3	350	819	0	819						
83LOC/MCI	7664-41-7	NH_3	350	819	0	819						
82PIE/HEH	7664-41-7	NH_3	350	819	0	819						
80MAU	7664-41-7	NH_3	550	819	0	819						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	34.7	811.4						
79LAU	7664-41-7	NH_3	650	819	0	819						
79CEY/UHE		threshold value							851.8			
78LAU/SAL	7664-41-7	NH_3	600	819	0	819						
77WOL/STA	7664-41-7	NH_3	350	819	0	819						
75TAF	7664-41-7	NH_3	350	819	0	819						
73YAM/KEB	7664-41-7	NH_3	600	819	0	819						
72HEN/TAA	7664-41-7	NH_3	350	819	0	819						
72ARN/JON	7664-41-7	NH_3	350	819	0	819						
[C_3H_5N]	**624-79-3**	**C_2H_5NC**				**818.9**			**851.3**			**0**
86MAU/KAR	142-96-1	(n-C_3H_9)$_2$O	335	818.3	0	818.9						
[$C_6H_8O_2$]	**765-87-7**	**c-hexane-1,2-dione**				**818.9**			**849.6**			**5.8**
87BOU/HOP	502-49-8	cyclooctanone	313	819.6	−3.8	815.9						
87BOU/HOP	693-03-2	(n-C_5H_{11})$_2$O	313	823.3	−2.5	822.9						
87BOU/HOP	108-94-1	cyclohexanone	313	811.2	3.8	815.0						
87BOU/HOP	1634-04-4	t-$C_4H_9OCH_3$	313	812.4	1.3	813.7						
83MAU	111-47-7	(n-C_3H_7)$_2$S	600	834.9	−15.9	820.0						
83MAU	624-89-5	$CH_3SC_2H_5$	600	815.3	10.5	825.2						
[CH_3N]	**2053-29-4**	**$CH_2{=}NH$**				**818.7**			**852.9**			**−5.8**
96BOU/SAL2	108-20-3; 123-54-6	(i-C_3H_7)$_2$O; $CH_3COCH_2COCH_3$				828-837						
	100-42-5; 108-20-3	$C_6H_5CH{=}CH_2$; (i-C_3H_7)$_2$O				809-828						
83TAF2												
[$C_6H_{12}O$]	**1003-17-4**	**2,2,-Dimethyltetrahydrofuran**				**818.5**			**847.7**			**11**
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	36.4	818.5						
[$C_4H_5N_3O_2$]	**54210-33-2**	**1-methyl-5-nitropyrazole**				**818.4**			**850.3**			**2**
92ABB/CAB	110-01-0	c-C_4H_8S	333	819.3	−2.3	817.3						
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	7.3	818.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
92ABB/CAB	123-19-3	$(n\text{-}C_3H_7)_2CO$	333	815.3	3.7	819.2						
[$C_8H_{18}O$]	**142-96-1**	**$(n\text{-}C_4H_9)_2O$**				**818.3**			**845.7**			**17**
86SAN/BAL	2868-37-3	$c\text{-}C_3H_4COOCH_3$	428	811.2	8.4	818.0						
86SAN/BAL	598-98-1	$t\text{-}C_3H_5\text{-}COOCH_3$	428	814.2	4.2	816.9						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	9.6	820.1						
82MAU	111-43-3	$(n\text{-}C_3H_7)_2O$	335	810.5	5.9	816.3						
79AUE/BOW	7664-41-7	NH_3	298	819	1.0	820.0						
[$C_5H_6F_3NO$]	**1547-87-1**	**$CF_3CON(CH_3)_2$**				**818.0**			**849.0**			**5**
87TAF	7664-41-7	NH_3	350	819	−0.5	818.0						
[CH_5P]	**593-54-4**	**CH_3PH_2**				**817.6**			**851.5**			**−5**
87TAF	7664-41-7	NH_3	350	819	−1.4	817.6						
74STA/BEA	7664-41-7	NH_3	320	819	−1.3	817.7						
[$C_{20}H_{20}$]	**4493-23-5**	**dodecahedrane**				**817.5**			**843.8**			**20.6**
86SAN/BAL	93-58-3	$C_6H_5CO_2CH_3$	428	819.5	−1.7	815.8						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	8.8	818.8						
[C_5H_8]	**3907-06-0**	**3,3-Dimethylcyclopropene**				**817.1**			**847.8**			**5.8**
76AUE/DAV	7664-41-7	NH_3	298	819	−2.0	817.1						
[$C_6H_{10}O$]	**279-49-2**	**Bicyclo[2.2.1]heptane,7-oxa**				**816.8**			**844.2**			**17**
86HOU/SCH	7664-41-7	NH_3	323	819	−1.7	816.8						
[C_3H_3NO]	**288-14-2**	**Isooxazole**				**816.8**			**848.6**			**2**
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	11.3	816.8						
[C_3H_6OS]	**21119-13-1**	**$CH_3C(=S)OCH_3$**				**816.5**			**846.0**			**10**
83CAS/KIM	111-43-3	$(n\text{-}C_3H_7)_2O$	323	810.5	5.9	816.5						
[$C_{10}H_{14}$]	**527-53-7**	**$1,2,3,5\text{-}(CH_3)_4\text{-}C_6H_2$**				**816.5**			**845.6**			**11.4**
86STO/LI	108-67-8	$1,3,5\text{-}(CH_3)_3\text{-}C_6H_3$	300	808.6	7.9	816.5	836.2	9.2	845.4	16.2	−4.5	11.7
[$C_6H_{18}OSi_2$]	**107-46-0**	**$(CH_3)_3SiOSi(CH_3)_3$**				**816.2**			**846.4**			**7.8**
87LI/STO	527-53-7	$1,2,3,5\text{-}(CH_3)_4\text{-}C_6H_2$	300	816.5	0.8	817.3	845.6	0	845.6	11.4	−2	9.4
87LI/STO	108-67-8	$1,3,5\text{-}(CH_3)_3\text{-}C_6H_3$	300	808.6	7.3	815.9	836.2	10.5	846.6	16.2	−10.5	5.7
87LI/STO	108-38-3	$1,3\text{-}(CH_3)_2\text{-}C_6H_4$	300	786.2	29.3	815.5	812.1	33.5	845.6	22	−13.8	8.2
75PIT/BUR	60-29-7; 108-20-3	$(C_2H_5)_2O$; $(i\text{-}C_3H_7)_2O$				801-828						
[$C_7H_{12}O$]	**502-42-1**	**cycloheptanone**				**815.9**			**845.6**			**9**
87TAF	7664-41-7	NH_3	350	819	−5.0	813.2						
84BOU/HOU	142-96-1	$(n\text{-}C_4H_9)_2O$	300	818.3	0.2	818.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_4H_5N_3O_2$]	**54210-32-1**	**1-methyl-3-nitropyrazole**				**815.7**			**847.6**			**2**
92ABB/CAB	565-80-0	(i-C_3H_7)$_2$CO	333	820.5	−5.2	815.5						
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	4.4	815.8						
[$C_6H_{10}O$]	**286-20-4**	**Cyclohexene oxide**				**815.6**			**848.1**			**0**
89KEN/PAC	75-97-8; 765-43-5	pinacolone; c-$C_4H_5COCH_3$				808-823						
[$C_7H_{10}O$]	**497-38-1**	**Bicyclo[2.2.1]heptan-2-one**				**815.5**			**847.4**			**2**
86HOU/SCH	7664-41-7	NH_3	323	819	−3.3	815.5						
[$C_{14}H_{18}$]	**5325-97-3**	**1,2,3,4,5,6,7,8-Octahydrophenanthrene**				**815.5**			**846.2**			**5.8**
80MAU	7664-41-7	NH_3	523	819	−0.8	815.4						
[$C_7H_{14}O$]	**123-19-3**	**(n-C_3H_7)$_2$CO**				**815.3**			**845.0**			**9**
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	3.3	814.6						
87TAF	7664-41-7	NH_3	350	819	−2.3	815.9						
[$C_8H_{14}O_2$]	**4630-82-4**	**c-$C_6H_{11}COOCH_3$**				**815.3**			**846.2**			**5**
87TAF	7664-41-7	NH_3	350	819	−3.2	815.2						
83TAF	7664-41-7	NH_3	350	819	−3.2	815.2						
[C_3H_8S]	**624-89-5**	**$CH_3SC_2H_5$**				**815.3**			**846.5**			**4**
87TAF	7664-41-7	NH_3	350	819	−4.1	814.4						
83TAF2	7664-41-7	NH_3	350	819	−4.1	814.4						
79AUE/BOW	7664-41-7	NH_3	298	819	−2.9	816.1						
[C_8H_7ClO]	**99-02-5**	**3-Cl-C_6H_4-$COCH_3$**				**815.1**			**846.9**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−14.2	815.1						
[C_3H_6ClNO]	**96-30-0**	**$ClCON(CH_3)_2$**				**814.8**			**845.8**			**5**
87TAF	7664-41-7	NH_3	350	819	−3.7	814.8						
[$C_{14}H_{18}$]	**1079-71-6**	**1,2,3,4,5,6,7,8-Octahydroanthracene**				**814.7**			**845.4**			**5.8**
80MAU	7664-41-7	NH_3	519	819	−1.7	814.7						
[$C_4H_{12}OSi$]	**1825-61-2**	**$(CH_3)_3SiOCH_3$**				**814.6**			**847.0**			**0**
75PIT/BUR	60-29-7; 108-20-3	(C_2H_5)$_2$O; (i-C_3H_7)$_2$O				801-828						
[$C_4H_{14}Si_2$]	**3277-26-7**	**$((CH_3)_2SiH)_2O$**				**814.6**			**845.3**			**5.8**
75PIT/BUR	60-29-7; 108-20-3	(C_2H_5)$_2$O; (i-C_3H_7)$_2$O				801-828						
[$C_7H_6N_2O_3$]	**619-80-7**	**4-NO_2-$C_6H_4CONH_2$**				**814.4**			**845.3**			**5**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94GRU/CAL	111-43-3; 142-96-1	$(n\text{-}C_3H_7)_2O$; $(n\text{-}C_4H_9)_2O$				810-818						
$[C_{10}H_{10}O_4]$	**1459-93-4**	**$3\text{-}CH_3COO\text{-}C_6H_4\text{-}COOCH_3$**				**814.3**			**843.5**			**10.8**
94DEC/IEXN2	2868-37-3	$c\text{-}C_3H_5COOCH_3$	338	811.2	2	812.9						
94DEC/IEXN2	111-43-3	$(n\text{-}C_3H_7)_2O$	338	810.5	4.9	815.6						
$[C_6H_{12}O_2]$	**598-98-1**	**$t\text{-}C_4H_9\text{-}COOCH_3$**				**814.2**			**845.2**			**5**
87TAF	7664-41-7	NH_3	350	819	−7.3	811.1						
86SAN/BAL	2868-37-3	$c\text{-}C_3H_5COOCH_3$	428	811.2	3.3	814.5						
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	5.0	817.0						
83TAF	7664-41-7	NH_3	350	819	−7.3	811.1						
[Si]	**7440-21-3**	**Si**				**814.1**			**837**			**32**
84ELK/ARM		See Refs.							837±4			
$[C_{10}H_{12}]$	**6921-43-3**	**Benzene,1-cyclopropyl-4-methyl-**				**813.8**			**846.3**			**0**
89GAL/SPE						813.8						
$[C_8H_7FO]$	**455-36-7**	**$3\text{-}F\text{-}C_6H_4COCH_3$**				**813.8**			**845.7**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−15.5	813.8						
$[C_5H_{12}O]$	**625-54-7**	**$C_2H_5O(i\text{-}C_3H_7)$**				**813.5**			**842.7**			**11**
87TAF	7664-41-7	NH_3	350	819	−4.1	814.0						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	30.5	812.6						
77WOL/STA	7664-41-7	NH_3	350	819	−4.1	814.0						
$[C_7H_8O]$	**694-98-4**	**Bicyclo[2.2.1]hept-2-ene-5-one**				**813.4**			**845.3**			**2**
86HOU/SCH	7664-41-7	NH_3	323	819	−5.4	813.4						
$[C_{18}H_{15}Sb]$	**603-36-1**	**$(C_6H_5)_3Sb$**				**813.1**			**845.5**			**0**
86TRA/MUN	100-66-3; 7664-41-7	$C_6H_5OCH_3$; NH_3				807-819						
$[C_7H_{12}O]$	**589-92-4**	**4-methylcyclohexanone**				**813.0**			**844.9**			**2**
84BOU/HOU	589-38-8	3-hexanone	300	811.3	1.7	813.0						
$[C_3H_7NO_2]$	**541-42-4**	**$i\text{-}C_3H_7ONO$**				**813**			**845.5**			**0**
78FAR/MCM	96-22-0; 7664-41-7	$(C_2H_5)_2O$; NH_3				807-819						
$[C_2H_4F_3N]$	**753-90-2**	**$CF_3CH_2NH_2$**				**812.9**			**846.8**			**−5**
91MAU/SIE	7664-41-7	NH_3	600				853.6	−4.2	849.4			
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	31.8	814.9	802.1	42.7	844.8	20	−18.0	2.0
91MAU/SIE	75-18-3	$(CH_3)_2S$	600	801.2	9.2	814.6	830.9	18.0	848.9	9.1	−14.6	−5.5
87TAF	7664-41-7	NH_3	350	819	−8.7	810.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
83TAF	7664-41-7	NH_3	350	819	−8.7	810.2						
79AUE/BOW	7664-41-7	NH_3	298	819	−7.3	811.7						
77STA/TAA	7664-41-7	NH_3	320	819	−7.9	811.0						
75TAF	7664-41-7	NH_3	350	819	−6.9	812.1						
75ARN	7664-41-7	NH_3	350	819	−6.9	812.1						
[C_8H_7Cl]	**2039-85-2**	**3-ClC$_6$H$_4$CH=CH$_2$**				**812.6**			**841.5**			**12**
87TAF	7664-41-7	NH_3	350	819	−5.5	812.6						
[C_8H_{12}]	**694-92-8**	**2-Methylbicyclo[2.2.1]hept-2-ene**				**812.5**			**846**			**0**
76SOL/FIE		See Refs.	300						845±6			
[CH_4N_2]	**26981-93-1:a**	**CH_3N=NH at terminal N**				**812.5**			845			**0**
92GAR/RUT		theory							845			
[$C_5H_{12}O$]	**1634-04-4**	**t-$C_4H_9OCH_3$**				**812.4**			**841.6**			**11**
87TAF	7664-41-7	NH_3	350	819	−9.6	808.5						
83TAF2	7664-41-7	NH_3	350	819	−10.1	808.1						
82MAU	111-43-3	(n-C_3H_7)$_2$O	335	810.5	0.8	811.5						
79AUE/BOW	7664-41-7	NH_3	298	819	−2.0	817.1						
75PTT/BUR	60-29-7; 108-20-3	(C_2H_5)$_2$O;(i-C_3H_7)$_2$O				801-828						
[CH_5NO]	**67-62-9**	**CH_3ONH_2**				**812.3**			**844.8**			**0**
87TAF	7664-41-7	NH_3	350	819	−6.4	812.3						
[$C_{10}H_{10}O_4$]	**120-61-6**	**4-CH_3COO-C_6H_4-$COOCH_3$**				**812.3**			**843.2**			**5**
94DEC/IEXN2	60-29-7	(C_2H_5)$_2$O	338	801	11.1	812.6						
94DEC/IEXN2	2868-37-3	c-$C_4H_5COOCH_3$	338	811.2	0.5	811.7						
94DEC/IEXN2	111-43-3	(n-C_3H_7)$_2$O	338	810.5	1.6	812.5						
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−7.1	812.4						
[$C_8H_8O_2$]	**591-31-1**	**3-$CH_3OC_6H_4CHO$**				**812.2**			**844.1**			**2**
87TAF	7664-41-7	NH_3	350	819	−6.4	812.2						
[C_8H_8O]	**6038-09-1**	**2-methyl-2-butenal(Z)**				**812.1**			**843.9**			**2**
88BOU/DJA	589-38-8	3-hexanone	313	811.3	0.8	812.1						
88BOU/DJA	111-43-3	(n-C_3H_7)$_2$O	313	810.5	2.1	812.8						
88BOU/DJA	589-92-4	4-methylcyclohexanone	313	813.0	−1.7	811.3						
[$C_5H_{10}O$]	**96-47-9**	**c-C_4H_7O(2-CH_3)**				**811.6**			**840.8**			**11**
87TAF	7664-41-7	NH_3	350	819	−5.9	812.2						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	28.9	811.0						
[$C_6H_{12}O$]	**589-38-8**	**3-hexanone**				**811.3**			**843.2**			**2**
84BOU/HOU	108-94-1	cyclohexanone	300	811.2	0	811.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_7H_{14}O$]	**931-56-6**	**c-$C_6H_{11}OCH_3$**				**811.3**			**840.5**			**11**
87TAF	7664-41-7	NH_3	350	819	−6.9	811.3						
[C_5H_8O]	**814-78-8**	**$CH_3C(=O)C(=CH_2)CH_3$**				**811.3**			**843.1**			**2**
84BOU/HOP	111-43-3	(n-$C_3H_7)_2O$	323	810.5	0.4	811.3						
[$C_6H_{10}O$]	**108-94-1**	**cyclohexanone**				**811.2**			**841.0**			**9**
87TAF	7664-41-7	NH_3	350	819	7.3	810.9						
86TAF/GAL	7664-41-7	NH_3	350	819	−7.3	810.9						
84BOU/HOU	111-43-3	(n-$C_3H_7)_2O$	300	810.5	0.4	810.9						
84BOU/HOU	502-42-1	cycloheptanone	300	815.9	−3.8	812.1						
83MAU	624-89-5	$CH_3SC_2H_5$	600	815.3	4.2	817.9						
83MAU	96-22-0	$(C_2H_5)_2CO$	600	807	10.5	817.5						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1		810.4						
79SAL/KEB	100-66-3	$C_6H_5OCH_3$	560	807.2	7.9	812.8						
[$C_5H_8O_2$]	**2868-37-3**	**c-$C_3H_5COOCH_3$**				**811.2**			**842.1**			**5**
87TAF	7664-41-7	NH_3	350	819	−6.9	811.6						
86SAN/BAL	111-43-3	(n-$C_3H_7)_2O$	428	810.5	1.7	813.7						
83TAF	7664-41-7	NH_3	350	819	−6.9	811.6						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	25.9	808.2						
[$C_8H_7ClO_2$]	**1126-46-1**	**4-Cl-C_6H_4-$COOCH_3$**				**811.1**			**842.1**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−8.4	811.1						
[$C_{12}H_{15}Cl$]	**146558-43-2**	**α-t-butylstyrene,3-Cl**				**811.0**			**839.8**			**12**
92NAK/NOM	141-78-6	$CH_3CO_2C_2H_5$	343	804.7	7.5	811.9						
92NAK/NOM	111-43-3	(n-$C_3H_7)_2O$	343	810.5	0	810.7						
92NAK/NOM	96-22-0	$(C_2H_5)_2CO$	343	807	3.8	810.6						
[$C_4H_8O_3$]	**623-53-0**	**$C_2H_5OCOOCH_3$**				**810.8**			**842.7**			**2**
87TAF	7664-41-7	NH_3	350	819	−7.8	810.8						
83TAF2	7664-41-7	NH_3	350	819	−7.8	810.8						
[C_9H_9F]	**3825-81-8**	**3-F$C_6H_4C(CH_3)=CH_2$**				**810.8**			**839.7**			**12**
87TAF	7664-41-7	NH_3	350	819	7.3	810.8						
[$C_9H_{10}O$]	**103-79-7**	**$C_6H_5CH_2COCH_3$**				**810.8**			**842.6**			**2**
93SZU/MCM	96-22-0	$(C_2H_5)_2CO$	600	807	1.7	810.8						
[C_9H_8]	**766-82-5**	**3-CH_3-C_6H_4-CCH**				**810.6**			**843.0**			**0**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	9.2	810.6						
[$C_6H_{14}O$]	**111-43-3**	**(n-$C_3H_7)_2O$**				**810.5**			**837.9**			**17**
87TAF	7664-41-7	NH_3	350	819	−7.8	810.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
86SAN/BAL	111-43-3	$(n\text{-}C_3H_7)_2O$	428	810.5	0	810.5						
83CAS/KIM	111-43-3	$(n\text{-}C_3H_7)_2O$	323	810.5	0	810.5						
82MAU	111-43-3	$(n\text{-}C_3H_7)_2O$	335	810.5	0	810.5						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	23.0	805.0						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	29.3	805.0						
79AUE/BOW	7664-41-7	NH_3	298	819	−3.9	815.1						
$[C_7H_6N_2]$	**2237-30-1**	**$3\text{-}NH_2\text{-}C_6H_4CN$**										
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−40.2	**810.4** 810.4			**842.3**			**2**
$[C_8H_7FO_2]$	**403-33-8**	**$4\text{-}F\text{-}C_6H_4\text{-}COOCH_3$**										
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−9.2	810.3 810.3			**841.3**			**5**
$[C_{18}H_{12}]$	**218-01-9**	**Chrysene**										
80MAU	7664-41-7	NH_3	550	819	−5.9	810.1 810.1			**840.9**			**5.8**
$[C_{12}H_{15}F]$	**146558-44-3**	**α-t-butylstyrene,3-F**										
92NAK/NOM	96-22-0	$(C_2H_5)_2CO$	343	807	2.9	**809.9**			**838.8**			**12**
92NAK/NOM	141-78-6	$CH_3CO_2C_2H_5$	343	804.7	5.9	809.8 810.3						
$[C_8H_7Br]$	**2039-82-9**	**$4\text{-}BrC_6H_4CH{=}CH_2$**										
84HAR/HOU	7664-41-7	NH_3	323	819	−8.8	**809.8** 809.8			**838.7**			**12**
$[C_9H_{11}]$	**19019-92-2**	**$C_6H_5(CHC_2H_5)$ radical**										
82MAU	96-22-0; 1634-04-4	$(C_2H_5)_2CO$;$(t\text{-}C_4H_9)OCH_3$				809.7 807-812			**842.2**			**0**
$[C_9H_{11}]$	**16804-70-9**	**$C_6H_5(CH_3)_2$ radical**										
82MAU	96-22-0; 1634-04-4	$(C_2H_5)_2CO$; $(t\text{-}C_4H_9)OCH_3$				**809.7** 807-812			**842.2**			**0**
$[C_8H_{14}O]$	**823-76-7**	**$c\text{-}C_6H_{11}COCH_3$**										
87TAF	7664-41-7	NH_3				809.5						
83TAF	7664-41-7	NH_3	350	819	−9.2	809.4			**841.4**			**2**
81BRO/ABB	67-64-1	$(CH_3)_2CO$	350	819	−9.2	809.4						
			320	782.1	26.8	809.1						
$[C_8H_8]$	**100-42-5**	**$C_6H_5CHCH_2$**										
91MAU/SIE	67-64-1	$(CH_3)_2CO$				**809.2**			**839.5**			**7.4**
91MAU/SIE	96-22-0	$(C_2H_5)_2CO$	600	782.1	26.4	808.9	812	23.8	835.8	8.7	4.2	12.9
89KAF/MAU	67-64-1	$(CH_3)_2CO$	600	807	3.8	811.2	836.8	1.7	838.4	9	3.3	12.3
89KAF/MAU	96-22-0	$(C_2H_5)_2CO$	570	782.1	26.2	808.7	812	23.8	835.8	8.7	4.2	12.9
89KAF/MAU	98-86-2	$C_6H_5COCH_3$	570	807	3.6	811.0	836.8	1.7	838.5	9	3.3	12.3
87TAF	7664-41-7	NH_3	570	829.3	−20.6	807.2	861.1	−23	838.1	2	4.2	6.2
84HAR/HOU	7664-41-7	NH_3	350	819	−10.5	807.8						
75WOL/HAR	7664-41-7	NH_3	323	819	−5.0	813.7						
			350	819	−11.0	807.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_9H_{12}]	**108-67-8**	**1,3,5-$(CH_3)_3$-C_6H_3**				**808.6**			**836.2**			**16.2**
86STO/LI	141-78-6	$CH_3CO_2C_2H_5$	300	804.7	4.8	809.5	835.7	1.5	837.1	5	11.2	16.2
80MAU	7664-41-7	NH_3	550	819	−5.9	807.5						
76DEV/WOL	71-43-2	C_6H_6	350	725.4	82.4	808.2						
[H_2OSi]	**22755-01-7:a**	**H_2SiO at O**				**808.5**			**841**			**0**
93LUC/CUR		theory	298						841			
[C_6H_4]	**462-80-6**	**ortho-benzyne**				**808.5**			**841**			**0**
91GUO/GRA		See Refs.	300						841			
80POL/HEH	107-47-1; 687-48-9	$(t\text{-}C_4H_9)_2S$; $(CH_3)_2NCOOC_2H_5$				864-866						
[CH_4N_2]	**26981-93-1:b**	**$CH_3N{=}NH$ at interior N**				**808.5**			**841**			**0**
92GAR/RUT		theory							841			
[$C_6H_{12}O$]	**75-97-8**	**$t\text{-}C_4H_9COCH_3$**				**808.2**			**840.1**			**2**
87TAF	7664-41-7	NH_3	350	819	−9.2	809.4						
83TAF	7664-41-7	NH_3	350	819	−9.6	809.0						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	24.3	806.5						
[$C_4H_6O_2$]	**96-48-0**	**γ-Butyrolactone**				**808.1**			**840.0**			**2**
87TAF	7664-41-7	NH_3	350	819	−10.5	808.1						
[C_8H_8O]	**620-23-5**	**3-$CH_3C_6H_4CHO$**				**808.1**			**840.0**			**2**
87TAF	7664-41-7	NH_3	350	819	−10.5	808.1						
[C_6H_8]	**628-41-1**	**1,4-c-C_6H_8**				**808.0**			**837**			**11.5**
83GAU/HOU		See Refs.							837			
[$C_{10}H_{12}$]	**27546-46-9**	**Benzene, 1-cyclopropyl-2-methyl-**				**807.9**			**840.4**			**0**
89GAL/SPE		See Refs.				807.9						
[$C_8H_8O_2$]	**118-90-1**	**Benzoic acid, 2-methyl**				**807.8**			**838.8**			**5**
91NOU/COO	563-80-4; 108-94-1	3-methyl-2-butanone; c-hexanone				804-811						
[C_6H_{10}]	**513-81-5**	**$CH_2{=}C(CH_3)C(CH_3){=}CH_2$**				**807.8**			**835.0**			**17.8**
79AUE/BOW	7664-41-7	NH_3	298	819	−11.2	807.8						
[H_2OSi]	**83892-34-6**	**HSiOH at Si**				**807.5**			**840**			**0**
93LUC/CUR		theory	298						840			
[C_9H_{10}]	**766-90-5**	**Benzene, cis-(2-methylethenyl)**				**807.5**			**836.4**			**12**
89GAL/SPE						807.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_5H_8]	**1489-60-7**	**1-Methylcyclobutene**				**807.3**			**841.5**			**−5.8**
76AUE/DAV	7664-41-7	NH_3	298	819	−11.7	807.3						
[C_6H_{10}]	**1501-58-2**	**1,2-Dimethylcyclobutene**				**807.3**			**838.0**			**5.8**
76AUE/DAV	7664-41-7	NH_3	298	819	−11.7	807.3						
[C_5H_8O]	**1576-87-0**	**2-pentenal(E)**				**807.2**			**839.0**			**2**
88BOU/DJA	109-60-4	$CH_3COOC_3H_7$	313	805.6	1.3	806.9						
88BOU/DJA	96-22-0	$(C_2H_5)_2CO$	313	807	−0.4	806.7						
88BOU/DJA	557-31-3	$C_2H_5OCH_2CH{=}CH_2$	313	804.5	3.3	807.9						
[C_7H_8O]	**100-66-3**	**$C_6H_5OCH_3$**				**807.2**			**839.6**			**0**
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−41.0	810.2						
79LAU	7664-41-7	NH_3	650	819	−11.3	805.5						
76LAU/KEB	71-43-2	C_6H_6	650	725.4	71.2	805.4						
[$C_5H_{10}O$]	**96-22-0**	**$(C_2H_5)_2CO$**				**807**			**836.8**			**9**
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	25.1	804.0	802.1	32.2	834.3	20	−12.1	7.9
93SZU/MCM	7664-41-7	NH_3	600	819	−5.9	808.5	853.6	−18.0	835.6	−6.4	20.5	14.1
93SZU/MCM	765-43-5	c-$C_3H_5COCH_3$	600	823	−15.1	805.8	854.9	−20.5	834.4	2	9.6	11.6
91SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	300	775.6	28.5	804.1	802.1	32.2	834.3	20	−12.1	7.9
91SZU/MCM	7664-41-7	NH_3	300	819	−11.7	807.3	853.6	−18.0	835.6	−6.4	20.5	14.1
91MAU/SIE	7664-41-7	NH_3	600	819	−8.8	805.6	853.6	−21.8	831.8	−6.4	21.8	15.4
91MAU/SIE	79-20-9	$CH_3CO_2CH_3$	600	790.7	16.3	805.8	821.6	18.8	840.5	5	−4.2	0.8
91MAU/SIE	90-12-0	1-methylnaphthalene	600	805.3			834.8	11.7	846.5			
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	26.4	805.3	802.1	31.0	833.1	20	−7.5	12.5
91MAU/SIE	75-18-3	$(CH_3)_2S$	600	801.2	4.6	805.8	830.9	7.5	838.4	9.1	−5.0	4.1
87TAF	7664-41-7	NH_3	350	819	−11.9	806.3						
84BOU/HOU	108-94-1	cyclohexanone	300	811.2	−3.8	807.5						
83TAF2	7664-41-7	NH_3	350	819	−12.8	805.4						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	25.1	801.2						
[$C_6H_{12}O$]	**592-90-5**	c-$C_6H_{12}O$(Oxepane)				**806.8**			**834.2**			**17**
87TAF	7664-41-7	NH_3	350	819	−12.4	805.5						
83MAU	624-89-5	$CH_3SC_2H_5$	600	815.3	1.3	812.6						
83MAU	142-68-7	c-$C_5H_{10}O$	600	795.4	7.9	803.3						
83MAU	109-99-9	Tetrahydrofuran	600	794.7	11.3	806.0						
[C_2H_3N]	**593-75-9**	**CH_3NC**				**806.6**			**839.1**			**0.1**
86MAU/KAR	96-22-0	$(C_2H_5)_2CO$	335	807	−7.5	799.8						
86MAU/KAR	109-99-9	Tetrahydrofuran	335	794.7	−0.4	794.9						
86KNI/FRE	60-29-7	$(C_2H_5)_2O$	303	801	5.0	806.1						
81AUE/PED	753-90-2	$CF_3CH_2NH_2$	298	812.9	−5.4	807.5						
81AUE/PED	141-78-6	$CH_3CO_2C_2H_5$	298	804.7	1.7	806.4						
[C_5H_7O]	**#1169**	**•$CH_2CH_2CH_2CH{=}CO$**				**806.2**			**838.6**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94SMI/CHY	75-18-3; 108-94-1	$(CH_3)_2S$; c-$C_6H_{10}(=O)$	300			801-811						
[$C_8H_8O_2$]	**99-94-5**	**Benzoic acid, 4-methyl**				**805.7**			**836.7**			**5**
91NOU/COO	563-80-4; 96-22-0	$(i\text{-}C_3H_7)COCH_3$; $C_2H_5OC_2H_5$				804-807						
[$C_5H_{10}O_2$]	**547-63-7**	**$i\text{-}C_3H_7COOCH_3$**				**805.7**			**836.6**			**5**
87TAF	7664-41-7	NH_3	350	819	−12.8	805.6						
83TAF	7664-41-7	NH_3	350	819	−12.8	805.6						
[$C_5H_{10}O_2$]	**108-21-4**	**isopropyl acetate**				**805.6**			**836.6**			**5**
86KAM/YOU	563-80-4	$(i\text{-}C_3H_7)COCH_3$	333	804.4	1.3	805.6						
[$C_5H_{10}O_2$]	**109-60-4**	**$CH_3COOC_3H_7$**				**805.6**			**836.6**			**5**
80MAU	7664-41-7	NH_3	550	819	−9.6	806.5						
79LAU	7664-41-7	NH_3	650	819	−10.4	804.6						
[$C_5H_{10}O_2$]	**623-42-7**	**$C_3H_7COOCH_3$**				**805.4**			**836.4**			**5**
87TAF	7664-41-7	NH_3	350	819	−14.2	804.2						
80MAU	7664-41-7	NH_3	550	819	−9.6	806.5						
79MAU	75-04-7	$C_2H_5NH_2$	550	878	−64.0	811.5						
[$C_{11}H_{10}$]	**90-12-0**	**1-methylnaphthalene**				**805.3**			**834.8**			**10**
91MAU/SIE	67-64-1	$(CH_3)_2CO$	600				812	15.1	827.1			
91MAU/SIE	96-22-0	$(C_2H_5)_2CO$	600				836.8	−11.7	825.1			
80MAU	7664-41-7	NH_3	550	819	−9.6	805.3						
[C_9H_{10}]	**873-66-5**	**Benzene, trans-(2-methylethenyl)**				**805.3**			**834.2**			**12**
89GAL/SPE		See Refs.				805.8						
89KAF/MAU	96-22-0	$(C_2H_5)_2CO$	570	807	−2.3	803.9	836.8	−1.3	835.5	9	6.3	15.3
89KAF/MAU	100-42-5	$C_6H_5CHCH_2$	500	809.2	−2.1	806.2						
[$C_4H_5F_6N$]	**407-01-2**	**$(CF_3CH_2)_2NH$**				**805.1**			**838.1**			**−2**
87TAF	7664-41-7	NH_3	350	819	−13.7	805.1						
[C_3H_6S]	**287-27-4**	**Thietane**				**805.0**			**834.8**			**9**
87TAF	7664-41-7	NH_3	350	819	−15.6	802.7						
79AUF/BOW	7664-41-7	NH_3	298	819	−11.7	807.3						
[$C_9H_7F_3O$]	**709-63-7**	**4-CF_3-C_6H_4-$COCH_3$**				**805.0**			**836.9**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−24.3	805.0						
[$C_4H_8O_2$]	**141-78-6**	**$CH_3CO_2C_2H_5$**				**804.7**			**835.7**			**5**
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	23.4	803.5	802.1	27.6	829.7	20	−7.1	12.9

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SZU/MCM	765-43-5	c-$C_3H_5COCH_3$	600	823	−17.6	804.5	854.9	−26.4	828.5	2	14.6	16.6
91SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	300	775.6	25.5	801.1	802.1	27.6	829.7	20	−7.1	12.9
91MAU/SIE	7664-41-7	NH_3	600	819	−13.4	802.2	853.6	−23.0	830.6	−6.4	15.9	9.5
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	27.2	807.3	802.1	32.2	834.3	20	−9.2	10.8
87TAF	7664-41-7	NH_3	350	819	−16.5	802.0						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	18.0	800.2						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	22.2	798.4						
79VAI/HAR	141-78-6	$CH_3CO_2C_2H_5$	373	804.7	0	804.7						
79AUE/BOW	7664-41-7	NH_3	298	819	14.2	804.8						
77WOL/STA	7664-41-7	NH_3	350	819	−16.9	801.5						
76YAM/KEB	7664-41-7	NH_3	600	819	−11.3	804.3						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	0	804.7						
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	8.4	790.8						
[C_6H_8O]	**6705-50-6**	**Bicyclo[2.2.1]hept-2-ene,7-oxa-**				**804.7**			**837.1**			**0**
86HOU/SCH	7664-41-7	NH_3	323	819	−14.2	804.6						
[C_6H_8]	**592-57-4**	**1,3-c-C_6H_8**				**804.5**			**837**			**0**
83GAU/HOU		See Refs.							837			
[$C_5H_{10}O$]	**557-31-3**	**$C_2H_5OCH_2CH{=}CH_2$**				**804.5**			**833.7**			**11**
86BOU/DJA	109-60-4	$CH_3COOC_3H_7$	313	805.6	−1	804.5						
[$C_8H_7ClO_2$]	**2905-65-9**	**3-Cl-C_6H_4-$COOCH_3$**				**804.4**			**835.4**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−15.1	804.4						
[$C_5H_{10}O$]	**563-80-4**	**(i-C_3H_7)$COCH_3$**				**804.4**			**836.3**			**2**
87TAF	7664-41-7	NH_3	350	819	−14.2	804.4						
83TAF	7664-41-7	NH_3	350	819	−14.2	804.4						
[C_5H_8]	**2004-70-8**	**(E)$CH_3CH{=}CHCH{=}CH_2$**				**804.4**			**834.1**			**9.1**
79AUE/BOW	7664-41-7	NH_3	298	819	−14.6	804.4						
[$C_5H_{12}Si$]	**754-05-2**	**$(CH_3)_3SiCH{=}CH_2$**				**804.1**			**833**			**12**
88HAJ/SQU		See Refs.							833±8			
[H_2Si]	**13825-90-6**	**SiH_2**				**804.1**			**839.2**			**−9.1**
86SHI/BEA	75-18-3; 96-22-0	$(CH_3)_2S$; $(C_2H_5)_2CO$				801-807						
[C_7H_{10}]	**498-66-8**	**Bicyclo[2.2.1]hept-2-ene**				**804.0**			**836.5**			**0**
86HOU/SCH	7664-41-7	NH_3	323	819	−13.4	805.5						
79SAL/KEB	100-66-3	$C_6H_5OCH_3$	560	807.2	−6.3	800.9	839.6	0.4	840.0	0	−11.7	−11.7
79AUE/BOW	7664-41-7	NH_3	298	819	−12.7	806.3						
77STA/WIE		$(C_2H_5)_2O$	320	801	2.1	803.4						
76SOL/FIE		See Refs.	300						829.1			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YtSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_7H_6F]	**2599-73-7**	**3-$FC_6H_4CH_2$ radical**				**804**			**836.5**			**0**
82MAU	60-29-7; 96-22-0	$(C_2H_5)_2O$; $(C_2H_5)_2CO$				801-807						
[C_8H_9]	**2348-51-8**	**$C_6H_5CHCH_3$ radical**				**804**			**836.5**			**0**
82MAU	60-29-7; 96-22-0	$(C_2H_5)_2O$; $(C_2H_5)_2CO$				801-807						
[$C_{13}H_{10}$]	**86-73-7**	**Fluorene**				**803.8**			**831.5**			**16**
80MAU	7664-41-7	NH_3	550	819	−9.6	803.8						
[$C_{11}H_{15}N$]	**23074-42-2**	**Tricyclo[3.3.1.1^{3,7}]decane-1-carbonitrile**				**803.8**			**834.4**			**6**
87TAF	7664-41-7	NH_3	350	819	−15.1	803.3						
87MAR/GAL	96-22-0	$(C_2H_5)_2CO$	350	807	−2.2	805.0						
87MAR/GAL	563-80-4	$(i\text{-}C_3H_7)COCH_3$	350	804.4	−1.2	803.0						
[$C_9H_7F_3O$]	**349-76-8**	**3-CF_3-C_6H_4-$COCH_3$**				**803.7**			**835.6**			**2**
87TAF	7664-41-7	NH_3	350	819	−18.3	800.3						
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−22.2	807.1						
[C_6H_{10}]	**1528-30-9**	**c-C_5H_8=CH_2**				**803.5**			**832.4**			**12**
77POL/WOL	7664-41-7	NH_3	350	819	−14.6	803.4						
[C_3H_4O]	**6004-44-0**	**CH_3CH=CO**				**803.4**			**834.1**			**6**
96BOU/SAL2	96-22-0; 565-80-0	$(C_2H_5)_2CO$; $(i\text{-}C_3H_7)_2CO$				807-821						
85TRA		threshold value							834.1			
80ARM/HIG	79-20-9	$CH_3CO_2CH_3$	320	790.7	6.7	797.3						
[$C_{10}H_{12}$]	**19714-73-9**	**Benzene, 1-cyclopropyl-3-methyl-**				**803.3**			**835.8**			**0**
89GAL/SPE						803.3						
[C_5HMnO_5]	**16972-33-1**	**$(CO)_5MnH$**				**803.0**			**835.5**			**0**
81STE/BEA	7664-41-7	NH_3	320	819	−15.9	803.0						
[$C_4H_8O_2S$]	**38103-96-7**	**$C_2H_5S(OCH_3)CO$**				**802.9**			**833.9**			**5**
87TAF	7664-41-7	NH_3	350	819	−15.6	802.9						
83TAF2	7664-41-7	NH_3	350	819	−15.6	802.9						
[C_4H_6O]	**78-94-4**	**CH_2=$CHCOCH_3$**				**802.8**			**834.7**			**2**
79VAJ/HAR	141-78-6	$CH_3CO_2C_2H_5$	373	804.7	−2.1	802.8						
[C_9H_{10}]	**873-49-4**	**c-C_3H_5-C_6H_5**				**802.4**			**834.9**			**0**
89GAL/SPE		See Refs.				802.4						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{11}H_{10}$]	**91-57-6**	**2-Methylnaphthalene**				**802.4**			**831.9**		**10**
80MAU	7664-41-7	NH_3	550	819	−12.6	802.3					
[$C_7H_{10}O$]	**10218-02-7**	**Bicyclo[2.2.1]heptan-7-one**				**802.4**			**832.1**		**9**
86HOU/SCH	7664-41-7	NH_3	323	819	−16.3	802.3					
[CH_3NO_2]	**4312-87-2**	**$HCOONH_2$**				**802.2**			**834.7**		**0**
87TAF	7664-41-7	NH_3	350	819	−16.5	802.2					
[$C_{13}H_{15}F_3$]	**146558-45-4**	**α-t-butylstyrene,3-CF_3**				**802.2**			**831.1**		**12**
92NAK/NOM	111-43-3	$(n\text{-}C_3H_7)_2O$	343	810.5	−9.2	801.5					
92NAK/NOM	60-29-7	$(C_2H_5)_2O$	343	801	1.7	802.9					
[C_7H_6O]	**100-52-7**	**C_6H_5CHO**				**802.1**			**834.0**		**2**
87TAF	7664-41-7	NH_3	350	819	16.0	802.6					
83TAF	7664-41-7	NH_3	350	819	−16.0	802.6					
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	17.6	799.8					
80MAU	7664-41-7	NH_3	550	819	−13.4	803.5					
79LAU	7664-41-7	NH_3	650	819	−13.6	802.5					
76LAU/KEB	71-43-2	C_6H_6	600	725.4	64.4	796.7					
[$C_9H_8O_3$]	**1571-08-0**	**4-HC(O)-C_6H_4-$COOCH_3$**				**801.9**			**832.9**		**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−17.6	801.9					
[$C_8H_7FO_2$]	**455-68-6**	**3-F-C_6H_4-$COOCH_3$**				**801.9**			**832.9**		**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−17.6	801.9					
[C_8H_5Cl]	**873-73-4**	**4-Cl-C_6H_4-CCH**				**801.7**			**832.4**		**5.8**
92MIS/ART	536-74-3	C_6H_5-CCH	323	801.3	0.4	801.7					
85MAR/MOD	109-99-9	Tetrahydrofuran	~300	794.7	1.3	796.0					
[$C_8H_{16}O$]	**19752-94-4**	**$C_6H_{11}CH_2OCH_3$**				**801.6**			**833.5**		**2**
87TAF	7664-41-7	NH_3	350	819	−16.9	801.6					
[CH_4N]	**10507-29-6**	**•CH_2NH_2**				**801.6**			**832.8**		**4**
96AUD/FOS	60-29-7; 100-	$(C_2H_5)_2O$; C_6H_5CHO				801-802					
89HOL/LOS		See Refs.	298						849.4		
81MCA/NIC	67-64-1; 60	$(CH_3)_2CO$; $(C_2H_5)_2O$				782-801					
[C_3H_6S]	**1072-43-1**	**2-Methylthiirane**				**801.5**			**833.3**		**2**
79AUE/BOW	7664-41-7	NH_3	298	819	−17.6	801.4					
[$C_9H_7MnO_3$]	**12108-13-3**	**$(CH_3C_5H_4)Mn(CO)_3$**				**801.3**			**833.8**		**0**
81STE/BEA	7664-41-7	NH_3	320	819	−17.6	801.3					
[C_8H_6]	**536-74-3**	**C_6H_5-CCH**				**801.3**			**832.0**		**5.8**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
96ZHA/STO	79-20-9	$CH_3CO_2CH_3$	588	790.7	9.2	799.6						
92MIS/ARI	7664-41-7	NH_3	323	819	−16.7	802.0						
85MAR/MOD	100-52-7	C_6H_5CHO	300	802.1	0	802.1						
[C_2H_6S]	**75-18-3**	**$(CH_3)_2S$**				**801.2**			**830.9**			**9.1**
97EAS/SMI		theory	298									9.1
93SMI/RAD		theory	600						834.2			
93SMI/RAD		theory	0						825.3			
93SMI/RAD		theory	298						830.9			9.1
91MAU/SIE	7664-41-7	NH_3	600	819	−16.3	798.0	853.6	−23.0	830.6	−6.4	10.9	4.5
91MAU/SIE	79-20-9	$CH_3CO_2CH_3$	600	790.7	11.7	801.1	821.6	12.1	833.8	5	−0.4	4.6
91MAU/SIE	115-11-7	$(CH_3)_2C=CH_2$	600	775.6	23.8	802.7	802.1	28.5	830.6	20	−8.8	11.2
87TAF	7664-41-7	NH_3	350	819	−16.9	801.3						
83TAF	7664-41-7	NH_3	350	819	−16.9	801.3						
79AUE/BOW	7664-41-7	NH_3	298	819	−14.6	804.4						
77WOL/STA	7664-41-7	NH_3	350	819	−16.9	801.3						
[$C_{15}H_{16}$]	**34403-06-0**	**3-CH_3-$C_6H_4(CH_2)_2C_6H_5$**				**801.0**			**833.5**			**0**
95CRE/FOR	67-64-1	$(CH_3)_2CO$	300	782.1	15.9	798.1						
95CRE/FOR	79-20-9	$CH_3CO_2CH_3$	300	790.7	10.5	801.1						
95CRE/FOR	141-78-6	$CH_3CO_2C_2H_5$	300	804.7	−0.8	803.9						
[$C_4H_{10}O$]	**60-29-7**	**$(C_2H_5)_2O$**				**801.**			**828.4**			**17**
93SZU/MCM	96-22-0	$(C_2H_5)_2CO$	600	807	−17	802.9	836.8	−7.1	829.7	9	8.8	17.8
91SZU/MCM	96-22-0	$(C_2H_5)_2CO$	300	807	−4.6	802.4	836.8	−7.1	829.7	9	8.8	17.8
87TAF	7664-41-7	NH_3	350	819	−19.7	798.2						
86MAU/LIE	60-29-7	$(C_2H_5)_2O$	600	801	0	801						
86KNI/FRE	7664-41-7	NH_3	303	819	−10.9	808.1						
86KNI/FRE	60-29-7	$(C_2H_5)_2O$	303	801	0	801						
83TAF	7664-41-7	NH_3	350	819	−17.8	800.0						
81LAU/NIS	62-53-3	$C_6H_5NH_2$	600	850.6	−42.3	803.8						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	14.6	796.6						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	20.5	796.2						
79AUE/BOW	7664-41-7	NH_3	298	819	−16.1	802.9						
78DAV/LAU	7664-41-7	NH_3	600	819	−11.7	800.3						
77WOL/STA	7664-41-7	NH_3	350	819	−17.8	800.0						
77STA/WIE	60-29-7	$(C_2H_5)_2O$	320	801	0	801						
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	9.2	790.8						
[$C_{16}H_{10}$]	**206-44-0**	**Fluoranthene**				**800.9**			**828.6**			**16**
80MAU	7664-41-7	NH_3	550	819	−12.6	800.8						
[$C_5H_{10}O$]	**107-87-9**	**n-$C_3H_7COCH_3$**				**800.9**			**832.7**			**2**
97HOM/HER	78-93-3	$CH_3COC_2H_5$	333	795.5	4.8	800.2						
97HOM/HER	60-29-7	$(C_2H_5)_2O$	333	801	2.8	804.4						
97HOM/HER	547-63-7	i-$C_3H_7COOCH_3$	333	805.7	−6.2	799.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
97HOM/HER	75-97-8	t-$C_4H_9COCH_3$	333	808.2	−9.2	799.0					
[C_7H_7]	**2154-56-5**	**$C_6H_5CH_2$**				**800.7**			**831.4**		**6**
82MAU	60-29-7; 111-43-3	$(C_2H_5)_2O$; (n-$C_4H_7)_2O$				801-810					
80DEF/MCI	79-20-9; 109-99-9	CH_3COOCH_3; c-C_4H_8O				791-795					
78HOU/BEA		threshold value							831.4		
[CH_3N_3]	**624-90-8**	**CH_3NNN**				**800.5**			**833**		**0**
89ATT/CAC		See Refs.; bracketed	358						833±12		
[ClLi]	**7447-41-8**	**LiCl**				**800.5**			**827**		**20**
87CRE/FAR		See Refs.							827±54		
[$C_5H_8O_2$]	**80-62-6**	**$CH_2=C(CH_3)COOCH_3$**				**800.5**			**831.4**		**5**
90WOL/GRU	79-20-9	$CH_3CO_2CH_3$	320	790.7	4	794.7					
90WOL/GRU	563-80-4	(i-C_3H_7)$COCH_3$	320	804.4	1.9	806.3					
[CSe]	**16674-18-3**	**CSe at C**				**800.2**			**831.8**		**3**
85JAS/STE		theory							831.8		
[$C_6H_{10}O$]	**557-40-4**	**$(CH_2=CHCH_2)_2O$**				**800.0**			**827.4**		**17**
87TAF	7664-41-7	NH_3	350	819	−17.8	800.0					
83TAF2	7664-41-7	NH_3	350	819	−18.3	799.5					
[C_7H_7]	**3551-27-7**	**c-C_7H_7 radical**				**800.0**			**832.4**		**0**
80DEF/MCI	78-93-3; 563-80-4	$CH_3COC_2H_5$; i-$C_3H_7COCH_3$				795-804					
[$C_9H_{10}O_4S$]	**22821-69-8**	**3-CH_3SO_2-C_6H_4-$COOCH_3$**				**799.5**			**830.5**		**5**
94DEC/EXN2	120-92-3	Cyclopentanone	338	794.0	3.2	797.3					
94DEC/EXN2	79-20-9	$CH_3CO_2CH_3$	338	790.7	9.1	799.8					
94DEC/EXN2	60-29-7	$(C_2H_5)_2O$	338	801	0	801.5					
[C_7H_5ClO]	**104-88-1**	**4-ClC_6H_4CHO**				**799.4**			**831.3**		**2**
87TAF	7664-41-7	NH_3	350	819	−19.2	799.4					
83TAF2	7664-41-7	NH_3	350	819	−19.2	799.4					
[$C_4H_8O_2$]	**504-12-1**	**$C_2H_5COOCH_3$**				**799.2**			**830.2**		**5**
87TAF	7664-41-7	NH_3	350	819	19.2	799.2					
83TAF	7664-41-7	NH_3	350	819	−19.2	799.2					
[$C_3H_6O_3$]	**616-38-6**	**$(CH_3O)_2CO$**				**799.2**			**830.2**		**5**
87TAF	7664-41-7	NH_3	350	819	−19.2	799.2					
77WOL/STA	7664-41-7	NH_3	350	819	−19.2	799.2					

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_5H_5]	**2143-63-5**	**c-C_5H_5 radical**				**799.1**			**831.5**			**0**
80DEF/MCI	598-53-8;	(i-C_3H_7)OOCH$_3$; $(C_2H_5)_2O$				797-801						
	60-29-7											
[C_4H_6O]	**4170-30-3**	**$CH_3CH{=}CHCHO$**				**799.0**			**830.8**			**2**
79VAJ/HAR	141-78-6	$CH_3CO_2C_2H_5$	373	804.7	−2.2	802.7						
79VAJ/HAR	67-64-1	$(CH_3)_2CO$	373	782.1	12.8	795.4						
79VAJ/HAR	79-20-9	$CH_3CO_2CH_3$	373	790.7	7.9	798.8						
[$C_8H_8O_2$]	**99-04-7**	**Benzoic acid, 3-methyl**				**798.8**			**829.8**			**5**
91NOU/COO	78-93-3;	$C_2H_5COCH_3$; C_6H_5CHO				795-802						
	100-52-7											
[C_5H_5NNiO]	**12071-73-7**	**(C_5H_5)NiNO**				**798.6**			**827.0**			**13.4**
81STE/BEA	7664-41-7	NH_3	320	819	−20.1	798.5						
[$C_8H_9NO_2$]	**89-87-2**	**2,4,-Dimethylnitrobenzene**				**798.5**			**831.0**			**0**
84ROL/HOU	1089-99-9	Tetrahydrofuran	320	794.7	2.1	797.1						
84ROL/HOU	60-29-7	$(C_2H_5)_2O$	320	801	−1.3	800.1						
[C_5FeO_5]	**13463-40-6**	**$(CO)_5Fe$**				**798.5**			**833.0**			**−7**
93EKE/HAG	7664-41-7	NH_3	300	819				5±5			−35±30	
91ALL/CRA	108-67-8	1,3,5,-$(CH_3)_3$-C_6H_3	300	808.6	−10.0	798.5	836.2	−2.9	833.3	16.2	−23	−6.8
75FOS/BEA3	616-38-6;	$(CH_3O)_2CO$; NH_3				799-819						
	7664-41-7											
75FOS/BEA2	7664-41-7	NH_3	320	819	−12.6	806.5						
[C_5H_6]	**542-92-7**	**1,3,c-C_5H_6**				**798.4**			**821.6**			**31**
81HOU/SCH	71-23-8;	n-C_3H_7OH; $(CH_3)_2O$				756-764						
	115-10-6											
80MAU	7664-41-7	NH_3	550	819	−11.3	798.4						
79AUE/BOW	7664-41-7	NH_3	298	819	−20.5	798.5						
75LOS/TRA		threshold value							827.6			
[C_7H_8O]	**694-71-3**	**Bicyclo[2.2.1]hept-2-ene-7-one**				**798.3**			**830.2**			**2**
86HOU/SCH	7664-41-7	NH_3	323	819	−20.5	798.3						
[C_3H_6OS]	**1534-08-3**	**$CH_3C(=O)SCH_3$**				**798.0**			**829.0**			**5**
87TAF	7664-41-7	NH_3	350	819	−21.1	797.4						
83CAS/KIM	79-20-9	$CH_3CO_2CH_3$	323	790.7	7.9	798.6						
[$C_6H_{12}O_2$]	**5515-64-0**	**trans-1,3-cyclohexanol**				**797.9**			**828.6**			**5.8**
85GUE/HOU	109-99-9;	tetrahydrofuran; $(C_2H_5)_2O$	323			795-801						
	60-29-7											

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_5H_8]	**78-79-5**	**CH_2=CHC(CH_3)=CH_2**				**797.6**			**826.4**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	−21.5	797.5						
[$C_4H_{12}Sn$]	**594-27-4**	**$(CH_3)_4Sn$**				**797.4**			**823.7**			**20.6**
84STO/SPL	108-38-3; 108-67-8	1,3-$C_6H_4(CH_3)_2$; 1,3,5-$C_6H_3(CH_3)_3$				786-809						
[Mg]	**7439-95-4**	**Mg**				**797.3**			**819.6**			**34**
77PO/POR	115-11-7; 7664-41-7	i-C_4H_8; NH_3				776-819						
[$C_4H_{10}O$]	**598-53-8**	**$(CH_3)_2CHOCH_3$**				**797.1**			**826.3**			**11**
87TAF	7664-41-7	NH_3	350	819	−21.1	797.1						
[$C_4H_6N_2O$]	**16703-51-8**	**$(CH_3)_2NCOCN$**				**797.1**			**829.0**			**2**
87TAF	7664-41-7	NH_3	350	819	21.5	797.1						
[$C_9H_{10}O_4S$]	**22821-70-1**	**4-CH_3SO_2-C_6H_4-$COOCH_3$**				**796.7**			**827.7**			**5**
94DEC/IEXN2	60-29-7	$(C_2H_5)_2O$	338	801	−2.6	798.9						
94DEC/IEXN2	120-92-3	Cyclopentanone	338	794.0	0.4	794.5						
94DEC/IEXN2	79-20-9	$CH_3CO_2CH_3$	338	790.7	6.1	796.8						
[C_8H_5F]	**766-98-3**	**4-FC_6H_4CCH**				**796.7**			**827.4**			**5.8**
85MAR/MOD	598-53-8	$(CH_3)_2CHOCH_3$	~300	797.1	−0.4	796.7						
[$C_6H_{13}O$]	**118-00-9**	**neo-$C_5H_{11}OCH_3$**				**796.7**			**825.8**			**11**
87TAF	7664-41-7	NH_3	350	819	−21.5	796.6						
[$C_{10}H_9F_3$]	**55186-75-9**	**4-$CF_3C_6H_4C(CH_3)CH_2$**				**796.6**			**825.5**			**12**
87TAF	7665-41-7	NH_3	350	819	−21.5	796.6						
83TAF2	7664-41-7	NH_3	350	819	−22.0	796.1						
[$C_9H_7F_3O_2$]	**2967-66-0**	**3-CF_3-C_6H_4-$COOCH_3$**				**796.5**			**827.5**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−23.0	796.5						
[$C_{13}H_{15}F_3$]	**22666-67-7**	**α-t-butylstyrene,4-CF_3**				**796.5**			**825.3**			**12**
92NAK/NOM	616-38-6	$(CH_3O)_2CO$	343	799.2	−2.9	796.0						
92NAK/NOM	109-99-9	Tetrahydrofuran	343	794.7	2.1	797.0						
[$C_4H_8O_2$]	**505-22-6**	**1,3-Dioxane**				**796.2**			**825.4**			**11**
83MAU	60-29-7	$(C_2H_5)_2O$	600	801	−5.9	797.0						
83MAU	109-99-9	Tetrahydrofuran	600	794.7	−0.8	795.7						
[C_4H_6O]	**1708-29-8**	**2,5-Dihydrofuran**				**796**			**823.4**			**17**
86BOU/DJA	60-29-7	$(C_2H_5)_2O$	313	801	−5	796						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_2H_6N_2O_2$]	**4164-28-7**	**$(CH_3)_2NNO_2$**				**795.8**			**828.3**			**0**
87TAF	7664-41-7	NH_3	350	819	−22.9	795.8						
[$C_9H_7F_3O_2$]	**2557-13-3**	**4-CF_3-C_6H_4-$COOCH_3$**				**795.7**			**826.6**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−23.8	795.7						
[$C_{13}H_{12}$]	**613-93-6**	**3-Methylbiphenyl**				**795.5**			**828.0**			**0**
89GAL/SPE		See Refs.				795.5						
[C_4H_8O]	**78-93-3**	**$CH_3COC_2H_5$**				**795.5**			**827.3**			**2**
87TAF	7664-41-7	NH_3	350	819	−22.0	796.6						
84BOU/HOU	120-92-3	Cyclopentanone	300	794.0	0.8	794.8						
83TAF	7664-41-7	NH_3	350	819	−21.5	797.1						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	18.4	794.7						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−0.4	805.2						
[C_2H_2S]	**18282-77-4**	**$CH_2{=}C{=}S$**				**795.4**			**826.2**			**5.8**
83CAS/KIM	463-51-4	$CH_2{=}C{=}O$	323	793.6	12.6	806.0						
83CAS/KIM	79-20-9; 1534-08-3	$CH_3CO_2CH_3$; $CH_3C(=O)SCH_3$	323			791-798						
[C_9H_7NO]	**6136-68-1**	**3-CN-C_6H_4-$COCH_3$**				**795.4**			**827.2**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−33.9	795.4						
[$C_5H_{10}O$]	**142-68-7**	**c-$C_5H_{10}O$**				**795.4**			**822.8**			**17**
87TAF	7664-41-7	NH_3	350	819	−19.7	798.2						
83MAU	67-64-1	$(CH_3)_2CO$	600	782.1	11.7	791.4						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	14.2	796.2						
77WOL/STA	7664-41-7	NH_3	350	819	−19.7	798.2						
[C_7H_5FO]	**459-57-4**	**4-FC_6H_4CHO**				**795.3**			**827.1**			**2**
87TAF	7664-41-7	NH_3	350	819	−23.3	795.2						
83TAF2	7664-41-7	NH_3	350	819	−23.3	795.2						
[$C_{14}H_{10}$]	**85-01-8**	**Phenanthrene**				**795.0**			**825.7**			**5.8**
85VAN/LEA		See Refs.										
80MAU	67-64-1	$(CH_3)_2CO$	547	782.1	12.1	795.0						
[C_9H_7NO]	**1443-80-7**	**4-CN-C_6H_4-$COCH_3$**				**795.0**			**826.8**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−34.3	795.0						
[$C_4H_6O_2$]	**96-33-3**	**$CH_2{=}CHCOOCH_3$**				**794.8**			**825.8**			**5**
90WOL/GRU	109-99-9	Tetrahydrofuran	320	794.7	0.3	795.2						
90WOL/GRU	120-92-3	Cyclopentanone	320	794.0	0.3	794.4						
[$C_{10}H_9F_3$]	**368-79-6**	**3-$CF_3C_6H_4C(CH_3){=}CH_2$**				**794.8**			**823.7**			**12**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	−23.3	794.7						
[$C_6H_{16}OSi$]	**597-52-4**	**$(C_2H_5)_3SiOH$**				**794.8**			**822.1**			**17**
88LI/STO	108-38-3	1,3-$(CH_3)_2$-C_6H_4	300	786.2	10.5	796.7	812.1	12.6	824.7	22	−7.1	14.9
88LI/STO	91-20-3	Naphthalene	300	779.4	13.4	792.8	802.9	16.7	819.7	30	−10.8	19.2
[C_4H_8O]	**109-99-9**	**Tetrahydrofuran**				**794.7**			**822.1**			**17**
87TAF	7664-41-7	NH_3	350	819	−23.8	794.0						
83TAF	7664-41-7	NH_3	350	819	−22.9	794.9						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	11.3	793.3						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	16.7	792.5						
79AUE/BOW	7664-41-7	NH_3	298	819	−20.0	799.0						
77WOL/STA	7664-41-7	NH_3	350	819	−22.9	794.9						
[$C_8H_7NO_3$]	**121-89-1**	**3-NO_2-C_6H_4-$COCH_3$**				**794.1**			**826.0**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−35.1	794.1						
[C_5H_8O]	**120-92-3**	**Cyclopentanone**				**794.0**			**823.7**			**9**
87TAF	7664-41-7	NH_3	350	819	−23.3	794.9						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	10.9	793.0						
79AUE/BOW	7664-41-7	NH_3	298	819	−19.0	800.0						
[C_2H_2O]	**463-51-4**	**$CH_2=C=0$**				**793.6**			**825.3**			**2.4**
97EAS/SMI		theory	298									2.4
96BOH/SAL	67-64-1; 141-78-6	$(CH_3)_2CO$; $CH_3CO_2C_2H_5$				782-805						
93SMI/RAD		theory	298						825			
93SMI/RAD		theory	600						829.8			
93SMI/RAD		theory	0						819.1			
84BEA/EYE		See Refs.							807.5			
82TRA/MCL		threshold value	298						825.3			
79LIA	67-64-1	$(CH_3)_2CO$	300	782.1	3.8	786.0						
79LIA	79-20-9	$CH_3CO_2CH_3$	300	790.7	0	790.7						
78DAV/LAU	7664-41-7	NH_3	600	819	−26.4	790.0						
[C_8H_7Br]	**2039-86-3**	**3-$BrC_6H_4CH=CH_2$**				**793.5**			**822.4**			**12**
84HAR/HOU	7664-41-7	NH_3	323	819	−25.1	793.5						
[$C_9H_{11}NO_2$]	**603-71-4**	**2,4,6-Trimethylnitrobenzene**				**793.1**			**823.8**			**5.8**
84ROL/HOU	89-87-2	2,4-Dimethylnitrobenzene	320	798.5	−5.4	793.0						
84ROL/HOU	79-20-9	$CH_3CO_2CH_3$	320	790.7	2.5	793.2						
[$C_4H_6O_2$]	**107-93-7**	**(E)-$CH_3CH=CHCOOH$**				**793**			**824.0**			**5**
84BOU/HOP	60-29-7	$(C_2H_5)_2O$	323	801	−6.3	795						
84BOU/HOP	109-99-9	Tetrahydrofuran	323	794.7	−3.8	791.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_7H_{12}O_2$]	**98-89-5**	**Cyclohexane carboxylic acid**				**792.8**			**823.8**			**5**
91NOU/COO	65-85-0; 78-93-3	C_6H_5COOH; $CH_3COC_2H_5$				790-795						
[$C_4H_8O_2$]	**543-75-9**	**Dihydro-1,4-dioxin**				**792.8**			**823.5**			**5.8**
86BOU/HAN	99-99-0	4-Nitrotoluene	313	782.7	3.3	786.0						
86BOU/HAN	79-20-9	$CH_3CO_2CH_3$	313	790.7	2.1	792.8						
[C_7H_{12}]	**591-49-1**	**1-Methylcyclohexene**				**792.6**			**825.1**			**0**
87TAF	7664-41-7	NH_3	350	819	−26.1	792.6						
77POL/WOL	7664-41-7	NH_3	350	819	−25.6	793.1						
[$C_5H_8O_2$]	**13991-37-2**	**(E)CH_3CH_2CH=CHCOOH**				**792.6**			**823.6**			**5**
88BOU/DJA	79-20-9	$CH_3CO_2CH_3$	313	790.7	2.5	793.2						
88BOU/DJA	109-99-9	Tetrahydrofuran	313	794.7	−3.8	791.1						
88BOU/DJA	60-29-7	$(C_2H_5)_2O$	313	801	−7.5	793.7						
[BrLi]	**7550-35-8**	**LiBr**				**792.5**			**819**			**20**
87CRE/FAR		See Refs.							819±54			
[$C_8H_7NO_3$]	**100-19-6**	**4-NO_2-C_6H_4-$COCH_3$**				**792.5**			**824.3**			**2**
86MIS/FUJ	98-86-2	$C_6H_5COCH_3$	343	829.3	−36.8	792.5						
[$C_5H_8O_2$]	**541-47-9**	**$(CH_3)_2C$=CHCOOH**				**791.9**			**822.9**			**5**
88BOU/DJA	120-92-3	Cyclopentanone	313	794.0	−2.9	791.1						
88BOU/DJA	78-93-3	$CH_3COC_2H_5$	313	795.5	−3.8	791.6						
88BOU/DJA	142-68-7	c-$C_5H_{10}O$	313	795.4	−2.5	793.0						
88BOU/DJA	60-29-7	$(C_2H_5)_2O$	313	801	−2.1	799.1						
[C_7H_{12}]	**765-47-9**	**c-C_5H_6-1,2-$(CH_3)_2$**				**791.9**			**822.6**			**5.8**
77POL/WOL	7664-41-7	NH_3	350	819	−26.5	791.8						
[$C_5H_8O_2$]	**565-63-9**	**(Z)CH_3CH=C(CH_3)COOH**				**791.5**			**822.5**			**5**
88BOU/DJA	109-99-9	Tetrahydrofuran	313	794.7	−3.3	791.6						
88BOU/DJA	120-92-3	Cyclopentanone	313	794.0	−2.5	791.5						
[$C_4H_9O_3P$]	**61580-09-4**	**4-Methyl-2,6,7-trioxa-1-phophabicyclo[2.2.1]heptane**				**791.5**			**823.9**			**0**
80HOD/HOU	79-20-9	$CH_3CO_2CH_3$	325	790.7	0.8	791.6						
80HOD/HOU	109-99-9	Tetrahydrofuran	325	794.7	−3.8	791.4						
[CH_3NO]	**75-12-7**	**$HCONH_2$**				**791.2**			**822.2**			**5**
83MAU	67-64-1	$(CH_3)_2CO$	600	782.1	7.9	791.2						
[$C_{18}H_{12}$]	**217-59-4**	**Triphenylene**				**791.2**			**819.2**			**14.9**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
80MAU	67-64-1	$(CH_3)_2CO$	530	782.1	10.5	791.2						
[$C_5H_{12}O$]	**628-28-4**	**n-$C_4H_9OCH_3$**				**791.2**			**820.3**			**11**
87TAF	7664-41-7	NH_3	350	819	−27.0	791.1						
[$C_6H_{12}O_2$]	**123-42-2**	**$(CH_3)_2C(OH)CH_2(C{=}O)CH_3$**				**791.1**			**822.9**			**2**
86KAM/YOU	78-93-3	$CH_3COC_2H_5$	330	795.5	−4.4	791.1						
[$C_2H_4N_2$]	**540-61-4**	**$NCCH_2NH_2$**				**791.0**			**824.9**			**−5**
87TAF	7664-41-7	NH_3	330	819	−28.4	790.6						
83TAF	75-04-7	$C_2H_5NH_2$	350	878	−86.5	791.5						
[$C_3H_6O_2$]	**79-20-9**	**$CH_3CO_2CH_3$**				**790.7**			**821.6**			**5**
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	10.9	791.0	802.1	14.2	816.3	20	−5.4	14.6
93SZU/MCM	109-86-4	$CH_3OCH_2CH_2OH$	600	729.8	−2.9	718.7	768.8	−20.1	748.7	−22	28.5	6.5
91SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	300	775.6	12.6	788.2	802.1	14.2	816.3	20	−5.4	14.6
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	15.1	795.2	802.1	13.0	815.1	20	3.8	23.8
91MAU/SIE	67-64-1	$(CH_3)_2CO$	600	782.1	7.9	791.2	812	2.9	814.9	8.7	8.4	17.1
87TAF	7664-41-7	NH_3	350	819	29.7	788.7						
83TAF	7664-41-7	NH_3	350	819	−29.7	788.7						
83CAS/KIM	79-20-9	$CH_3CO_2CH_3$	323	790.7	0	790.7						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	5.0	787.2						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	11.3	787.5						
80ARM/HIG	79-20-9	$CH_3CO_2CH_3$	320	790.7	0	790.7						
79LAU	7664-41-7	NH_3	650	819	−25.8	789.2						
79AUE/BOW	7664-41-7	NH_3	298	819	−28.8	790.2						
78AUS/LIA	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	11.3	787.5						
77WOL/STA	7664-41-7	NH_3	350	819	−29.7	788.7						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−12.1	792.6						
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	0.8	783.2						
[$C_3H_6O_2$]	**1759-53-1**	**Cyclopropane carboxylic acid**				**790.4**			**821.4**			**5**
91NOU/COO	65-85-0; 79-20-9	C_6H_5COOH; $CH_3CO_2CH_3$				790-791						
[$C_7H_6O_2$]	**65-85-0**	**C_6H_5COOH**				**790.1**			**821.1**			**5**
79LAU	7664-41-7	NH_3	650	819	−24.9	790.1						
[$C_3H_3N_3O_2$]	**26621-44-3**	**3(5)-nitropyrazole**				**789.0**			**820.8**			**2**
92ABB/CAB	109-99-9	Tetrahydrofuran	333	794.7	−5.1	790.1						
92ABB/CAB	67-64-1	$(CH_3)_2CO$	333	782.1	5.8	788.1						
[H_3O_3P]	**10294-56-1**	**H_3PO_3**				**788.8**			**821.3**			**0**
94DEP/OCC	67-64-1; 78-93-3	CH_3COCH_3; $CH_3COC_2H_5$				782-795						

J. Phys. Chem. Ref. Data, Vol. 27, No. 3, 1998

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_3H_3N_3O$]	**2075-46-9**	**4-NO_2-pyrazole**				**788.7**			**822.2**			**−3.8**
93NOT/HER	109-99-9	Tetrahydrofuran	333	794.7	−5.4	790.0						
94NOT/HER	67-64-1	$(CH_3)_2CO$	333	782.1	4.8	787.4						
[C_5H_8]	**698-23-2**	**$(CH_3)_2CHCCH$**				**787.8**			**814.9**			**18**
79AUE/BOW	7664-41-7	NH_3	298	819	−31.2	787.8						
[C_3H_4]	**2781-85-3**	**Cyclopropene**				**787.8**			**818.5**			**5.8**
76AUE/DAV	7664-41-7	NH_3	298	819	−31.2	787.8						
[$C_{15}H_{16}$]	**1081-75-0**	**$C_6H_5(CH_2)_3C_6H_5$**				**787.6**			**820.1**			**0**
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	12.6	785.4						
95CRE/FOR	67-64-1	$(CH_3)_2CO$	300	782.1	6.3	788.4						
95CRE/FOR	79-20-9	$CH_3CO_2CH_3$	300	790.7	−1.7	789.0						
[C_3H_5O]	**3122-07-4**	**•CH_2COCH_3**				**787.5**			**820**			**0**
89HOL/LOS			298						820			
[$C_6H_5N_3$]	**622-37-7**	**phenyl azide**				**787.5**			**820**			**0**
89ATT/CAC		See Refs.; bracketed	358						820±12			
[$C_9H_{10}O$]	**638-86-3**	**$C_6H_5CH_2OCH_3$**				**787.5**			**816.7**			**11**
87TAF	7664-41-7	NH_3	350	819	−30.7	787.5						
[C_5H_8]	**693-86-7**	**c-$C_3H_5CH{=}CH_2$**				**787.5**			**816.3**			**12**
87TAF	7664-41-7	NH_3	350	819	−30.7	787.4						
77WOL/STA	7664-41-7	NH_3	350	819	−30.7	787.4						
[C_6H_{10}]	**693-89-0**	**1-Methylcyclopentene**				**787.1**			**816.5**			**10**
87TAF	7664-41-7	NH_3	350	819	−33.9	784.3						
79AUE/BOW	7664-41-7	NH_3	298	819	−29.3	789.7						
77POL/WOL	7664-41-7	NH_3	350	819	−34.8	783.4						
76SOL/FIE		See Refs.	300						813.2			
[$C_8H_5Cl_3O$]	**2902-69-4**	**$C_6H_5COCCl_3$**				**787.0**			**818.9**			**2**
87TAF	7664-41-7	NH_3	350	819	−31.6	787.0						
[$C_7H_5CrNO_3$]	**36312-04-6**	**$(C_5H_5)Cr(CO)_2NO$**				**786.7**			**819.1**			**0**
81STE/BEA	7664-41-7	NH_3	320	819	−32.2	786.7						
[C_6H_5]	**116138-99-9**	**CH_3-CC-CC-CH_2·**				**786.6**			**819.1**			**0**
87KIN/BUR	67-56-1	CH_3OH		724.5			754.3	57.9	812.2			
87KIN/BUR	7732-18-5	H_2O		660.0			691	135	826			
[$C_9H_9NO_2$]	**1830-68-8**	**4-(NO_2)$C_6H_4C(CH_3){=}CH_2$**				**786.5**			**815.4**			**12**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	−31.6	786.5						
[$C_9H_7NO_2$]	**13531-48-1**	**3-CN-C_6H_4-$COOCH_3$**				**786.5**			**817.4**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−33.1	786.5						
[$C_2H_5NO_2$]	**109-95-5**	**C_2H_5ONO**				**786.4**			**818.9**			**0**
78FAR/MCM	67-64-1; 79-20-9	$(CH_3)_2CO$; CH_3COOCH_3				782-791						
[$C_6H_8N_2O$]	**1656-48-0**	**$O(CH_2CH_2CN)_2$**				**786.4**			**813.8**			**17**
84BOL/YVE	67-64-1; 79-20-9	$(CH_3)_2CO$; CH_3COOCH_3	298			782-791						
[$C_6H_{10}O_2$]	**3400-45-1**	**cyclopentane carboxylic acid**				**786.4**			**817.4**			**5**
91NOU/COO	67-64-1; 79-20-9	$(CH_3)_2CO$; CH_3COOCH_3				782-791						
[$C_5H_8O_2$]	**3721-95-7**	**Cyclobutane carboxylic acid**				**786.4**			**817.4**			**5**
91NOU/COO	67-64-1; 79-20-9	$(CH_3)_2CO$; CH_3COOCH_3				782-791						
[C_6H_6O]	**108-95-2**	**C_6H_5OH**				**786.3**			**817.3**			**5**
80MAU	7664-41-7	NH_3	550	819	−26.4	789.8						
79LAU	7664-41-7	NH_3	650	819	−32.2	782.8						
77DEF/MCI	74-90-81; 115-07-1	HCN; C_3H_6				682-723						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	47.3	778.7						
[C_8H_{10}]	**108-38-3**	**1,3-$(CH_3)_2$-C_6H_4**				**786.2**			**812.1**			**22**
87LI/STO	108-67-8	1,3,5-$(CH_3)_3$-C_6H_3	300	808.6	−23.4	785.1	836.2	−25.5	810.7	16.2	6	22.2
76DEV/WOL	71-43-2	C_6H_6	350	725.4	61.8	787.3						
72CHO/FRA2	115-10-6	$(CH_3)_2O$	340	764.5	3.3	767.6						
72CHO/FRA2	74-93-1	CH_3SH	340	742	10.8	752.1						
[C_6H_{12}]	**563-79-1**	**$(CH_3)_2C{=}C(CH_3)_2$**				**785.9**			**813.9**			**15**
75SOL/FIE		hydride transfer	300						813.9			
[$C_4H_6O_2$]	**79-41-4**	**$CH_3C(=CH_2)COOH$**				**785.7**			**816.7**			**5**
84BOU/HOP	109-99-9	Tetrahydrofuran	323	794.7	−8.4	786.6						
84BOU/HOP	79-20-9	$CH_3CO_2CH_3$	323	790.7	−5.9	784.8						
[$C_4H_{10}O$]	**557-17-5**	**n-$C_3H_7OCH_3$**				**785.7**			**814.9**			**11**
87TAF	7664-41-7	NH_3	350	819	−32.5	785.6						
[$C_9H_7NO_2$]	**1129-35-7**	**4-CN-C_6H_4-$COOCH_3$**				**785.6**			**816.6**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−33.9	785.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_{13}H_{12}$]	**644-08-6**	**4-Methylbiphenyl**				**785.4**			**817.9**			**0**
89GAL/SPE		See Refs.				785.4						
[C_5H_5P]	**289-68-9**	**Phosphabenzene**				**785.3**			**817.7**			**0**
85HOD/BEA	79-20-9	$CH_3CO_2CH_3$	320	790.7	−3.3	787.4						
85HOD/BEA	67-64-1	$(CH_3)_2CO$	320	782.1	0.8	783.2						
[$C_4H_{10}S$]	**75-66-1**	**t-C_4H_9SH**				**785.1**			**816.4**			**4**
87TAF	7664-41-7	NH_3	350	819	−33.4	785.1						
83TAF2	7664-41-7	NH_3	350	819	−34.8	783.7						
[$C_8H_7NO_4$]	**618-95-1**	**3-O_2N-C_6H_4-$COOCH_3$**				**784.7**			**815.7**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−35.1	784.4						
[$C_4H_{10}O$]	**78-92-2**	**$CH_3CH_2CH(OH)CH_3$**				**784.6**			**815**			**7**
78PAU/KIM		See Refs.							815			
[$C_3H_4O_3$]	**96-49-1**	**1,3-Dioxolane-2-one**				**784.4**			**814.2**			**9**
87TAF	7664-41-7	NH_3	350	819	−33.9	784.4						
[$C_7H_{11}N$]	**766-05-2**	**c-$C_6H_{11}CN$**				**784.4**			**815.0**			**6**
87TAF	7664-41-7	NH_3	350	819	−33.4	785.0						
87MAR/GAL	78-82-0	i-C_3H_7CN	320	772.8	12	784.8						
87MAR/GAL	5500-21-0	c-C_3H_5CN	320	777.5	6.5	784						
87MAR/GAL	100-47-0	C_6H_5CN	320	780.9	2.7	783.6						
[C_4H_4S]	**110-02-1**	**Thiophene**				**784.3**			**815.0**			**5.8**
86MAU	67-64-1	$(CH_3)_2CO$	600	782.1	−0.4	782.6						
83TAF2	7664-41-7	NH_3	350	819	−27.9	790.5						
83MAU	123-91-1	1,4-Dioxane	600	770.0	6.3	779.7						
83MAU	78-93-3	$CH_3COC_2H_5$	600	795.5	−10.5	783.9						
81HOU/SCH	71-23-8; 115-10-6	n-C_3H_7OH; $(CH_3)_2O$				756-764						
[C_6H_{12}]	**922-61-2**	**$CH_3CH{=}C(CH_3)C_2H_5$**				**784.0**			**812.9**			**12**
76GOR/MUN		hydride transfer	300						809.6			
75SOL/FIE		hydride transfer	300						816.1			
[$C_{18}H_{22}$]	**1087-49-6**	**$C_6H_5(CH_2)_6C_6H_5$**				**783.8**			**826.1**			**−33**
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	12.6	785.5						
95CRE/FOR	67-64-1	$(CH_3)_2CO$	300	782.1	0	782.2						
[$C_3H_5O_2$]	**‡1324**	**•CH_2COOCH_3**				**783.5**			**816**			**0**
89HOL/LOS			298						816			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_{13}H_{12}$]	**643-58-3**	**2-Methylbiphenyl**				**783.4**			**815.9**			**0**
89GAL/SPE		See Refs.				783.4						
[$C_3H_9B_3O$]	**121-43-7**	**$B(OCH_3)_3$**				**783.4**			**815.8**			**0**
93RAN/POU	78-92-2; 67-64-1	2-butanol; CH_3COCH_3				785-782						
[$C_9H_9NO_2$]	**64416-49-5**	**3-$(NO_2)C_6H_4C(CH_3)=CH_2$**				**783.3**			**812.2**			**12**
87TAF	7664-41-7	NH_3	350	819	−34.8	783.3						
[C_6H_{12}]	**625-27-4**	**$(CH_3)_2C=CHCH_2CH_3$**				**783.1**			**812**			**12**
78AUS/LIA	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	11.7	787.6						
76GOR/MUN		hydride transfer	300						811.1			
75SOL/FIE		hydride transfer	300						807.8			
[C_7H_{14}]	**625-65-0**	**$(CH_3)_2C=CHCH(CH_3)_2$**				**783.1**			**812**			**12**
76MAU/SOL		See Refs.							812			
[$C_4H_6O_2$]	**108-05-4**	**$CH_3COOCH=CH_2$**				**782.9**			**813.9**			**5**
86MAU	67-64-1	$(CH_3)_2CO$	600	782.1	−1.7	781.6						
86MAU	109-94-4	$HCO_2C_2H_5$	600	768.4	15.9	784.3						
[$C_{12}H_{10}$]	**92-52-4**	**Biphenyl**				**782.9**			**813.6**			**5.8**
80MAU	67-64-1	$(CH_3)_2CO$	550	782.1	0	782.9						
[$C_2H_6S_2$]	**624-92-0**	**CH_3SSCH_3**				**782.8**			**815.3**			**0**
81KIM/BON	115-10-6; 75-18-3	$(CH_3)_2O$; $(CH_3)_2S$				764-801						
[$C_7H_7NO_2$]	**99-99-0**	**4-Nitrotoluene**				**782.7**			**815.2**			**0**
84ROL/HOU	67-64-1	$(CH_3)_2CO$	320	782.1	0.4	782.7						
[$C_6H_8O_2$]	**637-88-7**	**c-hexane-1,4-dione**				**782.7**			**812.5**			**9**
87BOU/HOP	79-41-4	$CH_3C(=CH_2)COOH$	313	785.7	−2.9	782.7						
[C_7H_5FO]	**456-48-4**	**3-FC_6H_4CHO**				**782.5**			**814.3**			**2**
87TAF	7664-41-7	NH_3	350	819	−36.2	782.4						
83TAF2	7664-41-7	NH_3	350	819	−37.1	781.3						
[$C_7H_{14}S$]	**2550-37-0**	**c-$C_6H_{11}CH_2SH$**				**782.4**			**813.6**			**4**
87TAF	7664-41-7	NH_3	350	819	−36.2	782.3						
[$C_{17}H_{20}$]	**1718-50-9**	**$C_6H_5(CH_2)_5C_6H_5$**				**782.4**			**824.7**			**−33**
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	11.7	784.6						
95CRE/FOR	67-64-1	$(CH_3)_2CO$	300	782.1	−2.1	780.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_8H_7NO_4$]	**619-50-1**	**4-O_2N-C_6H_4-$COOCH_3$**				**782.3**			**813.2**			**5**
86MIS/FUJ2	93-58-3	$C_6H_5CO_2CH_3$	343	819.5	−37.2	782.3						
[C_3H_6O]	**67-64-1**	**$(CH_3)_2CO$**				**782.1**			**812**			**8.7**
97EAS/SMI		theory	298									8.7
95SMI/RAD		theory	298						811.9			
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	7.5	786.5	802.1	8.8	810.9	20	−2.1	17.9
93SZU/MCM	60-29-7	$(C_2H_5)_2O$	600	801	−16.3	787.2	828.4	−21.3	807.0	17	8.4	25.4
93SZU/MCM	96-22-0	$(C_2H_5)_2CO$	600	807	−18.0	789.1	836.8	−22.6	814.2	9	7.5	16.5
91SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	300	775.6	8.4	784.0	802.1	8.8	810.9	20	−2.1	17.9
91SZU/MCM	96-22-0	$(C_2H_5)_2CO$	300	807	−20.5	786.5	836.8	−22.6	814.2	9	7.5	16.5
91SZU/MCM	60-29-7	$(C_2H_5)_2O$	300	801	−18.8	782.2	828.4	−21.3	807.0	17	8.4	25.4
91MAU/SIE	91-20-3	Naphthalene	600	779.4	4.2	790.0	802.9	16.7	819.7	30	−20.9	9.1
91MAU/SIE	78-82-0	i-C_3H_7CN	600	772.8	12.1	784.1	803.6	14.6	818.2	5.7	−3.8	1.9
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	7.1	786.1	802.1	9.2	811.3	20	−2.9	17.1
87TAF	7664-41-7	NH_3	350	819	−35.2	783.0						
83MAU	67-64-1	$(CH_3)_2CO$	600	782.1	0	782.1						
81BRO/ABB	64-64-1	$(CH_3)_2CO$	320	782.1	0	782.1						
80MAU	7664-41-7	NH_3	550	819	−28.9	786.4						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	6.7	782.8						
79AUE/BOW	7664-41-7	NH_3	298	819	−31.7	787.3						
78DAV/LAU	7664-41-7	NH_3	600	819	−27.2	787.3						
78AUS/LIA	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	6.3	782.3						
77WOL/STA	7664-41-7	NH_3	350	819	−36.2	782.1						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−14.6	788.9						
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	0	782.1						
[C_8H_6ClN]	**874-86-2**	**4-(CH_2Cl)-C_6H_4-CN**				**782.1**			**812.8**			**6**
94DEC/EXN2	100-47-0	C_6H_5CN	338	780.9	0.8	781.7						
94DEC/EXN2	5500-21-0	c-C_3H_5CN	338	777.5	5.1	782.6						
[$C_{10}H_{17}$]	**119-64-2**	**1,2,3,4-Tetrahydronaphthalene**				**782.1**			**809.7**			**16**
80MAU	7664-41-7	NH_3	550	819	−31.4	782.0						
[$C_9H_7F_3$]	**402-24-4**	**3-$CF_3C_6H_4CH{=}CH_2$**				**781.8**			**810.7**			**12**
84HAR/HOU	7664-41-7	NH_3	323	819	−36.8	781.8						
[$C_4H_{10}S$]	**513-53-1**	**$CH_3CH_2CH(SH)CH_3$**				**781.7**			**813**			**4**
78PAU/KIM		See Refs.							813			
[$C_3H_{10}OSi$]	**1066-40-6**	**Silanol, trimethyl**				**781.5**			**814.0**			**0**
89ORL/ALL	95-47-6; 108-38-3	o-xylene; m-xylene				768-786						
85CLE/MUN	100-47-0; 109-99-9	C_6H_5CN; tetrahydrofuran	470			781-795						
75PIT/BUR		See Refs.										

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_3H_8O]	**540-67-0**	**$CH_3OC_2H_5$**				**781.2**			**808.6**			**17**
87TAF	7664-41-7	NH_3	350	819	−36.6	781.2						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	17.6	782.0						
77WOL/STA	7664-41-7	NH_3	350	819	−37.5	780.3						
[C_6H_{10}]	**764-35-2**	**2-hexyne**				**781.1**			**806.1**			**25**
96ZHA/STO	108-38-3	1,3-$(CH_3)_2$-C_6H_4	603	786.2	−4.2	781.1						
[C_7H_5ClO]	**587-04-2**	**3-ClC_6H_4CHO**				**781.1**			**813.0**			**2**
87TAF	7664-41-7	NH_3	350	819	−37.5	781.1						
[C_7H_5N]	**100-47-0**	**C_6H_5CN**				**780.9**			**811.5**			**6**
87TAF	7664-41-7	NH_3	350	819	−36.6	781.8						
86MAR/TOP	78-82-0	i-C_4H_7CN	300	772.8	7.9	780.8						
86MAR/TOP	74-90-8	HCN	300	681.6	96.2	777.9						
79LAU	7664-41-7	NH_3	650	819	−31.7	782.9						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	47.7	778.8						
[C_8H_6ClN]	**64407-07-4**	**3-(CH_2Cl)-C_6H_4-CN**				780.6			**811.2**			**6**
94DEC/EXN2	100-47-0	C_6H_5CN	338	780.9	−0.9	780.0						
94DEC/EXN2	5500-21-0	c-C_3H_5CN	338	777.5	3.7	781.2						
[$C_4H_8O_2$]	**625-55-8**	**$HCOOCH(CH_3)_2$**				**780.3**			**811.3**			**5**
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	−2.1	780.3						
[$C_7H_8O_2S$]	**3112-85-4**	**$C_6H_5SO_2CH_3$**				**780.3**			**812.7**			**0**
87TAF	7664-41-7	NH_3	350	819	−38.4	780.2						
[C_5H_9N]	**630-18-2**	**t-C_4H_9CN**				**780.2**			**810.9**			**6**
87TAF	7664-41-7	NH_3	350	819	−37.1	781.3						
86MAU/KAR	108-38-3	1,3-$(CH_3)_2$-C_6H_4	335	786.2	−2.9	783.9						
86MAU/KAR	67-64-1	$(CH_3)_2CO$	335	782.1	−4.2	778.1						
86MAR/TOP	78-82-0	i-C_4H_7CN	300	772.8	7.5	780.4						
86MAR/TOP	74-90-8	HCN	300	681.6	95.8	777.5						
[C_5H_{10}]	**513-35-9**	**$(CH_3)_2C{=}CHCH_3$**				**779.9**			**808.8**			**12**
79AUE/BOW	7664-41-7	NH_3	298	819	−33.7	785.3						
78AUS/LIA	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	5.4	781.4						
76GOR/MUN		hydride transfer	300						807.7			
75SOL/FIE		hydride transfer	300						809.8			
[C_8H_5Cl]	**766-83-6**	**3-ClC_6H_4CCH**				**779.8**			**812.3**			**0**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	−21.3	780.1						
85MAR/MOD	67-64-1	$(CH_3)_2CO$	~300	782.1	−2.5	779.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[$C_{16}H_{18}$]	**1083-56-3**	**$C_6H_5(CH_2)_4C_6H_5$**				**779.8**			822.0			**−33**
95CRE/FOR	78-82-0	i-C_4H_7CN	300	772.8	7.9	780.9						
95CRE/FOR	67-64-1	$(CH_3)_2CO$	300	782.1	−2.5	779.7						
80MAU/HUN	95-47-6	o-Xylene	350	768.3	7.5	778.3	796.0	24.7	820.7	16	−49	−33
[$C_{10}H_8$]	**91-20-3**	**Naphthalene**				**779.4**			**802.9**			**30**
88LI/STO	108-38-3	1,3-$(CH_3)_2$-C_6H_4	300	786.2	−3.8	782.5	812.1	−6.3	805.9	22	8	30
85VAN/LEA		See Refs.										
80MAU	7664-41-7	NH_3	550	819	−31.8	778.1						
78LAU/SAL	7664-41-7	NH_3	600	819	−30.1	778.0						
[$C_6H_{12}O_6$]	**26655-34-5**	**alpha-D-glucose**				**778.9**			**NE**			**NE**
96HEB/ZHA	115-11-7; 67-64-1	$(CH_3)_2C=CH_2$; $(CH_3)_2CO$				776-782						
[$C_6H_{12}O_6$]	**28905-12-6**	**beta-D-glucose**				**778.9**			**NE**			**NE**
96HEB/ZHA	115-11-7; 67-64-1	$(CH_3)_2C=CH_2$; $(CH_3)_2CO$				776-782						
[$C_5H_{12}S$]	**1679-08-9**	**neo-$C_5H_{11}SH$**				**778.2**			**809.5**			**4**
87TAF	7664-41-7	NH_3	350	819	−40.3	778.2						
[$C_7H_7NO_3$]	**619-73-8**	**4-NO_2-$C_6H_4CH_2OH$**				**778.0**			**810.5**			**0**
86SUN/KUL		See Refs.	300			778			812			
[C_5H_8]	**627-21-4**	**$C_2H_5CCCH_3$**				**778.0**			**810.2**			**1**
79AUE/BOW	7664-41-7	NH_3	298	819	−41	778						
74MCA	115-11-7; 67-64-1	i-C_4H_8; $(CH_3)_2CO$				776-782						
[C_3H_4S]	**420-12-2**	***c*-C_2H_4S(Thiirane)**				**777.6**			**807.4**			**9**
80AUE/WEB	79-20-9	$CH_3CO_2CH_3$	298	790.7	−8.8	781.9						
80AUE/WEB	115-11-7	$(CH_3)_2C=CH_2$	298	775.6	1.0	776.6						
80AUE/WEB	592-84-7	HCO_2(n-C_4H_9)	298	775	2.4	777.4						
80AUE/WEB	513-35-9	$(CH_3)_2C=CHCH_3$	298	779.9	−5.4	774.6						
[HOSi]	**97402-81-8;a**	**HSiO at O**				**777.5**			**810**			**0**
93LUC/CUR		theory	298						810			
[C_4H_5N]	**5500-21-0**	***c*-C_3H_5CN**				**777.5**			**808.2**			**6**
87TAF	7664-41-7	NH_3	350	819	−40.7	777.7						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−5.0	777.2						
76STA/KLE	7664-41-7	NH_3	320	819	−37.2	781.5						
[C_4H_6O]	**78-85-3**	**$CH_2=C(CH_3)CHO$**				**776.8**			**808.7**			**2**
79VAJ/HAR	123-91-1	1,4-Dioxane	373	770.0	4.6	775.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M - Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
79VAJ/HAR	592-84-7	HCO_2(n-C_4H_9)	373	775	2.5	777.7						
79VAJ/HAR	67-64-1	$(CH_3)_2CO$	373	782.1	−5.4	777.2						
[C_5H_9NO]	**2141-62-0**	**$C_2H_5CH(OC_2H_5)CH_2CN$**				**776.5**			**807.2**			**6**
87TAF	7664-41-7	NH_3	350	819	−42.1	776.3						
87MAR/GAL	100-47-0	C_6H_5CN	320	780.9	−3.3	777.6						
87MAR/GAL	78-82-0	i-C_3H_7CN	320	772.8	3	775.8						
87MAR/GAL	110-74-7	HCO_2(n-C_3H_7)	320	773.9	2.5	776.4						
[C_6H_{12}]	**592-41-6**	**1-hexene**				**776.3**			**805.2**			**12**
96ZHA/STO	108-38-3	1,3-$(CH_3)_2$-C_6H_4	580	786.2	−9.6	779.4						
96ZHA/STO	79-20-9	$CH_3CO_2CH_3$	573	790.7	−15.5	773.3						
[C_8H_5F]	**2561-17-3**	**3-FC_6H_4CCH**				**776.3**			**808.7**			**0**
85MAR/MOD	67-64-1	$(CH_3)_2CO$	~300	782.1	−5.9	776.3						
[C_4H_8]	**115-11-7**	**$(CH_3)_2C=CH_2$**				**775.6**			**802.1**			**20**
97EAS/SMI		theory	298									15.7
96TRA		threshold value	298						801.7			
93SZU/MCM	7664-41-7	NH_3	600	819	−32.2	778.9	853.6	−50.2	803.4	−6.4	30.5	24.1
93SMI/RAD		theory	0						798.7			
93SMI/RAD		theory	600						804.7			
93SMI/RAD		theory	298						802.1			
93KEI/RIL		appearance	298						802			
91SZU/MCM	7664-41-7	NH_3	300	819	−41.4	777.6	853.6	−50.2	803.4	−6.4	30.5	24.1
91MAU/SIE	7664-41-7	NH_3	600	819	−37.7	773.4	853.6	−53.6	800.0	−6.4	25.9	19.5
87TAF	7664-41-7	NH_3	350	819	−42.1	775.6						
80LIA/SHO	75-07-0	CH_3CHO	340	736.5	36.8	772.6						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	0	775.6						
79HOU/BEA		threshold value				783.7						
79AUE/BOW	7664-41-7	NH_3	298	819	−39.5	779.5						
78DAV/LAU	7664-41-7	NH_3	600	819	−33.9	777.2						
77WOL/STA	7664-41-7	NH_3	350	819	−42.1	775.6						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−21.3	778.9						
[C_6O_6V]	**20644-87-5**	**$(CO)_6V$**				**775.3**			**799.9**			**26.4**
81STE/BEA	7664-41-7	NH_3	320	819	−43.1	775.2						
[$C_8H_7FO_4S$]	**124397-36-0**	**3-SO_2F-C_6H_4-$COOCH_3$**				**775.1**			**806.1**			**5**
94DEC/EXN2	630-18-2	t-C_4H_9CN	338	780.2	−4.9	775.4						
94DEC/EXN2	5500-21-0	c-C_3H_5CN	338	777.5	−2.1	775.4						
94DEC/EXN2	109-94-4	$CHO_2C_2H_5$	338	768.4	6	774.4						
[$C_5H_{10}O_2$]	**592-84-7**	**HCO_2(n-C_4H_9)**				**775**			**806.0**			**5**
87TAF	7664-41-7	NH_3	350	819	−43.9	774.5						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	−1.7	774.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	11.7	776.2					
77WOL/STA	7664-41-7	NH_3	350	819	−43.9	774.5					
[CH_2N_2]	**420-04-2**	**NH_2-CN**				**774.9**			**805.6**		**6**
93CAC/DEP	78-82-0	i-C_3H_7CN	298	772.8	2.1	774.9					
84BEA/EYE		See Refs.							686		
[C_8H_7N]	**140-29-4**	**Benzyl cyanide**				**774.8**			**805.5**		**6**
87TAF	7664-41-7	NH_3	350	819	−43.5	774.9					
87MAR/GAL	5500-21-0	c-C_3H_5CN	350	777.5	−1.7	775.8					
87MAR/GAL	78-82-0	i-C_3H_7CN	350	772.8	1.7	774.5					
87MAR/GAL	107-12-0	C_2H_5CN	350	763.0	11	774.0					
[C_8H_{10}]	**693-02-7**	**1-hexyne**				**774.8**			**799.8**		**25**
96ZHA/STO	108-38-3	1,3-$(CH_3)_2$-C_6H_4	610	786.2	−8.8	776.5					
96ZHA/STO	79-20-9	$CH_3CO_2CH_3$	574	790.7	−12.1	773.0					
[Mn]	**7439-96-5**	**Mn**				**774.4**			**797.3**		**32**
86ELK/ARM2		See Refs.	298						797±13		
[$C_{14}H_{14}$]	**103-29-7**	**$C_6H_5(CH_2)_2C_6H_5$**				**774.1**			**801.8**		**16**
95CRE/FOR	115-10-6	$(CH_3)_2O$	300	764.5	11.3	775.8					
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	1.3	774.1					
80MAU/HUN	95-47-6	o-Xylene	350	768.3	3.8	772.1					
[C_3H_6O]	**503-30-0**	**c-C_3H_6O(Oxetane)**				**773.9**			**801.3**		**17**
87TAF	7664-41-7	NH_3	350	819	−43.9	773.9					
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	19.5	784.0					
[$C_4H_8O_2$]	**110-74-7**	**HCO_2(n-C_3H_7)**				**773.9**			**804.9**		**5**
87TAF	7664-41-7	NH_3	350	819	−44.8	773.6					
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−2.5	773.7					
79LAU	7664-41-7	NH_3	650	819	−43.1	771.9					
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	8.8	773.2					
77WOL/STA	7664-41-7	NH_3	350	819	−44.8	773.6					
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−27.6	777.1					
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	−8.4	774.0					
[$C_3H_5F_3$]	**705-28-2**	**3-CF_3-C_6H_4-CCH**				**773.8**			**806.2**		**0**
92MIS/ARI	536-74-3	C_6H_5-CCH	323	801.3	−27.6	773.8					
85MAR/MOD	115-10-6	$(CH_3)_2O$	~300	764.5	2.5	767.0					
[$C_8H_5F_3O$]	**455-19-6**	**p-$CF_3C_6H_4CHO$**				**773.8**			**805.6**		**2**
87TAF	7664-41-7	NH_3	350	819	−44.8	773.7					
87TAF	115-11-7	$(CH_3)_2C{=}CH_2$	350	775.6	−2.7	773.8					
83TAF2	7664-41-7	NH_3	350	819	−60.4	758.2					

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_2H_6O_2$]	**107-21-1**	**$HOCH_2CH_2OH$**				**773.6**			**815.9**			**−33**
95CHE/STO	108-88-3	$C_6H_5CH_3$	600	756.3	2.7	773.6	784.0	33.1	817.0	16	−50.6	−34.6
93BOU/JEZ	78-85-3; 67-64-1	CH_2=C(CH_3)CHO; $(CH_3)_2CO$	300			777-782			820			
[$C_{20}H_{24}$]	**128484-66-2**	***trans*-1,4-dibenzylcyclohexane**				**773.3**			**805.7**			**0**
95CRE/FOR	115-10-6	$(CH_3)_2O$	300	764.5	7.5	772.0						
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	1.7	774.5						
[C_4H_7N]	**78-82-0**	**i-C_3H_7CN**				**772.8**			**803.6**			**5.7**
93SZU/MCM	67-64-1	$(CH_3)_2CO$	600	782.1	−13.0	770.1	812	−1.7	810.3	8.7	−19.2	−10.5
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	−5.0	774.9	802.1	−3.8	798.3	20	−2.1	17.9
91MAU/SIE	107-12-0	C_2H_5CN	600	763.0	9.6	772.4	794.1	10.0	804.1	4.7	0.8	5.5
91MAU/SIE	91-20-3	Naphthalene	600	779.4	−9.6	777.1	802.9	2.1	805.0	30	−19.2	10.8
91MAU/SIE	108-88-3	$C_6H_5CH_3$	600	756.3	17.2	776.5	784.0	21.3	805.3	16	−7.1	8.9
87TAF	7664-41-7	NH_3	350	819	−45.3	773.1						
86MAR/TOP	78-82-0	i-C_3H_7CN	300	772.8	0	772.8						
77WOL/STA	7664-41-7	NH_3	350	819	44.8	773.5						
76STA/KLE	109-94-4	$HCO_2C_2H_5$	320	768.4	4.2	772.6						
[$B_3H_6N_3$]	**6569-51-3**	**Borazine**				**772.8**			**802.5**			**9.1**
79DOI/GRE	123-91-1	1,4-Dioxane	298	770.0	2.9	773.0						
79DOI/GRE	109-94-4	$HCO_2C_2H_5$	298	768.4	4.2	772.6						
[C_4H_6O]	**1191-95-3**	**cyclobutanone**				**772.7**			**802.5**			**9**
92ABB/CAN	110-74-7	HCO_2(n-C_3H_7)	333	773.9	0.3	774.0						
92ABB/CAN	109-74-0	n-C_3H_7CN	333	767.7	4.9	772.5						
92ABB/CAN	100-47-0	C_6H_5CN	333	780.9	−7.6	773.2						
87TAF	7664-41-7	NH_3	350	819	−46.7	771.6						
84BOU/HOU	115-10-6	$(CH_3)_2O$	300	764.5	5.0	769.5						
84BOU/HOU	79-09-4	C_2H_5COOH	300	766.2	0.4	766.7						
84BOU/HOU	75-65-0	t-C_4H_9OH	300	772.2	−1.7	770.5						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−10.5	771.7						
[C_3H_6O]	**75-56-9**	**2-Methyloxirane**				**772.7**			**803.3**			**6**
79AUE/BOW	7664-41-7	NH_3	298	819	−46.4	772.6						
[C_3H_8S]	**75-33-2**	**i-C_3H_7SH**				**772.3**			**803.6**			**4**
87TAF	7664-41-7	NH_3	350	819	−46.2	772.3						
83TAF2	7664-41-7	NH_3	350	819	−46.2	772.3						
[H_2N_2]	**3618-05-1**	**HN=NH**				**772.3**			**803**			**5.8**
92GAR/RUT		theory							803			
[$C_3H_6F_3N$]	**677-41-8**	**$CF_3N(CH_3)_2$**				**772.2**			**803.0**			**5.6**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	−45.3	773.1						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	6.8	771.3						
77STA/TAA	7664-41-7	NH_3	350	819	−47.6	770.8						
[$C_4H_{10}O$]	**75-65-0**	**t-C_4H_9OH**				**772.2**			**802.6**			**7**
79LAU	7664-41-7	NH_3	650	819	−41.7	772.6						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	6.8	771.3						
78TAF/TAA	67-56-1	CH_3OH	320	724.5	48.1	772.7						
77HIR/KEB		See Refs.							795			84
[C_5H_9N]	**110-59-8**	**n-C_4H_9CN**				**771.7**			**802.4**			**6**
87TAF	7664-41-7	NH_3	350	819	−46.7	771.7						
76STA/KLE	7664-41-7	NH_3	320	819	−42.7	776.1						
[$C_{18}H_{20}$]	**21072-42-4**	***trans*-1,4-diphenylcyclohexane**				**771.7**			**804.1**			**0**
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	−1.3	771.6						
[$C_7H_{14}O$]	**100-49-2**	**c-$C_6H_{11}CH_2OH$**				**771.7**			**802.1**			**7**
87TAF	7664-41-7	NH_3	350	819	−46.7	771.7						
[$C_9H_7FO_4S$]	**124397-38-2**	**4-SO_2F-C_6H_4-$COOCH_3$**				**771.6**			**802.6**			**5**
94DEC/EXN2	630-18-2	t-C_4H_9CN	338	780.2	−8.4	771.9						
94DEC/EXN2	5500-21-0	c-C_3H_5CN	338	777.5	−5.5	772.0						
94DEC/EXN2	109-94-4	$HCO_2C_2H_5$	338	768.4	2.4	770.8						
[$C_4H_{10}S$]	**513-44-0**	**i-C_4H_9SH**				**771.4**			**802.6**			**4**
87TAF	7664-41-7	NH_3	350	819	−47.1	771.3						
[C_4H_4O]	**110-00-9**	**Furan**				**770.9**			**803.4**			**0**
83MAU	108-88-3	$C_6H_5CH_3$	600	756.3	13.4	774.5						
83MAU	109-94-4	$HCO_2C_2H_5$	600	768.4	−2.5	767.4						
81HOU/SCH	71-23-8; 115-10-6	n-C_3H_7OH; $(CH_3)_2O$				756-764						
80HOU/SCH	67-64-1	$(CH_3)_2CO$	323	782.1	−2.5	779.8						
[$C_4H_7O_2$]	**4598-47-4**	**1,4-Dioxyl radical**				**770.7**			**803.2**			**0**
83AUS/LUT	123-91-1	1,4-Dioxane	340	770.0	~0	770.7						
[$C_3H_5O_3P$]	**279-53-8**	**2,6,7-Trioxa-1-phosphabicyclo[2.2.1]heptane**				**770.6**			**803.1**			**0**
80HOD/HOU	109-74-0	n-C_3H_7CN	320	767.7	1.7	769.5						
80HOD/HOU	5500-21-0	c-C_3H_5CN	320	777.5	−5.9	771.8						
[$B_3H_5N_3$]	**61110-11-0**	**B-Borazinyl radical**				**770.6**			**803.0**			**0**
76DES/POR	109-94-4; 6569-51-3	$HCO_2C_2H_5$; $H_3B_3N_3H_3$				768-773						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_4H_{10}S$]	**109-79-5**	**n-C_4H_9SH**				**770.5**			**801.7**			**4**
87TAF	7664-41-7	NH_3	350	819	−48.1	770.4						
[$C_4H_6O_2$]	**431-03-8**	**$CH_3COCOCH_3$**				**770.1**			**801.9**			**2**
87BOU/HOP	109-94-4	$HCO_2C_2H_5$	313	768.4	2.5	770.9						
87BOU/HOP	1191-95-3	cyclobutanone	313	772.7	−3.3	769.5						
87BOU/HOP	115-10-6	$(CH_3)_2O$	313	764.5	5.0	769.7						
83MAU	67-64-1	$(CH_3)_2CO$	600	782.1	−14.1	770.1	812	−7.5	804.5	8.7	−10.9	−2.2
[$C_4H_8O_2$]	**123-91-1**	**1,4-Dioxane**				**770.0**			**797.4**			**17**
87TAF	7664-41-7	NH_3	350	819	−48.1	769.8						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−11.7	770.3						
77WOL/STA	7664-41-7	NH_3	350	819	−47.6	770.2						
[$C_6H_5NO_2$]	**98-95-3**	**$C_6H_5NO_2$**				**769.5**			**800.3**			**5.8**
87TAF	7664-41-7	NH_3	350	819	−49.4	769.0						
84ROL/HOU	123-91-1	1,4-Dioxane	320	770.0	−1.3	769.0						
79LAU	7664-41-7	NH_3	650	819	−43.1	771.7						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	37.2	768.4						
[$C_{13}H_{12}$]	**101-81-5**	**$C_6H_5CH_2C_6H_5$**				**769.5**			**802.0**			**0**
95CRE/FOR	115-10-6	$(CH_3)_2O$	300	764.5	6.7	771.2						
95CRE/FOR	78-82-0	i-C_3H_7CN	300	772.8	−5.0	767.8						
[$C_6H_4O_2$]	**106-51-4**	**p-benzoquinone**				**769.3**			**799.1**			**9**
96IRI/MAU	107-12-0; 115-11-7	C_2H_5CN; i-C_5H_8				763-776						
[$C_8H_7NO_2S$]	**22821-75-6**	**3-(CH_3SO_2)-C_6H_4-CN**				**768.8**			**799.5**			**6**
94DEC/EXN2	109-74-0	n-C_3H_7CN	338	767.7	0.5	768.2						
94DEC/EXN2	109-94-4	$HCO_2C_2H_5$	338	768.4	1.1	769.5						
[$C_3H_6O_2$]	**109-94-4**	**$HCO_2C_2H_5$**				**768.4**			**799.4**			**5**
87TAF	7664-41-7	NH_3	350	819	−50.3	768.1						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−13.8	768.4						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−10.0	766.2						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	3.9	768.4						
78DAV/LAU	7664-41-7	NH_3	600	819	−41.8	773.7						
77WOL/STA	7664-41-7	NH_3	350	819	−50.3	768.1						
76STA/KLE	109-94-4	$HCO_2C_2H_5$	320	768.4	0	768.4						
76HAR/LIN	67-64-1	$(CH_3)_2CO$	370	782.1	−8.4	774.0						
[Cr]	**7440-47-3**	**Cr**				**768.4**			**791.3**			**32**
87ELK/ARM		See Refs.							791±9			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_8H_{10}]	**95-47-6**	**o-Xylene**				**768.3**			**796.0**			**16**
87TAF	7664-41-7	NH_3	350	819	−49.0	768.9						
80MAU/HUN	95-47-6	o-Xylene	350	768.3	0	768.3						
80MAU	108-88-3	$C_6H_5CH_3$	492	756.3	9.2	765.5						
76DEV/WOL	71-43-2	C_6H_6	350	725.4	43.9	769.8						
74HEH/MCI	7664-41-7	NH_3	350	819	−48.5	769.4						
72CHO/FRA2	115-10-6	$(CH_3)_2O$	340	764.5	3.3	767.7						
72CHO/FRA2	74-93-1	CH_3SH	340	742	10.4	751.9						
[C_2H_5P]	**6569-82-0**	**c-C_2H_4PH**				**768.3**			**802.5**			**−5.8**
80AUE/WEB	123-91-1	1,4-Dioxane	298	770.0	−2.4	767.6						
80AUE/WEB	115-10-6	$(CH_3)_2O$	298	764.5	2.4	766.9						
80AUE/WEB	110-74-7	HCO_2(n-C_3H_7)	298	773.9	−3.4	770.5						
[$C_8H_7NO_2S$]	**22821-76-7**	**4-(CH_3SO_2)-C_6H_4-CN**				**768.0**			**798.7**			**6**
94DEC/EXN2	109-74-0	n-C_3H_7CN	338	767.7	−0.3	767.4						
94DEC/EXN2	109-94-4	$HCO_2C_2H_5$	338	768.4	0.3	768.7						
[C_4H_7N]	**109-74-0**	**n-C_3H_7CN**				**767.7**			**798.4**			**6**
87TAF	7664-41-7	NH_3	350	819	−49.4	769.0						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	2.0	766.4						
76STA/KLE	7664-41-7	NH_3	320	819	−44.8	774.0						
[$C_8H_5F_3O$]	**434-45-7**	**$C_6H_5COCF_3$**				**767.4**			**799.2**			**2**
87TAF	7664-41-7	NH_3	350	819	−51.3	767.3						
[CH_2Te]	**43309-26-8**	**H_2C=Te**				**766.8**			**796**			**11**
85JAS/STE		theory							796			
[C_8H_{10}]	**106-42-3**	**p-Xylene**				**766.8**			**794.4**			**16**
76DEV/WOL	71-43-2	C_6H_6	350	725.4	40.7	766.6						
74HEH/MCI	7664-41-7	NH_3	350	819	−51.7	766.2						
72CHO/FRA2	74-93-1	CH_3SH	340	742	10.2	751.7						
72CHO/FRA2	115-10-6	$(CH_3)_2O$	340	764.5	3.0	767.5						
[C_2H_3NS]	**556-61-6**	**CH_3NCS**				**766.7**			**799.2**			**0**
85KAR/STE	109-74-0	n-C_3H_7CN	300	767.7	−1.3	766.5						
85KAR/STE	115-10-6	$(CH_3)_2O$	300	764.5	2.5	767.0						
74MCA	115-11-7; 67-64-1	i-C_4H_8; $(CH_3)_2CO$				776-782						
[CH_2OS]	**40100-16-1**	**CH_2=S=O**				**766.4**			**798.9**			**0**
96BOU/SAL	115-10-6; 109-94-4	$(CH_3)_2O$; $HCO_2C_2H_5$				764-768						
[CH_3NO_2]	**624-91-9**	**CH_3ONO**				**766.4**			**798.9**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
78FAR/MCM	115-10-6; 109-94-4	$(CH_3)_2O$; $HCOOC_2H_5$				764-768						
76MCA/PIT	64-17-5; 67-64-1	C_2H_5OH; CH_3COCH_3				746-782						
[$C_4H_7F_3S$]	**5187-62-2**	**$CF_3CH_2SC_2H_5$**				**766.4**			**797.6**			**4**
87TAF	7664-41-7	NH_3	350	819	−52.2	766.3						
[$C_5H_7F_3O_2$]	**352-23-8**	**$CF_3CH_2COOC_2H_5$**				**766.3**			**797.3**			**5**
87TAF	7664-41-7	NH_3	350	819	−52.2	766.3						
[C_8H_5NO]	**105-07-7**	**4-CNC_6H_4CHO**				**766.3**			**796.9**			**6**
87TAF	7664-41-7	NH_3	350	819	52.2	766.2						
83TAF2	7664-41-7	NH_3	350	819	−78.3	740.1						
[$C_3H_6O_2$]	**79-09-4**	**C_2H_5COOH**				**766.2**			**797.2**			**5**
76YAM/KEB	7664-41-7	NH_3	600	819	−49.4	766.2						
[C_2H_3NS]	**556-64-9**	**CH_3SCN**				**766.1**			**796.7**			**6**
85KAR/STE	115-10-6; 109-74-0	$(CH_3)_2O$; $n\text{-}C_3H_7CN$				764-768						
74MCA	115-11-7; 67-64-1	$i\text{-}C_4H_8$; $(CH_3)_2CO$				776-782						
[C_4H_3NO]	**57681-10-4**	**$NCC(CH_3)CO$**				**765.5**			**798**			0
94FLA/HAV		theory							798			
[C_4H_8O]	**78-84-2**	**$i\text{-}C_3H_7CHO$**				**765.5**			**797.3**			2
87TAF	7664-41-7	NH_3	350	819	−53.1	765.5						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	1.0	765.4						
77WOL/STA	7664-41-7	NH_3	350	819	−53.1	765.5						
[$C_5H_{12}O$]	**75-84-3**	**$neo\text{-}C_5H_{11}OH$**				**765.2**			**795.5**			7
78TAF/TAA	67-56-1	CH_3OH	320	724.5	40.6	765.2						
[C_3H_4O]	**107-02-8**	**$CH_2{=}CHCHO$**				**765.1**			**797.0**			2
79VAJ/HAR	109-94-4	$HCO_2C_2H_5$	373	768.4	−3.3	765.3						
[$C_5H_{10}O$]	**110-62-3**	**$n\text{-}C_4H_9CHO$**				**764.8**			**796.6**			2
87TAF	7664-41-7	NH_3	350	819	−53.1	765.5						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−0.5	764.0						
77WOL/STA	7664-41-7	NH_3	350	819	−53.1	765.5						
[C_2H_6O]	**115-10-6**	**$(CH_3)_2O$**				**764.5**			**792**			16.5
97EAS/SMI		theory	298									17.1
93SZU/MCM	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	−11.7	764.9	802.1	−8.8	793.3	20	−5.0	15.0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	298						792			
93SMI/RAD		theory	600						794.6			
93SMI/RAD		theory	0						787.3			
91MAU/SIE	115-11-7	$(CH_3)_2C{=}CH_2$	600	775.6	−12.6	764.1	802.1	−13.4	788.7	20	1.7	21.7
87TAF	7664-41-7	NH_3	350	819	−53.5	764.3						
86TAF/GAL	7664-41-7	NH_3	350	819	−53.0	764.8						
83TAF	7664-41-7	NH_3	350	819	−53.5	764.3						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−16.7	765.2						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−13.4	762.4						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	0	764.5						
77WOL/STA	7664-41-7	NH_3	350	819	−53.5	764.3						
76YAM/KEB	7664-41-7	NH_3	600	819	−46.4	765.7						
76KEB/YAM	141-78-6	$CH_3CO_2C_2H_5$	600	804.7	−32.2	769.0						
76HAR/LIN	75-07-0	CH_3CHO	370	736.5	18.4	753.9						
75SOL/HAR	75-07-0	CH_3CHO	373	736.5	18.8	754.2						
[$C_{10}H_{14}$]	**104-51-8**	**n-$C_4H_9C_6H_5$**				**764.2**			**791.9**			**16**
87TAF	7664-41-7	NH_3	350	819	−52.2	765.7						
76YAM/KEB	71-43-2	C_6H_6	600	725.4	33.1	761.2						
74HEH/MCI	7664-41-7	NH_3	350	819	−52.2	765.7						
[C_9H_{12}]	**98-82-8**	**i-$C_3H_7C_6H_5$**				**763.9**			**791.6**			**16**
76YAM/KEB	71-43-2	C_6H_6	600	725.4	33.1	761.2						
74HEH/MCI	7664-41-7	NH_3	350	819	−51.7	766.2						
[CHF]	**13453-52-6**	**CFH**				**763.8**			**797.9**			**−5.8**
85LIA/KAR	115-10-6; 107-12-0	$(CH_3)_2O$; C_2H_5CN				764-763						
[C_3H_8S]	**107-03-9**	**n-C_3H_7SH**				**763.6**			**794.9**			**4**
87TAF	7664-41-7	NH_3	350	819	−54.9	763.6						
83TAF2	7664-41-7	NH_3	350	819	−57.7	760.8						
[C_3H_5FO]	**430-61-3**	**CH_3COCH_2F**				**763.5**			**795.4**			**2**
81DRU/MCM	109-94-4	$HCO_2C_2H_5$	298	768.4	−5.4	763.0						
81DRU/MCM	115-10-6	$(CH_3)_2O$	298	764.5	−0.4	764.0						
[$C_7H_5NO_3$]	**555-16-8**	**4-$(NO_2)C_6H_4CHO$**				**763.2**			**795.1**			**2**
87TAF	7664-41-7	NH_3	350	819	−55.4	763.2						
[C_3H_5N]	**107-12-0**	**C_2H_5CN**				**763.0**			**794.1**			**4.7**
97EAS/SMI		theory	298									5.6
95SMI/RAD		theory	298						794.3			
91MAU/SIE	75-05-8	CH_3CN	600	748	17.6	765.5	779.2	15.9	795.1	4.3	2.5	6.8
91MAU/SIE	107-31-3	$HCOOCH_3$	600	751.5	10.5	762.1	782.5	13.0	795.5	5	−4.2	0.8
91MAU/SIE	108-88-3	$C_6H_5CH_3$	600	756.3	3.3	763.0	784.0	11.7	795.7	16	−14.2	1.8

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M – Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
91MAU/SIE	115-10-6	$(CH_3)_2O$	600				792	2.9	794.9			
87TAF	7664-41-7	NH_3	350	819	−55.4	763.1						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−14.2	762.0						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−2.9	761.5						
76STA/KLE	7664-41-7	NH_3	320	819	−50.2	768.6						
[C_3H_8O]	**67-63-0**	**i-C_3H_7OH**				**762.6**			**793.0**			**7**
79LAU	7664-41-7	NH_3	650	819	−53.0	761.3						
78TAF/TAA	67-56-1	CH_3OH	350	724.5	38.9	763.5						
[C_9H_{12}]	**103-65-1**	**n-$C_3H_7C_6H_5$**				**762.4**			**790.1**			**16**
87TAF	7664-41-7	NH_3	350	819	−54.0	763.9						
76YAM/KEB	71-43-2	C_6H_6	600	725.4	31.4	759.5						
74HEH/MCI	115-11-7	$(CH_3)_2C{=}CH_2$	350	775.6	−12.4	763.5						
[$C_4H_{10}O$]	**78-83-1**	**i-C_4H_9OH**				**762.2**			**793.7**			**3**
78TAF/TAA	67-56-1	CH_3OH	320	724.5	35.6	760.2						
78TAF/TAA	67-64-1	$(CH_3)_2CO$	320	782.1	−18.0	764.3						
[$C_7H_5O_3$]	**1124-18-1**	**$C_6H_5CD_3$**				**762**			**789.7**			**16**
77AUS/LIA		See Refs.	340			762						
[C_7H_7Cl]	**95-49-8**	**2-Cl-toluene**				**761.1**			**790.5**			**10**
87HER/JEN	352-70-5	3-F-toluene	478	756.0	5.1	761.1	785.4	23	808.4			
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−15.5	741.2						
[C_4H_8O]	**123-72-8**	**n-C_3H_7CHO**				**760.8**			**792.7**			**2**
87TAF	7664-41-7	NH_3	350	819	−57.7	760.9						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−15.5	760.8						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	1.0	765.4						
77WOL/STA	7664-41-7	NH_3	350	819	−57.7	760.9						
[$C_8H_4F_3N$]	**368-77-4**	**3-(CF_3)-C_6H_4-CN**				**760.8**			**791.4**			**6**
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	6.4	760.2						
94DEC/EXN2	123-72-8	n-C_3H_7CHO	338	760.8	0.7	761.3						
[C_8H_{10}]	**100-41-4**	**$C_2H_5C_6H_5$**				**760.3**			**788.0**			**16**
87TAF	7664-41-7	NH_3	350	819	−58.1	759.8						
79LAU	7664-41-7	NH_3	650	819	−50.3	760.8						
77WOL/STA	7664-41-7	NH_3	350	819	−58.1	759.8						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	30.5	758.7						
74HEH/MCI	7664-41-7	NH_3	350	819	−58.1	759.6						
[CS]	**2944-05-0**	**CS**				**760**			**791.5**			**3.3**
97EAS/SMI		theory	298									3.3
93SMI/RAD		theory	0						789.9			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	298						795.6			
93SMI/RAD		theory	600						799.1			
92CUR/NOB		theory	298						785			
85SMI/ADA		See Refs.	300			756.0						
85JAS/STE		theory							787.4			
85BOT/SEB		theory	0						793			
78MCA	74-96-4; 115-07-1	C_2H_5Br; C_3H_6				670-723						
[C_8H_8FeO]	**12080-06-7**	**$(C_5H_5)Fe(CO)_2CH_3$**				**759.5**			**792.0**			**0**
81STE/BEA	7664-41-7	NH_3	320	819	−59.4	759.5						
[$C_4H_5Cl_3O_2$]	**515-84-4**	**$CCl_3COOC_2H_5$**				**759.4**			**790.4**			**5**
87TAF	7664-41-7	NH_3	350	819	−59.0	759.4						
[$C_4H_{10}O$]	**71-36-3**	**n-C_4H_9OH**				**758.9**			**789.2**			**7**
87TAF	7664-41-7	NH_3	350	819	−59.5	758.8						
83TAF2	7664-41-7	NH_3	350	819	−59.9	758.4						
78PAU/KIM	7664-41-7	NH_3	320	819	−54.8	763.9						
[C_2H_6S]	**75-08-1**	**C_2H_5SH**				**758.4**			**789.6**			**4**
87TAF	7664-41-7	NH_3	350	819	−61.3	757.2						
83TAF2	7664-41-7	NH_3	350	819	−63.2	755.3						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−16.7	759.5						
[$C_8H_4F_3N$]	**455-18-5**	**4-(CF_3)-C_6H_4-CN**				**758.3**			**787.2**			**11.8**
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	5	758.6						
94DEC/EXN2	123-72-8	n-C_3H_7CHO	338	760.8	−2.5	757.9						
[C_4H_6]	**106-99-0**	**$CH_2{=}CHCH{=}CH_2$**				**757.6**			**783.4**			**22**
87LIA/AUS	75-05-08	CH_3CN	340	748	9.2	756.5						
87LIA/AUS	107-31-3	$HCOOCH_3$	340	751.5	3.8	754.6						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−2.9	761.5						
[$C_4H_4N_4O_4$]	**32683-48-0**	**1-methyl-3,5-dinitropyrazole**				**757.0**			**788.8**			**2**
92ABB/CAB	123-38-6	C_2H_5CHO	333	754.0	3.4	757.4						
92ABB/CAB	108-88-3	$C_6H_5CH_3$	333	756.3	−0.5	756.2						
92ABB/CAB	100-41-4	$C_2H_5C_6H_5$	333	760.3	−3.5	757.3						
[NP]	***17739-47-8***	***PN***				***757.0***			***789.4***			***0***
90ADA/MIC	7803-51; 2 107-12-0	PH_3; C_2H_5CN	300			751-763						
[C_6H_6O]	**6921-27-3**	**$(HCCCH_2)_2O$**				**756.5**			**783.9**			**17**
87TAF	7664-41-7	NH_3	350	819	−61.3	756.5						
83TAF2	7664-41-7	NH_3	350	819	−61.3	756.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_7H_8]	**108-88-3**	**$C_6H_5CH_3$**				**756.3**			**784.0**			**16**
97EAS/SMI		theory	298									11.5
93SZU/MCM	462-06-6	C_6H_5F	600	726.6	30.1	755.0	755.9	25.5	781.4	10.5	7.5	18.0
93SZU/MCM	78-82-0	i-C_3H_7CN	600	772.8	−15.1	754.7	803.6	−25.6	777.7	5.7	18.0	23.7
91MAU/SIE	71-43-2	C_6H_6	600	725.4	29.7	757.8	750.4	34.7	785.1	25	−8.4	16.6
91MAU/SIE	75-05-8	CH_3CN	600	748	12.1	756.6	779.2	6.7	785.9	4.3	9.2	13.5
87TAF	7664-41-7	NH_3	350	819	−62.2	755.6						
82STO/SPL	108-88-3	$C_6H_5CH_3$	478	756.3	0	756.3						
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	0	756.3						
80MAU	7664-41-7	NH_3	550	819	−46.0	767.4						
79LAU	7664-41-7	NH_3	650	819	−54.8	756.3						
77AUS/LIA		See Refs.	340			762						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	26.4	754.5						
76DEV/WOL	71-43-2	C_6H_6	350	725.4	30.2	756.1						
74HEH/MCI	7664-41-7	NH_3	350	819	−62.7	755.2						
72CHO/FRA2	74-93-1	CH_3SH	340	742	6.6	748.1						
[C_3H_8O]	**71-23-8**	**n-C_3H_7OH**				**756.1**			**786.5**			**7**
87TAF	7664-41-7	NH_3	350	819	−62.2	756.1						
81BRO/ABB	67-64-1	$(CH_3)_2CO$	320	782.1	−24.7	757.5						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−9.8	754.7						
78TAF/TAA	67-64-1	$(CH_3)_2CO$	320	782.1	−24.7	757.5						
78TAF/TAA	67-56-1	CH_3OH	320	724.5	28.9	753.4						
[C_7H_7F]	**352-70-5**	**3-F-toluene**				**756.0**			**785.4**			**10**
87FER/JEN	352-70-5	3-F-toluene	478	756.0	0	756.0	785.4	0	785.4			
82STO/SPL	108-88-3	$C_6H_5CH_3$	478	756.3	−0.8	756.5						
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−1.3	755.4						
[C_7H_7Cl]	**108-41-8**	**3-Cl-toluene**				**754.5**			**783.9**			**10**
87FER/JEN	352-70-5	3-F-toluene	478	756.0	−0.4	755.6	785.4	3	788.4			
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−3.3	753.3						
[C_4H_7]	**#1452**	**$CH_3CH{=}CHCH_2$•**				**754.4**			**785.1**			**6**
87LIA/AUS	64-19-7; 71-23-8	CH_3COOH; n-C_3H_7OH	340			753-756						
[C_3H_5NS]	**35120-10-6**	**CH_3SCH_2CN**				**754.1**			**784.8**			**6**
87TAF	7664-41-7	NH_3	350	819	−65.0	753.4						
87MAR/GAL	75-05-8	CH_3CN	320	748	5.8	753.8						
87MAR/GAL	75-08-1	C_2H_5SH	320	758.4	−3.8	754.5						
87MAR/GAL	123-38-6	C_2H_5CHO	320	754.0	1	754.9						
[C_3H_6O]	**123-38-6**	**C_2H_5CHO**				**754.0**			**786.0**			**1.5**
87TAF	7664-41-7	NH_3	350	819	−65.9	752.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	−23.4	752.9						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−9.8	754.7						
77WOL/STA	7664-41-7	NH_3	350	819	−65.9	752.7						
76YAM/KEB	7664-41-7	NH_3	650	819	−60.8	755.5						
75SOL/HAR	75-07-0	CH_3CHO	370	736.5	10.5	747.0						
68REF/CHU		threshold value	298						792			
[C_3H_3N]	**107-13-1**	**CH_2=CHCN**				**753.7**			**784.7**			**4.9**
97EAS/SMI		theory	298									4.9
93SMI/RAD		theory	600						787.3			
93SMI/RAD		theory	298						784.7			
93SMI/RAD		theory	0						779.4			
91MAU/SIE	115-10-6	$(CH_3)_2O$	600	764.5	−17.2	750.8	792	−14.2	777.8	16.5	−5.0	11.5
91MAU/SIE	107-31-3	$HCOOCH_3$	600	751.5	0.8	752.4	782.5	0.4	782.9	5	0.4	5.4
91MAU/SIE	108-88-3	$C_6H_5CH_3$	600	756.3	−8.4	751.2	784.0	0.4	784.4	16	−14.6	1.4
91MAU/SIE	75-05-8	CH_3CN	600	748	4.6	752.4	779.2	2.5	781.7	4.3	3.3	7.6
87TAF	7664-41-7	NH_3	350	819	−66.4	752.1						
76STA/KLE	7664-41-7	NH_3	320	819	−60.7	758.1						
[C_4H_6]	**822-35-5**	**Cyclobutene**				**753.6**			**784.4**			**5.8**
79AUE/BOW	7664-41-7	NH_3	298	819	−65.4	753.6						
[C_2D_6O]	**17222-37-6**	**$(CD_3)_2O$**				**753.0**			**780.4**			**17**
76HAR/LIn	75-07-0	CH_3CHO	370	736.5	17.6	753.0						
[$C_4H_2F_9N$]	**2809-92-9**	**$(CF_3)_3CNH_2$**				**752.9**			**783.7**			**5.6**
87TAF	7664-41-7	NH_3	350	819	−62.7	755.7						
80AUE/WEB	75-21-8	c-C_2H_4O	298	745.3	5.9	751.1						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−12.2	752.3						
[$C_2H_4O_2$]	**64-19-7**	**CH_3COOH**				**752.8**			**783.7**			**5**
90FEL/KIM		theory	300						823			
87TAF	7664-41-7	NH_3	350	819	−67.7	750.7						
77WOL/STA	7664-41-7	NH_3	350	819	−67.7	750.7						
76YAM/KEB	7664-41-7	NH_3	650	819	60.3	754.7						
[C_7H_7Br]	**591-17-3**	**3-Br-toluene**				**752.5**			**782.0**			**10**
82MAS/DOH	108-88-3	$C_6H_5CH_3$	360	756.3	−4.2	752.5						
[B_4H_8]	**12007-71-5**	**B_4H_8**				**752.4**			**784.9**			**0**
72SOL/POR	115-07-1; 67-64-1	C_3H_6; $(CH_3)_2CO$	~373			723-782						
[C_5H_5As]	**289-31-6**	**Arsabenzene**				**752.4**			**784.8**			**0**
85HOD/BEA	75-05-8	CH_3CN	320	748	3.8	751.9						
85HOD/BEA	107-31-3	$HCOOCH_3$	320	751.5	1.3	752.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_6H_{10}]	**110-83-8**	**c-C_6H_{10}**				**752.0**			**784.5**			**0**
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−24.3	752.1						
[$C_8H_4N_2$]	**623-26-7**	**1,4-$(CH)_2$-C_6H_4**				**751.8**			**779.0**			**17.5**
94DEC/EXN2	75-05-8	CH_3CN	338	748	2.4	749.9						
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	0.4	753.8						
[C_3HNO]	**4452-08-8**	**NCCHCO**				**751.5**			**784**			**0**
94FLA/HAV		theory							784			
[$C_2H_4O_2$]	**107-31-3**	**$HCOOCH_3$**				**751.5**			**782.5**			**5**
97EAS/SMI		theory	298									5.1
95SMI/RAD		theory	298						782.2			
93SZU/MCM	67-64-1	$(CH_3)_2CO$	600	782.1	−32.6	750.6	812	−23.4	788.6	8.7	−15.1	−6.4
91MAU/SIE	75-05-8	CH_3CN	600	748	5.9	753.6	779.2	2.5	781.7	4.3	5.4	9.7
87TAF	7664-41-7	NH_3	350	819	−67.3	751.2						
86KNI/FRE	75-07-0	CH_3CHO	303	736.5	8.4	744.9						
82STO/SPL	108-88-3	$C_6H_5CH_3$	478	756.3	−5.4	752.8						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−25.1	751.1						
79LAU	7664-41-7	NH_3	650	819	−61.2	753.8						
77WOL/STA	7664-41-7	NH_3	350	819	−67.3	751.2						
76HAR/LIN	75-07-0	CH_3CHO	370	736.5	8.4	744.6						
[Ru]	**7440-18-8**	**Ru**				**751.4**			**774**			**33**
84MAN/HAL		See Refs.							774±12			
[H_3P]	**7803-51-2**	**PH_3**				**750.9**			**785**			**−5.6**
97EAS/SMI		theory	298									−6.7
93SMI/RAD		theory	600						788.9			
93SMI/RAD		theory	0						778.9			
93SMI/RAD		theory	298						784.8			
87TAF	7664-41-7	NH_3	350	819	−73.2	745.7						
87POP/CUR		theory	298						785.3			
83TAF	7664-41-7	NH_3	350	819	−72.3	746.7						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−31.0	745.7						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−15.1	749.3						
78COR/BEA	7783-54-2; 684-16-2	NF_3; $(CF_3)_2CO$				539-640						
77WOL/STA	115-11-7	$(CH_3)_2C{=}CH_2$	350	775.6	−31.1	745.8						
77WOL/STA	7664-41-7	NH_3	350	819	−72.3	746.7						
[C_7H_7I]	**615-37-2**	**2-I-toluene**				**750.8**			**780.3**			**10**
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−5.9	750.8						
[$C_7H_4N_2O_2$]	**619-24-9**	**3-NO_2-C_6H_4-CN**				**750.7**			**781.4**			**6**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	−2.1	751.7						
94DEC/EXN2	75-05-8	CH_3CN	338	748	1.8	749.7						
[OSi]	**10097-28-6;a**	**SiO at O**				**750.4**			**777.8**			**17**
93LUC/CUR		theory	298						799			
89FOX/WLO	75-05-8; 64-19-7	CH_3CN; CH_3COOH	295			748-753						
85BOT/ROS			298						814±5			
[$C_8H_4N_2$]	**626-17-5**	**1,3-$(CN)_2$-C_6H_4**				**750.4**			**779.3**			**11.8**
94DEC/EXN2	75-05-8	CH_3CN	338	748	1.9	749.6						
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	−2.4	751.2						
[C_4H_6]	**590-19-2**	**CH_2=C=$CHCH_3$**				**749.8**			**778.9**			**11**
87LIA/AUS	75-05-8; 107-31-3	CH_3CN; $HCOOCH_3$	340			748-752						
[C_2H_3N]	**75-05-8**	**CH_3CN**				**748**			**779.2**			**4.3**
97EAS/SMI		theory	298									4.3
93SMI/RAD		theory	600						783.3			
93SMI/RAD		theory	0						775.4			
93SMI/RAD		theory	298						780.1			
91MAU/SIE	75-07-0	CH_3CHO	600	736.5	10.5	746.1	768.5	12.1	780.6	1.5	−2.5	−1.0
87TAF	7664-41-7	NH_3	350	819	−70.9	747.5						
86MAR/TOP	74-90-8	HCN	300	681.6	65.7	747.3						
86KNI/FRE	75-07-0	CH_3CHO	303	736.5	7.5	744.0						
84BEA/EYE		See Refs.							765			
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	−28.9	747.4						
79LAU	7664-41-7	NH_3	650	819	−65.7	749.5						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−12.2	752.3						
77WOL/STA	7664-41-7	NH_3	350	819	−70.9	747.5						
[C_7H_8O]	**100-51-6**	**$C_6H_5CH_2OH$**				**748.0**			**778.3**			**7**
78TAF/TAA	67-56-1	CH_3OH	350	724.5	23.3	748.0						
[CTe_2]	**12192-34-6**	**CTe_2**				**747.8**			**771**			**31**
85JAS/STE		theory							771			
[C_4H_7]	**15157-95-6**	**CH_2=C(CH_3)CH_2•**				**747.3**			**778**			**6**
89HOL/LOS			298						778			
87LIA/AUS	79-24-3; 352-32-9	$C_2H_5NO_2$; 4-$FC_6H_4CH_3$	340			733-736						
[C_2O]	**12071-23-7**	**CCO**				**747.0**			**774.7**			**16**
93MAC/SUD		theory	298						774.7			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_2H_6O]	**64-17-5**	**C_2H_5OH**				**746**			**776.4**			**7**
92PAR/FER	71-43-2	C_6H_6	550	725.4	11.4	741.3	750.4	24	774.4	25	−23	2
92PAR/FER	75-07-0	CH_3CHO	530	736.5	5.3	740.5						
92DOT/IRA	75-07-0	CH_3CHO	298	736.5	6.3	742.8						
90FEL/KIM		theory	300						810			
87TAF	7664-41-7	NH_3	350	819	−72.3	746.0						
83TAF	7664-41-7	NH_3	350	819	−72.3	746.0						
79LAU	7664-41-7	NH_3	650	819	−66.6	747.7						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	15.1	749.3						
78TAF/TAA	67-56-1	CH_3OH	350	724.5	22.0	746.6						
78TAF/TAA	67-64-1	$(CH_3)_2CO$	350	782.1	−38.9	743.3						
77WOL/STA	7664-41-7	NH_3	350	819	−72.3	746.0						
76HAR/LIN	75-07-0	CH_3CHO	370	736.5	5.4	741.5						
[$C_6H_5O_3Re$]	**14524-92-6**	**$(CO)_5ReCH_3$**				**745.9**			**774.9**			**11.5**
81STE/BEA	7664-41-7	NH_3	320	819	−72.8	745.8						
[C_3H_4]	**463-49-0**	**$H_2C{=}C{=}CH_2$**				**745.8**			**775.3**			**10**
AUS/LIA	75-07-0; 74-93-1	CH_3CHO; CH_3SH				736-742						
77ROS/DRA		threshold value							775.3			
[C_7H_7Br]	**106-38-7**	**4-Br-toluene**				**745.8**			**775.3**			**10**
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−10.9	745.8						
[C_7H_7Br]	**95-46-5**	**2-Br-toluene**				**745.8**			**775.3**			**10**
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−10.9	745.8						
[Rh]	**7440-16-6**	**Rh**				**745.4**			**768**			**33**
84MAN/HAL		See Refs.							768±12			
[C_2H_4O]	**75-21-8**	**c-C_2H_4O**				**745.3**			**774.2**			**12**
87TAF	7664-41-7	NH_3	350	819	−75.1	743.0						
80AUE/WEB	75-05-8	CH_3CN	298	748	−2.5	747.0						
80AUE/WEB	64-17-5	C_2H_5OH	298	746	−1.3	745.8						
[C_4H_6]	**503-17-3**	**CH_3-CC-CH_3**				**745.1**			**775.8**			**5.8**
87LIA/AUS	107-31-3	$HCOOCH_3$	340	751.5	−6.7	744.8						
87LIA/AUS	75-05-8	CH_3CN	340	748	−2.5	745.4						
79AUE/BOW	67-56-1	CH_3OH	298	724.5	9.3	733.8						
[$C_7H_4N_2O_2$]	**619-72-7**	**4-NO_2-C_6H_4-CN**				**745.1**			**775.7**			**6**
94DEC/EXN2	123-38-6	C_2H_5CHO	338	754.0	−6.9	746.9						
94DEC/EXN2	75-07-0	CH_3CHO	338	736.5	6.3	742.6						
94DEC/EXN2	75-05-8	CH_3CN	338	748	−2.3	745.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] / YrSquib	Reg No(M) / Reg No(R)	Base(M) / Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) / GB(M)	PA(R)	ΔPA(M,R)	PA(M) / PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) / ΔS_p(M)
[C_7H_7F]	**95-52-3**	**2-F-toluene**				**743.8**			**773.3**			**10**
82STO/SPL	108-88-3	$C_6H_5CH_3$	478	756.3	−13.4	744.0						
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−13.0	743.7						
[HOSi]	**71132-80-4:a**	**SiOH at Si**				**742.8**			**775.3**			**0**
93LUC/CUR		theory	298						775.3			
[C_3H_4ClN]	**542-76-7**	**$Cl(CH_2)_2CN$**				**742.4**			**773.1**			**6**
87TAF	7664-41-7	NH_3	350	819	−76.0	742.4						
76STA/KLE	7664-41-7	NH_3	320	819	−68.6	750.1						
[C_2H_5FSi]	**125413-85-6**	**$F(CH_3)Si{=}CH_2$**				**742.2**			**771.1**			**12**
90ALL/MCM	75-07-0; 75-05-8	CH_3CHO; CH_3CN				736-748						
[H_2N]	**15194-15-7**	**NH_2**				**742.0**			**773.4**			**3.4**
82DEF/HEH	74-93-1	CH_3SH	350	742	0	742.0						
[CH_4S]	**74-93-1**	**CH_3SH**				**742**			**773.4**			**3.5**
97EAS/SMI		theory	298									3.6
93SMI/RAD		theory	600						780.1			
93SMI/RAD		theory	0						770.6			
93SMI/RAD		theory	298						776.4			
92CUR/NOB		theory	298						776.6			
91MAU/SIE	71-43-2	C_6H_6	600	725.4	12.1	744.0	750.4	22.2	772.6	25	−16.7	8.3
87TAF	7664-41-7	NH_3	350	819	−77.3	741.2						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−33.1	743.2						
77WOL/STA	7664-41-7	NH_3	350	819	−76.0	742.5						
76HAR/LIN	75-07-0	CH_3CHO	370	736.5	1.7	738.0						
75SOL/HAR		See Refs.	370			749.4						
[C_2H_3O]	**4400-01-5**	**$\cdot CH_2CHO$**				**741.5**			**774**			**0**
89HOL/LOS			298						774			
[C_2H_6Hg]	**593-74-8**	**$(CH_3)_2Hg$**				**740.8**			**771.6**			**5.8**
80STO/CAM	71-43-2; 108-88-3	C_6H_6; $C_6H_5CH_3$				725-756						
[CClF]	**1691-88-9**	**CFCl**				**740.0**			**772.4**			**0**
85LIA/KAR	352-32-9; 95-52-3	4-$FC_6H_4CH_3$; 2-$FC_6H_4CH_3$				736-744						
[CHN]	**6914-07-4**	**HNC**				**739.8**			**772.3**			**0**
97EAS/SMI		theory	298									0.1
95SMI/RAD		theory	298						772.3			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
82PAU/HEH	123-38-6; 75-08-1	C_2H_5CHO; C_2H_5SH				754-758						
[$C_2HCl_3O_2$]	**76-03-9**	**CCl_3COOH**				**739.1**			**770.0**			**5**
76YAM/KEB	7664-41-7	NH_3	600	819	−76.6	739.0						
[C_6MoO_6]	**13939-06-5**	**$(CO)_6Mo$**				**738.1**			**762.6**			**26.4**
81STE/BEA	7664-41-7	NH_3	320	819	−80.3	738.0						
[$C_2H_3O_2$]	**#1498**	**$\cdot CH_2COOH$**				**737.5**			**770**			**0**
89HOL/LOS			298						770			
[C_2H_4O]	**75-07-0**	**CH_3CHO**				**736.5**			**768.5**			**1.5**
97EAS/SMI		theory	298									1.5
95BOG/NES		appearance	298						767.8			
94RUS/BER		appearance	298						768.5			
93SMI/RAD		theory	0						764.5			
93SMI/RAD		theory	298						770.2			
93SMI/RAD		theory	600						773.9			
87TAF	7664-41-7	NH_3	350	819	−82.4	736.2						
86TAF/GAL	7664-41-7	NH_3	350	819	−84.9	733.7						
86KNI/FRE	75-07-0	CH_3CHO	303	736.5	0	736.5						
79LAU	7664-41-7	NH_3	650	819	−73.0	743.3						
79AUE/BOW	115-10-6	$(CH_3)_2O$	298	764.5	−22.0	742.5						
77WOL/STA	7664-41-7	NH_3	350	819	−80.5	738.1						
76HAR/LIN	75-07-0	CH_3CHO	370	736.5	0	736.5						
75SOL/HAR	75-07-0	CH_3CHO	370	736.5	0	736.5						
68REF/CHU		threshold value	298						772.4			
[$C_3H_3Cl_3O$]	**918-00-3**	**CCl_3COCH_3**				**736.3**			**768.3**			**1.5**
87TAF	7664-41-7	NH_3	350	819	−82.4	736.2						
[C_3]	**12075-35-3**	**C_3**				**736.3**			**767.0**			**5.8**
83RAK/BOH	67-56-1; 75-05-8	CH_3OH; CH_3CN				725-748						
[C_7H_7F]	**352-32-9**	**4-CH_3-C_6H_4F**				**736.1**			**763.8**			**16**
92PAR/FER	71-43-2	C_6H_6	390	725.4	6.0	732.2	750.4	20	770.4	25	−36	−11
87FER/JEN	108-88-3	$C_6H_5CH_3$	478	756.3	−8.4	747.9						
82STO/SPL	108-88-3	$C_6H_5CH_3$	478	756.3	−16.7	739.5						
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−19.7	736.6						
[C_2H_5BrO]	**540-51-2**	**$BrCH_2CH_2OH$**				**735.7**			**766.1**			**7**
93HEC/DEK	71-43-2; 64-17-5	C_6H_6; C_2H_5OH				725-746						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_2H_5ClO]	**107-07-3**	**$ClCH_2CH_2OH$**				**735.7**			**766.1**			**7**
93HEC/DEK	71-43-2; 64-17-5	C_6H_6; C_2H_5OH				725-746						
[$C_6H_5MnO_5$]	**13601-24-6**	**$(CO)_5MnCH_3$**				**735.4**			**764.4**			**11.5**
81STE/BEA	7664-41-7	NH_3	320	819	−83.3	735.4						
79STE/BEA	115-07-1; 75-07-0	CH_3CHCH_2; CH_3CHO				723-736						
[C_7H_7Cl]	**106-43-4**	**4-Cl-toluene**				**735.2**			**762.9**			**16**
92PAR/FER	352-32-9	4-CH_3-C_6H_4F	390	736.1	−0.8	735.3	763.8	3.9	767.7	16	−12	**4**
92PAR/FER	71-43-2	C_6H_6	380	725.4	6.3	732.4	750.4	15	765.4	25	−23	2
87FER/JEN	352-70-5	3-F-toluene	369	756.0	13.5	742.1						
82MAS/BOH	108-88-3	$C_6H_5CH_3$	369	756.3	−18.4	737.9						
[$C_4H_7F_3O$]	**461-24-5**	**$C_2H_5OCH_2CF_3$**				**735.0**			**762.4**			**17**
87TAF	7664-41-7	NH_3	350	819	−82.8	735.0						
83TAF2	7664-41-7	NH_3	350	819	−81.0	736.8						
[CH_2Se]	**6596-50-5**	**$H_2C{=}Se$**				**734.9**			**764.0**			**11**
85KAR	79-24-3; 75-07-0	$C_2H_5NO_2$; CH_3CHO				733-736						
85JAS/STE		theory							781			
[CH_3FO_2]	**144-49-0**	**CH_2FCOOH**				**734.5**			**765.4**			**5**
76YAM/KEB	7664-41-7	NH_3	600	819	−81.2	734.4						
[$C_2H_3ClO_2$]	**79-11-8**	**$CH_2ClCOOH$**				**734.5**			**765.4**			**5**
76YAM/KEB	7664-41-7	NH_3	600	819	−81.2	734.4						
[$C_3H_3F_3OS$]	**41879-94-1**	**CF_3COSCH_3**				**734.3**			**765.2**			**5**
87TAF	7664-41-7	NH_3	350	819	−84.2	734.2						
[C_5H_8]	**142-29-0**	**c-C_5H_8**				**733.8**			**766.3**			**0**
HOU/BEA		threshold value							768.2			
80LIA/SHO	75-07-0	CH_3CHO	350	736.5	−3.8	732.8						
80LIA/SHO	79-24-3	$C_2H_5NO_2$	350	733.2	1.7	734.9						
76SOL/FIE		See Refs.	300						762.1			
[$C_3H_5ClO_2$]	**541-41-3**	**$ClCOOC_2H_5$**				**733.8**			**764.8**			**5**
87TAF	7664-41-7	NH_3	350	819	−84.7	733.8						
[$C_6H_9F_3O_2$]	**367-64-6**	**CF_3CO_2(n-C_4H_9)**				**733.8**			**764.8**			**5**
87TAF	7664-41-7	NH_3	350	819	−84.7	733.8						
77WOL/STA	7664-41-7	NH_3	350	819	−83.3	735.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[C_6O_6W]	**14040-11-0**	**$(CO)_6W$**				**733.4**			**758.0**			**26.4**
81STE/BEA	7664-41-7	NH_3	320	819	−84.9	733.4						
[$C_2H_5NO_2$]	**79-24-3**	**$C_2H_5NO_2$**				**733.2**			**765.7**			**0**
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−43.1	733.3						
[C_5F_5N]	**700-16-3**	**Pentafluoropyridine**				**733.0**			**764.9**			**2**
87TAF	7664-41-7	NH_3	350	819	−85.6	733.0						
[$C_3H_4F_2O$]	**453-14-5**	**CFH_2COCFH_2**				**733.0**			**762.8**			**9**
81DRU/MCM	75-07-0	CH_3CHO	298	736.5	−4.2	732.3						
81DRU/MCM	74-93-1	CH_3SH	298	742	−8.4	733.6						
[$C_5H_7F_3O_2$]	**383-66-4**	**$CF_3CO_2(n\text{-}C_3H_7)$**				**732.9**			**763.9**			**5**
87TAF	7664-41-7	NH_3	350	819	−85.6	732.9						
77WOL/STA	7664-41-7	NH_3	350	819	−84.2	734.2						
[CF_2]	**2154-59-8**	**CF_2**				**732.5**			**765**			**0**
91PAU/SQU		threshold value	298						765			
85LIA/KAR	7783-07-5; 109-77-3	H_2Se; $CH_2(CN)_2$				676-694						
77LIA/AUS		Bracketing				686						
75VOG/BEA	74-90-8; 50-00-0	HCN; CH_2O				682-683						
[C_2H_3NO]	**624-83-9**	**CH_3NCO**				**732.0**			**764.4**			**0**
85KAR/STE	383-63-1; 352-32-9	$CF_3COOC_2H_5$; 4-$FC_6H_4CH_3$				728-736						
[HNO_3]	**7697-37-2**	**HNO_3**				**731.5**			**751.4**			**42**
94CAC/ATT	598-58-3	CH_3ONO_2	298	714.8			733.6	16.7	750.3			
93SUN/SQU		See Refs.	298						744±10			
92LEE/RIC		theory	298						764±17			
90CAC/ATT	7732-18-5; 75-89-8	H_2O; CF_3CH_2OH	303			660-670						
[Fe]	**7439-89-6**	**Fe**				**731.1**			**754**			**32**
86ELK/ARM3		See Refs.							754±8			
84HAL/KLE		See Refs.							796±21			
[B_5H_8]	**65930-58-7**	**B_5H_8**				**731.0**			**763.4**			**0**
78WAN/DES	71-43-2; 75-07-0	C_6H_6; CH_3CHO				725-736						
[CH_2S]	**865-36-1**	**$H_2C{=}S$**				**730.5**			**759.7**			**11**
97EAS/SMI		theory	298									10.8

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	600						772.2			
93SMI/RAD		theory	0						762.8			
93SMI/RAD		theory	298						768.7			
85KAR	383-63-1; 79-24-3	$CH_3CO_2C_2H_5$; $C_2H_5NO_2$				728-733						
85JAS/STE		theory							776.6			
82ROY/MCM	383-63-1; 75-07-0	$CF_3CO_2C_2H_5$; CH_3CHO				728-736						
[CH_3BO_2]	**#1524**	**CH_3O-B=O**				**730.6**			**763.0**			**0**
87HET/COL	67-56-1; 75-07-0	CH_3OH; CH_3CHO				725-736						
[BHO_2]	**13460-50-9**	**HO-B=O**				**730.5**			**763.0**			**0**
92ATT/CAC	67-56-1; 75-07-0	CH_3OH; CH_3CHO	298			725-736						
[$C_3H_8O_2$]	**109-86-4**	**$CH_3OCH_2CH_2OH$**				**729.8**			**768.8**			**−22**
93SZU/MCM	115-11-7	$(CH_3)_2C=CH_2$	600	775.6	14.2	802.4	802.1	33.9	836.0	20	−33.5	−13.5
78TAF/TAA	67-56-1	CH_3OH	320	724.5	4.6	729.8						
[CH_4O_3S]	**75-75-2**	**CH_3SO_3H**				**728.9**			**761.3**			**0**
92PET/FOR	67-56-1; 79-24-3	CH_3OH; $C_2H_5NO_2$				725-733						
[$C_4H_5F_3O_2$]	**383-63-1**	**$CF_3CO_2C_2H_5$**				**727.9**			**758.8**			**5**
87TAF	7664-41-7	NH_3	350	819	−90.6	727.8						
77WOL/STA	7664-41-7	NH_3	350	819	−89.2	729.2						
[$C_3H_2N_4O_4$]	**38858-89-8**	**3,5-dinitropyrazole**				**727.5**			**759.4**			**2**
92ABB/CAB	71-43-2	C_6H_6	333	725.4	0.4	726.6						
92ABB/CAB	67-56-1	CH_3OH	333	724.5	3.7	728.5						
[C_3H_5NO]	**1738-36-9**	**CH_3OCH_2CN**				**727.4**			**758.1**			**6**
87MAR/GAL	383-63-1	$CF_3CO_2C_2H_5$	320	727.9	−0.4	727.4						
[C_6H_5F]	**462-06-6**	**C_6H_5F**				**726.6**			**755.9**			**10.5**
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−2.9	726.8	750.4	5.4	755.9	25	−14.2	10.8
92PAR/FER	71-43-2	C_6H_6	550	725.4	−2.4	726.6	750.4	5.8	756.2	25	−14.9	10.1
91MAU/SIE	67-56-1	CH_3OH	600	724.5	2.9	727.0	754.3	0.8	755.1	9	3.3	12.3
91MAU/SIE	71-43-2	C_6H_6	600	725.4	−4.2	725.6	750.4	5.0	755.4	25	−15.5	9.5
81BOH/STO	71-43-2	C_6H_6	334	725.4	0.8	726.7	750.4	5.9	756.3	25	−15	10
79LAU	7664-41-7	NH_3	650	819	−87.0	726.1						
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−0.8	726.0						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	−3.3	726.4						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_3H_5FO_2$]	**461-64-3**	**$FCO_2C_2H_5$**				**726.0**			**757.0**			**5**
87TAF	7664-41-7	NH_3	350	819	−92.4	726.0						
[C_6H_5Br]	**108-86-1**	**C_6H_5Br**				**725.8**			**754.1**			**14**
81BOH/STO	71-43-2	C_6H_6	334	725.4	0	725.8						
[CHNO]	**506-85-4**	**HCNO**				**725.5**			**758**			**0**
89HOP/HOL		Apperance							758			
[C_6H_6]	**71-43-2**	**C_6H_6**				**725.4**			**750.4**			**25**
93SZU/MCM	115-07-1	$CH_3CH{=}CH_2$	600	722.7	14.6	733.5	751.6	6.7	758.3	12	13.4	25.4
93SZU/MCM	108-88-3	$C_6H_5CH_3$	600	756.3	−28.0	725.5	784.0	−33.5	750.5	16	8.8	24.8
93SZU/MCM	67-56-1	CH_3OH	600	724.5	6.7	726.4	754.3	−7.5	746.8	9	23.0	32.0
93SZU/MCM	107-31-3	$HCOOCH_3$	600	751.5	−22.6	722.9	782.5	−33.9	748.6	5	18.8	23.8
93SZU/MCM	67-64-1	$(CH_3)_2CO$	600	782.1	−53.6	723.7	812	−55.2	756.8	8.7	2.5	11.2
92PAR/FER	75-07-0	CH_3CHO	550	736.5	−7.5	723.2	768.5	−19	749.5	1.5	21	22.5
92PAR/FER	67-56-1	CH_3OH	550	724.5	6.9	727.4	754.3	−3	751.3	9	18	27
91MAU/SIE	75-07-0	CH_3CHO	600	736.5	−10.9	718.6	768.5	−16.7	751.8	1.5	9.6	11.1
91MAU/SIE	75-05-8	CH_3CN	600	748	−15.9	725.9	779.2	−27.6	751.6	4.3	19.2	23.5
91MAU/SIE	67-56-1	CH_3OH	600	724.5	5.4	725.2	754.3	1.3	755.6	9	6.7	15.7
87TAF	7664-41-7	NH_3	350	819	−92.9	724.5						
85VAN/LEA		See Refs.										
81BOH/STO	71-43-2	C_6H_6	334	725.4	0	725.4						
80MAU	7664-41-7	NH_3	550	819	−79.1	732.1						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−50.6	724.8						
78LAU/SAL	7664-41-7	NH_3	600	819	−77.0	732.6						
78HAR/LIA	71-43-2	C_6H_6	400	725.4	0	725.4						
77WOL/STA	7664-41-7	NH_3	320	819	−84.9	733.4						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	0	725.4						
76DEV/WOL	71-43-2	C_6H_6	320	725.4	0	725.4						
[$H_2N_2O_2$]	**7782-94-7**	**H_2N-NO_2**				**725.0**			**757.4**			**0**
93ATT/CAC	67-56-1; 71-43-2	CH_3OH; C_6H_6	300			725-725						
[C_6H_5Cl]	**108-90-7**	**C_6H_5Cl**				**724.6**			**753.1**			**13.5**
81BOH/STO	462-06-6	C_6H_5F	334	726.6	−1.6	724.9	755.9	−2.5	753.4	10.5	2.8	13.3
81BOH/STO	71-43-2	C_6H_6	334	725.4	−0.8	725.0	750.4	3	753.4	25	−11	14
79LAU	7664-41-7	NH_3	650	819	−87.9	724.1						
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−2.1	724.5						
76LAU/KEB	71-43-2	C_6H_6	600	725.4	−4.2	724.7						
[CH_4O]	**67-66-1**	**CH_3OH**				**724.5**			**754.3**			**9**
97EAS/SMI		theory	298									7.3
93SZU/MCM	115-07-1	$CH_3CH{=}CH_2$	600	722.7	6.7	730.3	751.6	14.2	765.8	12	−12.6	−0.6
93SMI/RAD		theory	0						749.1			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	298						754.3			
93SMI/RAD		theory	600						757.3			
92PAR/FER	75-07-0	CH_3CHO	550	736.5	−13.3	721.4	768.5	−16	752.5	1.5	5	6.5
91MAU/SIE	115-07-1	$CH_3CH{=}CH_2$	600	722.7	8.4	732.0	751.6	11.3	762.9	12	−5.0	7.0
90FEL/KIM		theory	300						791.2			
87TAF	7664-41-7	NH_3	350	819	−94.7	723.5						
83TAF	7664-41-7	NH_3	350	819	−94.3	724.0						
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−54.0	722.1						
79LAU	7664-41-7	NH_3	650	819	−89.3	724.3						
77WOL/STA	7664-41-7	NH_3	350	819	−94.3	723.9						
[C_2H_5O]	**16520-04-0**	**•CH_2OCH_3**				**723.6**			**756.1**			**0**
96AUD/FOS	115-07-1; 67-56-1	$CH_3CH{=}CH_2$; CH_3OH				723-725						
[HN_3]	**7782-79-8**	**HNNN**				**723.5**			**756.0**			**0**
93CAC/ATT	75-52-5; 71-43-2	CH_3NO_2; C_6H_6	298			722-725						
90CAC/ATT2	598-58-3	CH_3ONO_2		714.8								
84BEA/EYE		See Refs.										
[C_3H_4]	**74-99-7**	**CH_3CCH**				**723.0**			**748**			**25**
83BUR/HOL		Appearance	300						748			
76AUE/DAV	7783-06-4	H_2S	298	673.8	8.8	682.6						
[C_3H_6]	**115-07-1**	**$CH_3CH{=}CH_2$**				**722.7**			**751.6**			**12**
97EAS/SMI		theory	298									11.7
93SMI/RAD		theory	600						747			
93SMI/RAD		theory	0						740.3			
93SMI/RAD		theory	298						744.3			
82ROS/BUF		threshold value	298						751			
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−58.6	717.4						
80LIA/SHO	115-07-1	$CH_3CH{=}CH_2$	340	722.7	0	722.7						
80BAE		threshold value	298						751.8			
76YAM/KEB	7664-41-7	NH_3	650	819	−93.8	718.7						
72CHO/FRA	67-56-1	CH_3OH	340	724.5	−3.1	721.3						
[C_3H_6]	**75-19-4**	**c-C_3H_6**				**722.2**			**750.3**			**14.9**
72CHO/FRA	67-56-1	CH_3OH	340	724.5	2.1	722.2						
[$C_6H_4F_2$]	**372-18-9**	**1,3-$C_6H_4F_2$**				**722**			**749.7**			**16**
93SZU/MCM	107-31-3	$HCOOCH_3$	600	751.5	−27.2	721.0	782.5	−34.3	748.2	5	12.1	17.1
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−5.9	722.3	750.4	0	750.4	25	−9.6	15.4
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−1.3	725.1						
76YAM/KEB	7664-41-7	NH_3	650	819	−92.0	719.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[CCl_2S]	**463-71-8**	**Cl_2CS**				**721.8**			**752.5**			**5.8**
93ABB/MO	108-90-7	C_6H_5Cl	333	724.6	−3.2	721.7						
93ABB/MO	75-19-4	c-C_3H_6	333	722.2	−0.6	721.9						
[CH_3NO_2]	**75-52-5**	**CH_3NO_2**				**721.6**			**754.6**			**−1.6**
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−59.0	717.5						
80LIA/SHO	115-07-1	$CH_3CH{=}CH_2$	340	722.7		717.1						
78MAC/BOH	115-07-1	$CH_3CH{=}CH_2$	297	722.7	2.5	725.2						
78MAC/BOH	67-56-1	CH_3OH	297	724.5	−0.7	723.8						
76MCA/PIT	67-56-1	CH_3OH	300	724.5	~0	724.5						
[C_2H]	**2122-48-7**	**HCC•**				**720.8**			**753.3**			**0**
93DOT/IRA	383-63-1	$CF_3CO_2C_2H_5$	298	727.9	−5.9	722.0						
93DOT/IRA	107-14-2	$CClH_2CN$	298	715.1	4.6	719.6						
88LIA/BAR									767			
[C_3HN]	**1070-71-9**	**HCC-CN**				**720.5**			**751.2**			**6**
87DEA/MAU	108-90-7	C_6H_5Cl	500	724.6	−6.3	719.9						
87DEA/MAU	75-07-0	CH_3CHO	500	736.5	−16.7	719.9						
87DEA/MAU	75-52-5	CH_3NO_2	500	721.6	−0.4	719.7						
87DEA/MAU	67-56-1	CH_3OH	500	724.5	−5.0	720.1						
87DEA/MAU	431-47-0	CF_3COOCH_3	500	709.6	2.9	712.3						
85KNI/FRE	75-52-5	CH_3NO_2	300	721.6	0.8	722.4						
85KNI/FRE	506-68-3	BrCN	300	719.2	3.9	723.1						
81BAK/BOH	75-52-5; 75-05-8	CH_3NO_2; CH_3CN				722-748						
[C_4H_8]	**624-64-6**	**E-$CH_3CH{=}CHCH_3$**				**719.9**			**747**			**18**
81TRA		threshold value	298						747			
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−59.0	716.7						
80LIA/SHO	115-07-1	$CH_3CH{=}CH_2$	340	722.7		718.0						
[C_2H_3]	**2669-89-8**	**C_2H_3**				**719.8**			**755.2**			**−10**
92PET/IRA	107-14-2; 67-56-1	$CClH_2CN$; CH_3OH	298			715-725						
80DEF/MCI	431-47-0; 67-56-1	CF_3COOCH_3; CH_3OH				710-725						
[Co]	**7440-48-4**	**Co**				**719.8**			**742.7**			**32**
86ELK/ARM4		See Refs.							742.7±6			
[$C_6H_2F_4$]	**2367-82-0**	**1,2,3,5-$C_6H_2F_4$**				**719.6**			**747.3**			**16**
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−6.7	719.6						
[CBrN]	**506-68-3**	**BrCN**				**719.2**			**749.8**			**6**
91PET/KNI	75-52-5	CH_3NO_2	300	721.6	−2.3	719.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
85KNI/FRE	75-52-5	CH_3NO_2	300	721.6	−2.6	719.0						
76STA/KLE	7664-41-7	NH_3	320	819	−96.7	722.1						
[CHNO]	**75-13-8**	**HNCO**				**718.8**			**753**			**−5.8**
89HOP/HOL		Appearance							753			
84BEA/EYE		See Refs.							740-753			
80WIG/BEA	50-00-0	$H_2C{=}O$	320	683.3	5.0	688.6						
[$C_6H_2F_4$]	**327-54-8**	**1,2,4,6-$C_6H_2F_4$**				**718.8**			**746.5**			**16**
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−7.5	718.8						
[CNS]	**15941-77-2**	**NCS**				**718.5**			**751**			**0**
94RUS/BER2		appearance							751			
[$C_3H_5F_3O$]	**460-43-5**	**$CF_3CH_2OCH_3$**				**718.4**			**747.6**			**11**
87TAF	7664-41-7	NH_3	350	819	−99.8	718.4						
[H_6OSi_2]	**13597-73-4**	**$H_3SiOSiH_3$**				**718.3**			**749**			**5.8**
91CUR/BRA		theory	0						749			
[C_6H_5]	**116139-00-5**	**$HCCCH_2CH(\bullet)CCH$**				**716.4**			**748.9**			**0**
87KIN/BUR	7732-18-5	H_2O		660.0			691	57.9	748.9			
[C_3H_3NO]	**631-57-2**	**CH_3COCN**				**716.2**			**746.9**			**6**
87TAF	7664-41-7	NH_3	350	819	−100.7	717.7						
86MAR/TOP	74-90-8	HCN	300	681.6	33.1	714.7						
[C_4NiO_4]	**13463-39-3**	**$(CO)_4Ni$**				**716.0**			**742.3**			**20.6**
81STE/BEA	7664-41-7	NH_3	320	819	−102.5	716.0						
[$C_6H_3F_3$]	**372-38-3**	**1,3,5-$C_6H_3F_3$**				**715.4**			**741.9**			**20**
93SZU/MCM	67-56-1	CH_3OH	600	724.5	−5.4	715.8	754.3	−14.2	740.1	9	14.6	23.6
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−12.6	714.4	750.4	−6.3	744.1	25	−8.8	16.2
79LAU	7664-41-7	NH_3	650	819	93.8	715.9						
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−2.9	723.0						
[C_2H_2ClN]	**107 14 2**	**$CClH_2CH$**				**715.1**			**745.7**			**6**
92DOT/IRA	67-56-1	CH_3OH	298	724.5	−4.8	719.7						
86MAR/TOP	74-90-8	HCN	300	681.6	31.8	713.4						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	17.6	712.0						
[CH_3NO_3]	**598-58-3**	**CH_3ONO_2**				**714.8**			**733.6**			**46**
93SUN/SQU		See Refs.	298						732±10			
93RIC	75-38-7; 67-56-1	CF_2CH_2; CH_3OH	298			705-725						
92LEE/RIC2		theory	298						740±21			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_4H_5NO_2$]	**623-49-4**	**$NCCOOC_2H_5$**				**714.7**			**745.7**		**5**
87TAF	7664-41-7	NH_3	350	819	−101.1	717.3					
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	17.6	712.1					
[$C_3H_3NO_2$]	**17640-15-2**	**CH_3COOCN**				**714.7**			**745.7**		**5**
86MAR/TOP	74-90-8	HCN	300	681.6	33.1	714.7					
[C_6CrO_6]	**13007-92-6**	**$(CO)_6Cr$**				**714.6**			**739.2**		**26.4**
81STE/BEA	7664-41-7	NH_3	320	819	−103.8	714.6					
[$C_3H_3F_3O_2$]	**32042-38-9**	**$HCOOCH_2CF_3$**				**714.6**			**745.5**		**5**
87TAF	7664-41-7	NH_3	350	819	−100.7	717.8					
77WOL/STA	109-77-3	$CH_2(CN)_2$	320	694.1	17.1	711.4					
[P_4]	**12185-10-8**	**P_4**				**714.3**			**742.3**		**14.9**
96ABB/HER	115-20-8	CCl_3CH_2OH	333	698.9	9.4	708.0					
96ABB/HER	32042-38-9	$HCOOCH_2CF_3$	333	714.6	−0.1	714.1					
96ABB/HER	463-71-8	Cl_2CS	333	721.8	−3.4	718.1					
96ABB/HER	75-19-4	c-C_3H_6	333	722.2	−5.8	716.5					
96ABB/HER	108-90-7	C_6H_5Cl	333	724.6	−10	714.6					
[Ni]	**7440-02-0**	**Ni**				**714.1**			**737**		**32**
86ELK/ARM4		See Refs.							737		
[H_4OSi]	**14475-38-8**	**H_3SiOH at O**				**713.9**			**746.4**		**0**
93LUC/CUR		theory	298						746.4		
91CUR/BRA		theory	0						742.2		
[CH_2F_2Si]	**51675-50-4**	**$F_2Si{=}CH_2$**				**713.4**			**742.3**		**12**
90ALL/MCM	75-38-7; 75-52-5	$CF_2{=}CH_2$; CH_3NO_2				705-722					
[C_4H_2]	**460-12-8**	**HCC-CCH**				**712.8**			**737.2**		**27**
91PET/KNI	506-68-3	BrCN	300	719.2	−6.4	712.8					
90BOT/KNI		theory	300						741		
87DEA/MAU	75-52-5; 2367-82-0	CH_3NO_2; 1,2,3,5-$C_6H_2F_4$	330			722-720					
[C_2H_5O]	**4422-54-2**	**•CH_2CH_2OH**				**712.5**			**745**		**0**
89HOL/LOS			298						745		
[AsH_3]	**7784-42-1**	**AsH_3**				**712.0**			**747.9**		**−11.5**
87TAF	7664-41-7	NH_3	350	819	−117.2	702.1					
80LIA/SHO	115-11-7	$(CH_3)_2C{=}CH_2$	340	775.6	−63.2	713.7					
80LIA/SHO	115-07-1	$CH_3CH{=}CH_2$	340	722.7	−3.3	720.3					

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	13.7	709.0						
[CH_2O_2]	**64-18-6**	**HCOOH**				**710.3**			**742.0**			**2.7**
97EAS/SMI		theory	298									2.7
93SMI/RAD		theory	600						746.7			
93SMI/RAD		theory	298						742.9			
93SMI/RAD		theory	0						737.1			
90FEL/KIM		theory	300						781			
87TAF	7664-41-7	NH_3	350	819	−120.4	698.2						
80LIA/SHO	115-11-7	$(CH_3)_2C=CH_2$	340	775.6	−64.4	711.9						
80LIA/SHO	115-07-1	$CH_3CH=CH_2$	340	722.7	−4.2	718.9						
79LAU	7664-41-7	NH_3	650	819	−115.9	699.9						
77WOL/STA	109-77-3	$CH_2(CN)_2$	320	694.1	11.7	706.0						
[$C_3H_3F_3O_2$]	**431-47-0**	**CF_3COOCH_3**				**709.6**			**740.5**			**5**
87TAF	7664-41-7	NH_3	350	819	−108.9	709.5						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	13.7	708.2						
[C_3H_3]	**2932-78-7**	**$HCCCH_2$•**				**708.5**			**741**			**0**
89HOL/LOS			298						741			
[C_3H_5]	**1981-80-2**	**$CH_2=CHCH_2$•**				**707.4**			**736**			**13**
89HOL/LOS		See Refs.	298						736			
80DEF/MCI	109-77-3; 431-47-0	$NCCH_2CN$; CF_3COOCH_3				694-710						
[H_3OSi]	**113648-09-2:a**	**H_2SiOH at O**				**705.5**			**738**			**0**
93LUC/CUR		theory	298						738			
[$C_2H_2F_2$]	**75-38-7**	**$CH_2=CF_2$**				**705.1**			**734**			**12**
76WIL/LEB		threshold value							734			
75RID	75-03-6; 67-56-1	C_2H_5I; CH_3OH				698-725						
[$C_4H_4F_4O_2$]	**1683-88-1**	**$CF_3COOCH_2CH_2F$**				**704.7**			**735.7**			**5**
87TAF	7664-41-7	NH_3	350	819	−117.2	701.3						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	13.7	708.1						
[H_2Te]	**7783-09-7**	**H_2Te**				**704.5**			**735.9**			**3.8**
86KAR/JAS	75-38-7	$CH_2=CF_2$	330	705.1	−0.8	704.5						
[C_3H_7O]	**31594-81-7**	**•$CH_2CH_2CH_2OH$**				**703.5**			**736**			**0**
89HOL/LOS			298						736			
[$C_6H_4F_2$]	**367-11-3**	**1,2-$C_6H_4F_2$**				**703.5**			**731.2**			**16**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−24.7	703.4	750.4	−17.6	732.8	25	−13.0	12.0
93SZU/MCM	67-56-1	CH_3OH	600	724.5	−18.8	703.6	754.3	−25.5	728.8	9	10.9	19.9
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−1.7	724.6						
[C_3H_5]	**2417-82-5**	**c-C_3H_5•**				**702.0**			**738.9**			**−14.9**
84LIA/BUC	421-50-1; 7784-42-1	CF_3COCH_3; AsH_3	330			692-712						
80DEF/MCI	75-07-0; 64-17-5	CH_3CHO; C_2H_5OH				736-746						
[C_3H_3]	**28933-84-8**	**c-C_3H_3•**				**701.8**			**734.3**			**0**
80DEF/MCI	109-77-3; 431-47-0	$NCCH_2CN$; CF_3COOCH_3				694-710						
[CH_3S]	**17032-46-1**	**•CH_2SH**				**701.5**			**733.9**			**0**
95CHO/SMI	545-06-2; 64-18-6	CCl_3CN; HCOOH				693-710						
[CSe_2]	**506-80-9**	**CSe_2**				**700.9**			**725**			**28**
85JAS/STE		theory							725			
[HOSi]	**71132-8-4:b**	**SiOH at O**				**700.1**			**732.6**			**0**
93LUC/CUR		theory	298						732.6			
[C_2H_3F]	**75-02-5**	**CH_2=CHF**				**700.1**			**729**			**12**
80KOP/COM									703			
76WIL/LEB		See Refs.							729			
75RID	7732-18-5; 7783-06-4	H_2O; H_2S				660-674						
[$C_6H_3F_3$]	**367-23-7**	**1,2,4-$C_6H_3F_3$**				**699.4**			**729.5**			**8**
93SZU/MCM	67-56-1	CH_3OH	600	724.5	−24.7	700.1	754.3	−31.0	723.3	9	10.5	19.5
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−31.8	698.7	750.4	−21.8	728.7	25	−17.2	7.8
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−5.0	722.1						
[$C_2H_3Cl_3O$]	**115-20-8**	**CCl_3CH_2OH**				**698.9**			**729.3**			**7**
87TAF	7664-41-7	NH_3	350	819	−122.6	695.7						
77WOL/STA	109-77-3	$CH_2(CH)_2$	350	694.1	7.8	702.2						
[BH_3O_3]	**10043-35-3**	**$B(OH)_3$**				**698.4**			**728.1**			**9.1**
92ATT/CAC	109-77-3	$CH_2(CN)_2$	298	694.1	−2.1	692.0						
92ATT/CAC	75-38-7	CH_2=CF_2	298	705.1	−0.4	704.7						
[C_2H_3I]	**75-03-6**	**C_2H_5I**				**698.3**			**724.8**			**20**
72BEA/HOL	7783-06-4; 115-07-1	H_2S; C_3H_6				674-723						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[$C_2H_4F_2O$]	**359-13-7**	**CF_2HCH_2OH**				**697.0**			**727.4**			**7**
87TAF	7664-41-7	NH_3	350	819	−128.1	690.2						
78TAF/TAA	67-56-1	CH_3OH	350	724.5	−21.0	703.6						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	2.7	697.1						
[$C_6H_3F_3$]	**1489 63 8**	**1,2,3 $C_6H_3F_3$**				**696.6**			**724.3**			**16**
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−28.5	699.7	750.4	−29.3	721.1	25	1.3	26.3
93SZU/MCM	7783-06-4	H_2S	600	673.8	24.3	694.6	705	16.7	721.7	4.3	12.6	16.9
93SZU/MCM	75-15-0	CS_2	600	657.7	31.4	692.7	681.9	47.7	729.5	28	−27.2	0.8
93SZU/MCM	67-56-1	CH_3OH	600	724.5	−23.0	699.4	754.3	−35.6	718.7	9	20.9	29.9
[$C_3H_2N_2$]	**109-77-3**	**$CH_2(CN)_2$**				**694.1**			**723.0**			**12**
87TAF	7664-41-7	NH_3	350	819	−128.6	689.5						
81DRU/MCM	109-77-3	$CH_2(CN)_2$	298	694.1	0	694.1						
81DOI/MCM	109-77-3	$CH_2(CN)_2$	298	694.1	0	694.1						
79LAU	7664-41-7	NH_3	650	819	−118.3	694.3						
78TAF/TAA	67-56-1	CH_3OH	320	724.5	−26.8	697.7						
77WOL/STA	7664-41-7	NH_3	350	819	−118.1	700.0						
77WOL/STA	67-56-1	CH_3OH	350	724.5	−28.8	695.5						
[$C_6H_4F_2$]	**540-36-3**	**1,4-$C_6H_4F_2$**				**692.8**			**718.7**			**22**
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−32.2	694.1	750.4	−36.0	714.4	25	6.3	31.3
93SZU/MCM	67-56-1	CH_3OH	600	724.5	−25.5	695.1	754.3	−41.8	712.5	9	27.2	36.2
93SZU/MCM	421-50-1	CF_3COCH_3	600	692.0	5.4	691.5	723.9	−8.4	715.5	2	23.0	25.0
93SZU/MCM	7783-06-4	H_2	600	673.8	22.2	690.7	705	11.3	716.3	4.3	18.0	22.3
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−4.2	721.5						
[C_2Cl_3N]	**545-06-2**	**CCl_3CN**				**692.6**			**723.2**			**6**
87TAF	7664-41-7	NH_3	350	819	−125.8	692.5						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	0.9	695.3						
[COTe]	**#1602**	**OCTe at Te**				**692.1**			**718**			**22**
85JAS/STE		theory							718			
[$C_3H_3F_3O$]	**421-50-1**	**CF_3COCH_3**				**692.0**			**723.9**			**2**
93SZU/MCM	75-15-0	CS_2	600	657.7	24.3	689.8	681.9	50.2	732.1	28	−43.1	−15.1
93SZU/MCM	367-23-7	1,2,4-$C_6H_3F_3$	600	699.4	−5.9	695.4	729.5	−4.2	725.3	8	−2.9	5.1
93SZU/MCM	540-36-3	1,4-$C_6H_4F_2$	600	692.8	−5.4	693.4	718.7	8.4	727.1	22	−23.0	−1.0
81DRU/MCM	109-77-3	$CH_2(CN)_2$	298	694.1	−4.2	689.9						
81DOI/MCM	109-77-3	$CH_2(CN)_2$	298	694.1	−2.5	691.6						
[CClN]	**506-77-4**	**ClCN**				**691.5**			**722.1**			**6**
87TAF	7664-41-7	NH_3	350	819	−130.4	688.0						
86MAR/TOP	74-90-8	HCN	300	681.6	13.4	695.0						
76STA/KLE	7664-41-7	NH_3	320	819	−107.5	711.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)		ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R) $\Delta\Delta S_p$(M,R)	ΔS_p(M)
[C_2HCl_3O]	**75-87-6**	**CCl_3CHO**				**690.5**			**722.3**		**2**
87TAF	7664-41-7	NH_3	350	819	−128.1	690.4					
[$C_2H_3F_3O$]	**421-14-7**	**CF_3OCH_3**				**690.0**			**719.2**		**11**
87TAF	7664-41-7	NH_3	350	819	−128.1	690.0					
[C_2H_5O]	**2348-46-1**	**$CH_3CH(\bullet)OH$**				**687.7**			**720.1**		**0**
96AUD/FOS	50-00-0; 421-50-1	$H_2C=O$; CF_3COCH_3				683-692					
[GeH_4]	**7782-65-2**	**GeH_4**				**687.1**			**713.4**		**20.6**
80SEN/ABE	74-85-1; 115-07-1	C_2D_4; CD_3CDCD_2				651-723					
[C_2H_5FO]	**371-62-0**	**FCH_2CH_2OH**				**685.2**			**715.6**		7
93HEC/DEK	392-56-3; 64-17-5	C_6F_6; C_2H_5OH				624-746					
[CH_3O]	**50-00-0**	**$H_2C=O$**				**683.3**			**712.9**		**9.5**
97EAS/SMI		theory	298								9.5
93TRA/HOL		threshold value	298						712.9		
93SMI/RAD		theory	0						705.8		
93SMI/RAD		theory	600						715.9		
93SMI/RAD		theory	298						711.8		
87TAF	7664-41-7	NH_3	350	819	−140.9	677.3					
85JAS/STE		theory							726.6		
84DIX/KOM		theory	300						730.1		
80WIG/BEA	50-00-0	$H_2C=O$	320	683.3	0	683.3					
78TAN/MAC	7732-18-5	H_2O	298	660.0	21.8	681.8					
78FRE/HAR	7783-06-4	H_2S	300	673.8	5.0	678.9					
77WOL/STA	109-77-3	$CH_2(CN)_2$	320	694.1	−11.2	683.0					
68REF/CHU		threshold value	298						709.2		
[CHN]	**74-90-8**	**HCN**				**681.6**			**712.9**		**4**
97EAS/SMI		theory	298								4
93SMI/RAD		theory	298						712		
93SMI/RAD		theory	0						706.2		
93SMI/RAD		theory	600						715.2		
87TAF	74-85-1	$CH_2=CH_2$	350	651.5	37.7	689.5					
86MAR/TOP	74-90-8	HCN	300	681.6	0	681.6					
78TAN/MAC	7732-18-5	H_2O	298	660.0	20.5	680.5					
78FRE/HAR2	7783-06-4	H_2S	340	673.8	4.2	678.0					
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	−13.7	680.9					
[$C_2HF_3O_2$]	**76-06-1**	**CF_3COOH**				**680.7**			**711.7**		**5**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
94KOP/ANV	74-85-1	$CH_2=CH_2$	373	651.5	28.0	680.0						
87TAF	74-85-1	$CH_2=CH_2$	350	651.5	33.1	684.9						
81DRU/MCM	360-52-1	CF_2HCOCF_2H	298	669.0	−1.7	667.3						
79LAU	7664-41-7	NH_3	650	819	−137.7	677.4						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	−20.1	674.3						
[SSi]	**113443-18-8**	**SiS**				**677.7**			**710.2**			**0**
89FOX/WLO	7783-06-4; 74-90-8	H_2S; HCN	295			674-682						
[H_2Se]	**7783-07-5**	**H_2Se**				**676.4**			**707.8**			**3.8**
87TAF	7664-41-7	NH_3	350	819	−143.7	674.8						
85KAR	7783-06-4	H_2S	340	673.8	4.2	678.0						
79AUE/BWO	67-56-1	CH_3OH	298	724.5	−37.6	686.9						
77WOL/STA	109-77-3	$CH_2(CN)_2$	320	694.1	−13.7	680.6						
[H_2P]	**13765-43-0**	**PH_2**				**675.7**			**709.2**			**−3.4**
86BER/CUR		thermo cycles	298						709.2			
[$C_4H_4F_6O$]	**333-36-8**	**$(CF_3CH_2)_2O$**				**674.9**			**702.3**			**17**
94KOP/ANV	74-85-1	$CH_2=CH_2$	373	651.5	23.8	674.9						
87TAF	74-85-1	$CH_2=CH_2$	350	651.5	29.7	680.9						
[H_2S]	**7783-06-4**	**H_2S**				**673.8**			**705**			**4.3**
97EAS/SMI		theory	298									3.4
93SZU/MCM	71-43-2	C_6H_6	600	725.4	−52.3	679.3	750.4	−44.8	705.6	25	−12.6	12.4
93SZU/MCM	540-36-3	1,4-$C_6H_4F_2$	600	692.8	−22.2	676.0	718.7	−11.3	707.4	22	−18.0	4.0
93SZU/MCM	367-23-7	1,2,4-$C_6H_3F_3$	600	699.4	−23.0	677.5	729.5	−23.4	706.1	8	0.8	8.8
93SMI/RAD		theory	600						712.2			
93SMI/RAD		theory	298						707.7			
93SMI/RAD		theory	0						701.6			
87TAF	7664-41-7	NH_3	350	819	−147.8	670.7						
87POP/CUR		theory	298						705			
85MCM/KEB	74-85-1	$CH_2=CH_2$	400	651.5	27.2	679.4						
84WAL/BLA		threshold value	298						704.4			
83PRE/TZE		threshold value	298						705.7			
79LAU	7664-41-7	NH_3	650	819	−144.1	671.1						
78TAN/MAC	7732-18-5	H_2O	298	660.0	15.9	675.9						
78FRE/HAR2	7783-06-4	H_2S	340	673.8	0	673.8						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	−17.6	676.9						
77MAU/FIE	7732-18-5	H_2O	550	660.0	16.3	676.5						
73HOP/BON	7732-18-5	H_2O	296	660.0	19.2	679.3						
[Pd]	**7440-05-3**	**Pd**				**673.4**			**696**			**33**
84MAN/HAL		See Refs.							696±12			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[$C_6H_2F_4$]	**551-62-2**	**1,2,3,4-$C_6H_2F_4$**				**672.7**			**700.4**			**16**
93SZU/MCM	7783-06-4	H_2S	600	673.8	3.3	673.7	705	−11.7	693.3	4.3	25.1	29.4
93SZU/MCM	75-15-0	CS_2	600	657.7	10.5	671.8	681.9	18.8	700.7	28	−14.2	13.8
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−6.3	720.0						
[C_4H_{10}]	**75-28-5**	**iso-C_4H_{10}**				**671.3**			**677.8**			**87**
78HIR	7732-18-5	H_2O		660.0			691	−16.3	674.7			
78HIR	7783-06-4	H_2S		673.8			705	−32.2	672.8			
76HIR/KEB		See Refs.							685.9			87
[CF_3NO]	**334-99-6**	**CF_3NO**				**670.8**			**703.3**			**0**
79FRE/HAR	7732-18-5; 74-90-8	H_2O; HCN				660-682						
[$C_2H_3F_3O$]	**75-89-8**	**CF_3CH_2OH**				**669.9**			**700.2**			**7**
94KOP/ANV	74-85-1	$CH_2{=}CH_2$	373	651.5	21.3	673.1						
87TAF	74-85-1	$CH_2{=}CH_2$	350	651.5	29.7	681.4						
85MCM/KEB	7732-18-5	H_2O	400	660.0	9.6	669.5						
83COL/MCM	7732-18-5	H_2O	298	660.0	9.2	669.2						
79LAU	7664-41-7	NH_3	650	819	147.3	667.0						
78TAF/TAA	67-56-1	CH_3OH	350	724.5	−48.8	675.8						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	−24.9	669.5						
[C_2H_5Br]	**74-96-4**	**C_2H_5Br**				**669.7**			**696.2**			**20**
72BEA/HOL	77-88-4; 7783-06-4	CH_3I; H_2S				666-674						
[$C_3H_2F_4O$]	**360-52-1**	**CF_2HCOCF_2H**				**669.0**			**698.8**			**9**
94KOP/ANV	74-85-1	$CH_2{=}CH_2$	373	651.5	18.4	670.1						
81DRU/MCM	7783-06-4	H_2S	298	673.8	−5.9	668.0						
[H_3OSi]	**81429-20-1**	**H_3SiO at O**				**667.5**			**700**			**0**
93LUC/CUR		theory	298						700			
[B_5H_9]	**19624-22-7**	**B_5H_9**				**666.9**			**699.4**			**0**
72SOL/POR	7732-18-5; 7783-06-4	H_2O; H_2S	~373			660-674						
[C_6H_{12}]	**110-82-7**	**c-C_6H_{12}**				**666.9**			**686.9**			**42**
82AUS/REB	7732-18-5; 7783-06-4	H_2O; H_2S				660-674						
[C_2H_5Cl]	**56-00-3**	**C_2H_5Cl**				**666.9**			**693.4**			**20**
72BEA/HOL	7732-18-5; 7783-06-4	H_2O; H_2H				660-674						
[H_2O_4S]	**7664-93-9**	**H_2SO_4**				**666.9**			**699.4**			**0**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
78SMI/MUN	7732-18-5; 7783-06-4	H_2O; H_2S				660-674						
[CHF_3O_3S]	**1493-13-6**	**CF_3SO_3H**				**666.6**			**699.4**			**0**
78MIN/MUN	7732-18-5; 7783-06-4	H_2O; H_2S				660-674						
[C_2HF_3]	**359-11-5**	**C_2F_3H**				**666.9**			**699.4**			**0**
75RID	7732-18-5; 7783-064	H_2O; H_2S				660-674						
[CHP]	**6829-52-3**	**HCP**				**666.5**			**699**			**0**
90ADA/MIC		Bracketing, See Refs.	300						699±8			
[CH_3I]	**74-88-4**	**CH_3I**				**665.5**			**691.7**			**21**
94GLU/SZU		theory	298						691.1			
94GLU/SZU	75-15-0	CS_2	600	657.7	5.2	665.0	681.9	8.4	690.3	28	−5.4	22.6
94GLU/SZU	363-72-4	C_6HF_5	600	662.7	4.9	666.1	690.4	−4.6	685.8	16	15.9	31.9
72BEA/HOL	7783-06-4	H_2S	300	673.8	0	673.8						
[PS]	**12281-56-6**	**PS**				**665.5**			**698**			**0**
90ADA/MIC		Bracketing, See Refs.	300						698±8			
[$C_2H_7B_5$]	**20693-69-0**	**2,4-$C_2B_5H_7$**				**665.0**			**697.4**			**0**
80DIX	7732-18-5; 75-89-8	H_2O; CF_3CH_2OH				660-670						
[F_3OP]	**13478-20-1**	**OPF_3**				**664.2**			**694.0**			**9.1**
83COL/MCM	7732-18-5	H_2O	298	660.0	4.2	664.2						
[F_3P]	**7783-55-3**	**PF_3**				**662.8**			**695.3**			**0**
87TAF	74-85-1	$CH_2{=}CH_2$	350	651.5	9.2	661.2						
83COL/MCM	74-85-1	$CH_2{=}CH_2$	298	651.5	13.0	664.4						
80DOI/MCM	7446-09-5; 74-85-1	SO_2; C_2H_4				643-651						
78COR/BEA	7783-54-2; 74-87-3	NF_3; CH_3Cl				539-621						
[C_8HF_5]	**363-72-4**	**C_8HF_5**				**662.7**			**690.4**			**16**
93SZU/MCM	7783-06-4	H_2S	600	673.8	−6.3	664.0	705	17.6	687.4	4.3	18.8	23.1
93SZU/MCM	75-15-0	CS_2	600	657.7	0	661.3	681.9	11.7	693.6	28	−19.2	8.8
78HAR/LIA	71-43-2	C_6H_6	400	725.4	−9.6	716.7						
[C_4F_7N]	**375-00-8**	**C_3F_7CN**				**662.6**			**693.2**			**6**
83COL/MCM	7732-18-5	H_2O	298	660.0	2.5	662.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[CH_3O]	**2597-43-5**	**•CH_2OH**				**662.5**			**695**			**0**
93MOU/AUD	363-72-4; 7783-06-4	C_6HF_5; H_2S				663-674						
89HOL/LOS		See Refs.	298						695			
[C_2HF]	**2713-09-9**	**HCCF**				**661.3**			**686**			**26**
84BEA/EYE		See Refs.							674			
74REI/BAU		threshold value							690			
73REI/KRA		threshold value							690			
[C_3F_5N]	**422-04-8**	**C_2F_5CN**				**661.3**			**692.0**			**6**
83COL/MCM	7732-18-5	H_2O	298	660.0	1.3	661.3						
[$C_4H_4F_6O$]	**1515-14-6**	**$(CF_3)_2C(CH_3)OH$**				**660.9**			**691.2**			**7**
83COL/MCM	7732-18-5	H_2O	298	660.0	0.8	650.9						
[SSi]	**12504-41-5:a**	**SiS at S**				**660.2**			**683**			**32.5**
92BRU/GRE		theory							683			
[H_2O]	**7732-18-5**	**H_2O**				**660.0**			**691**			**5**
97EAS/SMI		theory	298									4.8
93SZU/MCM	7783-06-4	H_2S	600	673.8	−14.6	659.0	705	−15.9	689.1	4.3	2.1	6.4
93SMI/RAD		theory	298						688.4			
93SMI/RAD		theory	600						692.8			
93SMI/RAD		theory	0						682.3			
93DEL		theory	298						687			
88MCI/ADA	74-85-1	CH_2=CH_2	300	651.5	9.2	660.7	680.5	10.5	691.0	11.5	−4.2	7.3
87TAF	7664-41-7	NH_3	350	819	−165.2	653.2						
87POP/CUR		theory	298						691.6			
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	13.8	665.9						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	14.2	665.7						
81BOH/MAC	74-85-1	CH_2=CH_2	298	651.5	7.5	659.0						
79LAU	7664-41-7	NH_3	650	819	−157.3	657.7						
78TAN/MAC	7732-18-5	H_2O	298	660.0	0	660.0						
77WOL/STA	109-77-3	$CH_2(CN)_2$	350	694.1	−35.1	659.3						
77NG/TRE		threshold value							702			
77MAU/FIE	7732-18-5	H_2O	550	660.0	0	660.0						
73HOP/BON	7732-18-5	H_2O	296	660.0	0	660.0						
69HAN/FRA		threshold value							690			
[$C_2H_2F_2$]	**1630-78-0**	**(E)-CHFCHF**				**657.9**			**688.6**			**5.8**
75RID	353-36-6; 7732-18-5	C_2H_3F; H_2O				656-660						
[CS_2]	**75-15-0**	**CS_2**				**657.7**			**681.9**			**28**
97EAS/SMI		theory	298									31.3

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SZU/MCM	540-36-3	1,4-$C_6H_4F_2$	600	692.8	−30.1	660.9	718.7	−43.5	675.2	22	22.6	44.6
93SZU/MCM	7783-06-4	H_2S	600	673.8	−5.9	660.9	705	−31.0	674.0	4.3	42.7	47.0
93SZU/MCM	7732-18-5	H_2O	600	660.0	8.4	661.5	691	−15.9	675.1	5	41.0	46.0
93SMI/RAD		theory	600						685.4			
93SMI/RAD		theory	298						681.9			
93SMI/RAD		theory	0						677.5			
88MCI/ADA	74-85-1	CH_2=CH_2	300	651.5	6.9	658.4	680.5	1.9	682.4	11.5	16.7	28.2
88MCI/ADA	7732-18-5	H_2O	300	660.0	−2.9	657.1	691	−9.6	681.4	5	23	28
87TAF	7664-41-7	NH_3	350	819	−168.9	648.4						
85WEI/PLA	463-58-1; 74-99-7	COS; CH_3CCH				603-723						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	18.8	668.7						
85JAS/STE		theory							689			
77MAU/FIE	7732-18-5	H_2O	550	660.0	6.3	660.6						
[C_2F_3N]	**353-85-5**	**CF_3CN**				**657.7**			**688.4**			**6**
94KOP/ANV	74-85-1	CH_2=CH_2	373	651.5	5.9	657.7						
93SZU/MCM	75-15-0	CS_2	600	557.7	−18.0	646.4	681.9	−8.4	673.5	28	−15.9	12.1
87TAF	74-85-1	CH_2=CH_2	350	651.5	6.7	658.4						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	5.0	657.0						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	11.7	663.2						
78COR/BEA	7664-41-7	NH_3	320	819	−155.2	663.5						
[$C_3H_2F_6O$]	**920-66-1**	**$(CF_3)_2CHOH$**				**656.2**			**686.6**			**7**
94KOP/ANV	74-85-1	CH_2=CH_2	373	651.5	2.5	654.3						
87TAF	74-85-1	CH_2=CH_2	350	651.5	2.3	654.0						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	6.7	658.2						
[C_2H_5F]	**353-36-6**	**C_2H_5F**				**655.8**			**683.4**			**16**
72BEA/HOL	74-85-1; 7732-18-5	CH_2=CH_2; H_2O				651-660						
[C_2HF_3O]	**75-90-1**	**CF_3CHO**				**653.6**			**685.5**			**2**
94KOP/ANV	74-85-1	CH_2=CH_2	373	651.5	0.8	653.0						
87TAF	74-85-1	CH_2=CH_2	350	651.5	2.3	654.2						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	6.7	658.2						
78COR/BEA	7664-41-7	NH_3	320	819	−159.8	659.0						
[C_2H_4]	**74-85-1**	**CH_2=CH_2**				**651.5**			**680.5**			**11.5**
97EAS/SMI		theory	298									12.2
93SMI/RAD		theory	0						676.5			
93SMI/RAD		theory	298						681.9			
93SMI/RAD		theory	600						685.6			
89RUS/BER		threshold value	298						680.3			
87TAF	7664-41-7	NH_3	350	819	−184.9	633.2						
85MCM/KEB	630-08-0;a	CO at C	400	562.8	72.8	634.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
85MCM/KEB	74-85-1	$CH_2=CH_2$	400	651.5	0	651.5						
83COL/MCM	74-85-1	$CH_2=CH_2$	298	651.5	0	651.5						
82ROS/BUF		threshold value	298						679.2			
81TRA/MCL		threshold value	298						680.3			
81DOI/MCM	74-85-1	$CH_2=CH_2$	298	651.5	0	651.5						
81BOH/MAC	74-85-1	$CH_2=CH_2$	298	651.5	0	651.5						
80BAE		threshold value	298						682.1			
[O_4Os]	**208-16-12-0**	**OsO_4**				**650.6**			**676.9**			**20.6**
89BRI/BEA	354-32-5; 74-85-1	CF_3COCl; C_2H_4				650-651						
[C_2ClF_3O]	**354-32-5**	**CF_3COCl**				**649.8**			**681.6**			**2**
94KOP/ANV	74-85-1	$CH_2=CH_2$	373	651.5	1.7	653.8						
87TAF	74-85-1	$CH_2=CH_2$	350	651.5	−6.9	645.1						
85MCM/KEB	74-85-1	$CH_2=CH_2$	400	651.5	−6.7	645.7						
[OP]	**14452-66-5**	**PO**				**649.5**			**682**			**0**
90ADA/MIC		Bracketing, See Refs.	300						682±8			
[C_4HF_9O]	**2378-02-1**	**$(CF_3)_3COH$**				**646.7**			**676.8**			**8**
94KOP/ANV	74-85-1	$CH_2=CH_2$	373	651.5	−5.0	646.7						
87TAF	74-85-1	$CH_2=CH_2$	350	651.5	−27.5	624.2						
83COL/MCM	74-85-1	$CH_2=CH_2$	298	651.5	−1.3	650.2						
[C_2N_2]	**460-19-5**	**NC-CN**				**645.8**			**674.7**			**11.8**
89PET/FRE	74-85-1	$CH_2=CH_2$	300	651.5	−5.7	645.8						
87DEA/MAU	354-34-7; 74-85-1	CF_3CFO; C_2H_4	~330			637-651						
84RAK/BOH	7446-09-5; 74-85-1	SO_2; C_2H_4				643-651						
[COSe]	**1603-84-5**	**OCSe AT S**				**644.1**			**670**			**22**
85KAR	463-58-1; 74-85-1	COS; C_2H_4				603-651						
85JAS/STE		theory							670			
[H_2O_2]	**7722-84-1**	**H_2O_2**				**643.8**			**674.5**			**5.8**
75LIN/ALB	3170-83-0; 7732-18-5	HO_2; H_2O				628-660						
[O_2S]	**7446-09-5**	**SO_2**				**643.3**			**672.3**			**11.5**
94KOP/ANV	74-85-1	$CH_2=CH_2$	373	651.5	10.5	641.0						
93SZU/MCM	630-08-0:a	CO at C	600	562.8	46.4	607.1	594	36.8	630.8	4.2	15.9	20.1
93SZU/MCM	75-15-0	CS_2	600	657.7	−55.6	607.0	681.9	−43.9	637.9	28	−18.8	9.2
93SZU/MCM	353-85-5	CF_3CN	600	657.7	−36.4	619.7	688.4	−35.1	653.3	6	−1.7	4.3

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
87TAF	7664-41-7	NH_3	350	819	−218.7	599.4						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	43.1	605.2						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−29.7	621.8						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	−5.9	645.6						
81DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−2	649.5						
[S]	**7704-34-9**	**S**				**640.2**			**664.3**			**28**
81SMI/ADA		threshold value							664.3			
[C_3F_6O]	**684-16-2**	**$(CF_3)_2CO$**				**639.7**			**670.4**			**5.8**
94KOP/ANV	74-85-1	CH_2=CH_2	373	651.5	−13.4	638.5						
93SZU/MCM	7446-09-5	SO_3	600	643.3	−9.2	635.8	672.3	−2.9	669.4	11.5	−11.3	0.2
85MCM/KEB	630-08-0:a	CO at C	400	562.8	35.1	597.8						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−37.7	614.4						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	−9.2	642.3						
83COL/MCM	7446-09-5	SO_2	298	643.00	−2.9	640.4						
81DRU/MCM	353-50-4	F_2CO	298	637.0	2.1	639.0						
81DRU/MCM	7446-09-5	SO_2	298	643.3	2.9	646.2						
81DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−11.3	640.2						
78COR/BEA	7664-41-7	NH_3	350	819	−179.8	638.5						
[HP]	**13967-14-1**	**PH**				**639.6**			**670.3**			**5.8**
86BER/CUR		thermo cycles	298						670.3			
[C_3H_7]	**2025-55-0**	**i-C_3H_7•**				**638.9**			**671.4**			**0**
88LIA/BAR		threshold value	298						671.4			
[CH_3Br]	**74-83-09**	**CH_3Br**				**638.0**			**664.2**			**21**
94GLU/SZU		theory	298						662.9			
94GLU/SZU	392-56-3	C_6F_6	600	624.4	10	637.1	648.0	18.8	666.8	30	−14.6	15.4
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	9.6	661.1						
72BEA/HOL	630-08-0:a; 7732-18-5	CO; H_2O				563-660						
[CF_2O]	**353-50-4**	**F_2CO**				**637.0**			**666.7**			**9**
94KOP/ANV	74-85-1	CH_2=CH_2	373	651.5	−18.8	632.8						
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	−11.3	640.2						
83COL/MCM	7446-09-5	SO_2	298	643.3	−5.9	637.5						
81DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−13.4	638.1						
[C_2F_4O]	**354-34-7**	**CF_3CFO**				**636.7**			**668.6**			**2**
83COL/MCM	74-85-1	CH_2=CH_2	298	651.5	−13.4	638.1						
83COL/MCM	7446-09-05	SO_2	298	643.3	−7.5	635.8						
81DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−15.1	636.4						
[Cu]	**7440-50-8**	**Cu**				**632.4**			**655.3**			**32**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
86ELK/ARM4		See Refs.							655±13			
[HO_2]	**3170-83-0**	**HO_2•**				**627.5**			**660**			**0**
88LIA/BAR		threshold value							660			
[C_6F_6]	**392-56-3**	**C_6F_6**				**624.4**			**648.0**			**30**
93SZU/MCM	7446-09-5	SO_2	600	643.3	20.1	657.8	672.3	12.1	684.5	11.5	13.4	24.9
93SZU/MCM	7732-18-5	H_2O	600	660.0	−28.5	624.1						
7BHAR/LIA	71-43-2	C_6H_6	400	725.4	−14.6	710.3						
[CH_3Cl]	**74-87-3**	**CH_3Cl**				**621.1**			**647.3**			**21**
94GLU/SZU		theory							649.8			
94GLU/SZU	392-56-3	C_6F_6	600	624.4	−6	621.1	648.0	7.1	655.1	30	−21.8	8.2
89PET/PRE	460-19-5	NC-CN	300	645.8	−1.1	644.7						
89PET/PRE	74-85-1	CH_2=CH_2	300	651.5	−6.5	645.0						
78COR/BEA		See Refs.	320			~659						
72BEA/HOL	74-86-2; 74-85-1	C_2H_2; C_2H_4				617-651						
[C_2H_3O]	**3170-69-2**	**CH_3CO•**				**620.5**			**653**			**0**
89HOL/LOS			298						653			
[C_2H_2]	**74-86-2**	**C_2H_2**				**616.7**			**641.4**			**26**
84SMI/ADA		thermochemical cycles	300						641.4			
84LIA/LIE		threshold value				611.3						
[H_4Si]	**7803-62-5**	**SiH_4**				**613.4**			**639.7**			**20.6**
92HU/SHE		theory							659.4			
87POP/CUR		theory	298						639.7			
73CHE/LAM	2025-56-1; 2025-55-0	C_2H_5; C_3H_7				584-639						
[F_3HOSi]	**91419-78-2**	**SiF_3OH**				**611.5**			**641.9**			**7**
84REE/MUJ	593-53-3; 74-85-1	CH_3F; C_2H_4				572-651						
[C_3H_8]	**74-98-6**	**C_3H_8**				**607.8**			**625.7**			**49**
75HIR/KEB		See Refs.							625.7			49
[P]	**7723-14-0**	**P**				**604.8**			**626.8**			**35**
86BER/CUR		thermo cycles	298						626.8			
[AsF_3]	**7784-35-2**	**AsF_3**				**604.2**			**636.7**			**0**
80DOI/MCM	593-53-3; 353-50-4	CH_3F; CF_2O				572-637						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[COS]	**463-58-1**	**OCS at S**				**602.6**			**628.5**			**22**
97EAS/SMI		theory	298									26.6
93SZU/MCM	630-08-0:a	CO at C	600	562.8	45.6	603.1	594	33.9	627.9	4.2	20.1	24.3
93SZU/MCM	7446-09-5	SO_2	600	643.3	−1.3	638.9	672.3	−3.8	668.6	11.5	3.8	15.3
85WEI/PLA	74-85-1; 7732-18-5	C_2H_4; H_2O				651-660						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	41.4	602.4						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−31.4	619.0						
85MCM/KEB	7446-09-5	SO_2	400	643.3	−1.7	640.6						
85JAS/STE		theory							636.4			
81SMI/ADA	630-08-0:a; 7704-34-9	CO; S				563-640						
[HOSi]	**97402-81-8:b**	**HSiO at Si**				**602.5**			**635**			**0**
93LUC/CUR		theory	298						635			
[CHO]	**2597-44-6**	**HCO**				**601.8**			**636**			**−5.8**
74WAR		threshold value							636			
[CFN]	**1495-50-7**	**FCN**				**601.3**			**632**			**6**
84BEA/EYE		See Refs.							632			
[HI]	**10034-85-2**	**HI**				**601.3**			**627.5**			**21**
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−43.1	607.4						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	29.7	590.8						
78POL/MUN	10035-10-6; 14362-44-8	HBr; I				558-583						
[CF_3I]	**2314-97-8**	**CF_3I**				**598.2**			**628.0**			**9.1**
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−45.2	606.5						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	27.6	589.9						
[SSi]	**12504-41-5:b**	**SiS at Si**				**596.6**			**627**			**7**
92BRU/GRE		theory							627			
[O_3]	**10028-15-6**	**O_3**				**595.9**			**625.5**			**9.5**
94CAS/SPE	593-53-3; 7446-09-5	CH_3F; SO_2	298			572-643						
91MER/QUE		theory	298						625.5			9.5
[CHO_2]	**2564-86-5**	**•COOH**				**590.9**			**623.4**			**0**
89HOL/LOS			298						623.4			
[CH_2F_2]	**75-10-5**	**CH_2F_2**				**589.7**			**620.5**			**5.8**
74BLI/MCM	630-08-0:a; 74-86-2	CO; C_2H_2				563-617						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[CHF_3]	**75-46-7**	**CHF_3**				**589.7**			**619.6**			**9.1**
74BLI/MCM	630-08-0:a; 74-86-2	CO; C_2H_2				563-617						
[Zn]	**7440-66-6**	**Zn**				**586.0**			**608.6**			**33**
78PO/RAD	74-82-8; 74-85-1	CH_4; C_2H_4				521-651						
[B_2H_6]	**19287-45-7**	**B_2H_6**				**586.0**			**615**			**11.5**
73PIE/POR		See Refs.							615±17			
[C_2H_5]	**2025-56-1**	**C_2H_5•**				**583.5**			**616**			**0**
88LIA/BAR		threshold value	298						616			
[I]	**14362-44-8**	**I**				**583.5**			**608.2**			**26**
88LIA/BAR		threshold value							608.2			
[F_2O_2S]	**2699-79-8**	**F_2SO_2**				**580.5**			**605.5**			**25**
93SZU/MCM	630-08-0:a	CO at C	600	562.8	24.7	581.2	594	12.1	606.1	4.2	20.9	25.1
85MCM/KEB2	630-08-0:a	CO at C	400	562.8	19.7	580.4						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	19.2	580.0						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−53.6	596.6						
81DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−15.9	635.6						
80DOI/MCM	74-85-1	CH_2=CH_2	298	651.5	−15.1	636.4						
[B_4H_{10}]	**18283-93-7**	**B_4H_{10}**				**572.5**			**605**			**0**
73PIE/POR		See Refs.							605±20			
[CH_3F]	**593-53-3**	**CH_3F**				**571.5**			**598.9**			**17**
94GLU/SZU		theory	298						597.2			
94GLU/SZU	630-08-0:a; 74-84-0	CO; C_2H_6				563-570						
85MCM/KEB2	630-08-0:a; 2699-79-8	CO; SO_2F_2	400			563-581						
72BEA/HOL	630-08-0:a; 74-86-2	CO; C_2H_2				563-617						
[C_2H_6]	**74-84-0**	**C_2H_6**				**569.9**			**596.3**			**20**
94CAR/SCH		theory	298						596.2			20
93SZU/MCM	74-85-1	CH_2=CH_2	600	651.5	−80.8	568.2	680.5	−83.3	597.2	11.5	5.0	16.5
93SZU/MCM	630-08-0:a	CO at C	400	562.8	7.5	568.8	594	3.3	597.3	4.2	10.9	15.1
85MCM/KEB	630-08-0:a	CO at C	400	562.8	7.1	568.3						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−65.7	584.9						
81MAC/SCH	10024-97-2:a	N_2O at O	298	548.7	18.1	566.8						
81MAC/SCH	630-08-0:a	CO at C	298	562.8	6	568.8						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
81BOH/MAC	630-08-0:a	CO at C	298	562.8	5.9	568.7						
76HIR/KEB		See Refs.	~200						561.4A			
76HIR/KEB		See Refs.	~400						593.1B			27.4
75FRE/KEB		See Refs.							589.3			
[HO]	**3352-57-6**	**OH**				**564.0**			**593.2**			**11**
88LIA/BAR		threshold							593.2			
[CN]	**2074-87-5**	**CN at N**				**>564**			**>596**			**4.2**
90PET/FRE		thermo cycles							>595			
[CO]	**630-08-0:a**	**CO at C**				**562.8**			**594**			**4.2**
97EAS/SMI		theory	298									3.8
93SZU/MCM	630-08-0:a	CO at C	600	562.8	0	562.8	594	0	594			
93SMI/RAD		theory	298						593			
93SMI/RAD		theory	0						587.1			
93SMI/RAD		theory	600						596.6			
92KOM/DIX		theory	298						593.3			
85TRA2		Appearance	298						594			
85MCM/KEB	630-08-0:a	CO at C	400	562.8	0	562.8						
85JAS/STE		theory							583.2			
84DIX/KOM		theory	300						591.6			
84BEA/EYE		See Refs.							577.4			
81BOH/MAC	630-08-0:a	CO at C	298	562.8	0	562.8						
80DYK/JON		threshold value							593.7			
76GUY/CHU		threshold value							604.2			
73HEM/RUN	630-08-0:a	CO at C	298	562.8	0	562.8						
69MAT/WAR		threshold value							594.5			
[NO_2]	**10102-44-0**	**NO_2**				**560.3**			**591.0**			**5.8**
84POL/MUN	10035-10-6; 630-08-0:a	HBr, CO				*558-563*						
[O_3S]	**7446-11-9**	**SO_3**				**560.3**			**588.3**			**14.9**
77MUN/SMI	10035-10-6; 630-08-0:a	HBr; CO				558-563						
[BrH]	**10035-10-6**	**HBr**				**657.7**			**584.2**			**20**
97EAS/SMI		theory	298									20.2
93SMI/RAD		theory	0						581			
93SMI/RAD		theory	298						585.9			
93SMI/RAD		theory	600						589.8			
89TIC/JAV	630-08-0:a	CO at C		562.8			594	−8.4	585.6			
89ADA/SMI	630-08-0:a	CO at C	298	562.8			594	−10.9	583.1			
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−78.2	572.4						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	−5.0	556.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
84POL/MUN	10024-97-2:a; 10102-44-0	N_2O; NO_2				549-560						
79TIE/AND		threshold value							589.9			
78POL/MUN	7647-01-0; 630-08-0:a	HCl; CO				530-563						
[H_3OSi]	**113648-09-2:b**	**H_2SiOH at Si**				**556.5**			**589**			**0**
93LUC/CUR		theory	298						589			
[F_6S]	**2551-62-4**	**SF_6**				**550.7**			**576.3**			**26.4**
94LAT/SMI	10024-97-2:a; 630-08-0:a	N_2O; CO	5			549-563						
92MAC/SCH	630-08-0:a	CO at C	298	562.8	−12.1	550.7						
[$CBrF_3$]	**75-63-8**	**CF_3Br**				**550.3**			**580.0**			**9.1**
95HIR/NAS		See Refs.							>553			
85MCM/KEB2	10024-97-2:a	N_2O at O	400	548.7	−1.3	548.6						
85MCM/KEB	74-82-8	CH_4	400	520.6	27.6	550.5						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	−10.5	551.8						
[N_2O]	**10024-97-2:a**	**N_2O at O**				**548.7**			**575.2**			**20**
93SZU/MCM	124-38-9	CO_2	600	515.8	32.6	550.2	540.5	35.1	575.6	26	−4.6	21.4
93SZU/MCM	630-08-0:a	CO at C	600	562.8	−6.3	551.8	594	−17.2	576.8	4.2	18.4	22.6
90JAV/GLO	74-82-8	CH_4					543.5	32.2	575.7			
89ADA/SMI	7647-01-0	HCl	298				556.9	17.2	574.1			
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−82.8	567.8						
84BEA/EYE		See Refs.							531.4			
80BOH/MAC	630-08-0:a	CO at C	296	562.8	−12.2	550.7						
80BOH/MAC	124-38-9	CO_2	296	515.8	33.9	549.7						
75LIN/MCF	630-08-0:a	CO at C	298	562.8	−13.4	549.4	594	−18.4	575.6	4.2	16.7	20.9
73HEM/RUN	630-08-0:a	CO at C	298	562.8	−12.6	550.3	594	−14.6	579.4	4.2	7.5	11.7
[$CClF_3$]	**75-72-9**	**CF_3Cl**				**541.5**			**571.3**			**9.1**
85MCM/KEB	74-82-8	CH_4	400	520.6	18.0	540.9						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	−20.1	542.2						
[F_3N]	**7783-54-2**	**NF_3**				**538.6**			**568.4**			**9.1**
92GRA/HRU		theory							578.2			
85MCM/KEB	74-82-8	CH_4	400	520.6	15.1	537.9						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	−23.0	539.3						
80DOI/MCM	630-08-0:a; 593-53-3	CO; CH_3F				563-572						
[Br]	**10097-32-2**	**Br**				**531.2**			**554.4**			**31**
78POL/MUN		threshold value							554.4			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[ClH]	**7647-01-0**	**HCl**				**530.1**			**556.9**			**19**
97EAS/SMI		theory	298									19.3
93SMI/RAD		theory	600						565.7			
93SMI/RAD		theory	298						561.5			
93SMI/RAD		theory	0						556.6			
89TIC/JAV	10035-10-6	HBr		557.7			584.2	−25.1	559.1			
89ADA/SMI	74-82-8	CH_4	298	520.6			543.5	13.4	556.9			
87POP/CUR		theory	298						556.5			
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	−100.4	550.3						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	−27.6	533.7						
79TIE/AND		threshold value							564.8			
78POL/MUN	10097-32-2; 10024-97-2:a	Br; N_2O				531-549						
74FEH/FER		thermochemical cycle				>519						
[N_2O]	**10024-97-2:b**	**N_2O at N**				**523.3**			**549.8**			**20**
90JAV/GLO	74-82-8	CH_4		520.6			543.5	6.3	549.8			
[CH_4]	**74-82-8**	**CH_4**				**520.6**			**543.5**			**32**
97EAS/SMI		theory	298									26.2
94CAR/SCH		theory	298						543.9			
93SZU/MCM	10024-97-2:a	N_2O at O	600	548.7	−25.5	519.6	575.2	−31.8	543.4	20	10.5	30.5
93SZU/MCM	630-08-0:a	CO at C	600	562.8	−31.4	523.1	594	−48.1	545.9	4.2	27.6	31.8
93SZU/MCM	74-84-0	C_2H_6	600	569.9	−39.3	526.9	596.3	−49.8	546.6	20	17.2	37.2
93SMI/RAD		theory	600						542.1			
93SMI/RAD		theory	0						535.5			
93SMI/RAD		theory	298						539.8			
92KOM/DIX		theory	298						542.2			
89TIC/JAV	10035-10-6	HBr		557.7			584.2	−38.1	546.1			
89ADA/SMI	124-38-9	CO_2	298				540.5	6.3	546.8			
87POP/CUR		theory	298						537.2			
85MCM/KEB	630-08-0:a	CO at C	400	562.8	-38.1	521.9						
85MCM/KEB	74-85-1	CH_2=CH_2	400	651.5	-110.9	538.5						
80BOH/MAC	124-38-9	CO_2	296	515.8	7.8	523.6						
77MAU/FIE	124-38-9	CO_2	550	515.8	5.4	519.7						
75STA/BEA	124-38-9	CO_2	320	515.8	8.8	524.5						
72KAS/FRA	124-38-9	CO_2	340	515.8	5.9	521.4						
73HEM/RUN	124-38-9	CO_2	296	515.8	7.8	523.6	540.5	6.2	546.7	26	5.8	31.8
73BOH/HEM	124-38-9	CO_2	300	515.8	7.9	523.7						
71CHU/BER		threshold value							592.3			
[CO_2]	**124-38-9**	**CO_2**				**515.8**			**540.5**			**26**
97EAS/SMI		theory	298									26.4
93SZU/MCM	74-82-8	CH_4	600	520.6	−6.3	516.1	543.5	−3.3	540.2	32	−5.0	27.0
93SMI/RAD		theory	600						542.7			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
93SMI/RAD		theory	298						539.3			
93SMI/RAD		theory	0						534.8			
92KOM/DIX		theory	298						541			
91TRA/KOM		Appearance	298						536.5		539.6	
89RUS/SCH		Appearance	298						540.5			
89ADA/SMI	10097-32-2	Br	298				554.4	−13.6	540.8			
85JAS/STE		theory							543.5			
85FRI/SCH		theory	298						547			
80BOH/MAC	630-08-0:a	CO at C	296	562.8	−46.0	516.9						
77MAU/FIE	124-38-9	CO_2	550	515.8	0	518.8						
76MEI/MIT	74-82-8	CH_4	298	520.6	−8.7	511.9	543.5	−6.6	536.9	32	−7.1	24.9
76FEH/LIN	124-38-9	CO_2	298	515.8	0	515.8						
75STA/BEA	124-38-9	CO_2	320	515.8	0	515.8						
72KAS/FRA	124-38-9	CO_2	340	515.8	0	515.8						
74WAR		threshold value							547.7			
73HEM/RUN	124-38-9	CO_2	298	515.8	0	515.8						
73BOH/HEM	124-38-9	CO_2	298	515.8	0	515.8						
[NO]	**10102-43-9**	**NO**				**505.3**			**531.8**			**20**
89TIC/JAV	75-73-0	CF_4	300	503.7	−2.2	501.6	529.3	2.5	531.8	23.3	−15.5	7.8
80KOP/COM									456			
71ROC/SUT	<74-82-8	CH_4		520.6	<0	<520						
[CF_4]	**75-73-0**	**CF_4**				**503.7**			**529.3**			**23.3**
89TIC/JAV	7647-01-0	HCl	300	530.1	−28.9	501.2	556.9	−29.3	527.6	19	1.3	20.3
89TIC/JAV	74-82-8	CH_4	300	520.6	−18.7	501.9	543.5	−16.7	526.8	32	−6.7	25.3
89TIC/JAV	124-38-9	CO_2	300	515.8	−7.6	508.2	540.5	−7.1	533.4	26	−1.7	24.3
71ROC/SUT	>7727-37-9	$>N_2$				>464						
[OSi]	**10097-28-6:b**	**SiO at Si**				**500.5**			**533**			**0**
93LUC/CUR		theory	298						533			
[Cl]	**22537-15-1**	**Cl**				**490.1**			**513.6**			**30.1**
88LIA/BAR		threshold value							513.6			
78POL/MUN		threshold value				488.7						
[FO]	**12061-70-0**	**OF**				**482.2**			**508.7**			**20**
88LIA/BAR									508.7			
80KOP/COM									582			
[Xe]	**7440-63-3**	**Xe**				**478.1**			**499.6**			**36.8**
80BOH/MAC	124-38-9	CO_2	800	515.8	−30.3	480.1						
76FEH/LIN	124-38-9	CO_2	800	515.8	−30.5	479.9						
76FEH/LIN	7727-37-9	N_2	298	464.5	9.9	474.4	493.8	2.6	496.4	10.5	24.3	34.8
[F_4Si]	**7783-61-1**	**SiF_4**				**476.6**			**502.9**			**20.6**

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
84REE/MUJ		See Refs.							502.9			
[N_2]	**7727-37-9**	**N_2**				**464.5**			**493.8**			**10.5**
97EAS/SMI		theory	298									10.5
93SZU/MCM	124-38-9	CO_2	600	515.8	−53.1	467.3	540.5	−44.8	495.7	26	−13.8	12.2
93SZU/MCM	7400-63-3	Xe	600	478.1	−20.9	465.1	499.6	−6.7	492.9	36.8	−23.8	13.0
93SMI/RAD		theory	0						488.3			
93SMI/RAD		theory	600						497			
93SMI/RAD		theory	298						493.9			
92KOM/DIX		theory	298						493.3			
91RUS/BER		appearance	298						<510			
80BOH/MAC	17778-80-2	O	296	459.6	1.3	460.8						
79WIB/FIS		threshold value							494			
78FON/HUD		threshold value							478.2			
76WIL/LOS		threshold value							469.4			
76FEH/LIN	17778-80-2	O	298	459.6	1.3	460.8						
76FEH/LIN	124-38-9	CO_2	298	515.8	−40.2	475.6						
[O]	**17778-80-2**	**O**				**459.6**			**485.2**			**23**
88LIA/BAR		threshold value							485.2			
81JON/BIR	7727-37-9	N_2	300	464.5	0	464.5						
80BOH/MAC	124-38-9	CO_2	296	515.8	−41.4	474.4						
80BOH/MAC	630-08-0:a	CO at C	296	562.8	−87.4	475.4						
80BOH/MAC	17778-80-2	O	296	459.6	0	459.6						
76MCC		threshold value							486.6			
[FH]	**7664-39-3**	**HF**				**456.7**			**484**			**17.3**
97EAS/SMI		theory	298									17.3
93SMI/RAD		theory	600						488.4			
98SMI/RAD		theory	298						484			
98SMI/RAD		theory	0						479.1			
93DEL		theory	298						486.2			
87POP/CUR		theory	298						483.2			
79TIE/AND		threshold value							397.5			
75FOS/BEA	7727-37-9	N_2	320	464.5	−2.9	461.4						
[Kr]	**7439-90-9**	**Kr**				**402.4**			**424.6**			**34.4**
80BOH/MAC	1333-74-0	H_2	296	394.7	8.3	403.1						
80BOH/MAC	7782-44-7	O_2	296	396.3	6.1	402.4						
79HUB/HER		threshold value							419.7			
75PAY/SCH	1333-74-0	H_2	296	394.7	7	401.8						
[CO]	**630-08-0;b**	**CO at O**				**402.2**			**426.3**			**28**
87FRE/KNI		See Refs.	300						427±8			
84DIX/KOM		theory	300						426.3			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M) ΔS_p(M)
[O_2]	**7782-44-7**	**O_2**				**396.3**			**421**			**26**
84ADA/SMI	1333-74-0	H_2	300	394.7	1.5	396.2	422.3	−1.3	421	16.3	9.2	25.5
81DYK/JON		threshold value							420.5			
80BOH/MAC	1333-74-0	H_2	296	394.7	1.7	396.4						
77MCC		threshold value							422.2			
75FEH/LIN	7782-44-7	O_2	298	396.3	0	396.3						
73FEN/HEM	7782-44-7	O_2	298	396.3	0	396.3						
73FEN/HEM	17778-80-2	O	298	459.6	−47.7	411.9						
[H_2]	**1333-74-0**	**H_2**				**394.7**			**422.3**			**16.3**
97EAS/SMI		theory	298									16.3
98SMI/RAD		theory	600						424			
93SMI/RAD		theory	298						419.1			
93SMI/RAD		theory	0						414.2			
84DIX/KOM		theory	300						423.8			
80BOH/MAC	17778-80-2	O	296	459.6	−49.4	410.2						
78PO/RAD		See Refs.							422.6			
75PAY/SCH	1333-74-0	H_2	296	394.7	0	394.7						
75FEH/LIN	7782-44-7	O_2	298	396.3	−1.3	395.0						
73HAR/CRO									400±14			
73FEN/HEM	7782-44-7	O_2	298	396.3	−1.7	394.6						
73FEN/HEM	17778-80-2	O	298	459.6	−49.4	410.2						
72COT/ROZ		threshold value							417.6			
[Ar]	**7440-37-1**	**Ar**				**346.3**			**369.2**			**32**
82VIL/FUT	1333-74-0	H_2		394.7			422.3	−53.1	369.2			
79HUB/HER		threshold value							>255			
71ROC/SUT	7722-84-1	H_2O_2		643.8		<644						
[N]	**17778-88-0**	**N**				**318.7**			**342.2**			**30**
88MAR/REB		See Refs.							339.7			
85ADA/SMI		See Refs.	300						344.7			
[F]	**14762-94-8**	**F**				**315.1**			**340.1**			**25**
88LIA/BAR		threshold value							340.1			
[F_2]	**7782-41-4**	**F_2**				**305.5**			**332**			**20**
97CIP/CRE		See Refs.							332±20			
[H_2OSi]	**22755-01-7:b**	**H_2SiO at Si**				**295.5**			**328**			**0**
93LUC/CUR		theory	298						328			
[Ne]	**7440-01-9**	**Ne**				**174.4**			**198.8**			**27**
91GLO/TWI	7440-59-7	He	300	148.5	25.9	174.4						
79HUB/HER		threshold value							200.8			
68CHU/RUS		threshold value							201.3			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)				GB(M)			PA(M)			ΔS_p(M)
YrSquib	Reg No(R)	Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS_p(R)	$\Delta\Delta S_p$(M,R)	ΔS_p(M)
[He]	**7440-59-7**	**He**				**148.5**			**177.8**			**10.5**
79HUB/HER		threshold value							177.8			

3. Annotated Refences to Tables 1 and 2

92ABB/CAB Abboud, J.-L. M., Cabildo, P., Canada, T., Catalan, J., Claramunt, R. M., de Paz, J. L. G., Elguero, J., Homan, H., Notario, R., Toiron, C., Yranzo, G. I., J. Org. Chem. **57**, 3938 (1992). ICR measurements of GB at 333 K.

92ABB/CAN Abboud, J.-L. M., Canada, T., Homan, H., Notario, R., Cativiela, C., Diaz de Villegas, M. D., Bordeje, M. C., Mo, O. Yanez, M., J. Am. Chem. Soc. **114**, 4728 (1992). ICR measurement of proton transfer equilibria at a single temperature.

96ABB/HER Abboud, J.-L. M., Herreros, M, Notario, R., Esseffar, M., Mo, O., Yanez, M., J. Am. Chem. Soc. **118**, 1126 (1996). ICR. Also G2 calculation of P_4 and P_4H^+.

93ABB/MO Abboud, J.-L. M., Mo, O., de Paz, J. L. G., Esseffar, M., Bouad, W., El-Mouhtadi, M., Mokhliss, R., Ballesteros, E., Herreros, M., Homan, H., Lopez-Mardomingo, C., Notario, R., J. Am. Chem. Soc. **115**, 12468 (1993). ICR measurements.

90ADA/MCI Adams, N. G., McIntosh, B. J., Smith, D., Astron. Astrophys. **232**, 443 (1990). Bracketing using SIFT technique. Bracketing partners indicated for PN but not for PO, PS nor HCP.

84ADA/SMI Adams, N. G., Smith, D., Chem. Phys. Lett. **105**, 604 (1984). Determination of enthalpy and entropy changes for reaction: $O_2H^+ + H_2 \rightleftarrows H_3^+ + O_2$ through determination of rate constants for forward and reverse reaction at 80 and at 300 K (SIFT).

85ADA/SMI Adams, N. G., Smith, D., Chem. Phys. Lett. **117**, 67 (1985). SIFDT. Study of the energy dependence of the reaction: $N^+(^3P) + H_2(X^1\Sigma_g^+) \rightarrow NH^+(X^2\Pi) + H(^2S_{1/2})$. Endothermicity determined to be 1 kJ mol^{-1}.

89ADA/SMI Adams, N. G., Smith, D., Tichy, M., Javahery, G., Twiddy, N. D., J. Chem Phys. **91**, 4037 (1989). Some PA values determined using variable temperature SIFT measurements and others determined using nonthermal SIFDT measurements.

81ALD/ARR Alder, R. W., Arrowsmith, R. J., Casson, A., Sessions, R. B., Heilbronner, E., Kovac, B., Huber, H., Taagepera, M., J. Am. Chem. Soc. **103**, 6137 (1981). ICR.

91ALL/CRA Allison, C. E., Cramer, J. A., Hop, C. E. C. A., Szulejko, J. E., McMahon, T. B., J. Am. Chem. Soc. **113**, 4469 (1991). HPMS. Temperature dependence of proton-transfer equilibria.

90ALL/MCM Allison, C. E., McMahon, T. B., J. Am. Chem. Soc. **112**, 1672 (1990). FT-ICR bracketing experiments.

96AME/TOR Amekraz, B., Tortajada, J., Morizur, J.-P., Gonzalez, A. I., Mo, O., Yanez, M., Leito, I., Maria, P.-C., Gal, J.-F., New J. Chem. **20**, 1011 (1996). ICR. Calculations at various levels of theory.

80ARM/HIG Armitage, M. A., Higgins, M. J., Lewars, E. G., March, R. E., J. Am. Chem. Soc. **102**, 5064 (1980). Time-resolved quadrupole ion store (quistor).

77ARM/HOD Armentrout, P., Hodges, R., Beauchamp, J. L., J. Am. Chem. Soc. **99**, 3162 (1977). Endothermicity of reactions: $\{U^- + D_2 \rightarrow UD^- + D\}$(1.7±0.1 eV) and $\{U^- + CD_4 \rightarrow UD^- + CD_3\}$ determined in an ion beam collision chamber apparatus. Using $\Delta_f H^0$(U,gas)=531.4 kJ mol^{-1}, IP(U) =6.19405 eV, $\Delta_f H^0$(D)=221.7 kJ mol^{-1} and $\Delta_f H^0(D^-)$ =1534.1 kJ mol^{-1} gives a deuteron affinity of 995.2 ± 10 kJ mol^{-1}.

75ARN Arnett, E. M., "Proton transfer and the solvation of ammonium ions," in Proton Transfer Reactions, Editors: E. F. Caldin and V. Gold, Chapman and Hall, London, pp. 79–101 (1975). A review which includes many results from the laboratory of R. W. Taft, some of which are not published elsewhere. See TAFT for discussion of this set of results, and how they have been treated in this evaluation.

77ARN/CHA Arnett, E. M., Chawla, B., Bell, L., Taagepera, M., Hehre, W. J., Taft, R. W., J. Am. Chem. Soc. **99**, 5729 (1977). ICR.

72ARN/JON Amett, E. M., Jones III, F. M., Taagepera, M., Henderson, W. G., Beauchamp, J. L., Holtz, D., Taft, R. W., J. Am. Chem. Soc. **94**, 4724 (1972). ICR. Data corrected from originally reported temperature of 300–350 K.

89ATT/CAC Attina, M., Cacace, F., De Petris, G., Grandinetti, F., Int. J. Mass Spectrom. Ion Processes **90**, 263 (1989). ICR bracketing measurements. No indication of which reference bases were used for bracketing, thus the tabulated value is just that given in this paper. Reservations about absolute accuracy, besides that due to the bracketing technique itself, because of the thermal instability of the compounds and their protonated ions. *Ab initio* calculations on methyl azide at 6-31G**//6-31G* level gives PA(CH_3N_3)=817.1 kJ mol^{-1}.

92ATT/CAC Attina, M., Cacace, F., Grandinetti, F., Occhiucci, G., Ricci, A., Int. J. Mass Spectrom. Ion Processes **117**, 47 (1992). FT-ICR. Thermochemistry for proton transfer equilibria inferred from Figs. 2 and 3. PA(HBO_2) bracketed between PA(CH_3OH) and PA(CH_3CHO).

93ATT/CAC Attina, M., Cacace, F., Ciliberto, E., de Petris, G., Grandinetti, F., Pepi, F., Ricci, A., J. Am. Chem. Soc. **115**, 12398 (1993). FT-ICR and calculations at G1 level of theory. Measured proton-transfer equilibria of $[H_2N{-}NO_2]H^+$ with CH_3OH and C_6H_6 as reference bases but no ΔG^0 values given for these systems, thus data are tabulated as if bracketed.

96AUD/FOS Audier, H. E., Fossey, J., Mourgues, P., Lablanc, D., Hammerun, S., Int. J. Mass Spectrom. Ion Processes **157/158**, 275 (1996). ICR. Bracketing measurements and *ab initio* calculations.

AUE Aue, D. H., personal communication, University of California, Santa Barbara, CA.

79AUE/BET Aue, D. H., Betowski, L. D., Davidson, W. R., Bowers, M. T., Beak, P., Lee, J., J. Am. Chem. Soc. **101**, 1361 (1979). ICR. Data relative to CH_3NH_2 or $(CH_3)_3N$ and expanded by the factor 350/298.

79AUE/BOW Aue, D. H., Bowers, M. T., in "Gas Phase Ion Chemistry," M. T. Bowers, Editor (Academic Press, New York), pp. 1–51. Chapter 9: "Stabilities of positive ions from equilibrium gas-phase basicity measurements." ICR. A review which includes many results from the laboratory of the authors, some of which have not been published elsewhere. Data relative to the nearest reference base shown in Table A, and expanded by the factor 350/298. More recently, one of the authors has re-interpreted the proton transfer equilibrium data for the following hydrocarbons: 1-methyl-cyclopropene [3100-04-7]; 2-butyne [503-17-3]; 3-methyl-1-butyne [598-23-2]; 2-pentyne [627-21-4]. Details are reported by D. H. Aue, in "Dicoordinated Carbocations and Related Species," Z. Rappoport and P. J. Stang, Editors, Wiley, New York (1997).

76AUE/DAV Aue, D. H., Davidson, W. R., Bowers, M. T., J. Am. Chem. Soc. **98**, 6700 (1976). ICR. Data relative to the nearest reference base shown in Table A and expanded by the factor 350/298. More recently, one of the authors has re-interpreted the proton transfer equilibrium data for cyclopropene [2781-85-3]. Details are reported by D. H. Aue, in "Dicoordinated Carbocations and Related Species," Z. Rappoport and P. J. Stang, Editors, Wiley, New York (1997).

81AUE/PED Aue, D. H., Pedley, M., Bowers, M. T., J. Am. Chem. Soc. **103**, 5674 (1981). GB(CH_3NC) 67 kJ mol^{-1} (16 kcal mol^{-1}) above GB(CH_3OH). No other details given.

72AUE/WEB Aue, D. H., Webb, H. M., Bowers, M. T., J. Am. Chem. Soc. **94**, 4726 (1972). ICR. Data relative to CH_3NH_2 and expanded by the factor 350/298.

73AUE/WEB Aue, D. H., Webb, H. M., Bowers, M. T., J. Am. Chem. Soc. **95**, 2699 (1973). ICR. Data relative to n-$C_3H_7NH_2$ and expanded by the factor of 350/298.

75AUE/WEB Aue, D. H., Webb, H. M., Bowers, M. T., J. Am. Chem. Soc. **97**, 4136 (1975). ICR. Data relative to CH_3NH_2 and expanded by the factor of 350/298.

75AUE/WEB2 Aue, D. H., Webb, H. M., Bowers, M. T., J. Am. Chem. Soc. **97**, 4137 (1975). ICR. Data relative to CH_3NH_2 included here and expanded by the factor 350/298; other data relative to CH_3CHO omitted because the "semiquantitative" values have been superseded by more recent equilibrium measurements.

76AUE/WEB Aue, D. H., Webb, H. M., Bowers, M. T., J. Am. Chem. Soc. **98**, 311 (1976). ICR. Data as relative to the nearest reference base shown in Table A and expanded by the factor of 350/298.

76AUE/WEB2 Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., Hopkins, Jr., H. P., J. Am. Chem. Soc. **98**, 854 (1976). ICR. Data given in graphic form, difficult to read: Values cited are from 79AUE/BOW review. Such data is tabulated relative to the nearest reference base shown in Table A, and is expanded by the factor 350/289.

80AUE/WEB Aue, D. H., Webb, H. M., Davidson, W. R., Vidal, M., Bowers, M. T., Goldwhite, H., Vertal, L. E., Douglas, J. E., Kollman, P. A., Kenyon, G. L., J. Am. Chem. Soc. **102**, 5151 (1980). ICR.

91AUE/WEB Aue, D. H., Webb, H. M., Davidson, W. R., Toure, P., Hopkins, Jr., H. P., Moulik, S. P., Jahagirdar, D. V., J. Am. Chem. Soc. **113**, 1770 (1991).

77AUS/LIA Ausloos, P., Lias, S. G., J. Am. Chem. Soc. **99**, 4198 (1977). ICR. Toluene relative to propionaldehyde and methyl formate.

78AUS/LIA Ausloos, P., Lias, S. G., J. Am. Chem. Soc. **100**, 1953 (1978). ICR. Entropy changes determined.

78AUS/LIA2 Ausloos, P., Lias, S. G., J. Am. Chem. Soc. **100**, 4594 (1978). ICR. Bracketing: $CCl_2 \leq C_2H_5OC_2H_5$.

AUS/LIA Ausloos, P., Lias, S. G., unpublished results. ICR. Bracketing: $CH_3CHO < CH_2=C=CH_2 < CH_3SH$.

83AUS/LUT Ausloos, P., Lutz, C., Schwarz, F., Lias, S. G., Radiat. Phys. Chem. **19**, 303 (1983). From the efficiency of the reaction: $C_4H_8O_2^+ + 1,4\text{-}C_4H_8O_2 \rightarrow C_4H_8O_2H^+ + C_4H_7O_2$, the proton affinity of the $C_4H_7O_2$ radical is within 4 kJ mol^{-1} (1 kcal mol^{-1}) of that of p-dioxane.

82AUS/REB Ausloos, P., Rebbert, R. E., Schwarz, F. P., Lias, S. G., Radiat. Phys. Chem. **19**, 27 (1982). ICR. Bracketing: $H_2O < c\text{-}C_6H_{12} < H_2S$.

80BAE Baer, T., J. Am. Chem. Soc. **102**, 2482 (1980). PIPECO measurements of $\Delta_f H^0(C_3H_5^+)$ and $\Delta_f H^0(C_3H_7^+)$ from C_3H_5I and C_3H_7I. For more detailed information see Sec. 3.4 for propene and Sec. 3.8 for ethene. Compare to 82ROS/BUF.

83BAR/BAS Bartmess, J. E., Basso, T., Georgiadis, R., J. Phys. Chem. **87**, 912 (1983). ICR. Temperature not specified but taken to be near 300 K.

84BEA/EYE Beach, D. B., Eyermann, C. J., Smit, S. P., Xiang, S. F., Jolly, W. L., J. Am. Chem. Soc. **106**, 536 (1984). The heat of formation of the M_2H^+ ion is estimated from the experimentally determined binding energies of isoelectronic neutral species. Cited proton affinities based on following data: N_2O from HNC*O (295.89 eV); CO from HN*CO (406.44 eV); HCCF from CH_2CO^* (540.25 eV); NCF from HNCO* (540.16 eV); NH_2CN from C*H_2CN (292.98 eV); CH_2N_2 from CH_2NC^* (292.37 eV) and CH_2C^*N292.44 eV); HNCO from C*H_2CO (291.13 eV) and NH_2C^*N (405.40 eV); CH_2CO from B*H_2CO (195.10 eV); HN_3 from NH_2C^*N (293.46 eV); and CH_3CN from CH_2C^*CH (291.0 eV) and CH_3CC^*H (290.4 eV). Asterisks indicate the core-ionized atom.

72BEA/HOL Beauchamp, J. L., Holtz, D., Woodgate, S. D., Patt, S. L., J. Am. Chem. Soc. **94**, 2798 (1972). ICR. Bracketing:

86BER/CUR Berkowitz, J., Curtiss, L. A., Gibson, S. T., Green, J. P., Hillhouse, G. L., Pople, J. A., J. Chem. Phys. **84**, 375 (1986). The tabulated PA values are derived only from experimental set of bond energies and ionization potentials. PA values derived from the corresponding theoretical set agree to within 8–12 kJ mol^{-1}.

91BER/DEC Berthelot, M., Decouzon, M., Gal, J.-F., Laurence, C., Le Questel, J.-Y., Maria, P.-C., Tortajada, J., J. Org. Chem. **56**, 4490 (1991). FT-ICR. The authors conclude that the substituted pyridines nornicotine and nicotine protonate on the pyrrolidine N atom, while the others are protonated on the pyridine N atom.

93BER/HEL Berthelot, M., Helbert, M., Laurence, C., Le Questel, J.-Y., Anvia, F., Taft, R. W., J. Chem Soc. Perkin Trans. **2**, 625 (1993). ICR. Temperature not indicated but assumed to be ~338 K.

87BIS/RUH Bisling, P. G. F., Ruhl, E., Brutschy, B., Baumgartel, H., J. Phys. Chem. **91**, 4310 (1987).

74BLI/MCM Blint, R. J., McMahon, T. B., and Beauchamp, J. L., J. Am. Chem. Soc. **96**, 1269 (1974). ICR. Bracketing: $C_2H_2 > CH_3F > CH_2F_2 = CHF_3 > CO > HCl > CH_4 > CF_4 > N_2$.

95BOG/NES Bogan, D. J., Nesbitt, F. L., Stief, L. J., Durant, J. L., Kuo, S. C., Zhang, Z., Klemm, R. B., "Photoionization and thermochemical study of radicals and ions derived from ethanol: Theory and experiment," presented at the 13th International Symposium on Gas Kinetics, Univ. College, Dublin, Ireland, Sept. 11–16, 1995. Discharge flow photoionization mass spectrometer.

94BOH/DEC Bohm, S., Decouzon, M., Exner, O., Gal, J.-F., Maria, P.-C., J. Org. Chem. **59**, 8127 (1994). FT-ICR.

73BOH/HEM Bohme, D. K., Hemsworth, R. S., Rundle, H. W., and Schiff, H. I., J. Chem. Phys. **58**, 3504 (1973). Flowing afterglow. Equilibrium constant determinations through measurements of forward and reverse rate constants.

80BOH/MAC Bohme, D. K., Mackay, G. I., Schiff, H. I., J. Chem. Phys. **73**, 4976 (1980). Flowing afterglow. Values first reported in 75SCH/BOH.

81BOH/MAC Bohme, D. K., Mackay, G. I., J. Am. Chem. Soc. **103**, 2173 (1981). Flowing afterglow.

81BOH/STO Bohme, D. K., Stone, J. A., Mason, R. S., Stradling, R. S., Jennings, K. R., Int. J. Mass Spectrom. Ion Phys. **37**, 283 (1981). HPMS. Entropy change determinations made.

86BOJ Bojesen, G., J. Chem. Soc., Chem. Commun. 244 (1986). MIKE analysis of proton bound dimer ions formed from the titled amino acids gave the following order of PA's Arg>His>Lys>Trp.

87BOJ Bojesen, G., J. Am. Chem. Soc. **109**, 5557 (1987). Proton-bound dimers composed of different amino acids were formed by FAB and their decomposition components analyzed by MIKE. Procedure gives only the relative order of PA's as follows: Gly<Ala<Cys<Ser<Val<Asp <Leu<Thr<Ile<Phe<Met<Tyr<Asn<Pro<Glu<Trp <Gln≈Lys<His<Arg.

84BOL/HOU Bollinger, J.-C., Houriet, R., Yvernault, T., Phosphorus Sulfur **19**, 379 (1984). ICR. Arguments are given supporting O atom protonation.

85BOL/HOU Bollinger, J.-C., Houriet, R., Kern, C. W., Perret, D., Weber, J., Yvernault, Y., J. Am. Chem. Soc. **107**, 5352 (1985). ICR.

84BOL/YVE Bollinger, J.-C., Yvernault G., Yvernault, T., Can. J. Chem. **62**, 361 (1984). ICR bracketing.

90BOR/HOU Borgarello, M., Houriet, R., Raczynska E. D., Drapala, T., J. Org. Chem. **55**, 38 (1990). FT-ICR.

89BOT Botschwina, P., J. Chem. Phys. **90**, 4301 (1989). *Ab initio* calculations using Meyer's coupled electron pair approximation (CEPA).

85BOT/ROS Botschwina P., Rosmus, P., J. Chem. Phys. **82**, 1420 (1985). Calculations employing Meyer's coupled electron pair approximation (CEPA).

90BOT/SCH Botschwina, P., Schramm, H., Sebald, P., Chem. Phys. Lett. **169**, 121 (1990).

85BOT/SEB Botschwina P., Sebald, P., J. Mol. Spectrosc. **110**, 1 (1985). *Ab initio* theory.

86BOU/DJA Bouchoux, G., Djazi, F., Hoppilliard, Y., Houriet, R., Rolli, E., Org. Mass Spectrom. **21**, 209 (1986). ICR.

88BOU/DJA Bouchoux, G., Djazi, F., Houriet R., Rolli, E., J. Org. Chem. **53**, 3498 (1988). ICR.

86BOU/HAN Bouchoux, G., Hanna, I., Houriet, R., Rolli, E., Can. J. Chem. **64**, 1345 (1986). ICR.

84BOU/HOP Bouchoux, G., Hoppilliard, Y., Jaudon, P., Houriet, R., Org. Mass Spectrom. **19**, 394 (1984). ICR. Protonation is at carbonyl site.

87BOU/HOP Bouchoux, G., Hoppilliard, Y., Houriet, R., New J. Chem. **11**, 225 (1987). ICR.

84BOU/HOU Bouchoux G., Houriet, R., Tetrahedron Lett. **25**, 5755 (1984). ICR.

93BOU/JEZ Bouchoux, G., Jezequel S., Penaud-Berruyer, F., Org. Mass Spectrom. **28**, 421 (1993). ICR bracketing.

95BOU/SAL Bouchoux, G., Salpin, J.-Y., Leblanc, D., Alcaraz, C., Dtuit O., Palm, H., Rapid Commun. Mass Spectrom. **9**, 1195 (1995). FT-ICR bracketing.

96BOU/SAL Bouchoux G., Salpin, J. Y., J. Am. Chem. Soc. **118**, 6516 (1996). Result is tabulated as a bracketing measurement, although the method of determination employs a "thermokinetic" approach that uses an observed correlation between the rate constant for proton transfer and the corresponding ΔG^0 value for reaction.

96BOU/SAL2 Bouchoux G., Salpin, J.-Y., J. Phys. Chem. **100**, 16555 (1996). FT-ICR. Results are tabulated as a bracketing measurement, although the method of determination employs a "thermokinetic" approach that uses an observed correlation between the rate constant for proton transfer and the corresponding ΔG^0 value for reaction. One of the bracketing partners for CH_3CHCHO was a unidentifiable "benzylacetone."

71BOW/AUE Bowers, M. T., Aue, D. H., Webb, H. M., McIver, R. T., J. Am. Chem. Soc. **93**, 4314 (1971). ICR. Data relative to $(CH_3)_3N$ and expanded by the factor of 350/298.

72BRI/YAM Briggs, J.-P., Yamdagni, R., Kebarle, P., J. Am. Chem. Soc. **95**, 5128 (1972). HPMS.

81BRO/ABB Bromilow, J., Abboud, J. L. M., Lebrilla, C. B., Taft, R. W., Scorrano, G., Lucchini, V., J. Am. Chem. Soc. **103**, 5448 (1981). ICR. Values of ΔG^0 for 41 proton transfer reactions. Compounds studied did not include ammonia or isobutene, but did include acetone. Acetone was used by the present authors to tie the thermochemical ladder to other results from the laboratory (see comments under TAFT).

89BRO/COO Brodbelt-Lustig, J. S., Cooks, R. G., Talanta **36**, 255 (1989).

92BRU/GRE Bruna, P. J., Grein, F. J. Phys. Chem. **96**, 6617 (1992). *Ab initio* calculations indicate that $HSiS^-$ is linear while $SiSH^-$ is bent. Compare with calculations of 89FOX/WLO.

91 BUK/GRU Buker, H.-H., Grutzmacher, H.-F., Int. J. Mass Spectrom. Ion Processes **109**, 95 (1991). FT-ICR study. Authors state that proton-transfer equilibria was observed between NH_3 and 3,5-di-t-butyl toluene and between N-methylformamide and 1,3,5-tri-t-butyl-benzene. Resultant GB values of the aromatic compounds were given but not ΔG^0 values for the reactions.

93BUR/GAS Burlet O., Gaskell, S. J., J. Am. Soc. Mass Spectrom. **4**, 461 (1993). CID study using the kinetic. GB(pyridylethylcysteine) was found to be considerably greater than GB(cysteine), and GB(dimethylpyrimidylornithine) was slightly less than GB(arginine).

82BUR/HAY Burdett, N. A., Hathurst, A. N., J. Chem. Soc., Faraday Trans. 1 **78**, 2997 (1982). Hydration enthalpies and entropies, respectively, for the reaction $M^+ + H_2O \rightleftarrows MOH_2^+$ and referred to 298 K were measured as follows: M=Na, -101 kJ mol^{-1} and -90.0 J (mol K)$^{-1}$; M=K, -71 kJ mol^{-1} and -86 J (mol K)$^{-1}$. Using $\Delta_f H^0(H_2O) = -241.8$ kJ mol^{-1}, $\Delta_f H^0(H^+) = 1530$ kJ mol^{-1}, $S^0(H_2O) = 188.7$ J (mol K)$^{-1}$, $\Delta_f H^0(NaOH) = -197.8$ kJ mol^{-1}, $\Delta_f H^0(Na^+) = 602.9$ kJ mol^{-1}, $S^0(Na^+) = 147.9$ J (mol K)$^{-1}$ and $S^0(NaOH) = 228.4$, yields $PA(NaOH) = 1072.1$ kJ mol^{-1} and $\Delta S_p(NaOH) = 18.2$ J (mol K)$^{-1}$. Using $\Delta_f H^0(KOH) = -234.3$ kJ mol^{-1}, $\Delta_f H^0(K^+) = 507.9$ kJ mol^{-1}, $S^0(K^+) = 154.6$ J (mol K)$^{-1}$ and $S^0(KOH) = 236.3$, yields $PA(KOH) = 1100.6$ kJ mol^{-1} and $\Delta S_p(KOH) - 21$ J (mol K)$^{-1}$.

83BUR/HOL Burgers, P. C., Holmes, J. L., Mommers, A. A., Szulejko, J. E., Org. Mass Spectrom. **18**, 596 (1983). Appearance energy measurements gave $\Delta_f H^0$(2-propenyl cation) $= (969 \pm 5)$ kJ mol^{-1}. This value combined with $\Delta_f H^0(CH_3CCH) = 187$ kJ mol^{-1} yields $PA(CH_3CCH) = (748 \pm 5)$ kJ mol^{-1}.

84BUT/KUD Butman, M. F., Kudin, L. S., Krasnov, K. S., Zh. Neorg. Khim. **29**, 2150 (1984); English translation, Russ. J. Inorg. Chem. **29**, 1228 (1984). Determinations of enthalpies of reactions of the type: $M_2OH^+ \rightleftarrows M^+ + MOH$(solid). Using $\Delta_f H^0(Li_2O,gas) = -167.4$ kJ mol^{-1}, $\Delta_f H^0(Li^+) = 679.6$ kJ mol^{-1} and $\Delta_f H^0$(LiOH, solid) $= -485$ kJ mol^{-1} gives $PA(Li_2O) = 1206$ kJ mol^{-1}. Using $\Delta_f H^0(Na_2O,gas) = -25.1$ kJ mol^{-1}, $\Delta_f H^0(Na^+) = 602.9$ kJ mol^{-1} and $\Delta_f H^0$(NaOH, solid) $= -425.9$ kJ mol^{-1} gives $PA(Na_2O) = 1375.9$ kJ mol^{-1}. Using $\Delta_f H^0(K_2O,gas) = -142.3$ kJ mol^{-1}, $\Delta_f H^0(K^+) = 507.9$ kJ mol^{-1} and $\Delta_f H^0$(KOH, solid) $= -424.7$ kJ mol-1 gives $PA(K_2O) = 1342.5$ kJ mol^{-1}. Using $\Delta_f H^0(Cs_2O,gas) = -92$ kJ mol^{-1}, $\Delta_f H^0(Cs^+) = 451.8$ kJ mol^{-1} and $\Delta_f H^0$(CsOH, solid) $= -416.7$ kJ mol^{-1} gives $PA(Cs_2O) = 1442.9$ kJ mol^{-1}.

89CAC/ATT Cacace, F., Attina, M., de Petris, G., Speranza, M., J. Am. Chem. Soc. **111**, 5481 (1989). Data from this reference are tabulated under 90CAC/ATT.

90CAC/ATT Cacace, F., Attina, M., de Petris, G., Speranza, M., J. Am. Chem. Soc. **112**, 1014 (1990). ICR. A more complete and detailed account of results first reported in 89CAC/ATT. $PA(H_2O) < PA(HNO_3) < PA(CF_3CH_2OH)$. Also found that $H_2NO_3^-$ dissociates to NO_2^- and H_2O under all conditions regardless of the protonating agent. Evidence of two isomeric structures, i.e., $(HO)_2NO^+$ and $H_2O{\cdot}NO_2^+$ with the latter structure being more stable.

90CAC/ATT2 Cacace, F., Attina, M., De Petris, G., Grandinetti, F., Speranza, M., Gazz. Chim. Ital. **120**, 691(1990). ICR proton-transfer equilibria. Temperature not explicitly stated but is said to be 298 K in a subsequent re-evaluation (93CAC/ATT). *Ab initio* calculations yield $PA(HN_3) = (731.7 \pm 16)$ kJ mol^{-1} at 0 K and (737 ± 16) kJ mol^{-1} at 298 K.

93CAC/ATT Cacace, F., Attina, M., Speranza, M., de Petris, G., Grandinetti, F., J. Org. Chem. **58**, 3639 (1993). ICR bracketing and MIKE measurements. *Ab initio* calculations yield $PA(HN_3) = (744.3 \pm 8)$ kJ mol^{-1} at 0 K and (750.6 ± 8) kJ mol^{-1} at 298 K.

94CAC/ATT Cacace, F., Attina, M. de Petris, G., Speranza, M., J. Am. Chem. Soc. **116**, 6413 (1994). FT-ICR study of the equilibrium $(HNO_3)H^+ + CH_3OH \rightleftarrows (CH_3ONO_2)H^+ + H_2O$ exploits the fact that protonated HNO_3 and CH_3ONO_2 are both structurally loosely bound complexes of H_2O and CH_3OH to NO_2^+ (see 92LEE/RIC, 92LEE/RIC2 and 90CAC/ATT) which readily transfer NO_2^+ between bases.

93CAC/DEP Cacace, F., de Petris, G., Grandinetti F., Occhiucci, G., J. Phys. Chem. **97**, 4239 (1993). ICR. The paper states that $GB(H_2N-CN)$ was determined by equilibrium proton transfer using $i\text{-}C_3H_7CN$ and o-xylene as reference bases but no data are given. A figure showing the time dependence of ion intensities associated with the equilibrium $NH_2\text{-}CNH^+ + i\text{-}C_3H_7CN \rightleftarrows NH_2\text{-}CN + i\text{-}C_3H_7CNH^+$ would suggest that $GB(NH_2\text{–}CN) = GB(i\text{-}C_3H_7CN) + 2$ kJ mol^{-1}. This is the value tabulated here. *Ab initio* calculations suggest that the most stable protonated form has the proton on the N of CN in a linear arrangement, while protonation at the amino N and at C are less stable by 94 kJ mol^{-1} (22.4 kcal mol^{-1}) and 226 kJ mol^{-1} (54 kcal mol^{-1}), respectively.

94CAC/SPE Cacace F., Speranza, M., Science **265**, 208 (1994). FT-ICR bracketing.

96CAR/CAS Carr S. R., Cassady, C. J., J. Am. Soc. Mass Spectrom. **7**, 1203 (1996). FT-ICR bracketing.

94CAR/SCH de M. Carneiro, J. W., von R. Schleyer, P., Saunders, M., Remington, R., Schaefer III, H. F., Rauk, A., Sorenson, T. S., J. Am. Chem. Soc. **116**, 3483 (1994). *Ab initio* study found the C–C protonated structure as global minimum.

83CAS/FRE Cassady, C. J., Freiser, B. S., Russell, D. H., Org. Mass Spectrom. **18**, 378 (1983).

84CAS/FRE Cassady, C. J., Freiser, B. S., J. Am. Chem. Soc. **106**, 6176 (1984). ICR. Bracketing: GB(Pyridine)<GB(FeO)<GB(1-Propylamine).

83CAS/KIM Caserio, M. C., Kim, J. K., J. Am. Chem. Soc. **105**, 6896 (1983). ICR. Equilibrium. Thioketene determined relative to ketene.

88CAT/CLA Catalan, J., Claramunt, R. M., Elguero, J., Laynez, J., Menendez, M., Anvia, F., Quian, J. H., Taagepera M., Taft, R. W., J. Am. Chem. Soc. **110**, 4105 (1988). ICR. Temperature assumed to be 300 K.

83CAT/ELG Catalan, J., Elguero, J., Flammang, R., Maquestiau, A., Angew. Chem. (Engl. Ed.) **22**, 323 (1983). Relative proton affinities of imidazole and benzimidazole (benzimidazole>imidazole) estimated by kinetic method, observation of the relative importances of modes of dissociation of proton-bound dimers (see 81MCL/CAM).

84CAT/PAZ Catalan, J., de Paz, J. L. G., Yanez, M., Elguero, J., J. Am. Chem. Soc. **106**, 6552 (1984). ICR. Data cited are from: J.-F. Gal and R. W. Taft (personal communication).

88CAU/CER Cauletti, C., Cerichelli, G., Grandinetti, F., Luchetti, L., Speranza, M., J. Phys. Chem. **92**, 2751 (1988). FT-ICR measurements. Some GB values obtained by the bracketing technique, others by observing proton transfer equilibrium. The reference bases used are indicated but not with which compounds. Since the GB values of the reference bases used are, on average, 7 kJ mol^{-1} greater in this current evaluation, the reported results in this paper are increased by 7 kJ mol^{-1}. Temperature not indicated but probably ~333 K, as per other papers from this group.

79CEY/TIE Ceyer, S. T., Tiedemann, P. W., Mahan, B. H., Lee, Y. T., J. Chem. Phys. **70**, 14 (1979). Absolute determination of the proton affinity of NH_3 from appearance potential of NH_4^+ from $(NH_3)_2$.

95CHE/KAS Chen, G., Kasthurikrishnan, N., Cooks, R. G., Int J. Mass Spectrom. Ion Processes **151**, 69 (1995). Result is tabulated here as a bracketing measurement; the method of determination is the kinetic method.

73CHE/LAM Cheng T. M. H., Lampe, F. W., Chem. Phys. Lett. **19**, 532 (1973). Bracketing: C_2H_2, C_2H_5<SiH_4<C_3H_8.

95CHE/STO Chen, Q.-F, Stone, J. A., J. Phys. Chem. **99**, 1442 (1995). HPMS from about 450 to 600 K.

93CHE/WU Cheng, X., Wu, Z., Fenselau, C., J. Am. Chem. Soc. **115**, 4844 (1993). MIKE and CID study of proton-bound dimers. Derived PA values are based on the 1984 scale but have been adjusted to this new scale.

72CHO/FRA Chong, S.-L., Franklin, J. L., J. Am. Chem. Soc. **94**, 6347 (1972). HPMS; equilibria relative to CH_3OH.

72CHO/FRA2 Chong, S.-L., Franklin, J. L., J. Chem. Soc. **94**, 6630 (1972). HPMS; equilibria relative to $(CH_3)_2O$.

95CHO/SMI Chou, P. K., Smith, R. L., Chyall, L. J., Kenttamaa, H. I., J. Am. Chem. Soc. **117**, 4374 (1995). ICR. Bracketing. Found that electron transfer occurred in competion with proton transfer with bases having ionization energies less than about 9.4 eV.

71CHU/BER Chupka W. A., Berkowitz, J., J. Chem. Phys. **54**, 4256 (1971). Threshold for photoionization efficiency curve of CH_5^+ in methane.

68CHU/RUS Chupka, W. A., Russell, M. E., J. Chem. Phys. **49**, 5426 (1968).

95CHY/SQU Chyall, L. J., Squires, R. R., Int. J. Mass Spectrom. Ion Processes **149**, 257 (1995). Determined translational energy thresholds for the endothermic proton transfer reactions; $C_5H_5NH^+ + NH_3 \rightarrow NH_4^+ + C_5H_5N$, $\Delta H^0(298\text{ K}) = (78.7 \pm 5.0)$ kJ mol^{-1}[(18.8±1.2) kcal mol^{-1}] and $c\text{-}C_3H_3^+ + NH_3 \rightarrow c\text{-}C_3H_2 + NH_4^+$ $\Delta H^0(298\text{ K}) = (97.5 \pm 8)$ kJ mol^{-1}[(23.3±1.8) kcal mol^{-1}].

97CIP/CRE Cipollini, R., Crestoni, M. E., Fornarini, S., J. Am. Chem. Soc. **119**, 9499 (1997). CID results on the reaction, $F_2H^+ \rightarrow HF^+ + F$, yielded a threshold dissociation energy of (1.6±0.2) eV. Combined with $\Delta H_f^0(HF^+) = 1273.3$ kJ mol^{-1} and $\Delta H_f^0(F) = 79.4$ kJ mol^{-1}, this yields $\Delta H_f^0(F_2H^+) = (1198 \pm 20)$ kJ mol^{-1} and finally $PA(F_2) = (332 \pm 20)$ kJ mol^{-1}.

85CLE/MUN Clemens, D., Munson, B., Anal. Chem. **57**, 2022 (1985). HPMS. Bracketing. GB(Benzonitrile)<GB[$(CH_3)_3SiOH$]<GB(Tetrahydrofuran).

83COL/MCM Collyer, S. M., McMahon, T. B., J. Phys. Chem. **87**, 909 (1983). ICR. Equilibrium reported between PF_3 and CF_3CN contradicts earlier bracketing results (80DOI/MCM and 78COR/BEA).

76COO/KAT Cook, M. J., Katrisky, A. R., Taagepera, M., Singh, T. D., Taft, R. W., J. Am. Chem. Soc. **98**, 6048 (1976). ICR. Data corrected to 350 K.

77COO/KRU Cooks, R. G., Kruger, T. L., J. Am. Chem. Soc. **99**, 1279 (1977). Dissociation of proton bound dimers indicates $C_4H_9NH_2$<$C_5H_{11}NH_2$; $C_6H_5NH_2$<3-$CH_3C_6H_4NH_2$; n-$C_4H_9NH_2$<c-C_5H_5N: Results not included.

76COR/BEA Corderman, R. R., Beauchamp, J. L., Inorg. Chem. **15**, 665 (1976). ICR. Data relative to $(CH_3)_3N$ and $(C_2H_5)_2NH$; $T = 350$ K assumed.

78COR/BEA Corderman, R. R., Beauchamp, J. L., Inorg. Chem. **17**, 1585 (1978). ICR. Equilibrium between PF_3 and CH_3Cl observed, but K could not be measured. Values marked with (*) are cited in this paper as "Koppel and Taft, unpublished data".

72COT/ROZ Cotter, R. J., Rozett, R. W., Koski, W. S., J. Chem. Phys. **57**, 4100 (1972). Measured onset of reaction: $(H_2O^- + H_2 \rightarrow H_3^- + OH)$ as (1.82±0.05) eV. Using $\Delta H_f^0(H_2O) = -241.8$ kJ mol^{-1}, $\Delta H_f^0(OH) = 38.9$ kJ mol^{-1} and $IP(H_2O) = 12.62$ eV, yields $PA(H_2) = (417.6 \pm 4.8)$ kJ mol^{-1}.

87CRE/FAR Creasy, W. R., Farrar, J. M., J. Chem. Phys. **87**, 5280 (1987). Determined the following dissociation energies: $DE(Li^+(HCl)\rightarrow Li^+ + HCl) = (0.83\pm0.04)$ eV, $DE(Li^+(HBr)\rightarrow Li^+ + HBr) = (0.88\pm0.04)$ eV, from which $\Delta_f H^0[Li^+(HCl)] = 506$ kJ mol^{-1}(121 kcal mol^{-1}) and $\Delta_f H^0[Li^+(HBr)] = 556$ kJ mol^{-1}(133 kcal mol^{-1}) are inferred. These lead to $PA(LiCl) = (827\pm54)$ kJ mol^{-1} and $PA(LiBr) = (819\pm54)$ kJ mol^{-1}. All other $\Delta_f H$ values are taken from 88LIA/BAR.

95CRE/FOR Crestoni, M. E., Fornarini S., Kuck, D., J. Phys. Chem. **99**, 3150 (1995). FT-ICR.

91CUR/BRA Curtiss, L. A., Brand, H., Nicholas, J. B., Iton, L. E., Chem. Phys. Lett. **184**, 215 (1991). PA values at 0 K calculated using GAUSSIAN-1 package.

92CUR/NOB Curtiss, L. A., Nobes, R. H., Pople J. A., Radom, L., J. Chem. Phys. **97**, 6766 (1992). The calculations indicate that protonation of CS is favored on the C end yielding a linear ion. Protonation at the S end yields a bridged structure and is 317 kJ mol^{-1} (75.8 kcal mol^{-1}) less stable.

76DAV/KEB Davidson, W. R., Kebarle, P., J. Am. Chem. Soc. **98**, 6133 (1976). HPMS measurements yielded $\Delta H^0 = -70.7$ kJ mol^{-1} (-16.9 kcal mol^{-1}) and $\Delta S^0 = -83.3$ J (mol K)$^{-1}$ for the reaction $K^+ + H_2O \rightleftarrows KOH_2^+$. Using $\Delta_f H^0(KOH) = -234.3$ kJ mol^{-1}, $\Delta_f H^0(K^+) = 507.9$ kJ mol^{-1}, $S^0(K^+) = 154.6$ J (mol K)$^{-1}$ and $S^0(KOH) = 236.3$, yields $PA(KOH) = 1100.3$ kJ mol^{-1} and $\Delta S_p(KOH) = 23.7$ J (mol K)$^{-1}$.

78DAV/LAU Davidson, W. R., Lau, Y. K., Kebarle, P., Can. J. Chem. **56**, 1016 (1978). HPMS.

87DEA/MAU Deakyne, C. A., Meot-Ner(Mautner), M., Buckley, T. J., Metz, R., J. Chem. Phys. **86**, 2334 (1987). HPMS and ICR spectrometer.

93DEC/ERT Decouzon, M., Ertl, P., Exner, O., Gal, J.-F., Maria, P.-C., J. Am. Chem. Soc. **115**, 12071 (1993). FT-ICR.

92DEC/EXN Decouzon, M., Exner, O., Gal, J.-F., Maria, P.-C., J. Org. Chem. **57**, 1621 (1992). FT-ICR. Authors suggest that protonation occurs on the carbonyl O atom.

94DEC/EXN Decouzon, M., Exner, O., Gal, J.-F., Maria, P.-C., J. Phys. Org. Chem. **7**, 511 (1994). FT-ICR.

94DEC/EXN2 Decouzon, M., Exner, O., Gal, J.-F., Maria, P.-C., J. Phys. Org. Chem. **7**, 615 (1994). FT-ICR proton transfer equilibrium.

96DEC/EXN Decouzon, M., Exner, O., Gal, J.-F., Maria, P.-C., J. Chem. Soc., Perkin Trans. **2**, 475 (1996). FT-ICR.

91DEC/GAL Decouzon, M., Gal, J.-F., Maria, P.-C., J. Org. Chem. **56**, 3669 (1991). FT-ICR.

93DEC/GAL Decouzon, M., Gal, J.-F., Maria P.-C., Raczynska, E. D., Rapid Commun. Mass Spectrom. **7**, 599 (1993). ICR measurements. GB's reported but no indication of the reference bases were given.

82DEF/HEH DeFrees, D. J., Hehre, W. J., McIver, Jr., R. T., McDaniel, D. H, J. Phys. Chem. **83**, 232 (1979). ICR. Bracketing: $NH_2 \sim CH_3SH$.

77DEF/MCI DeFrees, D. J., McIver, Jr., R. T., Hehre, W. J., J. Am. Chem. Soc. **99**, 3853 (1977). ICR. Bracketing. D^+ transfer from $C_6H_5OHD^+$ observed with propylene, not with HCN.

80DEF/MCI DeFrees. D. J., McIver. Jr.. R. T.. Hehre. W. J.. J. Am. Chem. Soc. **102**, 3334 (1980). ICR. Bracketing.

85DEF/MCL DeFrees D. J., McLean, A. D., J. Chem. Phys. **82**, 333 (1985).

93DEL Del Bene, J. E., J. Phys. Chem. **97**, 107 (1993). *Ab initio* calculation.

95DEN/ETI Denekamp, C., Etinger, A., Fokkens, R. H., Khaselev, N., Mandelbaum A., Nibbering, N. M. M., J. Mass Spectrom. **30**, 1174 (1995). Kinetic method estimate of GB differences isomers using isotopic labelling.

94DEP/OCC de Petris, G., Occhiucci, G., Pepi, F., Int. J. Mass Spectrom. Ion Processes **136**, 155 (1994). FT-ICR bracketing.

76DES/POR DeStefano, A. J., Porter, R. F., J. Phys. Chem. **80**, 2818 (1976). Photoionization mass spectrometer. Bracketing: $HCOOC_2H_5 < H_2B_3N_3H_3 < H_3B_3N_3H_3$.

76DEV/WOL Devlin, III, J. L., Wolf, J. F., Taft, R. W., Hehre, W. J., J. Am. Chem. Soc. **98**, 1990 (1976). ICR. Results related to TAFT scale. Temperature assumed to be 320 K.

77DIT/NIB Dits, H., Nibbering, N. M. M., Verhoeven, J. W., Chem. Phys. Lett. **51**, 95 (1977). ICR. Bracketing. Details not given. For this compilation, tabulated values are based on data given in ICR column of Table I, and compiled as GB data instead of PA data.

80DIX Dixon, D. A., Inorg. Chem. **19**, 593 (1980). ICR bracketing.

88DIX/GOL Dixon, D. A., Gole, J. L., Komornicki, A., J. Phys. Chem. **92**, 2134 (1988). PA's calculated from *ab initio* molecular orbital theory.

84DIX/KOM Dixon, D. A., Komornicki, A., Kraemer, W. P., J. Chem. Phys. **81**, 3603 (1984). PA's of CO at O, CO at C, H_2CO calculated at the CI-SDQ level of theory and $PA(H_2)$ at the CI-SD level.

79DOI/GRE Doiron, C. E., Grein, F., McMahon, T. B., Vasudevan, K., Can. J. Chem. **57**, 1751 (1979). ICR. Borazine vs $HCOOC_2H_5$, c-$C_4H_8O_2$.

80DOI/MCM Doiron, C. E., McMahon, T. B., Inorg. Chem. **19**, 3037 (1980). ICR. Bracketing.

81DOI/MCM Doiron, C. E., McMahon, T. B., Can. J. Chem. **59**, 2689 (1981). ICR. Data relative to ethylene and $CH_2(CN)_2$.

92DOT/IRA Dotan, I., Iraqi, M., Petrank, A., Lifshitz, C., Rapid Commun. Mass Spectrom. **6**, 579 (1992). SIFT. ΔG^0 values are determined for proton transfer reactions in two ways. First, the traditional way, forward and reverse rate constants are separately measured to obtain K_{eq}. Second, the rate constant in the endothermic direction is combined with the branching ratio for proton transfer and the calculated forward and reverse collision rates to derive K_{eq}. The results for both methods compare well. The tabulated values are those derived from equilibrium measurements.

93DOT/IRA Dotan, I., Iraqi, M., Lifshitz, C., Int. J. Mass Spectrom. Ion Processes. **124**, R21 (1993). ICR. ΔG^0 values obtained from the second method of 92DOT/IRA.

81DRU/MCM Drummond, D. F., McMahon, T. B., J. Phys. Chem. **85**, 3746 (1981). ICR.

80DYK/JON Dyke, J. M., Jonathan, N., Morris, A., Winter, M. J., Mol. Phys. **39**, 629 (1980).

81DYK/JON Dyke, J. M., Jonathan, N. B. H., Morris, A., Winter, M. J., Mol. Phys. **44**, 1059 (1981). Photoelectron spectroscopy. First adiabatic IP of $HO_2 = (11.35\pm0.01)$ eV.

70DZI/KEB Dzidic, I., Kebarle, P., J. Phys. Chem. **74**, 1466 (1970). Hydration enthalpies and entropies, respectively, for the reaction $M^+ + H_2O \rightleftarrows MOH_2^+$ were measured as follows: M=Li, -142.2 kJ mol^{-1} and -96.2 J (mol K)$^{-1}$; M=Na, -100.4 kJ mol^{-1} and -90.0 J (mol K)$^{-1}$; M=K, -74.9 kJ mol^{-1} and -90.4 J (mol K)$^{-1}$; M=Rb, -66.5 kJ mol^{-1} and -88.7 J (mol K)$^{-1}$; M=Cs, -57.3 kJ mol^{-1} and -81.2 J (mol K)$^{-1}$. Using $\Delta_f H^0(H_2O) = -241.8$ kJ mol^{-1}, $\Delta_f H^0(H^+) = 1530$ kJ mol^{-1}, $S^0(H_2O) = 188.7$ J (mol K)$^{-1}$, $\Delta_f H^0(LiOH) = -234.3$ kJ mol^{-1}, $\Delta_f H^0(Li^+) = 679.6$ kJ mol^{-1}, $S^0(Li^+) = 133.0$ J (mol K)$^{-1}$ and $S^0(LiOH) = 210.6$, yields $PA(LiOH) = 1000.1$ kJ mol^{-1} and $\Delta S_p(LiOH) = 14.9$ J (mol K)$^{-1}$. Using $\Delta_f H^0(NaOH) = -197.8$ kJ mol^{-1}, $\Delta_f H^0(Na^+) = 602.9$ kJ mol^{-1}, $S^0(Na^+) = 147.9$ J (mol K)$^{-1}$ and $S^0(NaOH) = 228.4$, yields $PA(NaOH) = 1071.5$ kJ mol^{-1} and $\Delta S_p(NaOH)$

=18.2 J (mol K)$^{-1}$. Using $\Delta_f H^0$(KOH)=−234.3 kJ mol^{-1}, $\Delta_f H^0(K^+)$=507.9 kJ mol^{-1}, $S^0(K^+)$=154.6 J (mol K)$^{-1}$ and S^0(KOH)=236.3, yields PA(KOH) =1104.5 kJ mol^{-1} and ΔS_p(KOH)=16.6 J (mol K)$^{-1}$. Using $\Delta_f H^0$(CsOH)=−259.4 kJ mol^{-1}, $\Delta_f H^0(Cs^+)$ =451.8 kJ mol^{-1}, $S^0(Cs^+)$=169.8 J (mol K)$^{-1}$ and S^0(CsOH)=254.7, yields PA(CsOH)=1117.9 kJ mol^{-1} and ΔS_p(CsOH)=22.6 J (mol K)$^{-1}$.

97EAS/SMI East, A. L. L., Smith, B. J., Radom, L., J. Am. Chem. Soc. **119**, 9014 (1997).

93EKE/HAG Ekeberg, D., Hagen, S. I., Hvistendahl, G., Schulze, C., Uggerud, E., Vedde, J., Org. Mass Spectrom. **28**, 1504 (1993). HPMS. Van't Hoff estimation of ΔH^0 and ΔS^0 over a rather limited temperature range in which clustering may have perturbed equilibrium. *Ab initio* calculations indicate $HFe(CO)_5^+$ is of C_{4v} symmetry with the proton attached to Fe.

84ELK/ARM Elkind, J. L., Armentrout, P. B., J. Phys. Chem. **88**, 5454 (1984). Determined $D^0(SiH^+)$=(3.23±0.04) eV. Using IP(Si)=8.15169 eV gives PA(Si)=(837.2±4) kJ mol^{-1}.

85ELK/ARM Elkind, J. L., Armentrout, P. B., J. Phys. Chem. **89**, 5626 (1985). Heats of formation of metal hydrides from determinations of the onset energies of endothermic rections. Derived $D^0(VH^+)$=(2.05±0.06) eV [(198±6) kJ mol^{-1}]. Using IP(V)=6.743 eV, PA(V)=(859.4±6) kJ mol^{-1}.

86ELK/ARM Elkind, J. L., Armentrout, P. B., Inorg. Chem. **25**, 1078 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions.

86ELK/ARM2 Elkind, J. L., Armentrout, P. B., J. Chem. Phys. **84**, 4862 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0_{298}(MnH^+)$=(2.10±0.15) eV [(206 ±15) kJ mol^{-1}]. Using IP(Mn)=7.434 eV gives PA(Mn)=(797±15) kJ mol^{-1}.

86ELK/ARM3 Elkind, J. L., Armentrout, P. B., J. Phys. Chem. **90**, 5736 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0(FeH^+)$=(2.12±0.06) eV [(204.5 ±6) kJ mol^{-1}]. Using IP(Fe)=7.9024 eV gives PA(Fe)=(754±8) kJ mol^{-1}.

86ELK/ARM4 Elkind, J. L., Armentrout, P. B., J. Phys. Chem. **90**, 6576 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0(CoH^+)$=(1.98±0.06) eV [(191.0 ±9) kJ mol^{-1}], $D^0(NiH^+)$=(1.68±0.08) eV [(162.1 ±8) kJ mol^{-1}] and $D^0(CuH^-)$=(0.92±0.13) eV [(88.8 ±13) kJ mol^{-1}]. Using IP(Co)=7.8810 eV gives PA(Co)=(742.7±6) kJ mol^{-1}. Using IP(Ni)=7.6398 eV gives PA(Ni)=(737±11) kJ mol^{-1}. Using IP(Cu) =7.72638 eV gives PA(Cu)=(655.3±13) kJ mol^{-1}.

87ELK/ARM Elkind, J. L., Armentrout, P. B., J. Chem. Phys. **86**, 1868 (1987). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0(CrH^+)$=(1.37±0.09) eV [(132.2 ±9) kJ mol^{-1}]. Using IP(Cr)=6.76664 eV gives PA(Cr)=(791.3±9) kJ mol^{-1}.

88ELK/ARM Elkind, J. L., Armentrout, P. B., Int. J. Mass Spectrom. Ion Processes **83**, 259 (1988). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0(TiH^+)$=(2.31±0.11) eV [(222.9±11) kJ mol^{-1}]. Using IP(Ti)=6.8282 eV gives PA(Ti)=(876±11) kJ mol^{-1}.

89ELK/SUN Elkind, J. L., Sunderlin L. S., Armentrout, P. B., J. Phys. Chem. **93**, 3151 (1989). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived $D^0(ScH^+)$=(2.44±0.09) eV [(235.4±9) kJ mol^{-1}], $D^0(YH^+)$=(2.66±0.06) eV [(256.6±6) kJ mol^{-1}], $D^0(LaH^+)$=(2.48±0.09) eV [(239.3±9) kJ mol^{-1}], and $D^0(LuH^+)$=(2.11±0.16) eV [(203.6±15) kJ mol^{-1}]. Using the following data, the corresponding PA values are deduced: IP(Sc) =6.56144 eV, PA(Sc)=(914.4±9) kJ mol^{-1}; IP(Y) =6.217 eV, PA(Y)=(967±6) kJ mol−1; IP(La)=5.577 eV, PA(La)=(1013.3±9) kJ mol^{-1}; IP(Lu)=5.42585 eV, PA(Lu)=(992.1±15) kJ mol^{-1}.

81ELL/DIX Ellenberger, M. R., Dixon, D. A., Farneth, W. E., J. Am. Chem. Soc. **103**, 5377 (1981). ICR, bracketing.

79ELL/EAD Ellenberger, M. R., Eades, R. A., Thomsen, M. W., Farneth, W. E., Dixon, D. A., J. Am. Chem. Soc. **101**, 7151 (1979). ICR. Bracketing.

96EWI/ZHA Ewing, N. P., Zhang, X., Cassady, C. J., J. Mass Spectrom. **31**, 1345 (1996). FT-ICR bracketing.

81FAH/FEH Fahey, D. W., Fehsenfeld, F. C., Ferguson, E. E., J. Chem. Phys. **75**, 669 (1981). Flowing afterglow. Observation of: $Si^+ + H_2O \rightarrow SiOH^+ + H$ gives $\Delta_f H$ of $SiOH^+$<778 kJ mol^{-1} (185.9 kcal mol^{-1}) or PA(SiO)>653 kJ mol^{-1} (156 kcal mol^{-1}). $SiOH^+$ transfers a proton to NH_3: PA(SiO)<PA(NH_3). Because these limits are so wide, data not given in the tables.

78FAR/MCM Farid, R., McMahon, T. B., Int. J. Mass Spectrom. Ion Phys. **27**, 163 (1978). ICR. Bracketing.

74FEH/FER Fehsenfeld, F. C., Ferguson, E. E., J. Chem. Phys. **60**, 5132 (1974). Flowing afterglow. Using $\Delta_f H^0$(HCl) =−92.5 kJ mol^{-1} and IP(HCl)=12.75 eV, and assumming the second titled reaction is exothermic, gives PA(HCl)≥519 kJ mol^{-1}.

75FEH/HOW Fehsenfeld, F. C., Howard, C. J., Schmeltekopf, A. L., J. Chem. Phys. **63**, 2835 (1975). Flowing afterglow. Bracketing: H_2O<HNO_3<NH_3. Because limits are so wide, results not included in table of relative gas phase basicities.

75FEH/LIN Fehsenfeld, F. C., Lindinger, W., Albritton, D. L., J. Chem. Phys. **63**, 443 (1975). Flowing afterglow.

76FEH/LIN Fehsenfeld, F. C., Lindinger, W. L., Schiff, H. I., Hemsworth, R. S., Bohme, D. K., J. Chem. Phys. **64**, 4887 (1976). Flowing afterglow. Entropy change determination.

90FEL/KIM von Nagy-Felsobuki, E. I., Kimura, K., J. Phys. Chem. **94**, 8041 (1990). Calculations at the 6-31G**//6-31G** level of theory.

73FEN/HEM Fennelly, P. F., Hemsworth, R. S., Schiff, H. I., Bohme, D. K., J. Chem. Phys. **59**, 6405 (1973). Flowing afterglow.

87FER/JEN Fernandez, M. T., Jennings, K. R., Mason, R. S., J. Chem. Soc., Faraday Trans. **83**, 159 (1987). HPMS. See 92PAR/FER for a reassessment of this paper's data.

94FLA/HAV Flammang, R., Haverbeke, Y. V., Wong, M. W., Ruhmann, A., Wentrup, C., J. Phys. Chem. **98**, 4818 (1994). Calulations at QCISD/6-311+G(2d,p) level of theory and indicate these molecules are C_2 protonated.

84FLA/MAQ Flammang, R., Maquestiau, A., Catalan, J., Perez, P., Elguero, J., Org. Mass Spectrom. **19**, 627 (1984). Relative proton affinities estimated by kinetic method, observation of the relative importances of modes of dissociation of proton-bound dimers (see 81MCL/CAM): PA(Pyrazole) <PA(Indazole)<PA(1-Methylindazole)<PA(Imidazole) <PA(2-Methylindazole)<PA(Benzimidazole).

78FON/HUD Foner, S. N., Hudson, R. L., J. Chem. Phys. **68**, 3169 (1978).

72FOS/BEA Foster, M. S., Beauchamp, J. L., J. Am. Chem. Soc. **94**, 2425 (1972). ICR. Bracketing.

75FOS/BEA Foster, M. S., Beauchamp, J. L., Inorg. Chem. **14**, 1229 (1975). ICR. Equilibrium observed between HF and N_2.

75FOS/BEA2 Foster, M. S., Beauchamp, J. L., J. Am. Chem. Soc. **97**, 4814 (1975). ICR. Bracketing.

75FOS/BEA3 Foster, M. S., Beauchamp, J. L., J. Am. Chem. Soc. **97**, 4808 (1975). ICR. Bracketing.

74FOS/WIL Foster, M. S., Williamson, A. D., Beauchamp, J. L., Int. J. Mass Spectrom. Ion Phys. **15**, 429 (1974). Temperature of 320 K assumed.

89FOX/WLO Fox, A., Wlodek, S., Hopkinson, A. C., Lien, M. H., Sylvain, M., Rodriquez, C., Bohme, D. K., J. Phys. Chem. **93**, 1549 (1989). Selected ion flow tube bracketing study. PA(SiO) bracketed with CH_3CN, allene and H_2S. PA(SiS) bracketed with HCN, H_2S and H_2O. Molecular orbital calculations (MP4/6-31G**//6-31G**) suggest that protonation preferrably occurs on the O and S ends, with $SiOH^+$ being linear and $SiSH^+$ being bent. Compare results of calculations with that of 92BRU/GRE.

78FRE/HAR Freeman, C. G., Harland, P. W., McEwan, M. J., Int. J. Mass Spectrom. Ion Phys. **28**, 19 (1978). Flowing afterglow.

78FRE/HAR2 Freeman, C. G., Harland, P. W., McEwan, M. J., Int. J. Mass Spectrom. Ion Phys. **27**, 77 (1978). Flowing afterglow.

79FRE/HAR Freeman, C. G., Harland, P. W., McEwan, M. J., Int. J. Mass Spectrom. Ion Phys. **30**, 285 (1979). Flowing afterglow. Bracketing.

75FRE/KEB French, M., Kebarle, P., Can. J. Chem. **53**, 2668 (1975). HPMS. Determination of activation energy of $(C_2H_7^+ + CH_4 \rightleftarrows C_2H_5^+ + H_2 + CH_4)$ as 44 kJ mol^{-1} (10.5 kcal mol^{-1}). Taking this as reaction enthalpy, $PA(C_2H_4)=681.7$ kJ mol^{-1}, $\Delta_f H^0(C_2H_4)=52.3$ kJ mol^{-1} and $\Delta_f H^0(C_2H_6)=-84.1$ kJ mol^{-1} yields $PA(C_2H_6)=589.3$ kJ mol^{-1}.

87FRE/KNI Freeman, C. G., Knight, J. S., Love, J. G., McEwan, M. J., Int. J. Mass Spectrom. Ion Processes **80**, 255 (1987). SIFT measurements. ΔG^0 values for HOC^- reacting with O_2 ($\approx$4 kJ mol^{-1}) and Kr ($\approx$0 kJ mol^{-1}) were inferred from a comparison of proton transfer reaction efficiencies. From these values and standard entropies of relevent species, ΔH^0 values were determined and a PA(CO at O)=(427 $\pm$8) kJ mol^{-1} was suggested.

85FRI/SCH Frisch, M. J., Schaefer III, H. F., Binkley, J. S., J. Phys. Chem. **89**, 2192 (1985). Optimizing structures at MP2/6-31G(d) level and computing energies at MP4/6-311+++G(d,p) level, gave $PA(CO_2, 298\ K)=547$ kJ mol^{-1} (130.7 kcal mol^{-1}).

89GAL/SPE Galli, C., Speranza, M., Org. Mass Spectrom. **24**, 139 (1989). Fourier transform ICR. GB's determined from proton transfer equilibria. Only the final measured GB values the arenes are tabulated. The reference bases employed in the GB measurements are listed, along with their GB values from the previous evaluation, but no thermochemical data is reported for the equilibria of any arene with these reference bases. Tabulated GB values for these arenes are adjusted according to the GB values of the reference bases in this present evaluation. Temperature not indicated.

92GAR/RUT van Garderen, H. F., Ruttink, P. J. A., Burgers, P. C., McGibbon, G. A., Terlouw, J. K., Int. J. Mass Spectrom. Ion Processes **121**, 159 (1992). *Ab initio* calculations at SDCI/6-31G**//6-31G** level of theory, including ZPVE corrections.

83GAU/HOU Gaumann, T., Houriet, R., Stahl, D., Tabet, J.-C., Heinrich, N., Schwarz, H., Org. Mass Spectrom. **18**, 215 (1983). ICR. Details not given. Authors conclude that $C_6H_7^+$ formed upon protonation of 1,3-C_6H_8 and 1,4-C_6H_8 has methylcyclopentenyl structure.

91GLO/TWI Glosik, J., Twiddy, N. D., Javahery, G., Ferguson, E. E., Int. J. Mass Spectrom. Ion Processes **109**, 75 (1991). Selected ion flow tube study. Direct measure of equilibrium constant, ΔS^0 calculated from known spectral data for the protonated ions and statistical thermodynamics to obtain ΔH^0 for titled reaction.

94GLU/SZU Glukhovtsev, M. N., Szulejko, J. E., McMahon, T. B., Gauld, J. W., Scott, A. P., Smith, B. J., Pross, A., Radom, L., J. Phys. Chem. **98**, 13099 (1994). HPMS measurements and G2 level calculations.

96GON/MO Gonzalez, A. I., Mo, O., Yanez, M., Leon, E., Tortajada, J., Morizur, J. P., Leito, I., Maria, P.-C., Gal, J. F., J. Phys. Chem. **100**, 10490 (1996). FT-ICR.

93GOR/AMS Gorman, G. S., Amster, I. J., J. Am. Chem. Soc. **115**, 5729 (1993). ICR bracketing using laser desorption techniques to volitilize either the dipeptides themselves or their protonated forms.

76GOR/MUN Goren, A., Munson, B., J. Phys. Chem. **80**, 2848 (1976). Relative values for heats of formation of alkyl ions from hydride transfer equilibrium constant determinations; absolute values assigned relative to $\Delta_f H^0(t\text{-}C_4H_9^+)=711$ kJ mol^{-1}. PA values derived using same data under 75SOL/FIE.

92GOR/SPE Gorman, G. S., Speir, J. P., Turner, C. A., Amster, I. J., J. Am. Chem. Soc. **114**, 3986 (1992). ICR bracketing using laser desorption techniques to volitilize either the amino acids themselves or their protonated forms.

92GRA/HRU Grandinetti, F., Hrusak, J., Schroder, D., Karrass, S., Schwarz, H., J. Am. Chem. Soc. **114**, 2806 (1992). The calculations estimated that the N site has a PA of 551.5 kJ mol^{-1} (131.8 kcal mol^{-1}), while the F site has a PA of 578.2 kJ mol^{-1} (138.2 kcal mol^{-1}).

90GRE/LIG Greco, F., Liguori, A., Sindona, G., and Uccella, N., J. Am. Chem. Soc. **112**, 9092 (1990). Kinetic method. The kinetic data in Tables II and III and Eq. (7) of this reference are used with the currently evaluated PA values for the reference bases to derive the tabulated values for this compilation.

94GRU/CAL Grutzmacher, H.-F., Caltapanides, A., Am Soc. Mass Spectrom. **5**, 826 (1994). Bracketing of PAs using MIKE spectra of proton-bound heterodimers. The observed substituent effects indicate O protonation for the benzamides examined.

85GUE/HOU Guenat, C., Houriet, R., Stahl, D., Winkler, J., Helv. Chim. Acta **68**, 1647 (1985). ICR measurements and CAD of proton-bound dimers containing NH_3.

91GUO/GRA Guo, Y., Grabowski, J. J., J. Am. Chem. Soc. **113**, 5923 (1991). Flowing afterglow bracketing measurement of gas phase acidity of the phenyl radical (1552 or 371 kcal mol^{-1}) by observing/not observing proton transfer from acids to o-benzyne radical anion (o-$C_6H_4^{\cdot-}$). From this value and an $EA(C_6H_4)=12.9$ kcal mol^{-1}, the values $\Delta_f H^0(\text{o-}C_6H_4^{\cdot-})=385$ kJ mol^{-1} (92 kcal mol^{-1}) and $\Delta_f H^0(\text{o-}C_6H_4)=439$ kJ mol^{-1} (105 kcal mol^{-1}) were derived and ultimately a $PA(\text{o-}C_6H_4)=841$ kJ mol^{-1} (201 kcal mol^{-1}). For comparison, see 91RIV/ING where $\Delta_f H^0(\text{o-}C_6H_4)=(440\pm10)$ kJ mol^{-1} is proposed. Refer also to 90KLO.

89GUR/VEY Gurvich, L. V., Veyts, I. V., Adcock, C. B., Editors, "Thermodynamic properties of individual substances," 4th ed., Hemisphere, New York (1989).

76GUY/CHU Guyon, P. M., Chupka, W. A., Berkowitz, J, J. Chem. Phys. **64**, 1419 (1976).

88HAJ/SQU Hajdasz, D., Squires, R., J. Chem. Soc. Chem. Commun. 1212 (1988). Authors suggest that protonation of $(CH_3)_3SiCH{=}CH_2$ occurs on the α-carbon of the vinyl group. Proton transfer equilibrium with n- or π-donor bases was not possible since $(CH_3)_3Si(CH_2CH_2)^+$ reacts by ethylene displacement instead. PA of $(CH_3)_3SiCH{=}CH_2$ estimated by monitoring kinetic energy dependence of proton transfer in a triple quadrupole collision chamber.

84HAL/KLE Halle, L. F., Klein, F. S., Beauchamp, J. L., J. Am. Chem. Soc. **106**, 2543 (1984). Determination of $D^0(Fe^+{-}H)$ $=(247\pm21)$ kJ mol^{-1} [(59 ± 5) kcal mol^{-1}]. Using IP(Fe)=7.9024 eV gives PA(Fe)$=(796\pm21)$ kJ mol^{-1}.

69HAN/FRA Haney, M. A., Franklin, J. L., J. Chem. Phys. **50**, 2028 (1969). Concluded 4.1 eV (386 kJ mol^{-1})$\leq$PA(H_2) $\leq$4.3 eV (414 kJ mol^{-1}).

73HAR/CRO Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., Leventhal, J. J., J. Chem. Phys. **59**, 6181 (1973). Measured onset of $H_3^+ + He \rightarrow H^+ + H_2 + He$.

84HAR/HOU Harrison, A. G., Houriet, R., Tidwell, T. T., J. Org. Chem. **49**, 1302 (1984). ICR. Details not given; gas basicities of compounds relative to ammonia listed. Values adjusted here for consistency with this compilation.

78HAR/LIA Hartman, K. G., Lias, S. G., Int. J. Mass Spectrom. Ion Phys. **28**, 213 (1978). ICR. Entropy change determinations included.

76HAR/LIN Harrison, A. G., Lin, P.-H., Tsang, C. W., Int. J. Mass Spectrom. Ion Phys. **19**, 23 (1976). Trapped ion mass spectrometry.

93HEC/DEK Heck, A. J. R., de Koning, L. J., Nibbering, N. M. M., Org. Mass Spectrom. **28**, 245 (1993). FT-ICR. Bracketing.

74HEH/MCI Hehre, W. J., McIver, Jr., R. T., Pople, J. A., Schleyer, P. v. R., J. Am. Chem. Soc. **96**, 7162 (1974). ICR. Data related to TAFT scale; temperature assumed to be 350 K.

86HEI/HON Heilbronner, E., Honegger, E., Lecoultre, J., Grob, C. A., Houriet, R., Rolli, E., Helv. Chim. Acta **69**, 2114 (1986). ICR.

73HEM/RUN Hemsworth, R. S., Rundle, H. W., Bohme, D. K., Schiff, H. I., Dunkin, D. B., Fehsenfeld, F. C., J. Chem. Phys. **59**, 61 (1973). ΔH° and ΔS° measurements for CO_2–CH_4 and N_2O–CO systems. Flowing afterglow. (196–553 K).

83HEN/FRE Hendewerk, M. L., Frey, R., Dixon, D. A., J. Phys. Chem. **87**, 2026 (1983). ICR. Bracketing: $(CH_3)_3N$ $<(CH_3)_3SiN(CH_3)_2$–$(C_2H_5)_2NH<$(iso-C_3H_7)$(CH_3)N$.

72HEN/TAA Henderson, W. G., Taagepera, M., Holtz, D., McIver, Jr., R. T., Beauchamp, J. L., Taft, R. W., J. Am. Chem. Soc. **94**, 4728 (1972). ICR. Temperature assumed to be 350 K.

82HEN/WEI Hendewerk, M. L., Weil, D. A., Stone, T. L., Ellenberger, M. R., Fameth, W. E., Dixon, D. A., J. Am. Chem. Soc. **104**, 1794 (1982). ICR. Bracketing.

95HER/ABB Hernandez-Laguna, A., Abboud, J.-L., Homan, H., Lopez-Mardomingo, C., Notario, R., Cruz-Rodriguez, Z., Haro-Ruiz, M. D., Botello, V., J. Phys. Chem. **99**, 9087 (1995). FT ICR and *ab initio* calculations. The titled molecule and all reference bases employed undergo proton bound cyclization, so entropy changes and PA values are uncertain.

87HET/COL Hettich, R. L., Cole, T., Freiser, B. S., Int. J. Mass Spectrom. Ion Processes **81**, 203 (1987). PA(CH_3O-B=O) was bracketed between CH_3OH and CH_3CHO. No experimental conditions were reported.

78HIR Hiraoka, K., Int. J. Mass Spectrom. Ion Phys. **27**, 139 (1978). HPMS. Arrhenius plots of k_{Rn} for $H_3O^+ + i\text{-}C_4H_8$ and $H_2S^+ + i\text{-}C_4H_8$. Reaction activation energies are taken as a measure of enthalpy changes for the proton transfers.

75HIR/KEB Hiraoka, K., Kebarle, P., Can. J. Chem. **53**, 970 (1975). HPMS. $\Delta H^0[C_2H_5^+ + CH_4 \rightleftarrows C_3H_9^+] = -27.6$ kJ mol^{-1} and $\Delta S^0[C_2H_5^+ + CH_4 \rightleftarrows C_3H_9^+] = -98$ J (mol K)$^{-1}$. Using PA(C_2H_4)=680.5 kJ mol^{-1}, $\Delta_f H^0(C_3H_8) = -104.6$ kJ mol^{-1}, $\Delta_f H^0(CH_4) = -74.5$ kJ mol^{-1} and $\Delta_f H^0(C_2H_4)$ $=52.3$ kJ mol^{-1} yields PA(C_3H_8)=625.7 kJ mol^{-1}. Using $\Delta S_p(C_2H_4)=11.5$ J (mol K)$^{-1}$, $S^0(C_3H_8)=270.0$ J (mol K)$^{-1}$, $S^0(CH_4)=186.2$ J (mol K)$^{-1}$ and $S^0(C_2H_4)$ $=219.5$ J (mol K)$^{-1}$, yields $\Delta S_p(C_3H_8)=49.2$ J (mol K)$^{-1}$.

76HIR/KEB Hiraoka, K., Kebarle, P., J. Am. Chem. Soc. **98**, 6119 (1976). HPMS. A and B: The enthalpy and entropy of reaction was determined from the equilibrium constant for the process: $C_2H_5^+ + H_2 \rightleftarrows C_2H_7^+$. Different values were obtained at low (-17 kJ mol^{-1}) (-4.0 kcal mol^{-1}) and -82 J (mol K)$^{-1}$ [-19.6 cal (mol K)$^{-1}$]) and at high (-49 kJ mol^{-1}) (-11.8 kcal mol^{-1}) and -104.6 [-25 cal (mol K)$^{-1}$]) temperature regimes. The authors interpret this as evidence for two $C_2H_7^+$ structures, indicated as A (associated with the low temperature measurement and having C–H protonated structure) and B (associated with the high temperature measurement and having a C–C protonated structure) in Table 2. Using $\Delta_f H^0(C_2H_6)$ $=-84.1$ kJ mol^{-1}, $\Delta_f H^0(C_2H_4)=52.3$ kJ mol^{-1} and PA(C_2H_4)=680.5 kJ mol^{-1} gives PA(C_2H_6–B)=593.1 kJ mol^{-1} and PA(C_2H_6–A)=561.4 kJ mol^{-1}. Using $S^0(C_2H_4)=219.5$ J (mol K)$^{-1}$, $\Delta S_p(C_2H_4)=11.4$ J (mol K)$^{-1}$, $S^0(C_2H_6)=229.6$ J (mol K)$^{-1}$ gives $\Delta S_p(C_2H_6)=27.4$ J (mol K)$^{-1}$. Also measured the thermochemistry for the association reaction of $sec\text{-}C_3H_7^+ + CH_4 \rightleftarrows iso\text{-}C_4H_{11}^+$ obtaining $\Delta H^0=$ -14.2 kJ mol^{-1} (-3.4 kcal mol^{-1}) and $\Delta S^0=$ -83.7 J (mol K)$^{-1}$ [-20 cal (mol K)$^{-1}$]. Using PA(C_3H_6)=751.6 kJ mol^{-1}, $\Delta_f H^0(CH_4) = -74.5$kJ mol^{-1}, $\Delta_f H^0(C_3H_6)=20.1$ kJ mol^{-1}, and $\Delta_f H^0(iso\text{-}C_4H_{10})$ $=-134.3$ kJ mol^{-1} yields PA(iso-C_4H_{10}) $=685.9$ kJ mol^{-1}. Using $S^0(CH_4)=186.2$ J (mol K)$^{-1}$, $S^0(C_3H_6)=267.1$ J (mol K)$^{-1}$, $S^0(iso\text{-}C_4H_{10})$ $=294.6$ J (mol K)$^{-1}$, and $\Delta S_p(C_3H_6)=12$ J (mol K)$^{-1}$ yields $\Delta S_p(iso\text{-}C_4H_{10})=87$ J (mol K)$^{-1}$.

77HIR/KEB Hiroaka, K., Kebarle, P., J. Am. Chem. Soc. **99**, 360 (1977). Measured $\Delta H^0=-46.9$ kJ mol^{-1} (-11.2 kcal mol^{-1}) and $\Delta S^0=-92$ J (mol K)$^{-1}$ (-22 cal (mol K)$^{-1}$) for the reaction $t\text{-}C_4H_9^+ + H_2O$ $\rightleftarrows C_4H_9OH_2^+$. Using PA($iso$-$C_4H_8$)$=802.1$ kJ mol^{-1}, $\Delta_f H^0(iso\text{-}C_4H_8) - 16.7$ kJ mol^{-1}, $\Delta_f H^0(H_2O) = -241.8$ kJ mol^{-1}, and $\Delta_f H^0(t\text{-}C_4H_9OH) = -312.5$ kJ mol^{-1}, yields PA(t-C_4H_9OH)$=795$kJ mol^{-1}. Using $S^0(iso\text{-}C_4H_8)=293.7$ J (mol K)$^{-1}$, $S^0(H_2O)=188.7$ J (mol K)$^{-1}$, $S^0(t\text{-}C_4H_9OH)=326.4$ J (mol K)$^{-1}$ and $\Delta S_p(iso\text{-}C_4H_8)=20$, yields $\Delta S_p(t\text{-}C_4H_9OH)=84$ J (mol K)$^{-1}$.

95HIR/NAS Hiraoka, K., Nasu, M., Fujimaki, S., Yamabe, S., J. Phys. Chem. **99**, 15822 (1995). Measured the activation energy for the reaction $(N_2)_2H^+ + NF_3 \rightleftarrows 2N_2 + NF_3H^+$ as 7.5 kJ mol^{-1} (1.8 kcal mol^{-1}). Combining this with PA(N_2)=493.8 kJ mol^{-1} and the dissociation energy for $(N_2)_2H^+ \rightleftarrows N_2H^+ + N_2$ of 67 kJ mol^{-1} yields PA(NF_3)$\geq$553.2 kJ mol^{-1}.

75HOD/BEA Hodges, R. V., Beauchamp, J. L., Inorg. Chem. **14**, 2887 (1975). ICR. Data related to TAFT scale.

85HOD/BEA Hodges, R. V., Beauchamp, J. L., Ashe, III, A. J., Chan, W.-T., Organometall. **4**, 457 (1985). ICR. Deuterium labelling experiments indicate that C_5H_5P is protonated at P and that C_5H_5As is C protonated.

80HOD/HOU Hodges, R. V., Houle, F. A., Beauchamp, J. L., Montag, R. A., Verkade, J. G., J. Am. Chem. Soc. **102**, 932 (1980). ICR.

80HOD/MCD Hodges, R. V., McDonnell, T. J., Beauchamp, J. L., J. Am. Chem. Soc. **102**, 1327 (1980). ICR.

94HOK/YAN Hoke, S. H., Yang, S. S., Cooks, R. G., Hrovat, D. A., Borden, W. T., J. Am. Chem. Soc. **116**, 4888 (1994). Kinetic method. Rate data was analyzed according to values of the current evaluation, but according to gas basicity values instead of proton affinity values.

89HOL/LOS Holmes, J. L., Lossing, F. P., Int. J. Mass Spectrom. Ion Processes **92**, 111 (1989). PA values are all derived from $\Delta_f H$ values of the corresponding free radicals and radical cations. For the keto radicals, protonation occurs on the carbonyl O atoms. For the hydroxy and amino radicals, protonation occurs on the hydroxy O and amino N atoms, respectively. For the following radicals, the site of protonation is underlined: $CH_2CH\underline{C}H_2\cdot$, $CH_2C(CH_3)\underline{C}H_2\cdot$, and $HCC\underline{C}H_2\cdot$.

97HOM/HER Homan, H., Herreros, M., Notario, R., Abboud, J.-L. M., Esseffar, M., Ma, O., Yanez, M., Foces-Foces, C., Ramos-Gallardo, A., Martinez-Ripoll, M., Vegas, A., Molina, M. T., Casanovas, J., Jimenez, P., Roux, M. V., Turrion, C., J. Org. Chem. **62**, 8503 (1997). ICR.

73HOP/BON Hopkins, J. M., Bone, L. I., J. Chem. Phys. **58**, 1473 (1973). HPMS.

89HOP/HOL Hop, C. E. C. A., Holmes, J. L., Ruttink, P. J. A., Schaftenaar, G., Terlouw, J. K., Chem. Phys. Lett. **156**, 251 (1989). Appearance energy measurements. N atom protonation of HNCO determined by comparison of CA mass spectra of protonated HNCO with the ion formed from dissociative ionization of CH_3CONH_2, i.e., $CH_3CONH_2 \rightarrow H_2NCO^+ + \cdot CH_3 + e^{-1}$. Also obtained $\Delta_f H^0(H_2NCO^+)=672$ kJ mol^{-1}; using $\Delta_f H^0(HNCO) = -104.6$ kJ mol^{-1} yields PA(HNCO)=753 kJ mol^{-1}. O atom protonation of HCNO determined by comparison of CA mass spectra of CI protonated HCNO with the ion generated from dissociative ionization of $CH_3CH{=}NOH$, i.e., $CH_3CH{=}NOH \rightarrow HCNOH^+ + \cdot CH_3 + e^{-1}$. Also obtained $\Delta_f H^0(HCNOH^+)=990$ kJ mol^{-1}; using $\Delta_f H^0(HCNO)=218$ kJ mol^{-1} yields PA(HCNO)=758 kJ mol^{-1}.

84HOP/JAH Hopkins, Jr., H. P., Jahagirdar, D. V., Moulik, P. S., Aue, D. H., Webb, H. M., Davidson, W. R., Pedley, M. D., J. Am. Chem. Soc. **106**, 4341 (1984). Gas basicities of 2,6-di-t-butylpyridine and 2,6-diisopropylpyridine estimated from relative intensities of ammonium ion fragments produced from the decomposition of metastable proton bound complexes with 2,2,6,6-tetramethylpiperidine and N-methyl-cis-3,5-dimethylpiperidine, respectively

94HOR/GLA Horan, C. J., Glaser, R, J. Phys Chem. **98**, 3989 (1994). Also reports calcualtions of methyl cation affinity of N_2.

78HOU/BEA Houle, F. A., Beauchamp, J. L., J. Am. Chem. Soc. **100**, 3290 (1978). Determination of ionization potentials of allyl and benzyl radicals.

79HOU/BEA Houle, F. A., Beauchamp, J. L., J. Am. Chem. Soc. **101**, 4067 (1979). Determination of ionization potentials of ethyl, isopropyl, and tert-butyl radicals.

89HOU/FEN Houriet, R., Feng, W., Vogel, E., Wolfrum, P., Schwartz, H., Int. J. Mass Spectrom. Ion Processes **91**, R1 (1989). ICR measurements of proton-transfer equilibrium constants at 313 K using various reference bases yielding GB values. The GB of N,N′-hexamethylene-syn-1,6:8,13-diimino[14]annulene was found by bracketing experiments to be equal to the GB of the corresponding pentamethylene compound, species 123524-79-8 and 123524-78-7, respectively.

85HOU/ROL Houriet, R., Rolli, E., Bouchoux, G., Hoppilliard, Y., Helv. Chim. Acta **68**, 2037 (1985). ICR. Authors suggest that protonation occurs at the α-C with the possible exception of 2,5-derivitives.

83HOU/RUF Houriet, R., Rufenacht, H., Carrupt, P.-A., Vogel, P., Tichu, M., J. Am. Chem. Soc. **105**, 3417 (1983). ICR. Temperature not specified but assumed to be 300 K.

80HOU/SCH Houriet, R., Schwarz, H., Zummack, W., Angew. Chem. Int. Ed. **19**, 905 (1980). ICR.

81HOU/SCH Houriet, R., Schwarz, H., Zummack, W., Andrade, J. G., Schleyer, P. v. R., Nouv. J. Chim. **5**, 505 (1981). ICR. Bracketing. All gas basicities lay between dimethyl ether and *n*-propanol.

86HOU/SCH Houriet, R., Schwitzguebel, T., Carrupt, P.-A., Vogel, P., Tetrahedron Lett. **27**, 37 (1986). ICR.

80HOU/VOG Houriet, R., Vogt, J., Haselbach, E., Chimia **34**, 277 (1980). ICR. Details not given.

79HUB/HER Huber, K. P., Herzberg, G., "Molecular Spectra and Molecular Structure Constants of Diatomic Molecules," Van Nostrand Reinhold, New York (1979).

92HU/SHE Hu, C.-H., Shen, M., Schaefer III, H. F., Chem. Phys. Lett. **190**, 543 (1992). *Ab initio* study at various levels of theory and basis sets. Tabulated PA(SiH_4) value used triple-zeta plus double polarization (TZ2P) basis set and single/double excitation coupled cluster (SDCC) as method.

88IKO/SUN Ikonomou, M. G., Sunner, J., Kebarle, P., J. Phys. Chem. **92**, 6308 (1988). High pressure mass spectrometry.

82IKU/KEB Ikuta, S., Kebarle, P., Bancroft, G. M., Chan, T., Puddephatt, R. J., J. Am. Chem. Soc. **104**, 5899 (1982). HPMS. Equilibria at 320 and 348 K: Entropy change assumed equal to zero.

89IRI/BEA Irikura, K. K., Beauchamp, J. L., J. Am. Chem. Soc. **111**, 75 (1989). FT-ICR.

96IRI/MAU Irikura, K. K., Meot-Ner, M., Sieck, L. W., Fant, A. D., Liebman, J. F., J. Org. Chem. **61**, 3167 (1996). HPMS; bracketing and *ab initio* calculations.

90ISA/OMO Isa, K., Omote, T., Amaya, M., Org. Mass Spectrom. **25**, 620 (1990). Combination of FAB to produce proton-bound dimers of amino acids and CAD to determine relative rates of formation of protonated amino acids which reflects the relative PAs. Only the relative PAs are determined as follows: Gly<Ala<Cys<Ser<Asp<Val<Leu<Thr<Ile <Phe<Met<Tyr<Glu<Asn<Trp<Pro<Gln<Lys<His <Arg.

89JAC Jacobson, D. B., J. Am. Chem. Soc. **111**, 1626 (1989). ICR bracketing.

89JAC/GOR Jacobson, D. B., Gord, J. R., Freiser, B. S., Organometallics **8**, 2957 (1989). ICR bracketing.

85JAS/STE Jasien, P. G., Stevens, W. J., J. Chem. Phys. **83**, 2984 (1985). *Ab initio* calculations yielding PA of CO, CS, CSe and CTe, all of which are C-protonated and linear. Tabulated PA values include ZPVE corrections but it is not clear if they refer to 0 or 298 K.

90JAV/GLO Javahery, G., Glosik, J., Twiddy, N. D., Ferguson, E. E., Int. J. Mass Spectrom. Ion Processes **98**, 225 (1990). ΔH^0 and ΔS^0 values for proton-transfer reactions obtained from "van't Hoff" plots of ratios of forward and reverse rate constants versus reciprocal average center of mass kinetic energies in a selected-ion flow drift tube.

96JEB/ZHA Jebber, K. A., Zhang, K., Cassady, C. J., Chung-Phillips, A., J. Am. Chem. Soc. **118**, 10515 (1996). FT-ICR, bracketing study.

84JEN/MOR Jenkins, H. D. B., Morris, D. F. C., J. Chem. Soc. Faraday Trans. II **80**, 1167 (1984). Derived from viscosity coefficients of ammonium halide salts in aqueous solution.

81JON/BIR Jones, J. D. C., Birkinshaw, K., Twiddy, N. D., Chem. Phys. Lett. **77**, 484 (1981). SIFT. PA(N_2)–PA(O).

89KAF/MAU Kafafi, S. A., Meot-Ner(Mautner), M., Liebman, J. F., Struct. Chem. **1**, 101 (1989). HPMS.

86KAM/YOU Kamar, A., Young, A. B., March, R. E., Can. J. Chem. **64**, 2368 (1986). QUISTOR measurement of proton transfer equilibria.

85KAR Karpas, Z., Chem. Phys. Lett. **120**, 53 (1985). ICR. Bracketing. GB($CF_3COOC_2H_5$)<GB(CH_2S) <GB($C_2H_5NO_2$)<GB($C_2H_5NO_2$)<GB(CH_2Se) <GB(CH_3CHO), GB(COS)<GB(SeCO)<GB(C_2H_2).

86KAR/JAS Karpas, Z., Jasien, P., Int. J. Mass Spectrom. Ion Processes **69**, 115 (1986). ICR. $GB(H_2S,H_2Se,HCN)<GB(H_2Te)\sim GB(CF_2CH_2)<GB(C_6F_6)$.

85KAR/STE Karpas, Z., Stevens, W. J., Buckley, T. J., Metz, R., J. Phys. Chem. **89**, 5274 (1985). ICR. Equilibria and bracketing. $GB(CF_3COOC_2H_5)<GB(CH_3NCO)-GB(C_2H_5NO_2)<GB(4\text{-}F\text{-}C_6H_4CH_3)$, $GB(CH_3SCN)-GB(CH_3)_2O<GB(n\text{-}C_3H_7CN)$.

72KAS/FRA Kaspar, S. F., Franklin, J. L., J. Chem. Phys. **56**, 1156 (1972). HPMS.

76KEB/YAM Kebarle, P., Yamdagni, R., Hiroaka, K., McMahon, T. B., Int. J. Mass Spectrom. Ion Phys. **19**, 71 (1976). HPMS. Only cited when data for a particular molecule has not been given in any subsequent papers from this laboratory. Values scaled to those from LAU papers.

93KEI/RIL Keister, J. W., Riley, J. S., Baer, T., J. Am. Chem. Soc. **115**, 12613 (1993). PEPICO measurement. At 298 K, derived quantities are $\Delta_f H^0(t\text{-}C_4H_9^+)=711$ kJ mol^{-1} and $PA(i\text{-}C_4H_8)=802$ kJ mol^{-1}.

89KEN/PAC Kenttamaa, H. I., Pachuta, R. R., Rothwell, A. P., Cooks, R. G., J. Am. Chem. Soc. **111**, 1654 (1989). PA of cyclohexene oxide determined by energy-resolved bracketing experiments, in which a proton-transfer reaction is judged as endothermic or exothermic on the basis of its dependence on the reactant ion kinetic energy. PA bracketed using pinacoline, diisopropyl ketone and cyclopropyl methyl ketone.

81KIM/BON Kim, J. K., Bonicamp, J., Caserio, M. C., J. Org. Chem. **46**, 4230 (1981). ICR. Bracketing.

87KIN/BUR Kinter, M. T., Bursey, M. M., Org. Mass Spectrom. **22**, 775 (1987). Endothermicity of proton transfer reactions estimated from the onset of proton transfer in an energy-resolved tandem mass spectrometry measurement.

96KIN/RID Kinser, R. D., Ridge, D. P., Hvistendahl, G., Rasmussen, B., Uggerud, E., Chem. Eur. J. **2**, 1143 (1996). Calculations indicate that the amino N atom is the most basic site.

90KLO Klots, C. E., J. Chem. Phys. **93**, 2513 (1990). $\Delta_f H^0(C_6H_5^+)=(1130\pm7)$ kJ mol^{-1} derived.

85KNI/FRE Knight, J. S., Freeman, C. G., McEwan, M. J., Adams, N. G., Smith, D., Int. J. Mass Spectrom. Ion Processes **67**, 317 (1985). SIFT measurement of proton transfer equilibria cyclically interlocking GB's of CH_3NO_2, HC_3N and BrCN.

86KNI/FRE Knight, J. S., Freeman, C. G., McEwan, M. J., J. Am. Chem. Soc. **108**, 1404 (1986). SIFT. The usual practice has been followed of allowing $GB(NH_3)$ to "float," and using the better established values for $GB(CH_3CHO)$ and $GB(C_2H_5)_2O$ as reference standards.

92KOM/DIX Kormornicki, A., Dixon, D. A., J. Chem. Phys. **97**, 1087 (1992). Tabulated PA values result from CCSD(T) (coupled cluster with single and double excitations and triple excitations included as a perturbational estimate) level of theory and includes basis set superposition error (BSSE) estimate. PA values expected to be within 4 kJ mol^{-1}.

94KOP/ANV Koppel, I. A., Anvia, F., Taft, R. W., J. Phys. Org. Chem. **7**, 717 (1994). FT-ICR.

80KOP/COM Koppel, I., Comisarow, M. B., "Ab Initio SCF LCAO MO Calculations of Molecules. I. Calculation of Proton Affinities. General Comparison with Experiment," Organic Reactivity, Engl. Ed. Tartu State University Press, Vol. XVII, p. 495 (1980). A review containing a table which lists experimental values for proton affinities of 70 compounds, cited as being "mostly from I. A. Koppel, U. H. Molder, and R. J. Pikver, Organic Reactivity, Tartu State University Press, Vol. XVII, p. 457 (1980). Because the latter paper was not available for this up-date when it was originally prepared, details of the cited values could not be evaluated. Since that time, I. Koppel has kindly made copies of his papers available to us; an evaluation of those data is in progress, but the data cited here are simply copied as given in the 1980 reference. The proton affinity values listed in 80KOP/COM for the most part are 2–5 kcal mol^{-1} higher than those recommended in this compilation (examples: NH_3, 866 kJ mol^{-1} (207 kcal mol^{-1}); pyridine, 932 kJ mol^{-1} (222.8 kcal mol^{-1}); ethanol 801 kJ mol^{-1} (191.4 kcal mol^{-1})). It must be emphasized that data from this reference have not yet been evaluated for internally consistency with other values given in this up-date, and to a first approximation, should be decreased by 8–21 kJ mol^{-1} in order to bring them into approximate consistency with the proton affinity scale used for this compilation.

93KUK/STR Kukol, A., Strehle, F., Thielking, G., Grutzmacher, H.-F., Org. Mass Spectrom. **28**, 1107 (1993). FT-ICR and kinetic method determination of GB values. Good agreement between both methods.

94LAT/SMI Latimer, D. R., Smith, M. A., J. Chem. Phys. **101**, 3410 (1994). Proton transfer chemistry performed within the core of a free jet flow reactor.

79LAU Lau, Y. K., Ph.D. thesis, University of Alberta (1979). HPMS. Some entropy change determinations.

76LAU/KEB Lau, Y. K., Kebarle, P., J. Am. Chem. Soc. **98**, 7452 (1976). HPMS. Some entropy change determinations.

81LAU/NIS Lau, Y. K., Nishizawa, K., Tse, A., Brown, R. S., Kebarle, P., J. Am. Chem. Soc. **103**, 6291 (1981). Data related to aniline. HPMS.

78LAU/SAL Lau, Y. K., Saluja, P. P. S., Kebarle, P., Alder, R. W., J. Am. Chem. Soc. **100**, 7328 (1978). HPMS.

92LEE/RIC Lee, T. J., Rice, J. E., J. Phys. Chem. **96**, 650 (1992). *Ab initio* study using variety of basis sets and computational methods and including zero point vibrational energy corrections. CCSD(T) method chosen as most accurate approach. Directly determined $PA(HNO_3)$ to be (763.6 ±17) kJ mol^{-1} [(182.5±4.0) kcal mol^{-1}]. The most stable form of $H_2NO_3^+$ was found to be a loosely bound planar complex of structure $H_2O\cdot\cdot NO_2^+$, with calculated $BE(H_2O\cdot\cdot NO_2^+)=(72.4\pm8)$ kJ mol^{-1} [(17.3±2.0) kcal mol^{-1}].

92LEE/RIC2 Lee, T. J., Rice, J. E., J. Am. Chem. Soc. **114**, 8247 (1992). Calculated $PA(CH_3ONO_2)=(740.1\pm21)$ kJ mol^{-1} (176.9 ±5 kcal mol^{-1}), using basis sets, methods and corrections similar to 92RIC/LEE. Most stable form of protonated CH_3ONO_2 consists of a loosely bound complex $CH_3OH\cdot\cdot NO_2^+$ with calculated $BE(CH_3OH\cdot\cdot NO_2^+)=(82\pm8)$ kJ mol^{-1} [(19.6±2) kcal mol^{-1}].

93LI/HAR Li, X., Harrison, A. G., Org. Mass Spectrom. **28**, 366 (1993). CID study of proton bound dimers of amines with amines and amino acids with amines. Relative rate data used with PA values of reference bases as determined for this compilation.

87LI/STO Li, X., Stone, J. A., Can. J. Chem. **65**, 2454 (1987). HPMS and temperature dependence of proton-transfer equilibrium constants between 330 and 600 K.

88LI/STO Li, X., Stone, J. A., Can. J. Chem. **66**, 1288 (1988). HPMS and temperature dependence of proton-transfer equilibrium constants.

79LIA Lias, S., in "Kinetics of Ion-Molecule Reactions," P. Ausloos, Editor, Thermochemistry of Polyatomic Cations, Plenum, New York, p. 223 (1979). ICR. Proton transfer equilibria of ketene with acetone and methyl acetate measured as a function of temperature.

77LIA/AUS Lias, S. G., Ausloos, P., Int. J. Mass Spectorm. Ion Phys. **23**, 273 (1977). ICR.

87LIA/AUS Lias, S. G., Ausloos, P., Int. J. Mass Spectrom. Ion Processes **81**, 165 (1987). ICR measurements of forward and reverse proton transfers.

88LIA/BAR Lias, S. G., Bartmess, J. E., Liebman, J. F., Holmes, J. L., Levin, R. D., Mallard, W. G., J. Phys. Chem. Ref. Data **17**, Supplement 1 (1988).

84LIA/BUC Lias, S. G., Buckley, T. J., Int. J. Mass Spectrom. Ion Processes **56**, 123 (1984). ICR. Bracketing. Based on the value $\Delta_f H^0(c\text{-}C_3H_6^-) = 1004.4$ kJ mol^{-1}, and a recommended value $\Delta_f H^0(c\text{-}C_3H_5) = 255$ kJ mol^{-1} [M. Rossi and D. M. Golden, J. Am. Chem. Soc. **101**, 2838 (1979)], a value $PA(c\text{-}C_3H_5) = 781$ kJ mol^{-1} is predicted. This is in close agreement with earlier bracketing experiments (80DEF/MCI). Another value of $\Delta_f H^0(c\text{-}C_3H_5) = (279.9 \pm 10.5)$ kJ mol^{-1} [D. F. McMillen and S. W. Golden, Ann. Rev. Phys. Chem. **33**, 493 (1982)], predicts $PA(c\text{-}C_3H_5) = (806 \pm 11)$ kJ mol^{-1}. However, the clear observation of proton transfer from $[C_3H_6^+]$ ions in cyclopropane to AsH_3 (PA=748 kJ mol^{-1}), $c\text{-}C_3H_6$ (PA=750 kJ mol^{-1}), and C_6F_6 (PA=654 kJ mol^{-1}), would appear to discredit the earlier result. The authors suggest that proton transfer to these molecules with lower proton affinities may be due to ring opening of the cyclopropane ion in the collision complex, or the occurrence of collisional rearrangement to $CH_3CH{=}CH_2^+$ followed by proton transfer from that ion.

85LIA/JAC. Lias, S. G., Jackson, J.-A., Argentar, H., Liebman, J. F., J. Org. Chem. **50**, 333 (1985). ICR.

85LIA/KAR Lias, S. G., Karpas, Z., Liebman, J. F., J. Am. Chem. Soc. **107**, 6089 (1985).

80LIA/SHO Lias, S. G., Shold, D. M., Ausloos, P., J. Am. Chem. Soc. **102**, 2540 (1980). ICR. Data relative to $i\text{-}C_4H_8$. Trans-$2\text{-}C_4H_8$ and $c\text{-}C_6H_{10}$ by bracketing. $2\text{-}C_4H_8$–CH_3NO_2; $c\text{-}C_6H_{10}$–$HCOOCH_3$.

94LIG/NAP Liguori, A., Napoli, A., Sindona, G., Rapid Commun. Mass Spectrom. **8**, 89 (1994). Kinetic method. Rate data was applied using the PA values in the present compilation, although the data in Table 1 of this paper did not agree completely with the final values presented in Table 2.

75LIN/ALB Lindinger, W., Albritton, D. L., Howard, C. J., Fehsenfeld, F. C., Ferguson, E. E., J. Chem. Phys. **63**, 5220 (1975). Flowing afterglow.

75LIN/MCF Lindinger, W., McFarland, M., Fehsenfeld, F. C., Albritton, D. L., Schmeltekopf, A. L., Ferguson, E. E., J. Chem. Phys. **63**, 2175 (1975). Drift tube flowing afterglow measurements.

93LIN/ROC Lin, H.-Y., Rockwood, A., Munson, M. S. B., Ridge, D. P., Anal. Chem. **65**, 2119 (1993). Temperature dependent FT-ICR.

92LIO/BRO Liou, C.-C., Brodbelt, J. S., J. Am. Chem. Soc. **114**, 6761 (1992). Kinetic method. The method, as applied to the molecules studied, could give only an "order" or "ladder" of relative proton affinities with no indication of how large the steps are in the "ladder." See third paragraph of this paper's Experimental Section for more details. As such, the method suggests the following order of relative PAs: PA(12-crown-4) $<PA(CH_3O[CH_2CH_2O]_3CH_3)<PA(15\text{-crown-}5)$ $<PA(CH_3O[CH_2CH_2CH_2O]_3CH_3)$ $<PA(CH_3O[CH_2CH_2O]_4CH_3)<PA(18\text{-crown-}6)$ $<PA(HO[CH_2CH_2O]_4H)<PA(21\text{-crown-}7)$ $<PA(HO[CH_2CH_2O]_5H)$.

79LOC/HUN Locke, M. J., Hunter, R. L., McIver, Jr., R. T., J. Am. Chem. Soc. **101**, 272 (1979). ICR. [382 K].

83LOC/MCI Locke, M. J., McIver, Jr., R. T., J. Am. Chem. Soc. **105**, 4226 (1983). ICR.

75LOS/TRA Lossing, F. P., Traeger, J. C., J. Am. Chem. Soc. **97**, 1579 (1975). Appearance potential of $C_5H_5^+$ from cyclopentene.

93LUC/CUR Lucas, D. J., Curtiss, L. A., Pople, J. A., J. Chem. Phys. **99**, 6697 (1993). *Ab initio* calculations using Gaussian-2 (G2) theory.

78MAC/BOH Mackay, G. I., Bohme, D. K., Int. J. Mass Spectrom. Ion Phys. **26**, 327 (1978). Flowing afterglow.

81MAC/SCH Mackay, G. I., Schiff, H. I., Bohme, D. K., Can. J. Chem. **59**, 1771 (1981). Flowing afterglow.

92MAC/SCH Mackay, G. I., Schiff, H. I., Bohme, D. K., Int. J. Mass Spectrom. Ion Processes **117**, 387 (1992). SIFT study of reactions of protonated molecules with SF_6 at 298 K. Protonated SF_6 only observed from the reaction of HCO^+ with SF_6, and is only 1% of the product ions. $PA(SF_6)$ bracketed between $PA(N_2O)$ and $PA(C_2H_6)$. Estimated $\Delta G^0 = GB(SF_6) - GB(CO) = -12.1$ kJ mol^{-1} (-2.9 kcal mol^{-1}) for the reaction $SF_6H^+ + CO \rightleftarrows SF_6 + HCO^+$ from the measured value of the reverse rate constant (5.5×10^{-12} cm^3 molecule^{-1} s^{-1}) and assuming the forward (and exothermic) rate constant to be equal to the collision rate (7.05×10^{-10} cm^3 molecule^{-1} s^{-1}).

92MAC/SUD Maclagan, R. G. A. R., Sudkeaw, P., Chem. Phys. Lett. **194**, 147 (1992). *Ab initio* study at various levels of theory and basis sets. Tabulated PA values obtained at the MP4SDQ/6-311G**//HF/6-311G** level of theory, including unscaled ZPVE and basis set superposition error corrections. Structures of C_2S and C_3S and their protonated forms (both preferred at C_1) are linear. The PA values for protonation as S for C_2S and C_3S calculated to be 567.7 and 598.4 kJ mol^{-1}, respectively, at the MP4SDQ/6-31G*//HF/6-31G* level of theory.

93MAC/SUD Maclagan, R. G. A. R., Sudkeaw, P., J. Chem. Soc. Faraday Trans. **89**, 3325 (1993). Calculations indicate that both C_3O and C_2O are C-terminal protonated, and that HC_3O^+ is linear and HC_2O^+ is bent. Values also given for O-terminal protonated forms at a somewhat lower level of theory.

84MAN/HAL Manlich, M. L., Halle, L. F., Beauchamp, J. L., J. Am. Chem. Soc. **6**, 4403 (1984). Determined $D^0(Ru^+\text{–}H) = (172 \pm 12)$ kJ mol^{-1} [(41 ± 3) kcal mol^{-1}], $D^0(Rh^+\text{–}H) = (176 \pm 12)$ kJ mol^{-1} [(42 ± 3) kcal mol^{-1}] and $D^0(Pd^+\text{–}H) = (188 \pm 12)$ kJ mol^{-1} [(45 ± 3) kcal mol^{-1}]. Using these data and the following ionization potentials gives the following PA values: IP(Ru)=7.3605 eV, PA(Ru)=(773.6±12) kJ mol^{-1}; IP(Rh)=7.4589 eV, PA(Rh)=(768±12) kJ mol^{-1}; IP(Pd)=8.3369 eV, PA(Pd)=(696±12) kJ mol^{-1}.

88MAQ/JOR Maquestiau, A., Jortay, C., Beuqnies, D., Flammang, R., Houriet, R., Rolli, E., Bouchoux, G., Int. J. Mass Spectrom. Ion Processes **82**, 33 (1988). ICR.

87MAR/GAL Maria, P.-C., Gal, J.-F., Taft, R. W., New J. Chem. **11**, 617 (1987). ICR.

96MAR/LEE Martin, J. M. L., Lee, T. J., Chem. Phys. Lett **258**, 136 (1996). Recommend a PA=(853.1±1.3) kJ mol^{-1} [(203.9±0.3) kcal mol^{-1}].

85MAR/MOD Marcuzzi, F., Modena, G., Paradisi, C., Giancaspro, C., Speranza, M., J. Org. Chem. **50**, 4973 (1985). ICR. Bracketing and equilibrium constant determinations. Temperature not indicated but assumed to be ~300 K.

88MAR/REB Marquette, J. B., Rebrion, C., Rowe, B. R., J. Chem. Phys **89**, 2041 (1988). CRESU measurement of endothermicity of the reaction $N^+(^3P) + H_2(X\,^1\Sigma_g^+, J=0) \rightarrow NH^+(X^2\Pi, J=0) + H(^2S)$ as (18 ± 2) meV, yielding a PA(N) = (3.524±0.003) eV or 340 kJ mol^{-1}.

86MAR/TOP Marriott, S., Topsom, R. D., Lebrilla, C. B., Koppel, I., Mishima, M., Taft, R. W., J. Mol. Struct.: THEOCHEM **137**, 133 (1986). ICR. Gas basicities relative to GB(HCN). Values high in scale related to local standards as follows: $(CH_3)_2NCN$, C_6H_5CN, t-C_4H_9CN relative to i-C_3H_7CN.

82MAS/BOH Mason, R. S., Bohme, D. K., Jennings, K. R., J. Chem. Soc., Faraday Trans. I **78**, 1943 (1982). HPMS.

69MAT/WAR Matthews, C. S., Warneck, P., J. Chem. Phys. **51**, 854 (1969).

79MAU Meot-Ner (Mautner), M., J. Am. Chem. Soc. **101**, 2396 (1979). HPMS [500–600 K].

80MAU Meot-Ner (Mautner), M., J. Phys. Chem. **84**, 2716 (1980). HPMS. [550 K].

82MAU Meot-Ner (Mautner), M., J. Am. Chem. Soc. **104**, 5 (1982). ICR. Bracketing: Proton transfer rate constants measured and thermoneutral point identified from fall-off of rate constant as reaction becomes progressively less exothermic.

83MAU Meot-Ner (Mautner), M., J. Am. Chem. Soc. **105**, 4906 (1983). HPMS.

86MAU Mautner, M. (unpublished results). HPMS.

89MAU Meot-Ner (Mautner), M., J. Am. Chem. Soc. **111**, 2830 (1989). High pressure mass spectometer. ΔH^0 and ΔS^0 values given for proton transfer.

77MAU/FIE Meot-Ner (Mautner), M., Field, F. H., J. Chem. Phys. **66**, 4527 (1977). HPMS.

80MAU/HAM Meot-Ner (Mautner), M., Hamlet, P., Hunter, E. P., Field, F. H., J. Am. Chem. Soc. **102**, 6393 (1980). HPMS. Observed the reaction, $(iso\text{-}C_5H_{11})_3NH^+ + H_2N(CH_2)_2NH(CH_2)_2NH_2 \rightleftarrows (iso\text{-}C_5H_{11})_3N + [H_2N(CH_2)_2NH(CH_2)_2NH_2]H^+$, and measured $\Delta H^0 = -0.8$ kJ mol^{-1} (-0.2 kcal mol^{-1}) and $\Delta S^0 = -20.9$ J (mol K)$^{-1}$ [-5.0 cal (mol K)$^{-1}$]. Also observed the reaction, $(iso\text{-}C_5H_{11})_3NH^+ + H_2N(CH_2)_3NH(CH_2)_3NH_2 \rightleftarrows (iso\text{-}C_5H_{11})_3N + [H_2N(CH_2)_3NH(CH_2)_3NH_2]H^+$, and measured $\Delta H^0 = -42.7$ kJ mol^{-1} (-10.2 kcal mol^{-1}) and $\Delta S^0 = -56.0$ J (mol K)$^{-1}$ [-13.4 cal (mol K)$^{-1}$]. Since no data connecting $(iso\text{-}C_5H_{11})_3N$ to any other base could be found, the PA and GB of $(iso\text{-}C_5H_{11})_3N$, $H_2N(CH_2)_2NH(CH_2)_2NH_2$, and $H_2N(CH_2)_3NH(CH_2)_3NH_2$ could not be evaluated and are not tabulated.

79MAU/HUN Meot-Ner (Mautner), M., Hunter, E. P., Field, F. H., J. Am. Chem. Soc. **101**, 686 (1979). HPMS.

80MAU/HUN Meot-Ner (Mautner), M., Hunter, E. P., Hamlet, P., Field, F. H., "Thermochemistry of Intramolecular Solvation in Protonated and Radical Ions: Diamines, Triamines, Amino Alcohols, Diphenyl Alkanes, and Normal Alkanes," Proceedings of the 28th Annual Conference on Mass Spectrometry and Allied Topics, May 25–30 p. 233 (1980). HPMS.

86MAU/KAR Meot-Ner (Mautner), M., Karpas, Z., Deakyne, C. A., J. Am. Chem. Soc. **108**, 3913 (1986). ICR.

86MAU/LIE Meot-Ner (Mautner), M., Liebman, J. F., Del Bene, J. E., J. Org. Chem. **51**, 1105 (1986). HPMS.

84MAU/NEL Meot-Ner (Mautner), M., Nelsen, S. F., Willi, M. R., Frigo, T. B., J. Am. Chem. Soc. **106**, 384 (1984). HPMS. Free energy changes at or near 600 K.

83MAU/SIE Mautner, M., Sieck, L. W., J. Am. Chem. Soc. **105**, 2956 (1983). HPMS. Includes entropy change measurements.

91MAU/SIE Mautner, M., Sieck, L. W., J. Am. Chem. Soc. **113**, 4448 (1991). HPMS and temperature dependence of proton transfer equilibrium constants.

91MAU/SMI Meot-Ner (Mautner), M., Smith, S. C., J. Am. Chem. Soc. **113**, 862 (1991). HPMS including some temperature dependence of proton-transfer equilibrium constants.

76MAU/SOL Mautner (Meot-Ner), M., Solomon, J. J., Field, F. H., J. Am. Chem. Soc. **98**, 1025 (1976). HPMS. Heats of formation of alkyl ions from hydride transfer equilibrium constant measurements; values calculated relative to a value of $\Delta_f H^0(t\text{-}C_4H_9^+) = 711$ kJ mol^{-1}.

74MCA McAllister, T., Int. J. Mass Spectrom. Ion Phys. **15**, 303 (1974). ICR. Bracketing.

77MCA McAllister, T., Int. J. Mass Spectrom. Ion Phys. **25**, 353 (1977). ICR. Bracketing: $CH_3OH < (CH_3)_2SO < C_2H_5OH$. Disagrees with equilibrium results.

78MCA McAllister, T., Astrophys. J. **222**, 857 (1978). ICR. Bracketing.

81MCA/NIC McAllister, T., Nicholson, J. C., Scott, J. D., Can. J. Chem. **59**, 1819 (1981).

76MCA/PIT McAllister, T., Pitman, P., Int. J. Mass Spectrom. Ion Phys. **19**, 241 (1976). ICR. Bracketing.

76MCC McCulloh, K. E., Int. J. Mass Spectrom. Ion Phys. **21**, 333 (1976). Appearance potential of OH^+ from H_2O.

77MCC McCulloh, K. E., "The Proton Affinity of O_2, from Photoionization Studies of H_2O_2," Proc. 25th Ann. Conf Mass Spectrom. Allied Topics, Washington, D.C. (1977). Also cited as data "To be published" in K. N. Hartman, S. Lias, P. Ausloos, H. M. Rosenstock, S. S. Schroyer, C. Schmidt, D. Martinsen, and G. W. A. Milne, "A Compendium of Gas Phase Basicity and Proton Affinity Measurements," NBSIR 79-1777 (1979). Measurement of the appearance potential of O_2H^+ from H_2O_2.

91MCE/CAL McElvany, S. W., Callahan, J. H., J. Phys. Chem. **95**, 6186 (1991). ICR bracketing indicated that $PA(NH_3) < PA(C_{60}, C_{70}) < PA(hexamethylbenzene)$. Reactivity data further suggested that $PA(C_{60}) < PA(C_{70})$.

88MCI/ADA McIntosh, B. J., Adams, N. G., Smith, D., Chem. Phys. Lett. **148**, 142 (1988). SIFT measurement of proton transfer equilibrium by measuring forward and reverse rate constants at a few temperatures.

94MCK/BEL McKiernam, J. W., Beltrame, C. E. A., Cassady, C. J., J. Am. Soc. Mass Spectrom. **5**, 718 (1994). FT-ICR bracketing.

72MCK/SAW McKnight, L. G., Sawina, J. M., J. Chem. Phys. **57**, 5156 (1972). Measured $\Delta H^0 = -49.7$ kJ mol^{-1} (-11.88 kcal mol^{-1}) and $\Delta S^0 = -61.5$ J (mol K)$^{-1}$ [-14.27 cal (mol K)$^{-1}$] for the reaction $Cs^+ + H_2O \rightleftarrows CsOH_2^+$. Using $\Delta_f H^0(H_2O) = -241.8$ kJ mol^{-1}, $\Delta_f H^0(H^+) = 1530$ kJ mol^{-1}, $S^0(H_2O) = 188.7$ J (mol K)$^{-1}$, $\Delta_f H^0(CsOH) = -259.4$ kJ mol^{-1}, $\Delta_f H^0(Cs^+) = 451.8$ kJ mol^{-1}, $S^0(Cs^+) = 169.8$ J (mol K)$^{-1}$ and $S^0(CsOH) = 254.7$, yields $PA(CsOH) = 1110.3$ kJ mol^{-1} and $\Delta S_p(CsOH) = 42.3$ J (mol K)$^{-1}$.

81MCL/CAM McLuckey, S. A., Cameron, D., Cooks, R. G., J. Am. Chem. Soc. **103**, 1313 (1981). Kinetic method.

85MCM/KEB McMahon, T. B., Kebarle, P., J. Am. Chem. Soc. **107**, 212 (1985). HPMS. A thermochemical ladder covering the span from H_2S to CH_4 at 400 K.

85MCM/KEB2 McMahon, T. B., Kebarle, P., Can. J. Chem. **63**, 3160 (1985). HPMS at 400 K. Paper includes several of the individual equilibrium constant measurements from 85MCM/KEB

76MEI/MIT Meisels, G. G., Mitchum, R. K., Freeman, J. P., J. Phys. Chem. **80**, 2845 (1976). HPMS. For the reaction $CO_2H^- + CH_4 = CO_2 + CH_5^-$, $\Delta H^0 = -6.6$ kJ mol^{-1} and $\Delta S^0 = 7.1$ J (mol K)$^{-1}$ was measured.

91MER/QUE Meredith, C., Quelch, G. E., Schaefer, III, H. F., J. Am. Chem. Soc. **113**, 1186 (1991). Ozone (O_3) found to be terminally protonated producing an open-chain and trans structure.

89MEY/BUR Meyerhoffer, W. J., Bursey, M. M., Org. Mass Spectrom. **24**, 169 (1989). PA(cis-1,2-pentanediol) determined from the onset [(0.34 ± 0.1) eV, center of mass coordinates] of proton transfer from the protonated diol to NH_3 (PA taken as 854 kJ mol^{-1}) in a TIKE experiment.

92MIS/ARI Mishima, M., Ariga, T., Fujio, M., Tsuno, Y., Kobayashi, S., Taniguchi, H., Chem. Lett., 1085 (1992). ICR.

92MIS/ARI2 Mishima, M., Ariga, T., Tsuno, Y., Ikenaga, K., Kikukawa, K., Chem. Lett., 489 (1992). ICR.

86MIS/FUJ Mishima, M., Fujio, M., Tsuno, Y., Tetrahedron Lett. **27**, 939 (1986). ICR.

86MIS/FUJ2 Mishima, M., Fujio, M., Tsuno, Y., Tetrahedron Lett. **27**, 951 (1986). ICR.

92MIS/KAN Mishima, M., Kang, C. H., Fujio, M., Tsuno, Y., Chem. Lett., **3**, 493 (1992). ICR.

92MIS/TER Mishima, M., Terasaki, T., Fujio, M., Tsuno, Y., Takai, Y., Sawada, M., Chem. Lett., 1081 (1992). ICR.

92MOR/MAR Morizur, J.-P., Martigny, I., Taphanel, M.-H., Tortajada, J., Geribaldi, S., Decouzon, M., Int. J. Mass Spectrom Ion Proc. **113**, 191 (1992). ICR study. CID studies and thermochemical considerations suggest that protonation of $CH_3C(OCH_3)=CHCOOCH_3$ occurs on the carbonyl O atom and that no internal ionic hydrogen bonding occurs.

93MOU/AUD Mourgues, P., Audier, H. E., Leblanc, D., Hammerum, S., Org. Mass Spectrom. **28**, 1107 (1993). ICR. Bracketing measurements.

77MUN/SMI Munson, B., Smith, D., Polley, C., Int. J. Mass Spectrom. Ion Phys. **25**, 323 (1977). HPMS. Bracketing.

80MUR Murad, E., J. Chem. Phys. **73**, 1381 (1980). Knudsen cell. Determinations of heats of formation of FeO and $FeOH^+$.

81MUR Murad, E., J. Chem. Phys. **75**, 4080 (1981). Determinations of appearance energies of MOH^+ ions, where M is Ca, Mg, Ba and Sr. Using $\Delta_f H^0(CaO)=(25.1\pm16.7)$ kJ mol^{-1} and $\Delta_f H^0(Ca)=178.2$ kJ mol^{-1} gives $PA(CaO)=(1187.4\pm25)$ kJ mol^{-1}. Using $\Delta_f H^0(BaO)=(-123.8\pm8.4)$ kJ mol^{-1} and $\Delta_f H^0(Ba)=1789.9$ kJ mol^{-1} gives $PA(BaO)=(1215.4\pm34)$ kJ mol^{-1}. Using $\Delta_f H^0(SrO)=(-13.4\pm16.7)$ kJ mol^{-1} and $\Delta_f H^0(Sr)=1789.9$ kJ mol^{-1} gives $PA(SrO)=(1207.3\pm31)$ kJ mol^{-1}.

83MUR Murad, E., J. Chem. Phys. **78**, 6611 (1983). Determinations of heats of formation of $CaOH^+$ and $SrOH^+$ through onset energies of endothermic reactions. Using $\Delta_f H^0(CaO)=(25.1\pm16.7)$ kJ mol^{-1} and $\Delta_f H^0(Ca^+)=768.1$ kJ mol^{-1} gives $PA(CaO)=(1193.7\pm22)$ kJ mol^{-1}. Using $\Delta_f H^0(SrO)=(-13.4\pm16.7)$ kJ mol^{-1} and $\Delta_f H^0(Sr^+)=712.6$ kJ mol^{-1} gives $PA(SrO)=(1210.7\pm20)$ kJ mol^{-1}.

92NAK/NOM Nakata, K., Nomura, H., Mishima, M., Saeki, Y., Nishimoto, K., Matsushita, T., Fujio, M., Tsuno, Y., "Substituent effect on gas phase stabilities of α-t-butyl-α-methylbenzyl cations," Memoirs of the Faculty of Science, Kyushu University, Ser. C. **18**, 287 (1992). ICR.

88NEL/RUM Nelsen, S. F., Rumack, D. T., Steck, L. W., Meot-Ner(Mautner), M., J. Am. Chem. Soc. **110**, 6303 (1988). High pressure mass spectrometry.

77NG/TRE Ng, C. Y., Trevor, D. J., Tiedemann, P. W., Ceyer, S. T., Kronebusch, P. L., Mahan, B. H., Lee, Y. T., J. Chem. Phys. **67**, 4235 (1977). Determination of proton affinities of H_2O and HF through appearance potential measurements on neutral dimers.

94NOT/HER Notario, R., Herreros, M., El Hammadi, A., Homan, H., Abboud, J.-L., Forfar, I., Claramunt, R. M., Elguero, J., J. Phys. Org. Chem. **7**, 657 (1994). FT-ICR measurements and AM1 calculations.

91NOU/COO Nourse, B. D., Cooks, R. G., Int. J. Mass Spectrom. Ion Processes **106**, 249 (1991). Proton affinities bracketed by measuring dissociation kinetics of proton-bound dimers ($ABH^+ \rightarrow AH^+ + B$ and/or $A + BH^+$). Relative abundances and proton affinities related by $\ln([AH^+]/[BH^+]) = \Delta PA/RT$. Quadrupole ion trap used to generate and mass select proton-bound dimers.

89ORL/ALL Orlando, R., Allgood, C., Munson, B., Int. J. Mass Spectrom. Ion Processes **92**, 93 (1989). Gas chromotography/chemical ionization mass spectrometry and bracketing technique.

89OSA/DEL Osapay, K., Delhalle, J., Nsunda, K. M., Rolli, E., Houriet, R., Hevesi, L., J. Am. Chem. Soc. **111**, 5028 (1989). ICR equilibrium proton transfer and bracketing.

92PAR/FER Parry, A., Fernandez, M. T., Garley, M., Mason, R., J. Chem. Soc. Faraday Trans. **88**, 3331 (1992). Variable temperature HPMS. The values reported for system XI of Table 1 are believed to be reversed and are thus reversed in this compilation. A reassessment of 87FER/JEN.

82PAU/HEH Pau, C.-F., Hehre, W. J., J. Phys. Chem. **86**, 321 (1982). ICR. Bracketing of deuteron transfer from protonated DCN: $C_2H_5CHO<HNC<C_2H_5SH$.

82PAU/HEH2 Pau, C.-F., Hehre, W. J., J. Phys. Chem. **86**, 1252 (1982). ICR. Bracketing of deuteron transfer from protonated D_2CO: $C_2H_5(i\text{-}C_3H_7)NH<DCOH<$N-Methylpiperidine.

78PAU/KIM Pau, J. K., Kim, J. K., Caserio, M. C., J. Am. Chem. Soc. **100**, 3831 (1978). Tables give values of proton affinities cited as being from 77WOL/STA. Proton affinities given here are compounds not actually found in that paper. Values have been adjusted for consistency with this scale.

91PAU/SQU Paulino, J. A., Squires, R. R., J. Am. Chem. Soc. **113**, 5573 (1991). The derived values of $\Delta_f H^0(CF_2)=(-164.8\pm14)$ kJ mol^{-1} [$-(39.4\pm3.4)$ kcal mol^{-1}] and $\Delta_f H^0(CCl_2)=(218\pm14)$ kJ mol^{-1} [(52.1 ± 3.4) kcal mol^{-1}], combined with $\Delta_f H^0(CHF_2^+)=(600\pm13)$ kJ mol^{-1} and $\Delta_f H^0(CHCl_2^+)=(887\pm13)$ kJ mol^{-1} yields $PA(CF_2)=(765\pm18)$ kJ mol^{-1} and $PA(CCl_2)=(861\pm18)$ kJ mol^{-1}.

75PAY/SCH Payzant, J. D., Schiff, H. I., Bohme, D. K., J. Chem. Phys. **63**, 149 (1975). Flowing afterglow.

90PEE/ING Peerboom, R. A. L., Ingemann, S., Nibbering, N. M. M., Liebman, J. F., J. Chem. Soc. Perkin Trans. 2, 1825 (1990). ICR bracketing measurements.

92PET/FOR de Petris, G., Fornarini, S., Occhiucci, G., Int. J. Mass Spectrom. Ion Processes **112**, 231 (1992). ICR and CI study. $PA(CH_3SO_3H)$ bracketed using CH_3NO_2, CH_3OH, $C_2H_5NO_2$ and C_2H_5OH as reference bases.

89PET/FRE Petrie, S. A. H., Freeman, C. G., McEwan, M. J., Meot-Ner(Mautner), M., Int. J. Mass Spectrom. Ion Processes **90**, 241 (1989). Selected-ion flow tube measurements.

90PET/FRE Petrie, S., Freeman, C. G., Meot-Ner(Mautner), M., McEwan, M. J., Ferguson, E. F., J. Am. Chem. Soc. **112**, 7121 (1990). Selected ion flow tube study. Estimated that $\Delta_f H^0(HNC^+)\leq1373$ kJ mol^{-1} and thus PA(CN at N) ≥595 kJ mol^{-1}.

92PET/IRA Petrank, A., Iraqi, M., Dotan, I., Lifshitz, C., Int. J. Mass Spectrom. Ion Processes **117**, 223 (1992). SIFT. PA value obtained from correlations between proton transfer reaction efficiency and reaction thermochemistry for reactions of $C_2H_4^+$ with a number of bases but with CH_3OH and $CClH_2CN$ in particular.

91PET/KNI Petrie, S., Knight, J. S., Freeman, C. G., Maclagan, R. G. A. R., McEwan, M. J., Sudkeaw, P., Int. J. Mass Spectrom. Ion Processes **105**, 43 (1991). Selected ion flow tube (SIFT) measurements.

82PIE/HEH Pietro, W. J., Hehre, W. J., J. Am. Chem. Soc. **104**, 4329 (1982). ICR. Bracketing: Identities of reference bases not specified; temperature correction of TAFT scale made by authors.

82PIE/HEH2 Pietro, W. J., Hehre, W. J., J. Am. Chem. Soc. **104**, 3594 (1982). ICR. Bracketing. D^- transfer from $(CH_3O)_2PDOH^+$ occurs with $3\text{-}CH_3C_6H_4NH_2$ but not with $(CH_3O)_3PO$. H^- transfer approximately thermoneutral with $CF_2HCON(CH_3)_2$ *Data cited in paper as "C. Lebrilla (unpublished work)", **Data cited in paper as "M. Berthelot (unpublished work)", ***Data cited in paper as "T. Gramstad (unpublished work)".

79PIE/POL Pietro, W. J., Pollack, S. K., Hehre, W. J., J. Am. Chem. Soc. **101**, 7126 (1979). ICR. Bracketing.

73PIE/POR Pierce, R. C., Porter, R. F., J. Am. Chem. Soc. **95**, 3849 (1973). HPMS.

75PIT/BUR Pitt, C. G., Bursey, M. M., Chatfield, D. A., J. Chem. Soc. Perkin Trans 1 **434** (1975). HPMS. Bracketing.

77PO/POR Po, P. L., Porter, R. F., J. Am. Chem. Soc. **99**, 4922 (1977). HPMS. Bracketing

77PO/POR2 Po, P. L., Porter, R. F., J. Phys. Chem. **81**, 2233 (1977). Observed equilibrium $MgH^+ + Mg(s) = Mg_2H^+$, $\Delta H^0 = (41 \pm 15)$ kJ mol^{-1}. Using $PA(Mg) = (820 \pm 22)$ kJ mol^{-1}, $\Delta_f H^0(Mg,g) = 147.7$ kJ mol^{-1} and $\Delta_f H^0(Mg_2,g) = 288.3$ kJ mol^{-1} yields $PA(Mg_2) = (919 \pm 30)$ kJ mol^{-1}.

78PO/RAD Po, P. L., Radus, T. P., Porter, R. F., J. Phys. Chem. **82**, 520 (1978). HPMS. Bracketing.

77POL/DEV Pollack, S. K., Devlin III, J. L., Summerhays, K. D., Taft, R. W., Hehre, W. J., J. Am. Chem. Soc. **99**, 4583 (1977). ICR. Data related to TAFT scale, corrected to 350 K.

80POL/HEH Pollack, S. K., Hehre, W. J., Tetrahedron Lett. **21**, 2483 (1980). ICR. Bracketing.

78POL/MUN Polley, C. W., Munson, B., Int. J. Mass Spectrom. Ion Phys. **26**, 49 (1978). High pressure mass spectrometry. Bracketing.

84POL/MUN Polley, Jr., C. W., Munson, B., Int. J. Mass Spectrom. Ion Proc. **59**, 333 (1984). Bracketing.

81POL/RAI Pollack, S. K., Raine, B. C., Hehre, W. J., J. Am. Chem. Soc. **103**, 6308 (1981). ICR. Bracketing.

77POL/WOL Pollack, S. K., Wolf, J. F., Levi, B. A., Taft, R. W., Hehre, W. J., J. Am. Chem. Soc. **99**, 1350 (1977). ICR. Data related to TAFT scale; temperature assumed to be 350 rather than 300 K.

87POP/CUR Pople, J. A., Curtiss, L. A., J. Phys. Chem. **91**, 155 (1987). *Ab initio* study.

83PRE/TZE Prest, H. F., Tzeng, W.-B., Brom, Jr., J. M., Ng, C. Y., J. Am. Chem. Soc. **105**, 7531 (1983). Heat of formation of H_3S^+ from appearance energy from $(H_2S)_2$; approximately corrected to 298 K by present authors.

92RAC/MAR Raczynska, E. D., Maria, P.-C., Gal, J.-F., Decouzon, M., J. Org. Chem. **57**, 5730 (1992). FT-ICR.

94RAC/MAR Raczynska, E. D., Maria, P.-C., Gal, J.-F., Decouzon, M., J. Phys. Org. Chem. **7**, 725 (1994). FT-ICR.

83RAK/BOH Rakshit, A. B., Bohme, D. K., Int. J. Mass Spectrom. Ion Phys. **49**, 275 (1983). Flowing afterglow. Bracketing.

84RAK/BOH Raksit, A. B., Bohme, D. K., Int. J. Mass Spectrom. Ion Processes **57**, 211 (1984). Flowing afterglow. Bracketing.

93RAN/POU Ranatunga, T. D., Poutsma, J. C., Squires, R. R., Kenttamaa, H. I., Int. J. Mass Spectrom. Ion Processes **128**, L1 (1993). FT-ICR bracketing.

80REE/FRE Reents, Jr., W. D., Freiser, B. S., J. Am. Chem. Soc. **102**, 271 (1980). ICR. Bracketing.

84REE/MUJ Reents, Jr., W. D., Mujsce, A. M., Int. J. Mass Spectrom. Ion Processes **59**, 65 (1984). Proton transfer equilibrium: SiF_4–N_2 observed; authors state that the proton affinity of SiF_4 is 2 kcal mol^{-1} above that of N_2, but do not give equilibrium constant or describe how entropy change was determined or derived. $GB(CH_3F) < GB(SiF_3OH) - GB(SO_2) < GB(C_2H_4)$.

68REF/CHU Refaey, K. M. A., Chupka, W. A., J. Chem. Phys. **48**, 5205 (1968). Determination of appearance potentials of fragment ions from alcohols.

74REI/BAU Reinke, D., Baumgartel, H., Cvitas, T., Klasinc, T., Gusten, H., Ber. Bunsenges. Phys. Chem. **78**, 1145 (1974).

73REI/KRA Reinke, D., Kraessig, R., Baumgartel, H., Z. Naturforsch. A **28**, 1021 (1973).

93RIC Ricci, A., Org. Mass Spectrom. **29**, 55 (1994). $GB(CH_3NO_3)$ bracketed between $GB(CH_2CF_2)$ and $GB(CH_3OH)$ and close to $GB(CH_3CHCH_2)$.

75RID Ridge, D. P., J. Am. Chem. Soc. **97**, 5670 (1975). ICR. Bracketing.

91RIV/ING Riveros, J. M., Ingemann, S., Nibbering, N. M. M., J. Am. Chem. Soc. **113**, 1053 (1991). ICR study of the reactions $RO^- + C_6H_5X$ (R=H, CH_3, C_2H_5; X=F, Cl, Br, I) lead to the suggestion of $\Delta_f H^0(C_6H_4) = (440 \pm 10)$ kJ mol^{-1}. Compare with 91GUO/GRA.

71ROC/SUT Roche, A. E., Sutton, M. M., Bohme, D. K., Schiff, H. I., J. Chem. Phys. **55**, 5480 (1971). Flowing afterglow, bracketing.

84ROL/HOU Rolli, E., Houriet, R., Spectrosc. Int. J. **3**, 177 (1984). ICR.

82ROS/BUF Rosenstock, H. M., Buff, R., Ferreira, M. A. A., Lias, S. G., Parr, A. C., Stockbauer, R. L., Holmes, J. L., J. Am. Chem. Soc. **104**, 2337 (1982). Appearance potentials of $C_2H_5^+$ and $C_3H_7^+$ from alkyl halides. For more details, see Sec. 3.4 for propene and Sec. 3.8 for ethene. Compare to 82BAE.

77ROS/DRA Rosenstock, H. M., Draxl, K., Steiner, B. W., Herron, J. T., J. Phys. Chem. Ref. Data **6**, Suppl. 1 (1977).

82ROY/MCM Roy, M., McMahon, T. B., Org. Mass Spectrom. **17**, 392 (1982). ICR. Bracketing.

89RUS/BER Ruscic, B., Berkowitz, J., Curtiss, L. A., Pople, J. A., J. Chem. Phys. **91**, 114 (1989). Determined $\Delta_f H^0(C_2H_5^+, 298\text{ K}) = (902 \pm 1.7)$ kJ mol^{-1}, and $PA(C_2H_4, 298\text{ K}) = (680.3 \pm 1.7)$ kJ mol^{-1}.

91RUS/BER Rusic, B., Berkowitz, J., J. Chem. Phys. **95**, 4378 (1991). Mass spectrometric photoion appearance potential measurement.

94RUS/BER Ruscic, B., Berkowitz, J., J. Chem. Phys. **101**, 10936 (1994). Photoionization mass spectrometry. From a measured appearance potential for CH_3CHOH^+ from C_2H_5OH, they deduced $\Delta H_f^0(CH_3CHOH^+, 298\text{ K}) \leq (595.4 \pm 0.9)$ kJ mol^{-1} [(142.3 ± 0.2) kcal mol^{-1}]. Using $\Delta H_f^0(CH_3CHO, 298\text{ K}) = -165.7$ kJ mol^{-1}, they conclude $PA(CH_3CHO) \geq (769.0 \pm 0.9)$ kJ mol^{-1} [(183.8 ± 0.2) kcal mol^{-1}]. The authors further indicate that "although this is rigorously a lower limit, it is very likely close to the true value, since it is based on an appearance potential of a first fragment resulting from a simple bond cleavage."

94RUS/BER2 Ruscic, B., Berkowitz, J., J. Chem. Phys. **101**, 7975 (1994). Estimated $\Delta H_f^0(HNCS^+) \approx 1087$ kJ mol^{-1} (259.8 kcal mol^{-1}). Using $\Delta H_f^0(NCS) < (305.9 \pm 3.3)$ kJ mol^{-1} [(73.1 ± 0.8) kcal mol^{-1}] yields $PA(NCS) \approx 751$ kJ mol^{-1}.

89RUS/SCH Ruscic, B., Schwarz, M., Berkowitz, J., J. Chem. Phys. **91**, 6772 (1989). Photoelectron-photoion coincidence experiment. Appearance energy for the process, $HCOOH = COOH^+ + H + e$, of (12.30 ± 0.02) eV gave $\Delta_f H^0(COOH^+, 0\text{ K}) = (599 \pm 2)$ kJ mol^{-1} [(143.3 ± 0.5) kcal mol^{-1}], using $\Delta_f H^0(HCOOH, 0\text{ K}) = -371.5$ kJ mol^{-1} (-88.79 kcal mol^{-1}) and $\Delta_f H^0(H) = 218$ kJ mol^{-1} (52.1 kcal mol^{-1}). From this, PA of CO_2 of (535.6 ± 2) kJ mol^{-1} [(128.0 ± 0.5) kcal mol^{-1}] at 0 K or (540.6 ± 2) kJ mol^{-1} [(129.2 ± 0.5) kcal mol^{-1}] at 298 K are derived. Compare with 91TRA/KOM.

79SAL/KEB Saluja, P. P. S., Kebarle, P., J. Am. Chem. Soc. **101**, 1084 (1979). HPMS.

86SAN/BAL Santos, I., Balogh, D. W., Doecke, C. W., Marshall, A. G., Paquette, L. A., J. Am. Chem. Soc. **108**, 8183 (1986). ICR. An interlocking thermochemical ladder.

75SCH/BOH Schiff, H. I., Bohme, D. K., Int. J. Mass Spectrom. Ion Phys. **16**, 167 (1975).

80SEN/ABE Senzer, S. N., Abernathy, R. N., Lampe, F. W., J. Phys. Chem. **84**, 3066 (1980). Ion beam scattering apparatus. Bracketing: $GB(C_2D_4) < GB(GeH_4) < GB(CD_3CD{=}CD_2)$, tabulated as bracketed between C_2H_4 and C_3H_6. See also: S. Kohda-Sudoh, S. Ikuta, O. Nomura, S. Katagiri, and M. Imamura, J. Phys. B: At. Mol. Phys. **16**, L529 (1983). The structure of GeH_5^-, is similar to CH_5^- and has C_s symmetry.

84SHA/BLA Sharma, R. B., Blades, A. T., Kebarle, P., J. Am. Chem. Soc. **106**, 510 (1984). HPMS. Entropy changes determined.

81SHA/KEB Sen Sharma, D. K., Kebarle, P., Can. J. Chem. **59**, 1592 (1981). Determination of equilibrium constant of reaction: $C_6H_5CH_2^+ + (CH_3)_3CCl \rightleftarrows (CH_3)_3C^+ + C_6H_5CH_2Cl$.

78SHE/GOB Shea, K. J., Gobeille, R., Bramblet, J., Thompson, E., J. Am. Chem. Soc. **100**, 1611 (1978). Data related to TAFT scale, but specific bases not identified. Data reported as "proton affinities" relative to ammonia: no information given about assumptions concerning entropy change or temperatures. Evaluated gas basicity data based on assumption that original authors simply added measured free energy change values to NH_3 proton affinity. Scale expanded to match the expanded TAFT scale.

97SHE/STE Shea, D. A., Steenvoorden, R. J. J. M., Chen, P., J. Phys. Chem. A **101**, 9728 (1997). PA values indicated as being the result of bracketing measurements, but the bracketing partners are not given.

86SHI/BEA Shin, S. K., Beauchamp, J. L., J. Phys. Chem. **90**, 1507 (1986). ICR. Bracketing.

81SMI/ADA Smith, D., Adams, N. G., Lindinger, W., J. Chem. Phys. **75**, 3365 (1981). SIFT. Bracketing. Also measured IP(HS)=(10.40±0.01) eV; using $\Delta_f H^0(S)=277$ kJ mol^{-1} gives PA(S)=664.3 kJ mol^{-1}.

84SMI/ADA Smith, D., Adams, N. G., Ferguson, E. E., Int. J. Mass Spectrom. Ion Processes **61**, 15 (1984). SIFT measurement of the reaction $C_2H_2^+ + H_2 = C_2H_3^+ + H$ yielded $\Delta H^0 = 6.7$ kJ mol^{-1}. This combined with data in 88LIA/BAR yields a $\Delta_f H^0(C_2H_3^+)=1116.7$ kJ mol^{-1}, which finally yields a $PA(C_2H_2)=641.4$ kJ mol^{-1}.

85SMI/ADA Smith, D., Adams, N. G., J. Phys. Chem. **89**, 3964 (1985). SIFT. Rate constant of proton transfer from HCS^+ to C_2H_5OH is 50% of collision rate constant; rate constant of proton transfer to CH_3SH is 30% of collision rate constant.

94SMI/CHY Smith, R. L., Chyall, L. J., Chou, P. K., Kenttamaa, H. I., J. Am. Chem. Soc. **116**, 781 (1994). FT-ICR bracketing. Title ion generated from ring opened ionized cyclo-butanone by $\cdot CH_2CH_2CH_2CO^+ - CH_2=C=O \rightleftarrows \cdot CH_2CH_2CH_2CH_2CO^+ + CO$.

78SMI/MUN Smith, D. E., Munson, B., J. Am. Chem. Soc. **100**, 497 (1978). Bracketing. $CH_3F < SO_2F_2 < SO_2 < HSO_3F < C_2H_4 H_2O < H_2SO_4 \sim CF_3SO_3H < H_2S$.

93SMI/RAD Smith, B. J., Radom, L., J. Am. Chem. Soc. **115**, 4885 (1993). *Ab initio* calculations at the G2 level.

95SMI/RAD Smith, B. J., Radom, L., J. Phys. Chem. **99**, 6468 (1995). Various *ab initio* procedures compared and evaluated. Tabulated values for each molecule correspond to the most rigorous method applied to that molecule.

75SOL/FIE Solomon, J. J., Field, F. H., J. Am. Chem. Soc. **97**, 2625 (1975). Heats of formation of alkyl ions from hydride transfer equilibria; related to the $\Delta_f H^0(t\text{-}C_4H_9^+) = 711$ kJl/mol and $\Delta_f H^0(\text{iso-}C_4H_{10}) = -134.3$ kJ mol^{-1}. Using $\Delta_f H^0$(2-methyl-2-pentene)$=-66.9$ kJ mol^{-1} and $\Delta_f H^0$(2-methyl pentane)$=-174.1$ kJ mol^{-1} gives PA(2-methyl-2-pentene)=807.8 kJ mol^{-1}. Using $\Delta_f H^0$(2,3-dimethyl-2-butene)$=-69.5$ kJ mol^{-1} and $\Delta_f H^0$(2,3-dimethyl butane)$=176.1$ kJ mol^{-1} gives PA(2,3-dimethyl-2-butene)=813.9 kJ mol^{-1}.

76SOL/FIE Solomon, J. J., Field, F. H., J. Am. Chem. Soc. **98**, 1567 (1976). Hydride transfer equilibrium constant determined for $t\text{-}C_4H_9^+$ and $i\text{-}C_3H_7^+$ with alkyl molecules. Using $\Delta_f H^0(t\text{-}C_4H_9^+)=711$ kJ mol^{-1}, $\Delta_f H^0(C_3H_7^+)=804.3$ kJ mol^{-1}, $\Delta_f H^0(i\text{-}C_4H_{10})=(-134.4\pm0.4)$ kJ mol^{-1} and $\Delta_f H\text{-}C_3H_8)=(-104.6\pm0.4)$ kJ mol^{-1} the following are derived: using $\Delta_f H^0$(1-methyl cyclopentene)$=-4.2$ kJ mol^{-1} and $\Delta_f H^0$(methyl cyclopentane)$=-105.9$ kJ mol^{-1} gives PA(1-methyl cyclopentene)=813.2 kJ mol^{-1}; using $\Delta_f H^0$(norborn-2-ene)$=(87.9\pm4.2)$ kJ mol^{-1} and $\Delta_f H^0$(norbornane)$=(-50.2\pm4.2)$ kJ mol^{-1} gives PA(norbornane)=829.1 kJ mol^{-1}; $\Delta_f H^0(c\text{-}C_5H_{10}) = -78.2$ kJ mol^{-1} and $\Delta_f H^0(c\text{-}C_5H_8)=36.0$ kJ mol^{-1} gives $PA[(c\text{-}C_5H_8)=762.1$ kJ mol$^{-1}]$. Values for *n* $\Delta_f H^0$(2-methyl norbornane) and $\Delta_f H^0$(2-methyl norborn-2-ene) were estimated in the following way. Since the difference $\Delta_f H^0(i\text{-}C_4H_{10})\{=(-134.4\pm0.4)$ kJ mol$^{-1}\}$ $-\Delta_f H^0(C_3H_8)\{=(-104.6\pm0.4)$ kJ mol$^{-1}\}=-30$ kJ mol^{-1}, the difference $\Delta_f H^0(c\text{-}C_5H_9CH_3)\{=(-105.9\pm0.4)$ kJ mol$^{-1}\}-\Delta_f H^0(c\text{-}C_5H_{10})\{=(-78.2\pm0.4)$ kJ mol$^{-1}\}=$ -28 kJ mol^{-1}, and the difference $\Delta_f H^0(c\text{-}C_4H_7CH_3)$ $\{=(-2.9\pm0.4)$ kJ mol$^{-1}\}-\Delta_f H^0(c\text{-}C_4H_8)\{=(28.5\pm0.4)$ kJ mol$^{-1}\}=-31$ kJ mol^{-1}, then the difference $\Delta_f H^0$(2-methyl norbornane)$-\Delta_f H^0$(norbornane)$\{=(-50.2$ $\pm0.4)$ kJ mol$^{-1}\}$ is estimated to be $=-30$ kJ mol^{-1} putting $\Delta_f H^0$(2-methyl norbornane)$=(-80\pm4)$ kJ mol^{-1}. Similarly, since the difference $\Delta_f H^0(i\text{-}C_4H_8)\{=(-16.7$ $\pm0.4)$ kJ mol$^{-1}\}-\Delta_f H^0(C_3H_6)\{=(20.1\pm0.4)$ kJ mol$^{-1}\}=$ -36.8 kJ mol^{-1}, the difference $\Delta_f H^0(c\text{-}C_5H_7CH_3)$ $\{=(-4.2\pm0.4)$ kJ mol$^{-1}\}-\Delta_f H^0(c\text{-}C_5H_8)\{=(36.0\pm0.4)$ kJ mol$^{-1}\}=-40.2$ kJ mol^{-1}, and the difference $\Delta_f H^0$(1-methyl cyclohexene)$\{=(-43.1\pm0.4)$ kJ mol$^{-1}\}$ $-\Delta_f H^0$(cyclo hexene)$\{=(-4.6\pm0.4)$ kJ mol$^{-1}\}=-38.5$ kJ mol^{-1}, then the difference $\Delta_f H^0$(2-methyl norborn-2-ene)$-\Delta_f H^0$(norborn-2-ene)$\{=87.9$ kJ mol$^{-1}\}$ is estimated as -38 kJ mol^{-1}, putting $\Delta_f H^0$(2-methyl norborn-2-ene) $=(50\pm4)$ kJ mol^{-1}. All of this puts PA(2-methyl norborn-2-ene)$=(845\pm6)$ kJ mol^{-1}.

75SOL/HAR Solka, B. H., Harrison, A. G., Int. J. Mass Spectrom. Ion Phys. **17**, 379 (1975). Equilibrium: $CH_3CHOH^+ + CH_3SH$, $\Delta G^0 = -2.1$ kJ mol^{-1}(−0.5 kcal mol^{-1}), $CH_3SH_2^+ + C_2H_5CHO$, $\Delta G^0 = -8.4$ kJ mol^{-1}(−2 kcal mol^{-1}), $CH_3SH_2^+ + (CH_3)_2O$, $\Delta G^0 = -16.7$ kJ mol^{-1}(−4 kcal mol^{-1}).

72SOL/POR Solomon, J. J., Porter, R. F., J. Am. Chem. Soc. **94**, 1443 (1972). Bracketing.

74STA/BEA Staley, R. H., Beauchamp, J. L., J. Am. Chem. Soc. **96**, 6252 (1974). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

74STA/BEA2 Staley, R. H., Beauchamp, J. L., J. Am. Chem. Soc. **96**, 1604 (1974). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

75STA/BEA Staley, R. H., Beauchamp, J. L., J. Chem. Phys. **62**, 1998 (1975). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

76STA/KLE Staley, R. H., Kleckner, J. E., Beauchamp, J. L., J. Am. Chem. Soc. **98**, 2081 (1976). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

77STA/TAA Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., Taft, R. W., J. Am. Chem. Soc. **99**, 326 (1977). ICR. Data related to TAFT scale; temperature assumed to be 320 K.

77STA/WIE Staley, R. H., Wieting, R. D., Beauchamp, J. L., J. Am. Chem. Soc. **99**, 5964 (1977). ICR. Data related to TAFT scale; temperature assumed to be 320 K.

79STE/BEA Stevens, A. E., Beauchamp, J. L., J. Am. Chem. Soc. **101**, 245 (1979). ICR. Bracketing: $CH_3CH=CH_2 < (CO)_5MnCH_3 - CH_3OH < CH_3CHO$.

81STE/BEA Stevens, A. E., Beauchamp, J. L., J. Am. Chem. Soc. **103**, 190 (1981). ICR. Compounds related to gas phase basicity scale, but no experimental details given; (bracketing or equilibrium?). From proton affinity cited here for $(C_5H_5)_2Ni$, also given in (76COR/BEA), it would appear that results given here correspond to the contracted 300 K scale, and therefore the usual correction to 320 has been made. However, there is still an unexplained discrepancy of 1.3 kcal mol^{-1} for $(C_5H_5)_2Ni$ results. Entropy corrections unknown.

80STO/CAM Stone, J. A., Camicioli, J. R. M., Baird, M. C., Inorg. Chem. **19**, 3128 (1980). ICR. Bracketing.

86STO/LI Stone, J. A., Li, X., Turner, P. A., Can. J. Chem. **64**, 2021 (1986). HPMS. Temperature dependence of proton-transfer equilibria.

82STO/SPL Stone, J. A., Splinter, D. E., Kong, S. Y., Can. J. Chem. **60**, 910 (1982). HPMS.

84STO/SPL Stone, J. A., Splinter, D. E., Int. J. Mass Spectrom. Ion Processes. **59**, 169 (1984). Bracketing.

77SUM/POL Summerhays, K. D., Pollack, S. K., Taft, R. W., Hehre, W. J., J. Am. Chem. Soc. **99**, 4585 (1977). ICR. Data related to TAFT scale; temperature assumed to be 350 K.

86SUN/KUL Sunner, J. A., Kulatunga, R., Kebarle, P., Anal. Chem. **58**, 1312 (1986). HPMS measurement of temperature-dependent proton transfer equilibria to obtain ΔG^0, ΔH^0 and ΔS^0 with respect to unspecified bases. Also estimated PA and GB of triethanolamine [102-71-6] to be 975 and 941 kJ mol^{-1}, respectively.

93SUN/SQU Sunderlin, L. S., Squires, R. R., Chem. Phys. Lett. **212**, 307 (1993). Energy-resolved CID used to obtain the dissociation energies of H_2O–NO_2^+ [(61.9±10) kJ mol^{-1}, (14.8±2.3) kcal mol^{-1}] and of CH_3OH–NO_2^+ [(80.3±10) kJ mol^{-1}, (19.2±2.3) kcal mol^{-1}]. Combined with $\Delta_f H^0(H_2O)$ and $\Delta_f H^0(CH_3OH)$ and a revised $\Delta_f H^0(NO_2^+)$ yielded $PA(HNO_3)=(743.5\pm10)$ kJ mol^{-1} and $PA(CH_3NO_3)=(732\pm10)$ kJ mol^{-1}. Compare with 94CAC/ATT.

91SZU/MCM Szulejko, J. E., McMahon, T. B., Int. J. Mass Spectrom Ion Processes **109**, 279 (1991). HPMS and temperature dependence of proton transfer equilibrium constants.

93SZU/MCM Szulejko, J. E., McMahon, T. B., J. Am. Chem. Soc. **115**, 7839 (1993). HPMS and temperature dependence of proton transfer equilibrium constants.

72TAA/HEN Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., Taft, R. W., J. Am. Chem. Soc. **94**, 1369 (1972).

81TAA/SUM Taagepera, M., Summerhays, K. D., Hehre, W. J., Topsom, R. D., Pross, A., Radom, L., Taft, R. W., J. Org. Chem. **46**, 891 (1981). ICR. See comments under TAFT.

TAFT ICR. Unpublished compiled list of values of gas phase basicities measured by several workers, notably including Taft, R. W., McIver, R., Hehre, W. J., and co-workers. Here referred to as the "TAFT list". Most of the data given on the list have been published elsewhere, and are listed here with the appropriate reference. (See: 75ARN, 72ARN/JON, 76COO/KAT, 82DEF/HEH, 80DEF/MCI, 76DEV/WOL, 74HEH/MCI, 72HEN/TAA, 79LOC/HUN, 83MCI, 82PAU/HEH, 82PAU/HEH(2), 82PIE/HEH, 82PIE/HEH(2), 79PIE/POL, 77POL/DEV, 80POL/HEH, 81POL/RAI, 77POL/WOL, 77SUM/POL, 75TAF, 83TAF, 73TAF/TAA, 77WOL/ABB, 75WOL/HAR, 77WOL/STA). Values cited as "TAFT" either have not been published, or the publication has not been identified for the current compilation. All data from these various publications have been assumed to have been taken at 320 K, rather than the originally reported 300 K (R. W. Taft, personal communication). As a result of the uncertainty in the actual temperature(s) at which measurements were made, and the great length of the free energy scale represented by these results, there may be some uncertainty in the length of the scale. To minimize this problem, sections of the scale have been related to local standards (i.e., H_2O, isobutene) wherever possible. Occasionally thermochemical scales from other laboratories have been related by the subsequent authors to this base scale; when this is the case, the notation given here is "Related to TAFT scale".

86TAFT Taft, R. W., Personal communication. A list (dated 10/9/86) of relative gas phase basicities of 310 compounds determined at the Department of Chemistry, University of California, Irvine, by R. W. Taft and collaborators. The list was submitted by R. W. Taft for inclusion in this update of proton affinity data. Experimental details of reference bases used in the measurements were not included. Many of the data have been published, or appeared in our 1984 published compilation of proton affinity data. Values appearing here represent only those species for which Taft *et al.* have revised their own earlier values, or for which determinations from the Irvine laboratory were not available previously. It is assumed that these data supersede any earlier values from this laboratory.

75TAF Taft, R. W., "Gas Phase Proton Transfer Equilibria", in "Proton Transfer Reactions," E. F. Caldin and V. Gold, Editors, p. 31 (1975). ICR. Data as reported corrected to 320 K. See comments under TAFT.

83TAF Taft, R. W., Prog. Phys. Org. Chem. **14**, 248 (1983). ICR. See comments under TAFT. Temperature correction of scale from 300 to 320 K were included in this 1983 review of the body of data referred to here as "TAFT scale".

86TAF/ANV Taft, R. W., Anvia, F., Taagepera, M., Catalan, J., Elguero, J., J. Am. Chem. Soc. **108**, 3237 (1986). ICR.

86TAF/GAL Taft, R. W., Gal, J.-F., Geribaldi, S., Maria, P.-C., J. Am. Chem. Soc. **108**, 861 (1986). ICR.

73TAF/TAA Taft, R. W., Taagepera, M., Summerhays, K. D., Mitsky, J., J. Am. Chem. Soc. **95**, 3811 (1973). ICR. See comments under TAFT.

78TAF/TAA Taft, R. W., Taagepera, M., Abboud, J. L. M., Wolf, J. F., DeFrees, D. J., Hehre, W. J., Bartmess, J. E., McIver, Jr., R. T., J. Am. Chem. Soc. **100**, 7765 (1978). Table I lists free energy changes for proton transfer relative to methanol. (Although data are cited as coming from 77WOL/STA, several compounds appear here that did not appear in that paper.) Data here corrected to 320 K and related to local standards.

78TAF/WOL Taft, R. W., Wolf, J. F., Beauchamp, J. L., Scorrano, G., Amett, E. M., J. Am. Chem. Soc. **100**, 1240 (1978). ICR. See comments under TAFT.

95TAN/ISB Tang, M., Isabel, J., Hodges B., Brodbelt, J., J. Mass Spectrom. **30**, 977 (1995). Ion trap mass spectrometer. Results of semi-empirical AMI calculations suggest that the proton is bridged by both the $-NH_2$ and $-COOH$ groups in o-isomer, is on the $-NH_2$ group in the m-isomer and is on the $-COOH$ group on the p-isomer.

76TAN/LIA Tang, I. N., Lian, M. S., Castleman, Jr., A. W., J. Chem. Phys. **65**, 4022 (1976). HPMS measurement of the equilibrium $Sr^+H_2O \rightleftarrows SrOH_2^+$ yielded $\Delta H^0 = -144.3$ kJ mol^{-1} (-34.5 kcal mol^{-1}) and $\Delta S^0 = -131$ J (mol K)$^{-1}$ (-31.1 cal (mol K)$^{-1}$). Using $\Delta_f H^0(SrOH) = -184.1$ kJ mol^{-1}, $\Delta_f H^0(Sr^+) = 712.6$ kJ mol^{-1}, $S^0(Sr^+) = 170.4$ J (mol K)$^{-1}$ and $S^0(SrOH) = 246.4$ J (mol K)$^{-1}$ gives PA(SrOH) = 1019.4 and $\Delta S_p = -18$ J (mol K)$^{-1}$.

78TAN/MAC Tanaka, K., Mackay, G. I., Bohme, D. K., Can. J. Chem. **56**, 193 (1978). Flowing afterglow.

89TIC/JAV Tichy, M., Javahery, G., Twiddy, N. D., Ferguson, E. E., Int. J. Mass Spectrom. Ion Processes **93**, 165 (1989). ΔH^0 and ΔS^0 values for proton-transfer reactions obtained from "van't Hoff" plots of ratios of forward and reverse rate constants versus reciprocal average center of mass kinetic energies in a selected-ion flow drift tube.

79TIE/AND Tiedemann, P. W., Anderson, S. L., Ceyer, S. T., Hirooka, T., Ng, C. Y., Mahan, B. H., Lee, Y. T., J. Chem. Phys. **71**, 605 (1979). Appearance energies of fragment ions from molecular clusters.

84TOL/BEA Tolbert M. A., Beauchamp, J. L., J. Am. Chem. Soc. **106**, 8117 (1984). Heat of formation of ScH^+ through determination of onset energies of the endothermic reaction $Sc^+ + H_2 = ScH^+ + H$. Using IP(Sc) = (6.56144 ±0.00006) eV gives PA(Sc) = 907.5 kJ mol^{-1}.

89TOM/ABB Tomas, F., Abboud, J.-L. M., Laynez, J., Notario, R., Santos, L., Nilsson, S. O., Catalan, J., Claramunt R. M., Elguero, J., J. Am. Chem. Soc. **111**, 7348 (1989). ICR.

81TRA Traeger, J. C., Org. Mass Spectrosc. **16**, 193 (1981). Appearance potential of sec-$C_4H_9^+$ from halogenated butanes, and correction to 298 K.

85TRA Traeger, J. C., Org. Mass Spectrom. **20**, 223 (1985). Appearance potential determinations of $C_3H_5O^+$ by photoionization mass spectrometry.

85TRA2 Traeger, J. C., Int. J. Mass Spectrom. Ion Processes **66**, 271 (1985). AE measurements for HCO^+ derived from H_2CO, CH_3CHO, C_2H_5CHO, glyoxal and HCOOH. A value of $\Delta_f H^0(HCO^+, 298\ K) = (825.6 \pm 2.7)$ kJ mol^{-1} is deduced from the formation of HCO^+ from HCOOH, yielding PA(CO) = (594 ± 3) kJ mol^{-1}.

96TRA Traeger, J. C., Rapid Commun. Mass Spectrom. **10**, 119 (1996). Threshold photoionization mass spectrometry. Determined $\Delta_f H^0(t\text{-}C_4H_9^+, 298\ K) = (711.4 \pm 1.1)$ kJ mol^{-1}, yielding PA(i-C_4H_8) = (801.7 ± 1.4) kJ mol^{-1}.

93TRA/HOL Traeger, J. C., Holmes, J. L., J. Phys. Chem. **97**, 3453 (1993). Photoionization mass spectrometric appearance energy of CH_2OH^+ from CH_3OH as 11.578 eV.

91TRA/KOM Traeger, J. C., Kompe, B. M., Org. Mass Spectrom. **26**, 209 (1991). Dissociative photoionization mass spectrometry of HCOOH and CF_3COOH used to obtain $\Delta_f H^0(COOH^+, 298\ K) = (600 \pm 3)$ kJ mol^{-1} [(143.5 ±0.7) kcal mol^{-1}] from appearance energy measurements (12.31 eV for HCOOH and 11.82 eV for CF_3COOH) and using the following ΔH_f^0 values at 298 K: HCOOH, -378.7 kJ mol^{-1}; H, 218 kJ mol^{-1}; CF_3COOH, -1030.5 kJ mol^{-1} and CF_3, -460.2 kJ mol^{-1}. Compare with 89RUS/SCH.

81TRA/MCL Traeger, J. C., McLoughlin, R. G., J. Am. Chem. Soc. **103**, 3647 (1981). Appearance potentials of CH_3^+, $C_2H_5^+$, sec-$C_3H_7^+$, and t-$C_4H_9^+$: evaluation and correction to 298 K.

82TRA/MCL Traeger, J. C., McLoughlin, R. G., Nicholson, A. J. C., J. Am. Chem. Soc. **104**, 5318 (1982). Appearance potentials of CH_3CO^+ ions; correction to 298 K.

86TRA/MUN Tran, V. T., Munson, B., Org. Mass Spectrom. **21**, 41 (1986). HPMS. Bracketing.

78TSA Tsang, W., Int. J. Chem. Kinet. **10**, 41 (1978). Heats of formation of benzyl, tert-butyl radicals.

79VAJ/HAR Vajda, J. H., Harrison, A. G., Int. J. Mass Spectrom. Ion Phys. **30**, 293 (1979). HPMS.

85VAN/LEA Vandiver, V. J., Leasure, C. S., Eiceman, G. A., Int. J. Mass Spectrom. Ion Proc. **66**, 223 (1985). Ordering of proton affinities from ion mobility measurements (non-quantitative): Benzophenone~Pyrene>Anthracene >Phenanthrene>Acetophenone>Naphthalene>Benzene. (The ordering derived from equilibrium constant measurements is: Benzophenone>Anthracene>Pyrene >Acetophenone>Phenanthrene>Naphthalene>Benzene.)

82VIL/FUT Villinger, H., Futrell, J. H., Howorka, F., Duric, N., Lindinger, W., J. Chem. Phys. **76**, 3529 (1982).

75VOG/BEA Vogt, J., Beauchamp, J. L., J. Am. Chem. Soc. **97**, 6682 (1975). ICR. Bracketing.

84WAL/BLA Walters, E. A., Blais, N. C., J. Chem. Phys. **80**, 3501 (1984).

78WAN/DES Wang, J.-S., DeStefano, A. J., Porter, R. F., Inorg. Chem. **17**, 1374 (1978). HPMS. Bracketing.

74WAR Wameck, P., Z. Naturforsch. **29a**, 350 (1974).

88WEB/HOU Weber, J., Houriet, R., J. Phys. Chem. **92**, 5926 (1988). ICR study of proton transfer equilibria. *Ab initio* calculations suggest that protonation occurs on the chalcogen atom in each case.

85WEI/PLA Weil, D. A., Platzner, I., Miller, L. L., Dixon, D. A., Org. Mass Spectrom. **20**, 115 (1985). ICR. Bracketing. GB(C_2H_4)<GB(COS)<GB(H_2O). GB(COS)<GB(CS_2) –GB(H_2S)<GB(CH_3CCH): This basicity value for CS_2 is in good agreement with the value one would predict for a temperature of 320 K from the results of 77MAU/FIE.

79WIB/FIS Wiberg, N., Fischer G., Bachhuber, H., Z. Naturforsch. **34b**, 1385 (1979). Ionization and appearance potentials in HN=NH, $H_2N{=}N$, and N_2H_4.

80WIG/BEA Wight, C. A., Beauchamp, J. L., J. Phys. Chem. **84**, 2503 (1980). ICR: Related to TAFT scale; temperature corrected to 320 K.

76WIL/LEB Williamson, A. D., LeBreton, P. R., Beauchamp, J. L., J. Am. Chem. Soc. **98**, 2705 (1976). Thermochemical cycles based on appearance potentials of CH_2CFX^+ and CH_3CFX (X=H,F) from CH_3CFXCH_3, and IP(CH_2CFX). Measured AE($CH_3CHFCH_3 \rightarrow CH_3CHF^+ + CH_3 + e^-$) = 11.75 eV and AE($CH_3CHFCH_3 \rightarrow CH_2CHF^+ + CH_4 + e^-$) = 11.53 eV; combining these quantities with IP(CH_2CHF) = 10.363 eV and $D_e(CH_3{-}H) = 438.1$ kJ mol^{-1} yields PA(CH_2CHF) = 729 kJ mol^{-1}. Measured AE($CH_3CF_2CH_3 \rightarrow CH_3CF_2^+ + CH_3 + e^-$) = 11.81 eV and AE($CH_3CF_2CH_3 \rightarrow CH_2CF_2^+ + CH_4 + e^-$) = 11.57 eV; combining these quantities with IP(CH_2CF_2) = 10.29 eV gives PA(CH_2CF_2) = 734 kJ mol^{-1}.

76WIL/LOS Willis, C., Lossing, F. P., Back, R. A., Can. J. Chem. **54**, 1 (1976). Heat of formation of N_2H^+ as a fragment ion in N_2H_2.

75WIL/MCC Wilson, M. S., McCloskey, J. A., J. Am. Chem. Soc. **97**, 3436 (1975). HPMS. Bracketing: All compounds bracketed relative to NH_3, CH_3NH_2, $(CH_3)_2NH$, and $(CH_3)_3N$.

88WLO/ROD Wlodek, S., Rodriquez, C. F., Lien, M. H., Hopkinson, A. C., Bohme, D. K., Chem. Phys. Lett. **143**, 385 (1988). Selected ion flow tube measurement. An approximate empirical relationship between reaction efficiency and ΔG^0 suggested that proton transfer from $SiNH_2^-$ to NH_3 was close to isoergic. Also observed no proton transfer from $SiNH_2^-$ to $(CH_3)_2S$ nor $(CH_3)_2CO$.

77WOL/ABB Wolf, J. F., Abboud, J. L. M., Taft, R. W., J. Org. Chem. **42**, 3316 (1977). ICR. Results given in figure form.

76WOL/DEV Wolf, J. F., Devlin, J. L., DeFrees, D. J., Taft, R. W., Hehre, W. J., J. Am. Chem. Soc. **98**, 5097 (1976).

90WOL/GRU Wolf, R., Grutzmacher, H. F., New J. Chem. **14**, 379 (1990). FT-ICR. GB values obtained from proton-transfer equilibria at an assumed temperature of 320 K.

75WOL/HAR Wolf, J. F., Harch, P. G., Taft, R. W., J. Am. Chem. Soc. **97**, 2904 (1975). ICR: Related to TAFT scale. Data corrected from 300 to 350 K.

77WOL/STA Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, Jr., R. T., Beauchamp, J. L., Taft, R. W., J. Am. Chem. Soc. **99**, 5417 (1977). ICR. Data corrected from 300 to 350 K (R. W. Taft, personal communication).

92WU/FEN Wu, Z., Fenselau, C., Rapid Commun. Mass. Spectrom. **6**, 403 (1992). PA(arginine) reported using the kinetic method employing 1,1,3,3-tetramethylguanidine (TMG), 1,5-diazabicyclo[4.3.0]non-5-ene (DBN) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as reference bases. The relevant rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation.

92WU/FEN2 Wu, Z., Fenselau, C., J. Am. Soc. Mass Spectrom. **3**, 863 (1992). Proton affinities are reported from measured dissociation kinetics of proton-bound dimers. The relevent rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation. The results are tabulated as GB values at an unknown effective temperature.

93WU/FEN Wu, Z., Fenselau, C., Tetrahedron **49**, 9197 (1993). GB values obtained from MIKE measurements and by applying the kinetic method. The relevent rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation. GB values are reported at unknown effective T.

94WU/FEN Wu, Z., Fenselau, C., Rapid Commun. Mass Spectrom. **8**, 777 (1994). Kinetic method. As much as possible, the relevent rate data were reanalyzed using the current PA values of reference bases as determined in this present evaluation. ΔS_p values also determined.

93WU/LEB Wu, J., Lebrilla, C. B., J. Am. Chem. Soc. **115**, 3270 (1993). ICR bracketing. Also molecular orbital calculations using the semi-empirical AM1 package.

73YAM/KEB Yamdagni, R., Kebarle, P., J. Am. Chem. Soc. **95**, 3504 (1973). HPMS.

76YAM/KEB Yamdagni, R., Kebarle, P., J. Am. Chem. Soc. **98**, 1320 (1976). HPMS. Data assumed to have been superseded by data in 79LAU, when species studied have been duplicated. Other data corrected to 79LAU scale; free energy change values multiplied by 1.05.

96ZHA/STO Zhang, W., Stone, J. A., Brook, M. A., McGibbon, G. A., J. Am. Chem Soc. **118**, 5764 (1996). HPMS.

93ZHA/ZIM Zhang, K., Zimmerman, D. M., Chung-Phillips, A., Cassady, C. J., J. Am. Chem. Soc. **115**, 10812 (1993). FT-ICR. Bracketing by gas-basicity. Calculations indicate glycine protonates at the amino group and that diglycine protonates on N-terminal amino group with H bonding to carbonyl of amide moiety.