Evaluated Gas Phase Basicities and Proton Affinities of Molecules; Heats of Formation of Protonated Molecules

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The available data on gas phase basicities and proton affinities of molecules are compiled and evaluated. Tables giving the molecules ordered (1) according to proton affinity and (2) according to empirical formula, sorted alphabetically are provided. The heats of formation of the molecules and the corresponding protonated species are also listed.

Key words: basicity, heats of formation, ion-molecule reaction, proton affinity, proton transfer.

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1. Introduction

1.1. Definitions

The gas phase basicity and proton affinity of a molecule, M, are both defined in terms of the hypothetical reaction:

$$M + H^+ \rightarrow MH^+. \qquad (1)$$

The gas phase basicity is the negative of the free energy change associated with this reaction, while the proton affinity is the negative of the corresponding enthalpy change.

1.2. Proton Affinities and Gas Phase Basicities: An Overview

Proton transfer reactions are of considerable importance in chemistry. Acid-base reactions have been studied extensively in solution for decades, but it is only in the past twenty years or so that experimental techniques have been devised to permit the quantitative study of the thermochemistry of proton transfer reactions in the gas phase. Particularly in the years since 1971, when the first gas phase ion-molecule equilibrium studies on proton transfer appeared, there has been a burgeoning of data in the literature, and consequently, a great interest in using information from such gas phase studies to distinguish between the chemical effects of solvation and the effects of intrinsic molecular properties. To date, although several excellent reviews of this active field of research have appeared[1-7], and two unevaluated compilations of data are available[8-9], there was, until the current publication, no single reference which presented a comprehensive collection of data on gas phase proton affinities evaluated for internal consistency.

The vast majority of proton affinities presented here are based on measurements of the equilibrium constants of gas phase proton transfer reactions:

$$MH^+ + N \rightleftharpoons NH^+ + M \qquad (2)$$

where:

$$-RT \ln K_{eq} = \Delta G_{Rn} = \Delta H_{Rn} - T\Delta S_{Rn} \qquad (3)$$

and the equilibrium constant for reaction 2 is obtained from a mass spectrometric observation of the relative abundances of equilibrated ions, MH^+ and NH^+, in a mixture of known composition of compounds M and N:

$$K_{eq} = [NH^+]/[MH^+]\cdot[M]/[N] \qquad (4)$$

The observed equilibrium constant of reaction 2 directly leads to a value for the Gibbs free energy change of reaction, which represents the relative gas phase basicities of compounds M and N; if the entropy change of the reaction is determined, or can be reliably estimated, a value for the enthalpy change of reaction, or relative proton affinity, is obtained. Thus, the extensive scales of data presented here based on equilibrium constant measurements provide relative gas phase basicities and relative proton affinities, but do not directly give any information about absolute values of proton affinities, i.e., about the actual enthalpy changes of reaction 1 for the various compounds. Absolute values must be assigned based on some comparison standard incorporated in the thermochemical ladder for which heats of formation of both M and MH^+ are independently available. These species will necessarily be limited to those for which an MH^+ ion of known structure can be generated in a mass spectrometer, so that a reliable independent gas phase heat of formation will be known.

Thus, it must be emphasized that for data derived from equilibrium constant measurements, absolute values for proton affinities cited by authors depend on the proton affinity value selected for a comparison standard, and these may vary considerably from year to year, and from paper to paper. (For example, proton affinities varying from 202 kcal/mol to 210 kcal/mol have been cited for ammonia, which is often used as a comparison standard for scales of proton affinities). Although researchers working in the field are usually acutely aware of these arbitrary fluctuations in absolute values assigned to gas phase proton affinities, workers in related fields who seek to use these data often fall unwarily into the trap of using proton affinities from the literature without realizing that the experimental results actually lead only to relative thermochemical relationships, and that the absolute values assigned to proton affinities may have changed because of subsequent re-evaluations of the thermochemistry of a primary standard. The current publication seeks to provide a complete and internally-consistent set of gas phase proton affinity values based mainly on the vast body of data generated by equilibrium constant measurements, and to assign absolute values to the resulting proton affinity scale using the best current information about the thermochemistry of positive ions, imposing the requirement of internal consistency.

2. Types of Experiment Leading to Proton Affinity/Gas Basicity Data

In this compilation, as discussed above, most of the information is derived from scales of relative values for the gas basicities and proton affinities, based on (1) measurements of equilibrium constants of proton transfer reactions, or (2) use of the so-called "bracketing" technique. Absolute values are assigned to the scale using certain primary standards (discussed in detail below), whose position in the proton affinity scale is known and for which well-established values of the heats of formation of both M and MH^+ are available.

2.1. Absolute Proton Affinity Values from Ionization Thresholds

Experiments in which the heat of formation of MH^+ is determined lead directly to values for the proton affinity when combined with a heat 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^+ exists as a fragmentation product from some larger molecular species, absolute values for the heat of formation of MH^+ may be obtained through determinations of the ionization potential of MH:

$$MH \rightarrow MH^+ + e, \tag{5}$$

or the appearance potential of MH^+ from a larger molecule:

$$N \rightarrow MH^+ + A + e. \tag{6}$$

Because the heats of formation of MH^+ are known from ionization potential or appearance potential determinations, such "absolute" proton affinity determinations are labelled "Threshold Value" in Table 1. Such absolute values for proton affinities are available for only a very few species of the 780 compounds on which data is reported here, largely because in most cases the neutral MH molecule does not exist, and the energetics of formation of an MH^+ ion of the required structure in ionic fragmentation processes is not reliably established.

2.2. Proton Affinity Values from Thermochemical Information Derived from Hydride Transfer Equilibrium Constant Determinations

Values for heats of formation of a number of carbonium ions, $C_nH_{2n+1}{}^+$, are known from measurements of hydride transfer equilibrium constants in alkane mixtures:

$$C_nH_{2n+1}{}^+ + C_mH_{2m+2} \rightleftharpoons C_nH_{2n+2} + C_mH_{2m+1}{}^+. \tag{7}$$

In systems for which the heats of formation of three reactant species have been independently established, the heat of formation of the fourth can be determined. Since a knowledge of the heat of formation of the $C_mH_{2m+1}{}^+$ carbonium ion can be used to calculate an absolute proton affinity value for the corresponding olefin, C_mH_{2m}, several values based on hydride transfer equilibria are also included in the compilation; the heats of formation of ions from such experiments are all related to the heat of formation of the tert-butyl ion as a primary standard. (See below for a discussion of the heat of formation of this standard.)

2.3. Relative Gas Basicity Values from Proton Transfer Equilibrium Constants

During the past decade, there has been extensive use of gas phase ion-molecule equilibrium constant measurements to establish the relative basicities of chemical compounds in the absence of solvent effects. In these studies, carried out in a number of laboratories using mainly high pressure mass spectrometry, ion cyclotron resonance spectroscopy, and flowing afterglow experiments, the equilibrium constants associated with proton transfer reactions such as (2) are measured, yielding the relative gas basicities of M and N from the free energy change associated with the reaction at a given temperature (Eq. 3). If assumptions are made about the entropy changes associated with reaction 2, or if experimental determinations of the entropy change have been made (Sec. 3.1.1), values for relative gas phase basicities obtained in this way can be translated into scales of relative proton affinities. Although these equilibrium constants are determined mass spectrometrically at pressures of 10^{-6} torr to approximately 1 torr, there is abundant evidence[1-7] that thermodynamic equilibrium is achieved in this type of experiment.

2.4. Relative Gas Basicity/Proton Affinity Values from "Bracketing"

There are certain species for which measurements of equilibrium constants for proton transfer reactions are difficult or impossible. These include free radicals and species for which the MH^+ ion undergoes fast reactions with M or alternate reaction channels with N. In these cases, the basicity is usually estimated using the technique known as "bracketing". In this approach, one reacts MH^+ with a series of bases, observing whether or not proton transfer occurs:

$$MH^+ + B_1 \rightarrow B_1H^+ + M, \tag{8}$$

$$MH^+ + B_2 \rightarrow \text{No proton transfer.} \tag{9}$$

The basicity of M is assumed to lie between those of B_1 and B_2, and where these species have known gas basicity values, a value can be assigned to M. Results obtained through bracketing experiments are generally less reliable than those obtained through other methods because of numerous possible complications. For instance, exothermic proton transfer reactions sometimes do not occur when there is an energetically favorable alternate channel open to the reactants. Furthermore, endothermic proton transfer reactions can be observed if the reaction has a negative Gibbs free energy change, or if the reaction is not endothermic by more than ~8 kJ/mol (~2 kcal/mol). Finally, if there are several isomeric structures of B_1H^+, the observed proton transfer reaction may involve a rearrangement of the B_1 or B_1H^+ species in the reaction complex to a more stable structure, so that the observed "bracketing" does not necessarily reflect the thermochemistry of a straightforward or even unique proton transfer reaction.

2.5. Other Sources of Proton Affinity/Gas Basicity Data

The compilation includes a few pieces of data originating from measurements which do not fall into any of the above categories. Quantitative information about relative proton affinities has 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 constants. Also, determinations of the equilibrium constants of processes such as:

$$B + AH^+ \rightleftharpoons ABH^+ \tag{10}$$

lead to values of heats of formation of the condensation or association ions, ABH^+, if the heats of formation of AH^+ and B are known; this information can then be used to derive the proton affinity of AB.

Qualitative information about relative proton affinities has been derived from observations of the modes of dissociation of $(ABH)^+$ ions into $(AH^+ + B)$ or $(BH^+ + A)$; a semi-quantitative relationship between the ratios of the two product ions and relative proton affinities has been reported[10].

3. Description of the Evaluation

3.1. Thermodynamic Ladders

In the compilation of gas phase basicity and proton affinity data presented here, the available thermodynamic ladders giving relative gas phase basicities of series of compounds were made the initial basis for the evaluation, using consistency between sets of data from different laboratories and matching of the intervals of the scale with those predicted from widely separated primary standards as the criteria for judgement. To minimize problems due to uncertainties in the temperature at which measurements were made, the thermodynamic ladders were related to as many local standards over the course of the scale as possible. Results obtained from "bracketing" experiments were then related to the evaluated scale. A specific example of this procedure and the mode of presentation in Table 1 is given in Sec. 5.1. Finally, the experimentally-determined scale of relative gas basicities was translated into a scale of proton affinities by evaluating the entropy change associated with reaction 1.

3.1.1. Entropy Changes

For most polyatomic species, the entropy change of the half reaction ($M \rightarrow MH^+$) was estimated by making the usual simplifying assumption[1-7] that this quantity can be adequately approximated by the expression:

$$\Delta S = R \ln[\sigma(M)/\sigma(MH^+)] \tag{11}$$

(where $\sigma(M)$ and $\sigma(MH^+)$ are the rotational symmetry numbers of M and MH^+). The use of this expression is obviously inexact, in some cases enough so that a more exact calculation of the entropy change from the complete partition function is warranted. This is especially true for species in which internal rotations are lost or gained upon protonation, or in which there is a significant difference in the moments of inertia of the protonated and unprotonated species. In such cases, the entropy change was calculated from the complete partition function. In all cases for which experimental entropy change determinations of reaction 2 have been made, the experimental results were made the basis of the evaluation of the relevant entropy changes.

3.1.2. Temperature

Several of the data sets constituting the backbone thermodynamic ladder for Table 1 are very extensive, covering energy ranges of up to 300 kJ/mol (72 kcal/mol). Uncertainties of only a few percent in the operating temperature used in the original experiments may translate into differences of tens of kJ (or several kcal) in the absolute values assigned to gas basicities or proton affinities when applied across such an energy range relative to a single absolute standard. One must be particularly aware of this problem in dealing with data sets from ion cyclotron resonance experiments originally reported to have been carried out at "300 K". More recent work has shown that unless special precautions are taken, the operating temperature of an ICR cell at "ambient" temperature is higher than 300 K by 20 to 50 degrees. In such cases, the free energy changes originally calculated from the observed equilibrium constant (Eq. 3) have been corrected by multiplying by T(corrected)/300. Where such changes in the original data have been made, the magnitude of the correction factor is indicated in the notes under the literature citation. A comparison of data from these sets with analogous results from experiments in which the temperature was measured generally confirms that the magnitudes of these corrections are at least approximately correct. (It is obvious that for the data sets considered here, the distinction between "300 K" and the temperature corresponding to STP conditions, 298.15 K, is essentially irrelevant; the two numbers, 298 and 300, will be used in this discussion and in the tables essentially interchangably, depending mainly on which number was used in a particular paper.)

3.2. Assignment of Absolute Values to the Scale: Reference Standards

Although absolute values have been assigned to the relative proton affinity scale here, these values can be considered really well-established only for the lower part of the scale (i.e., for proton affinities lower than about 750 kJ/mol or 180 kcal/mol), which is based on numerous primary comparison standards. The upper part of the scale is based primarily on the proton affinity of isobutene, which in turn depends on the heat of formation of the tert-butyl ion; other standards, which appear to give a consistent assignment to the scale, are ketene and ammonia. However, none of these standards can be considered to have a firmly-enough established proton affinity that it can be stated with certainty that future variations in absolute assignments will not occur.

To minimize problems due to uncertainties in the temperature, long thermodynamic ladders have been related to as many local standards over the course of the scale as possible. In such cases, the same data are listed twice in Table 1, once as originally reported and a second time in evaluated form, as described in more detail in Sec. 5.1. Similarly, in the single thermodynamic ladder available for the low end of the scale (H_2 to C_2H_6), in agreement with an evaluation of these data from the laboratory where the original work was done[11], we have chosen to relate segments of the scale to well-established local standards, rather than accept the originally-reported relationships between widely separated portions of the scale.

In the following section, we present details of the evaluations of the proton affinities of the compounds which served as the primary standards for assigning absolute values to the gas basicity and proton affinity scales. In this process, for all but the lowest part of the scale (H_2 to C_2H_6), the greatest weight was given to the proton affinities of ethylene, propylene, and isobutene. The heats of formation of $C_2H_5^+$ and $CH_3C^+HCH_3$ have been carefully studied in numerous laboratories, and are now rather well established. The heat of formation of the tert-butyl ion is somewhat less well established, but recent evaluations of this heat of formation give a proton affinity value for isobutene which is in fairly good agreement with information from other comparison standards in the immediate vicinity in the scale (ketene and ammonia). The relevant heats of formation, and evaluated 300 K proton affinity values of the standard compounds are summarized in Sec. 3.3. It should be noted that the heats of formation of positive ions cited here are given using the so-called "stationary electron convention" commonly used by mass spectrometrists[12], and described in detail below (Sec. 5.2.1).

3.2.1. Ammonia

For reasons which appear to have more to do with tradition than with science, the scale of gas phase proton affinities is often related to the proton affinity of ammonia as a standard. This proton affinity is defined by the reaction:

$$NH_3 + H^+ \rightarrow NH_4^+. \quad (12)$$

An experimental determination of the heat of formation of NH_4^+ based on its appearance energy from a $(NH_3)_2$ dimer[13]:

$$(NH_3)_2 \rightarrow NH_4^+ + NH_2 + e. \quad (13)$$

leads to a value of the proton affinity of ammonia of 846.3 kJ/mol (202.3 kcal/mol) at 0 K, and assuming that all rotational degrees of freedom are excited and that no vibrational degrees of freedom are excited at 298 K, this corresponds to a value of 852 kJ/mol (203.6 kcal/mol) for the proton affinity of ammonia at 298 K. Although the authors of that paper cite error limits of ±5 kJ/mol (1.3 kcal/mol) for this value of the proton affinity, an examination of the error limits associated with the appearance energy measurement (±2 kJ/mol or 0.5 kcal/mol), the heat of formation of NH_2 (±12 kJ/mol or 3 kcal/mol) and the assumed well depth for formation of the $(NH_3)_2$ dimer (±4 kJ/mol or 1 kcal/mol) leads one to assign error limits of at least ±13 kJ/mol (3.2 kcal/mol) to this value. Substitution of the dimer well depth used in reference 13 (-14.6 kJ/mol or 3.5 kcal/mol) with a value from a more recent ab initio calculation[14] (-7.9 kJ/mol or 1.9 kcal/mol) leads to a modification of the proton affinity derived from this experimental result to a value of 845 kJ/mol (202.0 kcal/mol). More direct ab initio calculations of the proton affinity of ammonia[15,16] lead to values of 858 kJ/mol (205.0 kcal/mol) and 879 kJ/mol (210 kcal/mol), respectively.

In fact, the exact value for the proton affinity of ammonia is of less importance than it is usually accorded, since the position of ammonia in the scale of relative gas phase basicities is not well established. In fact results from various laboratories show considerable variation in measurements involving this molecule. For instance, relative to the proton affinity of isobutene, one would assign values for the proton affinity of ammonia ranging from 851 to 858 kJ/mol (203.5 to 205.0 kcal/mol), depending on which set of measurements one selected. (Although this range is not really large in terms of absolute quantities, the reproducibility of measurements of proton transfer equilibrium constants often allows one to assign error limits of <0.4 kJ/mol (0.1 kcal/mol) to any particular directly-measured interval in the free energy scale. The apparently poor quality of the measurements involving this compound is easy to rationalize, since ammonia tends to adsorb on surfaces making accurate pressure measurements difficult.) The selected value for the proton affinity of ammonia, 853.5 kJ/mol (204.0 kcal/mol), which is in good agreement with the experimental determination[13] and one theoretical calculation[15], is an intermediate value taken from the several thermochemical ladders which have been reported relating the proton affinity of ammonia to that of the primary standard isobutene. Because the agreement between the different thermochemical scales is generally good except for the position of ammonia, the exact value of the proton affinity of ammonia was given little weight in carrying out the evaluation reported here. This proton affinity was treated as a secondary standard, and, in fact, was allowed to "float" relative to the rest of the scale in evaluating different data sets, in order to maintain the overall agreement between the different experimentally-determined thermodynamic ladders.

The entropy change associated with the half reaction ($NH_3 \rightarrow NH_4^+$) is -7.5 J/mol K (-1.8 cal/mol K), calculated from the complete partition function. This leads to a value of 818 kJ/mol (195.6 kcal/mol) for the 300 K gas phase basicity.

3.2.2. Ketene

The proton affinity is defined by the reaction:

$$CH_2{=}C{=}O + H^+ \rightarrow CH_3CO^+. \qquad (14)$$

A recent determination[17] of the heat of formation of CH_3CO^+ at 298 K led to a value of 657 kJ/mol (157 kcal/mol). Accepting a value of -47.7 kJ/mol (-11.4 kcal/mol) for the heat of formation of ketene[18], this would correspond to a proton affinity of 825.5 kJ/mol (197.3 kcal/mol). A re-evaluation of the data of that reference by the present authors gives a heat of formation for CH_3CO^+ of 653 kJ/mol (156 kcal/mol) which corresponds to a proton affinity of 830 kJ/mol (198.3 kcal/mol). However, from the onset of 9.6035 eV determined[19] for the occurrence of the reaction:

$$CH_2CO^+ + CH_2CO \rightarrow C_2H_4^+ + 2\ CO, \qquad (15)$$

one calculates a slightly less negative heat of formation for CH_2CO, -36.4 kJ/mol (-8.7 kcal/mol), which would correspond to a proton affinity[17] of 832 kJ/mol (198.8 kcal/mol), or 836 kJ/mol (199.8 kcal/mol), respectively.

The position of ketene in the thermochemical ladder of proton affinities has been established[12,20], and relative to the value chosen above for isobutene, leads to a proton affinity for ketene of 828 kJ/mol (198.0 kcal/mol).

3.2.3. Isobutene

The proton affinity of isobutene is defined by the reaction:

$$\text{iso-}C_4H_8 + H^+ \rightarrow \text{tert-}C_4H_9^+. \qquad (16)$$

The heat of formation of the tert-$C_4H_9^+$ ion is less well established than those of the ethyl and sec-propyl ions discussed below. A recent analysis of the 298 K heat of formation of this ion as derived from appearance energy measurements led to a value of $<695\pm3$ kJ/mol (166.2 ± 0.8 kcal/mol)[21]. A value of 697 kJ/mol (166.5 kcal/mol) is obtained for this heat of formation taking a value of 50.2 ± 4 kJ/mol ($12.0\pm1.$ kcal/mol) for the heat of formation of the tert-butyl radical[22] and a value of 6.7 eV for the ionization potential[23]. However, the latter value can not be considered well-established without additional corroborating evidence, since experimentally-determined values for the heat of formation of the radical ranging from 44 to 35 kJ/mol (10.5 to 8.4 kcal/mol)[24-27] have also been reported, and a value of 6.58 eV has been reported for the ionization potential[28]. The corroborating evidence is derived from measurements[29-31] of the equilibrium constant of the reaction:

$$C_6H_5CH_2^+ + (CH_3)_3CCl \rightleftharpoons C_6H_5CH_2Cl + \text{tert-}C_4H_9^+ \qquad (17)$$

which give a value of -5.4 kJ/mol (-1.3 kcal/mol) for the enthalpy change at 300 K; from these data the heat of formation of the tert-butyl ion would be estimated to be 694 kJ/mol (165.8 kcal/mol) accepting a value of 899 kJ/mol (214.8 kcal/mol) for the heat of formation of the benzyl ion. This is based on a value for the heat of formation of the benzyl radical of 204 kJ/mol (48.8 kcal/mol)[22,32] and an ionization potential of the radical of 7.20 eV[33]. (The heat of formation of $(CH_3)_3CCl$ is taken as -182 kJ/mol or -43.5 kcal/mol[34]; the heat of formation of $C_6H_5CH_2Cl$ is derived from a liquid phase heat of formation[34] and a heat of vaporization[35] taken to be 4.1 kcal/mol.) Based on this result, the proton affinity of isobutene is 820 kJ/mol (195.9 kcal/mol).

Taking into account changes in external rotational symmetry numbers, the gain of an internal rotation upon protonation, and the change in the moments of inertia, the entropy change for the half reaction

$$(\text{i-}C_4H_8 \rightarrow \text{tert-}C_4H_9^+)$$

is about +3 J/mol K (+0.7 cal/mol K)[36]. This leads to a value of 784 kJ/mol (187.3 cal/mol) for the 298 K gas phase basicity.

3.2.4. Propylene

The proton affinity of propylene is defined by the reaction:

$$CH_3CH=CH_2 + H^+ \rightarrow \text{sec-}C_3H_7^+. \qquad (18)$$

The heat of formation of the sec-$C_3H_7^+$ ion at 298 K has been determined to be 798 kJ/mol (190.8 kcal/mol)[37], 799 kJ/mol (190.9 kcal/mol)[38], or 802.5 kJ/mol (191.8 kcal/mol)[21]. Taking a value of 799 kJ/mol (191.0 kcal/mol) for this heat of formation, the proton affinity of propylene is 751 kJ/mol (179.5 kcal/mol).

A calculation of the rotational entropy change associated with changes in the moments of inertia and rotational symmetry numbers for the half reaction ($CH_3CH=CH_2 \rightarrow$ sec-$C_3H_7^+$) leads to a value of -3.8 J/mol K (-0.9 cal/mol K); this estimate fails to take into account the predicted positive entropy change brought about by the loss of the double bond. (The methyl group in the ion can be taken to be essentially a free rotor[39].) In the evaluation of the gas basicity of propylene, it has been assumed that the entropy change of this half reaction is close to zero, as discussed before[36]. On this basis, the gas basicity of propylene is taken to be 718 kJ/mol (171.7 kcal/mol).

The gas basicity of propylene has been related through thermochemical ladders to several of the other comparison standards listed here. If one estimates the proton affinity through such data using ethylene as the primary standard for the proton affinity scale (i.e. using the data from reference 40 for the interval C_2H_4-H_2O and from reference 41 for the interval H_2O-C_3H_6), one obtains a value of 752 kJ/mol (179.7 kcal/mol) for the proton affinity of propylene, in excellent agreement with the conclusion presented above. On the other hand, the interval in the thermochemical ladder between isobutene and propylene appears to be somewhat constricted, an effect which may result from the fact that small inaccuracies in temperature measurement may cause noticable errors in such a scale if the scale covers a wide energy range, as discussed above, or may possibly reflect uncertainties in the heat of formation of the tert-butyl ion, also discussed above.

3.2.5. Formaldehyde

Approximately following the recent discussion of Collyer and McMahon[40], an analysis of the proton affinity of formaldehyde is given. Although this compound was not used as a primary reference standard in the evaluation of the thermochemical ladder, this proton affinity provides an additional reference point to verify the assignment of absolute values to the proton affinity scale. Values for the heat of formation of CH_2OH^+ derived from the appearance energy of this ion from CH_3OH range from 711 kJ/mol (170.0 kcal/mol) to 714 kJ/mol (170.7 kcal/mol)[42-44] corresponding to proton affinity values of 711–715 kJ/mol (170–171 kcal/mol). Since the proton affinity of formaldehyde is 22 kJ/mol (5.2 kcal/mol) above that of water[45], the value predicted from the evaluated proton affinity scale is 718 kJ/mol (171.7 kcal/mol), in reasonably good agreement with that obtained from threshold measurements.

3.2.6. Water

A value for the heat of formation of H_3O^+ has been obtained from a measurement of the appearance energy of this ion from a hydrogen-bonded dimer[46]:

$$(H_2O)_2 \rightarrow H_3O^+ + OH + e. \qquad (19)$$

From this experiment, one obtains a value for the proton affinity of H_2O of 694 kJ/mol (165.8 kcal/mol) at 0 K, and assuming that all rotational degrees of freedom are excited and that no vibrational degrees of freedom are excited at 298 K, this corresponds to a value of 697 kJ/mol (166.5 kcal/mol) for the proton affinity of water at 298 K. The error limits cited by the authors for this proton affinity are ±7.5 kJ/mol (1.8 kcal/mol), with the major uncertainty being the well depth for formation of the water dimer. A recent state-of-the-art ab initio calculation[47], which included corrections for the change in the zero point energy upon protonation, correction to 298 K, and vibrational mode corrections, verifies the well depth of -17 kJ/mol (-4 kcal/mol) assumed in the interpretation of those results; these authors also calculate a value for the proton affinity of water of 689 kJ/mol (164.8 kcal/mol), in good agreement with the experimental result.

Recent equilibrium studies[40,48] have tied the proton affinity of H_2O to that of ethylene. The experimental results from those studies indicate that the Gibbs free energy change of the reaction:

$$C_2H_5^+ + H_2O \rightarrow H_3O^+ + C_2H_4 \qquad (20)$$

is -7.5 kJ/mol (-1.8 kcal/mol)[48] or -14 kJ/mol (-3.4 kcal/mol)[40]. In one of these studies[48], the direct measurement of the free energy change of reaction 20 was complicated by clustering of H_3O^+ to C_2H_4, and therefore, more weight is given to the latter result, which is based on a low pressure measurement of a thermodynamic ladder linking the gas basicities of the two compounds through several interlocking steps. Accepting a value for the proton affinity of C_2H_4 of 680 kJ/mol (162.6 kcal/mol) (see Discussion below) this result leads to a proton affinity of water of 697 kJ/mol (166.7 kcal/mol) if one calculates the entropy change for reaction 20 taking into account only the changes in the rotational symmetry numbers of the reactants and products; a more complete calculation of the entropy change for this reaction leads to a value of 696 kJ/mol (166.3 kcal/mol). Both estimates of the entropy change give proton affinity values which are in agreement with the value derived from the threshold determination of the heat of formation of H_3O^+[46] and with the ab initio calculation[47].

The entropy change associated with the half reaction ($H_2O \rightarrow H_3O^+$) is 4.3 J/mol K (1.03 cal/mol K)[49]. The evaluated proton affinity of water, 697 kJ/mol (166.5 kcal/mol), thus corresponds to a gas phase basicity of 665 kJ/mol (159.0 kcal/mol).

3.2.7. Ethylene

The proton affinity of ethylene is defined by the reaction:

$$C_2H_4 + H^+ \rightarrow C_2H_5^+. \quad (21)$$

The heat of formation of $C_2H_5^+$ at 298 K has been determined from photoion–photoelectron coincidence experiments to be 901±4 kJ/mol (215.3±1.0 kcal/mol)[37], or 903±2 kJ/mol (215.9±0.5 kcal/mol)[38], and from photoionization mass spectrometric appearance potentials, to be 904±2 kJ/mol (216.0±0.5 kcal/mol)[21]. In agreement with recent analyses of these data[40,48], we take an average value of 902 kJ/mol (215.6 kcal/mol) for this heat of formation, and on that basis, take a value for the proton affinity of ethylene of 680 kJ/mol (162.6 kcal/mol).

Assuming the $C_2H_5^+$ ion to have a non-classical bridged structure of C_{2v} symmetry[16] (which has been calculated[50] to be 21.6 kJ/mol or 5.2 kcal/mol lower in energy than the classical structure), the entropy change calculated from the complete partition function for the half reaction ($C_2H_4 \rightarrow C_2H_5^+$) is -10 J/mol K (-2.4 cal/mol K). The gas basicity of this compound is 651 kJ/mol (155.6 kcal/mol).

3.2.8. Carbon monoxide

The heat of formation of HCO^+ derived from appearance potential measurements in formaldehyde is 824 kJ/mol (196.9 kcal/mol) corresponding to a proton affinity of 596 kJ/mol (142.4 kcal/mol)[51], or 827 kJ/mol (197.6 kcal/mol) corresponding to a proton affinity of 593 kJ/mol (141.7 kcal/mol)[52]. The selected value is the average of these two and some other values from appearance potential measurements[53], or 594 kJ/mol (141.9 kcal/mol). Accepting a recent recommended value for the heat of formation of HCO[27] of 37±5 kJ/mol (8.9±1.2 kcal/mol), an ionization potential determination[53] for this radical of 8.27±0.01 eV leads to a heat of formation of the HCO^+ ion of 835 kJ/mol (199.6 kcal/mol), and a corresponding proton affinity of 584.5±6 kJ/mol (139.7±1.4 kcal/mol), in good agreement with the values derived above.

Following the recommendation of Bohme et al.[11], the entropy change associated with the half reaction ($CO \rightarrow HCO^+$) is taken as 3 J/mol K (0.8 cal/mol K).

3.2.9. Carbon dioxide

From the appearance potential of HCO_2^+ in formic acid (12.29 eV)[54], one can derive a heat of formation of the ion of 589 kJ/mol (140.8 kcal/mol), which corresponds to a proton affinity of 548 kJ/mol (130.9 kcal/mol).

Following the recommendation of Bohme et al.[11], the entropy change associated with the half reaction ($CO_2 \rightarrow HCO_2^+$) is taken as 19 J/mol K (4.5 cal/mol K).

3.2.10. Oxygen atom

The heat of formation of the OH^+ ion has been determined from its appearance potential in H_2O (18.115±0.008 eV) to be 1293 kJ/mol (308.96 kcal/mol)[55]. A value for the ionization potential of the OH radical has been derived from appearance energy measurements in HOF to be 12.88 eV[56] in good agreement with the value of 13.01 eV[57] obtained from a direct experimental measurement. These values correspond to heats of formation of the OH^+ ion of 1281.5 or 1294 kJ/mol (306.3 or 309.3 kcal/mol), respectively. Accepting the value of 1293 kJ/mol (308.96 kcal/mol)[55], the proton affinity of the O atom is taken as 487 kJ/mol (116.3 kcal/mol).

Bohme et al.[11] recommend a value of 27 J/mol K (6.5 cal/mol K) for the entropy change associated with the half reaction ($O \rightarrow OH^+$). On this basis, the gas basicity of the O atom at 298 K is taken as 463 kJ/mol (110.7 kcal/mol).

3.2.11. Molecular Oxygen

The ionization potential of O_2H has been determined to be 11.35±0.01 eV[58]. Accepting values for the heat of formation of O_2H of 13 kJ/mol (3.2 kcal/mol) at 0 K, or 10.5 kJ/mol (2.5 kcal/mol) at 298 K[59], one obtains a value for the heat of formation of O_2H^+ ion of 1108 or 1098 kJ/mol (264.9 or 262.4 kcal/mol) at 0 or 298 K, respectively, leading to a value for the proton affinity of oxygen of 420 kJ/mol (100.5 kcal/mol). This result is in good agreement with a value of 422 kJ/mol (100.9 kcal/mol) which has been cited[60] for this proton affinity, based on the appearance potential of O_2H^+ in H_2O_2.

The entropy change associated with the half reaction ($O_2 \rightarrow O_2H^+$) is taken to be 27 J/mol K (6.5 cal/mol K)[11]. The gas basicity of O_2 is taken as 397 kJ/mol (95.0 kcal/mol).

3.3. Summary of Thermochemical Data on Comparison Standards for Proton Affinity Scale

Standard(M)	$\Delta_f H$(M)(298 K)			$\Delta_f H(MH^+)^b$			Proton Affinity^c	
	kcal/mol	kJ/mol		kcal/mol	kJ/mol		kcal/mol	kJ/mol
NH_3	-11.02	-46.11	59	151.0	632.	13	203.6	852.
				153.6	643.	13,14	202.0	845.
	Ab initio calculation		15				205.0	858.
	Ab initio calculation		16				210.0	879.
							204.0±3*	853.5±12*
$CH_2=C=O$	-11.4	-47.7	18	156.0	653.	17	198.3	830.
	-8.7	-36.4	19				198.8	832.
	From thermochemical ladder, relative to isobutene:						198.0±2*	828.±8*
$(CH_3)_2C=CH_2$	-4.04	-16.9	34	⩽166.2	⩽695.	21	⩾195.5	⩾818.
				166.5	697.	22,23	195.2	817.
				165.8	694.	22,31,32,33	195.9±1.5*	819.5±6*
$CH_3CH=CH_2$	4.83	20.2	34	190.8	798.	37	179.7	752.
				190.9	799.	38	179.6	752.
				191.8	802.5	21	178.7	748.
	From thermochemical ladder, relative to ethylene:						179.7	752.
				191.0	799.		179.5±0.8*	751.±3*
H_2O	Ab initio calculation		47				164.8	689.
	From thermochemical ladder, relative to ethylene:						166.3	695.8
	-57.8	-241.8	59	141.4	592.	46	166.5±2*	697.±8*
$CH_2=CH_2$	12.48	52.2	34	215.3	901	37	162.9	681.5
				215.9	903	38	162.3	679.
				215.6	902		162.6±1*	680.±4*
CO	-26.4	110.5	59	196.9	824.	51	142.4	596.
				197.6	827.	52	141.7	593.
				199.6	835.	27,53	139.7	584.5
							141.9±2*	594.±8*
CO_2	-94.05	-393.5	59	140.8	589.	54	130.9*	548.*
O				306.3	1281.5	56	118.9	498.
				309.3	1294.	57	115.9	485.
	59.56	249.2	54	308.96	1293.	55	116.3±1*	491.±4*
O_2	0.00	0.00		262.4	1098.	58,59	100.5	420.
				264.8	1108.	60	100.9±0.5*	422.±2*

*Selected value.

[a] See Sec. 3.2 for detailed discussion and error limits.

[b] Heats of formation using "stationary electron convention" (described in Sec. 5.2.1)

[c] 298 K heat of formation of H^+ (Eq. 1) in "stationary electron convention" = 365.7 kcal/mol, 1530.0 kJ/mol.

4. Experimental Error Limits

As shown in Sec. 3.3, the heats of formation of the MH^+ ions used for establishing absolute values for the proton affinity scale have error limits which are larger than ±4 kJ/mol (±1 kcal/mol), sometimes considerably larger (e.g., NH_4^+). In general, absolute values assigned to the proton affinities of species determined through equilibrium measurements can be considered to be known to within ±8 kJ/mol (±2 kcal/mol) if the proton affinity lies in the region of the scale between water and ammonia (i.e. if the proton affinity is in the range 700–850 kJ/mol). In the region of the scale below water (proton affinities less than about 700 kJ/mol), the absolute values of proton affinities can be assumed to be known to within 4–6 kJ/mol for species determined through equilibrium measurements. In the region of the scale above ammonia (proton affinities greater than 850 kJ/mol), the absence of reliable absolute standards makes it impossible to check on the reliability of assigned proton affinity values. In particular, if the temperatures at which measurements were made were not well known, the thermochemical ladders generated from equilibrium constant determinations could be too long or too short, causing proton affinity values at the top end of the scale to vary considerably from their correct absolute values. Some confidence in the assigned values is gained from the general agreement observed in the reported thermochemical ladders generated in different laboratories. However, the lack of reference proton affinities in the upper part of the scale necessitates the assignment of relatively large error limits in this region, ±16 kJ/mol. Throughout the scale, relative values derived from equilibrium constant measurements can be considered to be known to within ±1 kJ/mol (0.2 kcal/mol) or less when ΔG is small ($\leqslant$4–6 kJ/mol). Since the experimentally measured free energy changes are given in Table 1, users of this compilation can identify for themselves species for which larger or smaller error limits on relative gas basicities are warranted. Proton affinities derived from bracketing measurements have error limits which are determined by the size of the bracket (given under the appropriate literature reference).

In Table 2, the values given for the heats of formation of the positive ions include, of course, the error limits associated with the assignment of absolute values to the proton affinity scale (described above in Sec. 3.2) as well as the error limits associated with the heat of formation of the neutral molecule.

Nearly all of the data compiled here were originally reported in units of kcal/mol; the cited values in these units are given to tenths of a kcal/mol, in order to preserve the originally-reported information about relative ordering. On the other hand, in order to emphasize the large absolute uncertainties in cited proton affinity values, the columns giving data in kJ/mol show values only to within the nearest kilojoule per mole.

5. Explanation of the Tables

5.1. Explanation of Table 1

Table 1 presents a summary of the data from the literature, an evaluation of those data, and evaluated values for the gas basicities at 300 K and the proton affinities, in units of both kcal/mol and kJ/mol (where one kcal/mol is defined as 4.184 kJ/mol). The data in Table 1 are presented in order of descending proton affinity. Data from proton transfer equilibrium measurements are given in considerable detail, with (as described below) reference bases and temperatures specifically noted in most cases. The bracketing experiments, denoted by (br), have been related to the evaluated thermodynamic ladders from equilibrium constant measurements. Details of bracketing and hydride transfer experiments are provided in annotations under the appropriate literature references, as is information about equilibrium measurements related to reference bases not included in the standard list given below in Sec. 5.1.1; these latter experiments are identified in Table 1 by the notation (Key) appearing in the column usually used to identify the reference base.

In order to understand the structure of Table 1 (as well as the thought processes which went into the evaluation) it is best to consider specific examples of data sets, and illustrate how they are presented in Table 1. Table A represents a small portion of an extensive set of data originally published in J. F. Wolf, R. H. Staley, I. Koppel, M. Taagepera, R. T. McIver, Jr., J. L. Beauchamp, and R. W. Taft, J. Am. Chem. Soc. **99**, 5417 (1977) (denoted by 77WOL/STA in Table 1).

TABLE A.

	ΔG kcal/mol	Reference
NH_3	0.0	77WOL/STA
CH_3COCH_3	-7.2	77WOL/STA
iso-C_4H_8	-8.6	77WOL/STA
H_2S	-27.8	77WOL/STA
H_2O	-31.4	77WOL/STA

In Table A, ΔG represents the free energy changes (in kcal/mol) derived for the process ($MH^+ + NH_3 \rightarrow NH_4^+ + M$) from interlocking series of equilibrium constant determinations at a temperature assumed to be 300 K. As one can find in the comments under 77WOL/STA in the annotated references, the authors of this paper subsequently found that the operating temperature at which the original measurements were made was actually approximately 320 K, and therefore, from Eq. (3), the experimentally determined values of ΔG were increased by a factor of 320/300. These data then would appear in Table 1 as shown in Table B with the temperature-corrected values of ΔG (these are surrounded by parentheses) in the column labelled "Relative gas basicity, kcal/mol". The "Relative gas basicity" is the negative of the Gibbs free energy change associated with the reaction:

$$BH^+ + M \rightleftharpoons MH^+ + B(Ref) \qquad (22)$$

where B(Ref) is the reference base corresponding to the one- or two- alphabetic character denoter given in the list in Sec. 5.1.1.

TABLE B.

	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Reference
NH_3	A	(0.0)	195.6	77WOL/STA
CH_3COCH_3	A	(-7.9)	187.9	77WOL/STA
iso-C_4H_8	A	(-9.2)	186.4	77WOL/STA
H_2S	A	(-29.6)	167.0	77WOL/STA
H_2O	A	(-33.5)	163.1	77WOL/STA

The entry "A" in Table B in the column labelled "Reference base" identifies ammonia as the species to which the original authors referred their basicity data. The "Gas basicity" values displayed here next to the corresponding "Relative gas basicity" are taken relative to the absolute gas basicity of ammonia derived in Sec. 3.2.1 and obtained using the relative ΔG values cited here.

Since, as described in Secs. 3.2.3 and 3.2.6, the gas basicities of iso-C_4H_8 and water are taken to be, respectively, 187.3 and 159.0 kcal/mol, it appears that in this data set cumulative errors exist in the overall thermochemical ladder over the span of more than 30 kcal/mol. Therefore, the data from this paper are related to several local standards. In the example set shown here, iso-C_4H_8 and H_2O happen to be species for which well-established values for the gas basicity and proton affinity can be assigned (Sec. 3.2), and therefore, these are chosen as local standards. In Table 1, data from any given reference are always reproduced in their original form (or, as here, their original form corrected for temperature) in addition to appearing in their evaluated form (if the two differ); original thermochemical ladders have been preserved in the presentation so that users of the compilation can examine the information as it appeared in the literature and re-evaluate the data for themselves if future experimental results bring about changes in values assigned to particular reference gas basicities or proton affinities. Thus, any given piece of data from 77WOL/STA could appear twice, once as given above and once with the cited gas basicity value as derived in relation to the appropriate local standard. The example data would be given in Table 1 as shown in Table C.

TABLE C.

	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Reference
NH_3	A	(0.0)	195.6	77WOL/STA
	H		196.6	
CH_3COCH_3	A	(-7.9)	187.9	77WOL/STA
	H		188.9	
iso-C_4H_8	A	(-9.2)	186.4	77WOL/STA
	H	(0.0)	187.3	
H_2S	A	(-29.6)	167.0	77WOL/STA
	N		162.9	
H_2O	A	(-33.5)	163.1	77WOL/STA
	N	(0.0)	159.0	

In Table C (see the list in Sec. 5.1.1) the symbols H and N identify iso-C_4H_8 and H_2O as respective local standards; the gas basicity values taken relative to these standards are shown in the appropriate column. In Table 1, when two entries appear together without a repetition of the "Reference" identifier, the second entry represents the same data item as the first but, as in the example given here, the "Gas basicity" in the second instance is that relative to a local standard not used by the original authors. In cases where such dual entries occur, only the second "evaluated" gas basicities were taken into account in the final evaluation of the gas basicity of the particular compound. The local standards used for particular data sets are identified in the list in Sec. 5.1.1 and also can be located in Table 1 by the appearance of the entry "(0.0)" in the "Relative gas basicity" column.

The evaluation of the gas basicity and proton affinity of a particular compound and its reconstruction from the entries in Table 1, can be illustrated by considering a single molecule from our example data set, H_2S. All the entries from Table 1 relating to H_2S are reproduced in Table D. However, for clarity of presentation we want the gas basicity values taken into account in the final evaluation to stand out and therefore, all the entries of "unevaluated" gas basicities (e.g. the basicity of H_2S relative to that of ammonia in the example given above) are here replaced by a row of dots.

TABLE D.

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Reference
H_2S					
	340	Y	(0.0)	162.8	78FRE/HAR(2)
	296	N	(4.6)	163.6	73HOP/BON
	298	N	(3.8)	162.8	78TAN/MAC
	320	A	(-29.6)	....	77WOL/STA
	320	N		162.9	
	550	N	(3.9)	162.7	77MAU/FIE
	600	A	(-31.8)	....	79LAU
	600	N		162.2	

In Table D, the absence of entries in the "Reference" column indicates that the particular experimental result comes from the reference cited immediately above; such a result has been related to a local standard (water, N, in this case) which is different from the comparison standard used by the original authors. In all such cases, it is the second entry which is taken into account in the final evaluation of the absolute gas basicity of the compound. Other entries shown here (73HOP/BON, 78TAN/MAC, 77MAU/FIE) are clearly results derived from studies in which the authors related their experimentally-determined thermochemical ladders to water. The first entry, with a Y in the "Reference base" column and (0.0) under "Relative gas basicity" shows that in the paper 78FRE/HAR(2), the authors have related the gas basicities of some other compound(s) to that of H_2S (symbol, Y); the gas basicity given opposite this entry is the evaluated value, 162.8 kcal/mol, derived from the five determinations relative to an H_2O standard.

A final example will illustrate how results from bracketing experiments are evaluated and listed in Table 1. In J. J. Solomon and R. F. Porter, J. Am. Chem. Soc. **94**, 1443 (1972) (72SOL/POR) it was seen that H_3O^+ transfers a proton to B_5H_9 but H_3S^+ does not. Therefore, the gas basicity of B_5H_9 is assumed to lie between those of water and hydrogen sulfide. The entry for B_5H_9 is shown in Table E. The gas basicity given is the average of that of the two bracketing compounds; these are listed in the comments under the appropriate reference.

TABLE E.

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Reference
B_5H_9		(br)		161	72SOL/POR

In many instances, investigators have determined proton transfer equilibrium constants of pairs which do not include any of the standards listed above in Secs. 3.2 and 3.3., nor even any of the more commonly-used secondary standards listed in Sec. 5.1.1. In such cases, the data have been tied in to the scale in the usual way by relating to evaluated thermochemical ladders, and the identities of the particular reference compounds are given in comments under the appropriate reference at the end of Table 1. Such cases are identified by the designation (Key) appearing in the "Reference base" column.

In some cases, "proton affinities" have been reported in the literature without any information about the details of the experiment leading to the cited value; such data are usually reported here as they originally appeared since evaluation is impossible. Unevaluated data are denoted by a double asterisk (**). Other papers have presented revisions by original authors of data published earlier; in such cases the details of the original experiments are available, but the nature of the revisions are not; these data also have not been evaluated, and are denoted by a single asterisk (*).

The entries in the column labelled "Gas basicity" are actual gas phase basicities only for measurements made at temperatures close to 300 K. The gas basicities listed for experiments at higher temperatures have been normalized to those at 300 K in order to make intercomparison easier; that is, in the defining reaction, that part of the term $T\Delta S$ which is associated with the proton is taken as 32.6 kJ/mol (7.8 kcal/mol)[61] in all cases, so that actual differences in the free energy change of the defining reaction due to entropy changes associated with the half reaction ($M \rightarrow MH^+$) may be discerned.

Literature references, identified by the eight-character identifier at the end of a data-containing line, are given at the end of the Table 1, sorted alphabetically according to the characters appearing in the identifying tag. The individual references contain annotations giving any special remarks pertaining to the particular paper.

5.1.1. Explanation of Symbols Used in Table 1

Symbol used in Table 1	Reference base	Evaluated gas basicity (300 K)		Evaluated proton affinity	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol
A	NH_3	195.6	818.	204.0	853.5
B	CH_3NH_2	205.7	861.	214.1	896.
C	n-$C_3H_7NH_2$	210.1	879.	217.9	912.
D	Pyridine	213.1	892.	220.8	924.
E	$(CH_3)_3N$	217.3	909.	225.1	942.
F	$C_6H_5NH_2$	202.5	847.	209.5	876.5
G	$C_2H_5NH_2$	208.5	872.	217.0	908.
H	$(CH_3)_2C{=}CH_2$	187.3	784.	195.9	820.
I	$C_6H_5N(CH_3)_2$	215.4	901.	223.4	935.
J	C_6H_6	174.6	730.5	181.3	758.5
K	C_2H_4	155.6	651.	162.6	680.
L	$CH_2(CN)_2$	167.4	700.	175.6	735.
M	H_2CO	164.3	687.	171.7	718.
N	H_2O	159.0	665.	166.5	697.
O	O	110.7	463.	116.3	487.
O′	O_2	95.0	397.	100.9	422.
P	$(C_2H_5)_2O$	192.4	805.	200.2	838.
Q	$HCO_2C_2H_5$	185.3	775.	193.1	808.
R	1,2-$C_6H_4(CH_3)_2$	186.1	779.	193.3	809.
S	CO_2	124.4	520.	130.9	548.
T	CH_3CHO	178.6	747.	186.6	781.
U	$(CH_3)_2CO$	188.9	790.	196.7	823.
V	CH_3COOCH_3	190.0	795.	197.8	828.
W	$C_6H_5CH_3$	182.0	761.	189.8	794.
X	$CH_3COOC_2H_5$	192.9	807.	200.7	840.
Y	H_2S	162.8	681.	170.2	712.
Z	CO	134.4	562.	141.9	593.
AA	$CH_3CH{=}CH_2$	171.7	718.	179.5	751.
BB	H_2	94.6	396.	101.3	424.
EE	$(CH_3)_3P$	219.3	917.5	227.1	950.
XX	$(n\text{-}C_3H_7)_2O$	194.5	814.	202.3	846.
ZZ	$(CH_3)_6C_6$	200.0	837.	207.3	867.

(Key) — Identity of reference base or other experimental details (in the case of hydride transfer equilibrium constant determinations, for instance) are given in a comment under the appropriate literature citation. (In the case of proton transfer equilibria, usually used for small data sets which were experimentally related to unusual reference bases.)

(br) — Bracketing result.

* — Asterisk appearing after gas basicity value indicates that original authors reevaluated the original data in a subsequent publication, but without giving sufficient information for relating the reevaluation to the present scale. Data as cited are the reevaluated values of the authors.

** — Double asterisks appearing after gas basicity or proton affinity values indicate that insufficient information is available to evaluate the data. Proton affinity values are given as reported by the original authors, and are not necessarily internally consistent with the evaluated proton affinity scale.

RN — CAS Registry Number.

5.2. Explanation of Table 2

Table 2 presents the evaluations from Table 1 sorted according to the empirical formula of the appropriate compound. The empirical formulas are given at the beginning of each new data item enclosed in square brackets; component atoms are listed alphabetically, with no concessions to chemical meaning (except that lower case letters are given a lower priority than upper case letters), and the compounds are given simply according to an alphabetical ordering of these empirical formulas. Table 2 also lists the heat of formation at 298 K of the compound, and a 298 K heat of formation of the protonated molecule derived from the evaluated proton affinity, using the "stationary electron convention".

5.2.1. Conventions Used

As mentioned above, the heats of formation of protonated molecules given in Table 2 are given according to the so-called "stationary electron" convention[12]. According to this convention, the integrated heat capacity of the electron in eqs. (5) and (6) is taken as zero at all temperatures, and the thermal energy of the electron is not taken into account in calculating the heat of formation of the ion at temperatures other than zero kelvin. Obviously, since ionic species occur on both sides of equation (1), the absolute value for the proton affinity does not change with the convention, but one must take care to use consistent data in calculating a proton affinity from ionic heats of formation. If the heats of formation of ions given here are to be used in conjunction with heats of formation of ions taken from a compilation of thermodynamic data (such as "The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units"[59] or the "JANAF Thermochemical Tables"[61]) in which the electron is treated as a conventional chemical element, the 298 K values given here must be increased by 1.48 kcal/mol or 6.2 kJ/mol in order to achieve consistency. The existence of two different conventions does not matter for neutral species. For the defining eq. (1), the 298 K heat of formation of the proton using this convention is 1530.0 kJ/mol or 365.7 kcal/mol. Relevant heats of formation of reference ions used to standardize the scale were taken at 298 K in all cases where sufficient information was available that this was possible.

5.2.2. Heats of Formation of Neutral Molecules

Heats of formation of the neutral molecule, M, in eq. (1) are listed in Table 2. The experimental data in Table 1 lead to a value for the proton affinity of M, and if the heat of formation of M is known or, as described below, can be estimated, one can thereby obtain a value for the heat of formation of the protonated molecul MH^+. In a few cases, a reliable value for the heat o formation of MH^+ was available from other sources, and the proton affinity determination led to a determination of the heat of formation of the neutral molecule or radical. No distinction is made between these cases in Table 2, but in the latter case, the cited reference will be to the paper describing the proton affinity determination.

Values for the heats of formation of neutral molecules were taken from the experimental literature wherever possible. If data for a particular compound could be obtained from an evaluated data compilation, this value was selected for inclusion. Such compilations included, for organic compounds:

(1) J. B. Pedley and J. Rylance, "Sussex-N. P. L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds," University of Sussex (1977)[34]. The numerous data from this evaluated compilation of 300 K heats of formation of organic compounds are identified as [77PED/RYL]. Where condensed phase data from this reference have been used in conjunction with experimental or estimated heats of vaporization or sublimation, the source of the heat of formation is identified simply by an asterisk (*) in the first space of the reference identification.

and for inorganic compounds (in order of preference):

(2) D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, "The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units," J. Phys. Chem. Ref. Data, Vol. 11, Suppl. 2 (1982), hereafter referred to as 82/TN270 from the original publication of this compilation as a series of NBS Technical Notes called the 270-series[59].

(3) (a) D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," NSRDS-NBS 37 (1971); (b) M. W. Chase, J. L. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, "JANAF Thermochemical Tables, 1975 Supplement, J. Phys. Chem. Ref. Data 4, 1 (1975); (c) M. W. Chase, Jr., J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela, J. Chem. Phys. Ref. Data **11**, 695 (1982). Information from these sources is hereafter referred to as JANAF[61].

The preferential use of these compilations as sources of experimental data recognizes that these data have been evaluated for internal consistency insofar as possible. Experimental information about heats of formation of compounds not included in these sources was obtained from scientific articles presenting relevant thermochemical determinations; when more than one such article was available for a given piece of data, the most recent value was usually arbitrarily chosen in the possibly naive hope that improved instrumentation and compound purity, as well as a greater awareness of the problems inherent in particular measurements or of the thermochemistry of particular classes of compounds, should contribute to improved values. In such cases, it should be noted, the cited references are not always the primary references for the determination, but may represent a choice by a subsequent author. Heats of formation of deuterated or partially deuterated molecules were assumed to be the same as the heats of formation of the non-deuterated analogues. Also, gas phase heats of formation of racemic mixtures are the same as the heats of formation of the optically pure enantiomers.

Implicitly, in assigning gas phase heats of formation to the neutral species, the compounds are assumed to be ideal gases at STP. Few of the species are, in fact, gases under these conditions — most are liquids or solids. Numerous methods exist for measuring and interpreting experimental heats of sublimation [ΔH(solid $\rightarrow$ gas)] and of vaporization [ΔH(liquid $\rightarrow$ gas)], and, so need not be discussed here. Where available, such measurements were used to translate condensed phase data into gas phase information. However, such measurements do not exist for many compounds of interest here, either because of lack of adequate volatility, purity, or thermal stability, or even, seemingly because of a lack of interest in the species in the gas phase. Estimation methods for heats of vaporization, and occasionally sublimation, have been described in the literature. Some require other experimental data (e.g., critical constants), while others are limited to well-defined, however large, classes of compounds. Some of these methods have been used to generate values of gas phase molecular heats of formation from corresponding liquid or solid phase data; although such heats of formation are based on an estimation of one parameter, comparisons indicate that the resulting gas phase data are usually within 4 kJ/mol (1 kcal/mol) of accepted values, at least for heats of vaporization. Therefore, these entries are not labelled "Est" for "Estimate" (see below), but are rather identified by a two-part reference, the first segment giving the source of the liquid or solid phase heat of formation of the compound (abbreviated to an asterisk (*) when that source is the often-referred to [77PED/RYL]), and the second segment, listing a reference describing the technique of determining the heat of vaporization or sublimation.

Heats of formation of compounds for which no experimental data were available were estimated, and are labelled "Est". Several estimation approaches were utilized. Only brief descriptions of these will be given here; a detailed discussion will be presented elsewhere[62].

One approach utilizes experimental information about isomerization processes for the formation of two or more isomeric species in a particular reaction. The assumption is made that $\Delta\Delta_f H = \Delta\Delta_f G$ for a pair of isomers (ΔS is assumed negligible) in the experimentally observed process, so that a heat of formation of an unknown species can be predicted from thermochemical information about isomeric molecules. This approach, which is not well characterized and so is less trustworthy than other approaches used here, utilizes various types of information including direct equilibration studies on isomers and the more casual observation that two isomers are formed in comparable quantities in a particular process, and so have comparable Gibbs free energies and enthalpies of formation.

A related approach to estimation is based on the assumption that $\Delta\Delta_f H$ can be equated with ΔE_{tot} for two isomers, where ΔE_{tot} is the total energy of the molecule calculated quantum chemically. For this assumption, as well as all other estimation approaches employing quantum chemical studies, only ab initio calculations were considered as opposed to any of the plethora of semi-empirical studies at a wide variety of levels and approximations to the correct Hamiltonian and wavefunction. In all cases, care was taken to compare isomeric species with the same basis set and degree of geometry optimization. Built into this last assumption that $\Delta\Delta_f H = \Delta E_{tot}$ are the requirements that the zero point energy and enthalpy function H°-H_0° are essentially equal for an arbitrary pair of isomers, and that conformational isomerism and relative energies hardly affect heats of formation. None of these assumptions is rigorously true, but experience indicates that they represent a good first guess as to molecular energetics.

There remain three related approaches which were employed to estimate heats of formation of molecules here. The first and best characterized is Benson's "group increment" approach[63,64] in which the molecule of interest is defined as a collection of groups, and a "group", in turn, is defined as a polyvalent atom (ligancy $\geqslant 2$) with all its ligands in a molecule. The heat of formation of the molecule is obtained by summing statistically-determined contributions from the heats of formation of the various "groups", and correcting for various higher order interaction and other "correction" terms. These corrections include such things as the presence of gauche configurations in substituted alkanes, and the presence of heterocyclic and/or non-six membered rings.

A related approach consists of formulating the molecule of interest as a substituted derivative of a well-characterized species. The unknown heat of formation is taken to be the sum of the known heat of formation and a suitable correction term associated with the exchange of the substituent and parent components. For example, the heat of formation of an arbitrary aliphatic azoxy compound may be determined[65] from the heat of formation of the related (E)-olefin by:

$$\Delta_f H(\text{R-NN(O)-R}') = \Delta_f H(\text{R-CH=CH-R}') + 14.6\ \text{kcal/mol}, \qquad (23)$$

where the 14.6 kcal/mol for the $[\Delta_f H(\text{-NN(O)-}) - \Delta_f H(\text{-CH=CH-})]$ correction term was obtained by averaging the difference of the heats of formation of R–NN(O)–R′ and (E)R–CH=CH–R′ for R=R′=tert-butyl and n-propyl.

The final estimation approach, termed "macroincrementation reactions"[66], assumes that "if for each of two sets of molecules the total number of bonds, atoms and structural types is the same, then the total heat of formation of each set of molecules is the same. Then, if all but one of the heats are available, the remaining one can be estimated by simple arithmetic. It deals with ring strain, resonance energy and other interactions much more explicitly but less universally by embedding these corrections in the heat of formation of the individual molecules which among them possess the desired bonding characteristics. Further, it maximizes the direct use of available experimental data."[66].

Quite clearly, the last three approaches described here are interrelatable, and "were they flawless, they would agree with each other and with experiment"[67]. Furthermore, macroincrementation considerations, when coupled with the earlier assumption, $\Delta\Delta_f H = \Delta E_{tot}$, result in "isodesmic reactions"[68] and "group separation reactions"[69], widely employed here and elsewhere.

5.2.3. References

The reference citations given in Table 2 refer to the sources of data on the heats of formation of the neutral molecules. The references having to do with proton affinity determinations are given at the end of Table 1. In the column labelled "Reference" in Table 2, the appropriate literature reference is given as an eight-character identifier showing the year the paper appeared and the first three letters of the names of the first two authors. In addition, as discussed above in part, the following specialized notations and abbreviations are used:

Notation	Definition
82/TN270	D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, "The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units," J. Phys. Chem. Ref. Data **11**, Suppl. 2 (1982).
JANAF	(a) D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," NSRDS-NBS 37 (1971). (b) M. W. Chase, J. L. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, "JANAF Thermochemical Tables," 1975 Supplement, J. Phys. Chem. Ref. Data **4**, 1 (1975); (c) M. W. Chase, Jr., J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela, J. Phys. Chem. Ref. Data **11**, 695 (1982).
*00ABC/DEF	A condensed phase heat of formation was obtained from 77PED/RYL (J. B. Pedley and J. Rylance, "Sussex-N. P. L. Computer Analysed Thermochemical Data: Organic and Organometallic Comppounds," University of Sussex (1977)) and translated into a gas phase heat of formation using heat of vaporization or sublimation data from the reference 00ABC/DEF.
Est	The gas phase heat of formation was estimated using the approaches described in the previous section.
DEF	A defined heat of formation.
(E) or (Z)	In the absence of other information, the most stable isomeric configuration (usually E) has been assumed.

6. Literature Coverage

Data from literature which appeared before June 1983, are included. A number of researchers who were aware that this compilation was in progress made available to the authors preprints of work which was in press or in preparation, and these more recent data are also included. Older data, which have been superseded by newer, better, measurements have been omitted. These include primarily bracketing measurements which have been replaced by results from equilibrium studies. In some cases where an author has repeated his own measurements in a later study and obtained different results, both sets of data are included, with preference generally given to the more recent set in carrying out the evaluation. Exceptions to this policy are specifically mentioned under the description of the evaluation of a paper in the annotated reference. Particularly in laboratories which have been very active in determinations of proton affinities from ion–molecule equilibrium constant measurements, one sees that closely similar or identical results on a particular molecule or set of molecules often appear in various publications from the laboratory without specific reference to earlier appearances of the data in print. In these cases, we do not presume to try to judge who the "original" author was, but simply present all the reincarnations of the data set.

In a few cases, authors have bracketed the gas phase basicities of molecules between limits which are so widely spaced (i.e., ammonia and water) that the result is difficult to present in the more quantitative scale given here; in such cases, the paper is listed in the bibliography, but the result is not included in the Tables 1 and 2. Other authors have given only an upper or lower limit to a gas basicity; these results have not been included.

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As specifically noted, Mahnaz Motevalli-Aliabadi collaborated in the preparation of Table 2, carrying out estimates of the heats of formation of neutral molecules. In addition, the authors gratefully acknowledge the work of Carol Martin and Clairemarie Lanthier who critically proofread the Tables, and Ricardo Metz, Nathan Seidenman, Carlo Messina, and Dr. Thomas J. Buckley who carried out the computer processing leading to the production of the final manuscript.

We would also like to acknowledge those colleagues, notably Dr. Michael Mautner, who made available to the authors experimental data which was in various stages of preparation, so that the compilation could be as complete and up-to-date as possible.

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7. References

[1] D. K. Bohme, "The Kinetics and Energetics of Proton Transfer," in *Interactions between Ions and Molecules,* P. Ausloos, Editor, pp. 489–504, Plenum Press, New York (1975).

[2] R. W. Taft, "Gas Phase Proton Transfer Equilibria," in *Proton Transfer Reactions*, E. F. Caldin and V. Gold, Editors, pp.31–78, John Wiley & Sons, New York (1975).

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

[4] P. Kebarle, "Ion Thermochemistry and Solvation from Gas Phase Ion Equilibria," Ann. Rev. Phys. Chem. **28**, 445 (1977).

[5] D. H. Aue and M. T. Bowers, "Stabilities of Positive Ions from Equilibrium Gas Phase Basicity Measurements," in *Gas Phase Ion Chemistry*, M. T. Bowers, Editor, pp. 1–51, Academic Press, New York (1979).

[6] R. W. Taft, "Protonic Acidities and Basicities in the Gas Phase and in Solution: Substituent and Solvent Effects," Prog. Phys. Org. Chem. **14**, 248 (1983).

[7] C. R. Moylan and J. I. Brauman, "Gas Phase Acid-Base Chemistry," Ann. Rev. Phys. Chem. **34**, 187 (1983).

[8] 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).

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

[10] S. A. McLuckey, D. Cameron, and R. G. Cooks, "Proton Affinities from Dissociations of Proton Bound Dimers," J. Am. Chem. Soc. **103**, 1313 (1981).

[11] D. K. Bohme, G. I. Mackay, and H. I. Schiff, "Determination of Proton Affinities from the Kinetics of Proton Transfer Reactions. VII. The Proton Affinities of O_2, H_2, Kr, O, N_2, Xe, CO_2, CH_4, N_2O, and CO," J. Chem. Phys. **73**, 4976 (1980).

[12] (a) S. G. Lias, "Thermochemistry of Polyatomic Cations," in Kinetics of Ion-Molecule Reactions (P. Ausloos, Editor), Plenum Publishing Corp. (1979), p. 223; (b) H. M. Rosenstock, ibid., p. 246.

[13] S. T. Ceyer, P. W. Tiedemann, B. H. Mahan, and Y. T. Lee, "Energetics of Gas Phase Proton Solvation by NH_3," J. Chem. Phys. **70**, 14 (1979).

[14] M. J. Frisch, J. A. Pople, and J. E. Del Bene, unpublished results, personal communication.

[15] R. A. Eades, K. Scanlon, M. R. Ellenberger, D. A. Dixon, and D. S. Marynick, "The Proton Affinity of Ammonia. A Theoretical Determination," J. Phys. Chem. **84**, 2840 (1980).

[16] J.E. Del Bene, M. J.Frisch, K. Raghavachari, and J. A. Pople, "Molecular Orbital Study of Some Protonated Bases," J. Phys. Chem. **86**, 1529 (1982).

[17] J. C. Traeger, R. G. McLoughlin, and A. J. C. Nicholson, "Heat of Formation for Acetyl Cation in the Gas Phase," J. Am. Chem. Soc. **104**, 5318 (1982).

[18] R. L. Nuttall, A.H. Laufer, and M. V. Kilday, "The Enthalpy of Formation of Ketene," J. Chem. Thermodyn. **3**, 167 (1971).

[19] J. Vogt, A. D. Williamson, and J. L. Beauchamp, "Properties and Reactions of Ketene in the Gas Phase by Ion Cyclotron Resonance Spectroscopy and Photoionization Mass Spectrometry. Proton Affinity, Site Specificity of Protonation, and Heat of Formation of Ketene," J. Am. Chem. Soc. **100**, 3478 (1978).

[20] W. R. Davidson, Y. K. Lau, and P. Kebarle, "Gas Phase Dissociation of Protonated Acetic Acid to the Acyl Cation and Water. Heat of Formation of CH_3CO^+ and Proton Affinity of Ketene," Can. J. Chem. **56**, 1016 (1978).

[21] J. C. Traeger and R. G. McLoughlin, "Absolute Heats of Formation for Gas Phase Cations," J. Am. Chem. Soc. **103**, 3647 (1981).

[22] W. Tsang, "Thermal Stability of Primary Amines," Int. J. Chem. Kinet. **10**, 41 (1978).

[23] F. A. Houle and J. L. Beauchamp, "Photoelectron Spectroscopy of Methyl, Ethyl, Isopropyl, and tert-Butyl Radicals. Implications for the Thermochemistry and Structures of the Radicals and Their Corresponding Carbonium Ions," J. Am. Chem. Soc. **101**, 4067 (1979).

[24] C. E. Canosa and R. M. Marshall, "The Rate Constant for $t\text{-}C_4H_9 \rightarrow H + i\text{-}C_4H_8$ and the Thermodynamic Parameters of $t\text{-}C_4H_9$," Int. J. Chem. Kinet. **13**, 303 (1981).

[25] A. L. Castelhano, P. R. Marriott, and D. Griller, "Heats of Formation of tert-Butyl and Ethyl Radicals," J. Am. Chem. Soc. **103**, 4262 (1981).

[26] J. L. Holmes and F. P. Lossing, "Heats of Formation of Organic Radicals from Appearance Energies," Int. J. Mass Spectrom. Ion Phys. in press.

[27] D. F. McMillen and D. M. Golden, "Hydrocarbon Bond Dissociation Energies," Ann. Rev. Phys. Chem. **33**, 493 (1982).

[28] J. Dyke, N. Jonathan, E. Lee, A. Morris, and M. Winter, "Vacuum Ultraviolet Photoelectron Spectroscopy of Transient Species: Part 8, The t-Butyl Radical," Phys. Scr. **16**, 197 (1977).

[29] J.-L. M. Abboud, W. J. Hehre, and R. W. Taft, "Benzyl Cation. A Long Lived Species in the Gas Phase?," J. Am. Chem. Soc. **98**, 6072 (1976).

[30] J.-A. A. Jackson, S. G. Lias, and P. Ausloos, "An Ion Cyclotron Resonance Study of the Structures of $C_7H_7^+$ Ions," J. Am. Chem. Soc. **99**, 7515 (1977).

[31] D. K. Sen Sharma and P. Kebarle, "Stability and Reactivity of the Benzyl and Tropylium Cations in the Gas Phase," Can. J. Chem. **59**, 1592 (1981).

[32] M. Rossi and D. M. Golden, "Absolute Rate Constants for Metathesis Reactions of Allyl and Benzyl Radicals with HI(DI). Heat of Formation of Allyl and Benzyl Radicals," J. Am. Chem. Soc. **101**, 1230 (1979).

[33] F. A. Houle and J. L. Beauchamp, "Detection and Investigation of Allyl and Benzyl Radicals by Photoelectron Spectroscopy," J. Am. Chem. Soc. **100**, 3290 (1978).

[34] J. B. Pedley and J. Rylance, "Sussex-N. P. L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds," University of Sussex (1977).

[35] S. J. Ashcroft, "Vapor Pressures and Enthalpies of Vaporization of Benzyl Halides," J. Chem. Eng. Data **21**, 397 (1976).

[36] S. G. Lias, D. M. Shold, and P. Ausloos, "Proton Transfer Reactions Involving Alkyl Ions and Alkenes. Rate Constants, Isomerization Processes, and the Derivation of Thermochemical Data", J. Am. Chem. Soc. **102**, 2540 (1980).

[37] T. Baer, "Gas Phase Heats of Formation of $C_2H_5^+$ and $C_3H_7^+$," J. Am. Chem. Soc. **102**, 2482 (1980).

[38] H. M. Rosenstock, R. Buff, M. A. A. Ferreira, S. G. Lias, A. C. Parr, R. L. Stockbauer, and J. L. Holmes, "Fragmentation Mechanism and Energetics of Some Alkyl Halide Ions," J. Am. Chem. Soc. **104**, 2337 (1982).

[39] D. Cremer, J. S. Binkley, J. A. Pople, and W. J. Hehre, "Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XXI. Rotational Potentials for Geminal Methyl Groups," J. Am.

Chem. Soc. **96**, 6900 (1974).

[40] S. M. Collyer and T. B. McMahon, "Proton Affinity of Water. A Scale of Gas Phase Basicities Including Ethylene and Water from Ion Cyclotron Resonance Proton Transfer Equilibria Measurements," J. Phys. Chem. **87**, 909 (1983).

[41] R. Yamdagni and P. Kebarle, "Gas Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements," J. Am. Chem. Soc. **98**, 1320 (1976).

[42] K. M. A. Refaey and W. A. Chupka, "Photoionization of the Lower Aliphatic Alcohols with Mass Analysis," J. Chem. Phys. **48**, 5205 (1968).

[43] I. Omura, T. Kaneko, Y. Yamada, and K. Tanaka, "Mass Spectrometric Studies of Photoionization. V. Methanol and Methanol-d," J. Phys. Soc. Japan **27**, 981 (1969).

[44] F. P. Lossing, "Heats of Formation of Some Isomeric $[C_nH_{2n+1}O]^+$ Ions. Substitutional Effects on Ion Stability," J. Am. Chem. Soc. **99**, 7526 (1977).

[45] K. Tanaka, G. I. Mackay, and D. Bohme, "Rate and Equilibrium Constant Measurements for Gas-Phase Proton Transfer Reactions Involving H_2O, H_2S, HCN, and H_2CO," Can. J. Chem. **56**, 193 (1978).

[46] C. Y. Ng, D. J. Trevor, P. W. Tiedemann, S. T. Ceyer, P. L. Kronebusch, B. H. Mahan, and Y. T. Lee, "Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H_2O and HF," J. Chem. Phys. **67**, 4235 (1977).

[47] J. E. Del Bene, H. D. Mettee, M. J. Frisch, B. T. Luke, and J. A. Pople, "Ab Initio Computation of the Enthalpies of Some Gas-Phase Hydration Reactions," J. Phys. Chem. **87**, 3279 (1983).

[48] D. K. Bohme and G. I. Mackay, "Gas Phase Proton Affinities for H_2O, C_2H_4, and C_2H_6," J. Am. Chem. Soc. **103**, 2173 (1981).

[49] R. Clair and T. B. McMahon, "A Statistical Thermodynamic Analysis of the Entropy Change for the Equilibrium: $H_3O^+ + H_2S \rightleftharpoons H_3S^+ + H_2O$," Int. J. Mass Spectrom. Ion Phys. **39**, 27 (1981).

[50] K. Raghavachari, R. A. Whiteside, J. A. Pople, and P. v. R. Schleyer, "Molecular Orbital Theory of the Electronic Structure of Organic Molecules. 40. Structures and Energies of C_1-C_3 Carbocations, Including Effects of Electron Correlation," J. Am. Chem. Soc. **103**, 5649 (1981).

[51] P. M. Guyon, W. A. Chupka, and J. Berkowitz, "Photoionization Mass Spectrometric Study of Formaldehyde H_2CO, HDCO and D_2CO," J. Chem. Phys. **64**, 1419 (1976).

[52] C. Matthews and P. Warneck, "Heats of Formation of CHO^+ and $C_3H_3^+$ by Photoionization," J. Chem. Phys. **51**, 854 (1969).

[53] J. M. Dyke, N. Jonathan, A. Morris, and M. J. Winter, "The First Ionization Potential of the Formyl Radical Studied with U.V. Photoelectron Spectroscopy," Molecular Physics **39**, 629 (1980).

[54] P. Warneck, "Heat of Formation of the HCO Radical," Z. Naturforsch. **29a**, 350 (1974).

[55] K. E. McCulloh, "Energetics and Mechanisms of Fragment Ion Formation in the Photoionization of Normal and Deuterated Water and Ammonia," Int. J. Mass Spectrom. Ion. Phys. **21**, 333 (1976).

[56] J. Berkowitz, E. H. Appelman, and W. A. Chupka, "Photoionization of HOF with Mass Analysis," J. Chem. Phys. **58**, 1950 (1973).

[57] S. Katsumata and D. R. Lloyd, "The Photoelectron Spectra of the OH and OD Radicals," Chem. Phys. Letters **45**, 519 (1977).

[58] J. M. Dyke, N. Jonathan, A. Morris, and M. J. Winter, "The He I Photoelectron Spectrum of the Hydroperoxy Radical," Molecular Physics **44**, 1059 (1981).

[59] D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, "The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units," J. Phys. Chem. Ref. Data **11**, Suppl. 2 (1982).

[60] K. E. McCulloh, "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).

[61] (a) D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," NSRDS-NBS 37 (1971); (b) M. W. Chase, J. L. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, "JANAF Thermochemical Tables, 1975 Supplement, J. Phys. Chem. Ref. Data 4, 1 (1975); (c) M. W. Chase, Jr., J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela, J. Chem. Phys. Ref. Data, 11, 695 (1982).

[62] J. F. Liebman and M. Motevalli-Aliabadi, in preparation.

[63] S. W. Benson and J. H. Buss, "Additivity Rules for the Estimation of Molecular Properties. Thermodynamic Properties," J. Chem. Phys. **29**, 546 (1958).

[64] S. W. Benson, "Thermochemical Kinetics: Methods for the Estimation of Thermochemical Data and Rate Parameters," John Wiley & Sons, New York (1976).

[65] K. Bystrom, "Enthalpies of Combustion, Vaporization and Formation for Di-n-propyldiazene N-oxide and Di-t-butyldiazene N-oxide," J. Chem. Thermodyn. **13**, 139 (1981).

[66] H. M. Rosenstock, J. Dannacher, and J. F. Liebman, "The Role of Excited Electronic States in Ion Fragmentation: $C_6H_6^+$," Radiat. Phys. Chem. **20**, 7 (1982).

[67] S. W. Benson, personal communication.

[68] W. J. Hehre, R. Ditchfield, L. Radom, and J. A. Pople, "Molecular Orbital Theory of the Electronic Structure of Organic Compounds. V. Molecular Theory of Bond Separation," J. Am. Chem. Soc. **92**, 4796 (1970).

[69] J. D. Dill, A. Greenberg, and J. F. Liebman, "Substituent Effects on Strain Energies," J. Am. Chem. Soc. **101**, 6814 (1979).

Table 1. Gas phase basicities and proton affinities

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_{14}H_{18}N_2]$ N,N,N',N'-Tetramethyl-1,8-naphthalenediamine RN 20734-58-1					234.8	982.	241.8	1012	
	320	ZZ	(34.9)	234.9					83TAF
	600	A	(39.2)	234.8					78LAU/SAL
$[C_8H_{20}N_2]$ $(CH_3)_2N(CH_2)_4N(CH_3)_2$ RN 111-51-3					232.6	973.	240.4	1006.	
	320	A	(37.9)	233.5					TAFT
	300			231.7**					79AUE/BOW
$[C_{14}H_{27}N]$ 1-Methyl-2,6-t-butylpiperidine RN xxxxx					231.4	968.	239.2	1001.	
	320	ZZ	(31.4)	231.4					83TAF
$[C_7H_{18}N_2]$ $(CH_3)_2N(CH_2)_3N(CH_3)_2$ RN 110-95-2					231.0	967.	238.8	999.	
	320	A	(36.2)	231.8					TAFT
	300			230.2**					79AUE/BOW
$[C_5H_{14}N_2]$ 1,5-Diaminopentane RN 462-94-2					223.0	933.	238.1	996.	
	298	A	(30.4)	225.0					73YAM/KEB
	300	C	(12.9)	223.0					73AUE/WEB
	300			221.9*					79AUE/BOW
	600	A	(26.2)	221.3					78LAU/SAL
$[C_7H_{18}N_2]$ 1,7-Diaminoheptane RN 646-19-5					224.2	938.	238.	996.	
	298	E	(6.9)	224.2					73YAM/KEB
$[C_{10}H_{24}N_2]$ $(CH_3)_2N(CH_2)_6N(CH_3)_2$ RN 111-18-2					230.1	963.	237.9	995.	
	320	A	(35.3)	230.9					TAFT
	300			229.3**					79AUE/BOW
$[C_6H_{16}N_2]$ 1,6-Diaminohexane RN 124-09-4					223.0	933.	237.7	994.5	
	300	C	(12.9)	223.0					73AUE/WEB
	300			221.9**					79AUE/BOW
$[C_4H_{12}N_2]$ 1,4-Diaminobutane RN 110-60-1					225.0	941.	237.6	994.	
	330	D	(12.2)	225.3					80MAU/HAM
	300	C	(14.6)	224.7					73AUE/WEB
	300			223.9*					79AUE/BOW
$[C_5H_{14}N_2]$ $(CH_3)_2N(CH_2)_3NH_2$ RN 109-55-7					229.4	959.	237.2	992.	
	320	A	(33.8)	229.4					TAFT
	300			228.0**					79AUE/BOW
$[C_6H_{13}N]$ $(CH_3)_2NC(CH_3)=CHCH_3$ RN 52113-79-8					~229	~958	~237	~991	
		(br)		~229					81ELL/DIX
$[C_6H_{16}N_2]$ $(CH_3)_2N(CH_2)_2N(CH_3)_2$ RN 110-18-9					228.6	956.5	236.4	989.	
	320	A	(33.0)	228.6					75TAF
	300			227.2**					79AUE/BOW
$[C_7H_{15}N]$ $(CH_3)_2NC(C_2H_5)=CHCH_3$ RN 78733-73-0					228.6	956.	236.4	989.	
		(br)		228.6					81ELL/DIX

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_7H_{10}N_2$] N,N-Dimethyl-4-pyridinamine RN 1122-58-3					228.4	956.	236.2	988.	
	320	A	(33.3)	228.9					TAFT
	300			227.9*					76AUE/WEB(2)
[$C_{13}H_{16}N_2$] N,N,N'-Trimethyl-1,8-naphthalenediamine RN 20723-57-0					227.8	953.	235.6	986.	
	600	A	(32.2)	227.8					78LAU/SAL
[$C_8H_{19}N$] $(i\text{-}C_3H_7)_2(C_2H_5)N$ RN 7087-68-5					227.5	952.	235.3	984.	
	320	A	(31.9)	227.5					TAFT
[$C_{10}H_{16}N_2$] 1,2-$(N(CH_3)_2)_2C_6H_4$ RN 704-01-8					227.4	951.	235.2	984.	
	600	A	(31.8)	227.4					78LAU/SAL
[$C_9H_{21}N$] $(t\text{-}C_4H_9)C(CH_3)_2N(CH_3)_2$ RN 3733-36-6					227.3	951.	235.1	984.	
	320	A	(31.7)	227.3					78SHE/GOB
[$C_{12}H_{27}N$] $(n\text{-}C_4H_9)_3N$ RN 102-82-9					227.0*	950.*	234.8*	982.*	
	300	B	(21.3)	227.0*					79AUE/BOW
[$C_{13}H_{25}N$] 2,6-Di-t-butylpiperidine RN xxxxx					226.5	948.	234.3	980.	
	320	ZZ	(26.5)	226.5					83TAF
[$C_8H_{15}N$] 1,4,4-Trimethyl-1,2,3,4-tetrahydropyridine RN 35079-50-6							234.2**	980.**	80HOU/VOG
[$C_3H_{10}N_2$] 1,3-Diaminopropane RN 109-76-2					222.0	929.	234.1	979.	
	298	A	(30.1)	225.7					73YAM/KEB
	330	D	(8.8)	221.9					80MAU/HAM
	300	C	(12.0)	222.1					73AUE/WEB
	300			220.9*					79AUE/BOW
[$C_9H_{21}N$] $(n\text{-}C_3H_7)_3N$ RN 102-69-2					226.2	946.	234.0	979.	
	320	ZZ	(27.1)	227.1					83TAF
	320	A	(31.3)	226.9					TAFT
	320	A	(30.6)	226.2					75TAF-75ARN
	300	B	(19.9)	225.6*					79AUE/BOW
	300	B	(20.5)	226.2					72AUE/WEB
[$C_4H_{11}NO$] $NH_2(CH_2)_4OH$ RN 13325-10-5					220.7	923.	233.8	978.	
		D	(7.6)	220.7					80MAU/HAM
[$C_{13}H_{21}N$] 2,6-Di-t-butylpyridine RN 585-48-4					224.7	940.	233.4	976.	
	320	ZZ	(24.4)	224.4					83TAF
	320	A	(28.8)	224.4					TAFT
	320	A	(29.8)	225.4					75TAF-75ARN
	320	A	(28.2)	223.8					75WOL/HAR
	300			223*					76AUE/WEB(2)
	425	D	(13.6)	226.7					83MAU/SIE
[$C_8H_{19}N$] $(t\text{-}C_4H_9)_2NH$ RN 21981-37-3					225.4	943.	233.2	976.	
	320	A	(29.8)	225.4					TAFT

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_9H_{17}N$] 1-Cyclopentylpyrrolidine RN 18707-33-0						233.1**	975.**	
								79AUE/BOW
[$C_{15}H_{18}$] 1,4-Dimethyl-7-isopropylazulene RN 489-84-9				225.	941.	233.	975.	
320	ZZ	(25.)	225.					77WOL/ABB
[$C_{11}H_{17}N$] 2,6-Diisopropylpyridine RN 6832-21-9				225.1	942.	232.9	974.	
425	D	(12.0)	225.1					83MAU/SIE
[$C_9H_{19}N$] N-Isobutylpiperidine RN 10315-89-6						232.9**	974.**	
								80HOU/VOG
[$C_9H_{21}N$] (t-C_5H_{11})(t-C_4H_9)NH RN 58471-09-3				224.7*	940.	232.5*	973.	
300	B	(19.0)	224.7*					79AUE/BOW
[$C_9H_{18}N_2$] 1,5-Diazabicyclo[3.3.3]-undecane RN 283-58-9				224.6	940.	232.4	972.	
320	A	(29.0)	224.6					81ALD/ARR
[$C_6H_{15}N$] $(C_2H_5)_3N$ RN 121-44-8				224.5	939.	232.3	972.	
320	A	(29.3)	224.9					83TAF
320	A	(28.9)	224.5					72ARN/JON
320	A	(28.5)	223.9					77STA/TAA-75TAF
320	A	(28.8)	224.5					83MCI
320	E	(7.3)	225.1					74STA/BEA(2)
300	B	(17.7)	223.4*					79AUE/BOW
300	B	(18.2)	223.9					72AUE/WEB
550	C	(14.7)	224.8					79MAU
[$C_7H_{13}N$] 1-Azabicyclo[2.2.2]octane (Quinuclidine) RN 100-76-5				224.3	938.	232.1	971.	
320	ZZ	(25.5)	225.5					83TAF
320	A	(28.9)	224.5					77STA/TAA-75TAF
300	B	(17.9)	223.6*					79AUE/BOW
320	E	(7.7)	225.5					74STA/BEA(2)
						232.1**	971.**	80HOU/VOG
[$C_6H_{15}N$] $(CH_3)_2(t$-$C_4H_9)N$ RN 918-02-5				224.2	938.	232.0	971.	
320	A	(28.6)	224.2					TAFT
[$C_{11}H_{13}N$] 1,4-Dihydro-1,4-ethanoquinoline RN 4363-25-1				224.2	938.	232.0	971.	
320	A	(28.6)	224.2					TAFT
[$C_7H_{17}N$] $(C_2H_5)_2(n$-$C_3H_7)N$ RN 4458-31-5				224.2**	938.**	232.0**	971.**	
300	B	(18.5)	224.2*					79AUE/BOW
[$C_9H_{17}NO_2$] 3,3-Dimethoxy--1-azabicyclo[2.2.2]octane RN xxxxx				224**	937**	232**	971**	
300			224**					79AUE/BOW
[$C_{13}H_9N$] Acridine RN 260-94-6				224.1	938.	231.9	970.	
550	C	(14.0)	224.1					79MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_6H_9N_3O_2]$ L-Histidine RN xxxxx					224.1	938.	231.9	970.	
		A	(28.5)	224.1					83MCI
$[C_7H_{19}NSi]$ $(CH_3)_3Si(CH_2)_2N(CH_3)_2$ RN 23138-94-5					224.0	937.	231.8	970.	
	320	A	(28.4)	224.0					78SHE/GOB
$[C_8H_{21}NSi]$ $(CH_3)_3Si(CH_2)_3N(CH_3)_2$ RN 28247-29-2					224.0	937.	231.8	970.	
	320	A	(28.4)	224.0					78SHE/GOB
$[C_8H_{19}N]$ $(sec\text{-}C_4H_9)_2NH$ RN 626-23-3					223.6	935.5	231.8	970.	
	300	B	(17.0)	223.6					72AUE/WEB
$[C_7H_{14}N_2]$ 3-Amino-1-azabicyclo[2.2.2]octane RN 6238-14-8					224.0**	937.**	231.8**	970.**	
	300			224.0**					79AUE/BOW
$[C_8H_{15}N]$ 3-Methyl-1-azabicyclo[2.2.2]octane RN 695-88-5					223.9**	937.**	231.7**	969.**	
	300			223.9**					79AUE/BOW
$[C_6H_{15}P]$ $(C_2H_5)_3P$ RN 554-70-1					223.9**	937.**	231.7**	969.**	
	300			223.9**					79AUE/BOW
$[C_9H_{19}N]$ 2,2,6,6-Tetramethylpiperidine RN 768-66-1					223.9**	937.**	231.7**	969.**	
	300			223.9**					79AUE/BOW
$[C_6H_{17}NSi]$ $(CH_3)_3SiCH_2N(CH_3)_2$ RN 18182-40-6					223.6	936.	231.5	968.	
	320	A	(28.0)	223.6					TAFT
	320	A	(27.9)	223.5					78SHE/GOB
$[C_{13}H_{21}N]$ Pyridine,2,4-di-t-butyl RN 29939-31-9					223.6*	935.5**	231.4**	968.**	
	300			223.6*					76AUE/WEB(2)
$[C_9H_{13}N]$ 2,6-Diethylpyridine RN 935-28-4					223.3	934.	231.1	967.	
	425	D	(10.2)	223.3					83MAU/SIE
$[C_8H_{13}N]$ 1-Azabicyclo[2.2.2]-oct-2-ene,3-methyl RN xxxxx					223.2**	934.**	231.0**	966.5**	
	300			223.2**					79AUE/BOW
$[C_6H_{15}NO]$ $NH_2(CH_2)_6OH$ RN 4048-33-3					216.0**	904.**	231.0**	966.5**	
	300			216.0**					79AUE/BOW
$[C_8H_{17}N]$ 1,4,4-Trimethylpiperidine RN 1003-84-5							230.8**	966.**	
									80HOU/VOG
$[C_{12}H_{21}N]$ $(CH_2{=}C(CH_3)CH_2)_3N$ RN xxxxx					222.9**	932.6**	230.7**	965.**	
	300			222.9**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_9H_{17}N$] c-$C_5H_{10}NCH=C(CH_3)_2$ RN 673-33-6				222.9**	932.6**	230.7**	965.**	
300			222.9**					79AUE/BOW
[$C_8H_{19}N$] $(CH_3)_3C(CH_2)_2N(CH_3)_2$ RN 15673-04-8				222.6	931.	230.4	964.	
320	A	(27.0)	222.6					78SHE/GOB
[$C_{13}H_{13}P$] $(C_6H_5)_2(CH_3)P$ RN 1486-28-8				222.5	931.	230.3	963.5	
320	EE	(3.2)	222.5					82IKU/KEB
[$C_6H_{14}N_2O_2$] L-Lysine RN 56-87-1				222.5	931.	230.3	963.5	
	A	(26.9)	222.5					83MCI
[$C_6H_{15}N$] $(i\text{-}C_3H_7)_2NH$ RN 108-18-9				222.0	929.	230.2	963.	
320	A	(26.4)	222.0					TAFT
320	A	(25.5)	221.1					75ARN
	A	(26.4)	222.0					83MCI
300	B	(15.0)	220.7*					79AUE/BOW
300	B	(16.2)	221.9					72AUE/WEB
[$C_{10}H_{19}N$] 1-Azabicyclo[3.3.3]undecane (Manxine) RN 31023-92-4				222.3	930.	230.1	963.	
300	B	(16.6)	222.3					75AUE/WEB
300			223**					79AUE/BOW
[$C_8H_{13}N$] 1-Azabicyclo[2.2.2]-octane,3-methylene RN 22207-84-7				222.3**	930.**	230.1**	963.**	
300			222.3**					79AUE/BOW
[$C_5H_{13}N$] $(CH_3)(C_2H_5)_2N$ RN 616-39-7				222.2	930.	230.0	962.	
320	A	(26.9)	222.5					TAFT
320	A	(26.3)	221.9					75TAF-75ARN
[$C_{12}H_{24}O_6$] 1,4,7,10,13,16-Hexaoxacyclooctadecane (18-Crown-6) RN 17455-13-9				216.0	904.	230.0	962.	
300	(Key)		211.3					83MAU
300	A	(20.4)	216.0					84SHA/BLA
[$C_{12}H_{14}N_2$] N,N'-Dimethyl-1,8-naphthalenediamine RN 20734-56-9				223.0	933.	230.0	962.	
600	A	(27.9)	223.0					78LAU/SAL
[$C_9H_{15}N$] $(CH_2=CHCH_2)_3N$ RN 102-70-5				222.2	930.	230.0	962.	
320	A	(27.0)	222.6					TAFT
320	A	(26.4)	222.0					75TAF-75ARN
300			221.5**					79AUE/BOW
[$C_5H_6N_2$] 4-Pyridinamine RN 504-24-5				222*	929*	230*	962*	
300			222*					76AUE/WEB(2)
[$C_{18}H_{15}P$] $(C_6H_5)_3P$ RN 603-35-0				222.5	931.	~230.	~962.	
320	EE	(~3.2)	222.5					82IKU/KEB
[$C_7H_{17}N$] $(CH_3)_2(neo\text{-}C_5H_{11})N$ RN 10076-31-0				222.1	929.	229.9	962.	
320	A	(26.6)	222.1					TAFT
320	A	(26.5)	222.0					78SHE/GOB

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[$C_7H_{10}N_2$] N,N-Dimethyl-3-pyridinamine RN 18437-57-5					222.1**	929.**	229.9**	962.**	
	300			222.1**					76AUE/WEB(2)
[$C_5H_{13}N$] $(CH_3)_2(i\text{-}C_3H_7)N$ RN 996-35-0					222.0	929.	229.8	961.	
	320	A	(26.9)	222.5					TAFT
	300	B	(15.4)	221.1*					79AUE/BOW
[$C_8H_{21}NSi$] $(CH_3)_2(t\text{-}C_4H_9)SiN(CH_3)_2$ RN 66365-05-7					221.9	928.	229.7	961.	
	320	A	(26.3)	221.9					78SHE/GOB
[$C_6H_{13}N$] 1-Methylpiperidine RN 626-67-5					221.9	928.	229.7	961.	
	320	A	(26.8)	222.4					TAFT
	320	A	(27.4)	223.0					75ARN
	300	B	(15.3)	221.0					76AUE/WEB
[$C_8H_{11}P$] $C_6H_5P(CH_3)_2$ RN 672-66-2					221.8	928.	229.6	961.	
	320	EE	(2.5)	221.8					82IKU/KEB
[$C_5H_{11}N$] $(CH_3)_2C{=}NC_2H_5$ RN 15673-04-8					221.7**	927.5**	229.5**	960.**	
	300			221.7**					79AUE/BOW
[$C_6H_{13}N$] $(CH_3)_2C{=}CHN(CH_3)_2$ RN xxxxx					221.7	928.	229.5	960.	
		(br)		221.7					81ELL/DIX
[$C_5H_{11}N$] $CH_3CH{=}CHN(CH_3)_2$ RN 6163-56-0					221.7	928.	229.4	960.	
		(br)		221.7					81ELL/DIX
[$C_{12}H_{19}N$] $C_6H_4N(CH_3)_2$,2-t-C_4H_9 RN 22025-87-2					221.5	927.	229.3	959.	
	320	A	(25.9)	221.5					TAFT
[$C_7H_{10}N_2$] N,N-Dimethyl-2-pyridinamine RN 5683-33-0					221.4*	926.*	229.2*	959.*	
	300			221.4*					76AUE/WEB(2)
[$C_6H_{12}N_2$] 1,4-Diazabicyclo[2.2.2]octane RN 280-57-9					221.2	925.5	229.0	958.	
	320	A	(25.1)	220.6					75ARN
	320	E	(3.8)	221.6					74STA/BEA(2)
	300	B	(15.0)	220.7					76AUE/WEB
	300			220**					79AUE/BOW
[CH_2O] HCOH RN xxxxx					221.	925.	229.	958.	
		(br)		221.					82PAU/HEH(2)
[$C_4H_6N_2$] 1-Methylimidazole RN 616-47-7					221.1	925.	228.9	958.	
	320	A	(25.1)	220.7					TAFT
		(br)		221.4					81ELL/DIX
	600	(Key)		220.					83MAU
[$C_{11}H_{17}N$] 2-C_6H_{13}(c-C_5H_4N) RN 1129-69-7					221.1	925.	228.9	958.	
	425	D	(8.0)	221.1					83MAU/SIE

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_{11}H_{17}N$] 3-$CH_3C_6H_4N(C_2H_5)_2$ RN 91-67-8					220.9	924.	228.9	958.	
	320	I	(5.5)	220.9					LIA/JAC
[$C_5H_{11}N$] N-Methylpyrrolidine RN 120-94-5					220.9	924.	228.7	957.	
	320	A	(25.7)	221.3					75TAF-75ARN
	300	B	(14.3)	220.0					76AUE/WEB
		D	(8.3)	221.4					73TAF/TAA-78TAA/WOL
[C_3H_9NO] $NH_2(CH_2)_3OH$ RN 156-87-6					217.3	909.	228.6	956.5	
	330	D	(4.2)	217.3					80MAU/HAM
				216.0**					79AUE/BOW
[$C_8H_{19}N$] $(i-C_4H_9)_2NH$ RN 110-96-3					220.4	922.	228.6	956.	
	300	B	(14.7)	220.4*					72AUE/WEB
	320	A	(25.2)	220.4					75ARN
[$C_{11}H_{17}N$] 4-$CH_3C_6H_4N(C_2H_5)_2$ RN 613-48-9					220.6	923.	228.6	956.	
		I	(5.2)	220.6					LIA/JAC
[$C_{12}H_{19}N$] $C_6H_5N(C_3H_7)_2$ RN 2217-07-4					220.6	923.	228.6	956.	
	320	I	(5.2)	220.6					LIA/JAC
[$C_7H_{11}N$] 1-Azabicyclo[2.2.2]oct-2-ene RN 13929-94-7					220.7**	923.**	228.5**	956.**	
	300			220.7**					79AUE/BOW
							229.3**	959.**	80HOU/VOG
[$C_8H_{19}N$] $(n-C_4H_9)_2NH$ RN 111-92-2					220.3	922.	228.4	956.	
	300	B	(14.5)	220.2*					76AUE/WEB
	300	B	(14.6)	220.3					72AUE/WEB
	320	A	(24.6)	220.2					75ARN
[C_7H_9N] 2,6-Dimethylpyridine RN 108-48-5					220.4	922.	228.2	955.	
	300			219.2*					76AUE/WEB(2)
	320	A	(24.3)	219.9					75ARN
	425	D	(7.8)	220.9					83MAU/SIE
[$C_6H_{11}NO$] c-$C_5H_8N(2-OCH_3)$ RN 53687-79-9					220.3*	922.*	228.1*	954.*	
	300	B	(14.6)	220.3*					79AUE/BET
[$C_7FH_{12}N$] 3-Fluoro-1-azabicyclo[3.2.1]octane RN xxxxx					220.3**	922.**	228.1**	954.**	
	300			220.3**					79AUE/BOW
[$C_9H_{13}N$] $C_6H_5CH_2N(CH_3)_2$ RN 103-83-3					220.3**	922.**	228.1**	954.**	
	300			220.3**					79AUE/BOW
[C_4H_9N] $(CH_3)_2NCH=CH_2$ RN 5763-87-1					220.0	920.	227.8	953.	
		(br)		220.0					81ELL/DIX
[$C_9H_{11}N$] 2,3-Cyclohexenopyridine RN 10500-57-9					219.9**	920.**	227.7**	953.**	
	300			219.9**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

Compound	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_9H_{11}N$] 3,4-Cyclohexenopyridine RN 36566-06-6					219.9**	920.**	227.7**	953.**	
	300			219.9**					79AUE/BOW
[$C_7ClH_{14}N$] c-C_5H_9N,2-CH_2Cl,1-CH_3 RN 49665-74-9					219.8**	920.**	227.6**	952.**	
	300			219.8**					79AUE/BOW
[$C_{10}H_{15}N$] $C_6H_5N(C_2H_5)_2$ RN 91-66-7					219.6	919.	227.6	952.	
	600	A	(26.9)	222.0					73YAM/KEB
	325	I	(4.2)	219.6					LIA/JAC
[C_6H_7NO] 4-Methoxypyridine RN 620-08-6					219.8	920.	227.6	952.	
	320	D	(8.7)	221.7					72TAA/HEN
	320	A	(24.8)	220.4					81TAA/SUM
	320	A	(24.2)	219.8					75TAF-75ARN
	300			218.8*					76AUE/WEB(2)
[$C_4H_{11}N$] $(CH_3)_2(C_2H_5)N$ RN 598-56-1					219.7	919.	227.5	952.	
	320	A	(24.5)	220.1					TAFT
	320	A	(23.9)	219.5					75TAF-75ARN
	300	B	(13.1)	218.8*					76AUE/WEB
[$C_6H_{15}N$] $(n-C_3H_7)_2NH$ RN 142-84-7					219.7	919.	227.5	952.	
	320	A	(24.3)	219.9					75TAF-83TAF
	300	B	(13.5)	219.2*					79AUE/BOW
	300	B	(13.8)	219.5					72AUE/WEB
	535	C	(9.6)	219.7					79MAU
[$C_9H_{13}N$] 2-t-Butylpyridine RN 5944-41-2					219.6**	919.**	227.4**	951.**	
	300			218.6**					79AUE/BOW
	425	D	(7.4)	220.5					83MAU/SIE
[$C_5H_{13}N$] $(C_2H_5)(i-C_3H_7)NH$ RN 19961-27-4					219.4	918.	227.4	951.	
	320	A	(23.8)	219.4					TAFT
[C_7H_9N] 2,4-Dimethylpyridine RN 108-47-4					219.5*	918.*	227.3*	951.*	
	300			219.5*					76AUE/WEB(2)
[$C_8H_{11}N$] 2-Isopropylpyridine RN 75981-47-4					219.4	918.	227.2	951.	
	425	D	(6.3)	219.4					83MAU/SIE
[$C_{10}H_{22}O_5$] $CH_3(OCH_2CH_2)_4OCH_3$ RN 143-24-8					213.2	892.	227.2	951.	
	300	A	(17.6)	213.2					84SHA/KEB
[C_3H_9P] $(CH_3)_3P$ RN 594-09-2					219.3	917.5	227.1	950.	
	320	EE	(0.0)	219.3					82IKU/KEB
	320	E	(1.6)	219.3					74STA/BEA
	320	A	(23.4)	219.0					75TAF
[$BrC_7H_{12}N$] 3-Bromo-1-azabicyclo[2.2.2]-octane RN xxxxx					219.3**	917.5**	227.1**	950.**	
	300			219.3**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
		kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_9H_{13}N]$ $C_6H_5N(CH_3)(C_2H_5)$ RN 613-97-8				219.3	917.5	227.1	950.	
600	A	(24.2)	219.3					73YAM/KEB-78LAU/SAL
$[C_{10}H_{15}N]$ 3,5-$(CH_3)_2C_6H_3N(CH_3)_2$ RN 4913-13-7				219.0	916.	227.0	950.	
320	I	(3.6)	219.0					LIA/JAC
$[C_8H_9N]$ 3,4-Cyclopentenopyridine RN xxxxx				219.0**	916.**	226.8**	949.**	
300			219.0**					79AUE/BOW
$[C_9H_7N]$ Quinoline RN 91-22-5				218.7	915.	226.5	948.	
425	(Key)					225.8		81MCL/CAM
535	C	(8.6)	218.7					79MAU
$[C_3H_8Si]$ $(CH_3)_2Si{=}CH_2$ RN 4112-23-6				218.0	912.	226.4	947.	
320	A	(22.4)	218.0					82PIE/HEH
320	(br)		~219.0					79PIE/POL
$[C_5H_{15}NSi]$ $(CH_3)_3SiN(CH_3)_2$ RN 18135-05-2						226.4	947.	
	(br)							83HEN/FRE
$[C_5H_{11}N]$ Piperidine RN 110-89-4				218.2	913.	226.4	947.	
320	A	(22.3)	217.9					75TAF-75ARN-83TAF
300	E	(1.0)	218.8					71BOW/AUE
300	C	(8.3)	218.4					73AUE/WEB
300	B	(11.9)	217.4					75AUE/WEB(2)
300	B	(11.5)	217.2*					76AUE/WEB
600	A	(23.1)	218.2					78LAU/SAL
600	A	(24.5)	219.6					73YAM/KEB
$[C_3H_7N]$ $CH_2{=}C(CH_3)NH_2$ RN 4427-28-5				218.5	914.	226.3	947.	
	(Key)		218.5					81ELL/DIX
$[C_7H_9N]$ 2-Ethylpyridine RN 100-71-0				218.4	914.	226.2	946.	
300			217.1*					76AUE/WEB(2)
425	D	(5.3)	218.4					83MAU/SIE
$[C_7H_9N]$ 2,3-Dimethylpyridine RN 583-61-9				218.4*	914.*	226.2*	946.*	
300			218.4*					76AUE/WEB(2)
$[C_7H_9N]$ 3,4-Dimethylpyridine RN 583-58-4				218.4*	914.*	226.2*	946.*	
300			218.4*					76AUE/WEB(2)
$[C_6H_{13}O_3P]$ cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane RN 7735-82-2				218.4	914.	226.2	946.	
320	(Key)		218.4					80HOD/HOU
$[C_{12}H_{24}N_2]$ 1,6-Diazabicyclo[4.4.4]-tetradecane RN 71058-67-8				218.9	916.	226.0	946.	
320	A	(23.3)	218.9					81ALD/ARR
$[C_7H_9N]$ 2,5-Dimethylpyridine RN 589-93-5				218.2*	913.*	226.0*	946.*	
300			218.2*					76AUE/WEB(2)

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_7H_9NO]$ Pyridine-2-methoxymethyl RN 23579-92-2					218.2**	913.**	226.0**	945.5**	
	300			218.2**					79AUE/BOW
$[C_5H_9NO]$ c-$C_4H_6N(2\text{-}OCH_3)$ RN 5264-35-7					218.1	912.5	225.9	945.	
	300	B	(12.4)	218.1					79AUE/BET
$[C_2H_8N_2]$ 1,2-Diaminoethane RN 107-15-3					219.2	917.	225.9	945.	
	298	A	(24.1)	219.2					73YAM/KEB
	330	D	(3.4)	216.6					80MAU/HAM
	300	C	(6.5)	216.6					73AUE/WEB
$[C_4H_{11}N]$ $(C_2H_5)_2NH$ RN 109-89-7					217.7	911.	225.9	945.	
	320	A	(22.0)	217.6					83TAF
	320	A	(21.6)	217.2					75TAF-75ARN
	320	A	(22.0)	217.6					72ARN/JON
	300	B	(12.0)	217.7					72AUE/WEB
	300	B	(11.7)	217.4					75AUE/WEB(2)
	300	B	(11.2)	216.9*					76AUE/WEB
	550	C	(7.6)	217.7					79MAU
$[C_9H_7N]$ Isoquinoline RN 119-65-3					218.1	912.	225.9	945.	
	535	C	(8.0)	218.1					79MAU
$[C_9H_{13}N]$ 4-t-Butylpyridine RN 3978-81-2					218.1	913.	225.9	945.	
	300			218.1*					76AUE/WEB(2)
$[C_7H_7N]$ 3,4-Cyclobutenopyridine RN xxxxx					218.1**	912.**	225.9**	945.**	
	300			218.1**					79AUE/BOW
$[C_{11}H_{15}N]$ 1-Phenylpiperidine RN 4096-2-2					219.5	918.	225.8	945.	
	320	A	(23.9)	219.5					TAFT
$[C_8H_9N]$ 2,3-Cyclopentenopyridine RN xxxxx					218.0**	912.**	225.8**	945.**	
	300			218.0**					79AUE/BOW
$[C_7ClH_{12}N]$ 3-Chloro-1-azabicyclo[2.2.2]-octane RN 42332-45-6					218.0**	912.**	225.8**	945.**	
	300			218.0**					79AUE/BOW
$[C_9H_{13}N]$ 4-$CH_3C_6H_4N(CH_3)_2$ RN 99-97-8					217.6	910.	225.6	944.	
	320	I	(2.2)	217.6					LIA/JAC
$[C_{10}ClH_{14}N]$ 4-$ClC_6H_4N(C_2H_5)_2$ RN 2873-89-4					217.8	911.	225.6	944.	
	320	I	(-2.4)	213.0					LIA/JAC
$[C_7H_9N]$ 3,5-Dimethylpyridine RN 591-22-0					217.7*	911.*	225.5*	943.*	
	300	B	(12.0)	217.7*					76AUE/WEB
$[C_6H_7NS]$ 4-(Methylthio)-pyridine RN 22581-72-2					217.7**	911.**	225.5**	943.**	
	300			217.7**					79AUE/BOW
$[C_{11}H_{12}N_2O_2]$ L-Tryptophan RN 54-12-6					217.6	910.	225.4	943.	
		A	(22.0)	217.6					83MCI

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_6H_{13}N$] n-$C_3H_7CH{=}NC_2H_5$ RN 1611-12-7					217.5**	910.**	225.3**	943.**	
	300			217.5**					79AUE/BOW
[C_6H_7N] 4-Methylpyridine RN 108-89-4					217.4	909.	225.2	942.	
	320	D	(+5.4)	218.4					72TAA/HEN
	320	A	(21.1)	216.7					83TAF
	320	A	(21.4)	217.0					75TAF-75ARN
[C_4H_9N] Pyrrolidine RN 123-75-1					217.3	909.	225.2	942.	
	320	A	(21.3)	216.9					83TAF-81TAA/SUM
	320	A	(21.4)	217.0					75TAF-75ARN
	300	B	(10.4)	216.1*					76AUE/WEB
	320	E	(-0.3)	217.5					71BOW/AUE
[C_3H_9N] $(CH_3)_3N$ RN 75-50-3					217.3	909.	225.1	942.	
	320	E	(0.0)	217.3					74STA/BEA
	320	E	(0.0)	217.3					74STA/BEA(2)
	300	E	(0.0)	217.3					71BOW/AUE
	300	B	(11.5)	217.2					72AUE/WEB
	300	B	(10.7)	216.4					75AUE/WEB(2)
	300	B	(10.8)	216.5*					76AUE/WEB
	320	A	(21.9)	217.4					TAFT
	320	A	(21.4)	216.9					75TAF-75ARN
	320	A	(21.8)	217.3					72HEN/TAA-72ARN/JON
		A	(22.0)	217.6					83MCI-83TAF
	330	D	(4.4)	217.5					80MAU/HAM
	600	A	(23.3)	218.4					72BRI/YAM
[C_6H_7N] 2-Methylpyridine RN 109-06-8					217.2	909.	225.0	942.	
	320	A	(21.5)	217.1					TAFT
				215.9*					76AUE/WEB(2)
	425	D	(4.1)	217.2					83MAU/SIE
[$C_6H_{13}O_3P$] trans-2-Methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane RN 41821-91-4					216	904	225	941	
	320	A		216					80HOD/HOU
[$C_{10}H_{13}N$] N-Phenylpyrrolidine RN 4096-21-3					216.9	907.	224.7	940.	
	320	A	(21.3)	216.9					TAFT
[$C_6H_{11}N$] $(CH_2{=}CHCH_2)_2NH$ RN 124-02-7					216.9	907.	224.7	940.	
	320	A	(21.3)	216.9					TAFT
[C_9H_7NO] Quinoline-1-oxide RN 1613-37-2					216.8	907.	224.6	940.	
	526	C	(6.7)	216.8					79MAU
[C_7H_9N] 4-Ethylpyridine RN 536-75-4					216.8**	907.**	224.6**	940.**	
	300			216.8*					76AUE/WEB(2)
[$C_9H_{13}N$] 3-$CH_3C_6H_4N(CH_3)_2$ RN 121-72-2					216.7	907.	224.5	939.	
	320	F	(14.3)	216.7					77POL/DEV
[$C_6H_{11}NO_3$] $CH_3CONHCH(CH_3)COOCH_3$ (N-Acetyl L-alanine methyl ester) RN xxxxx					211.	883.	224.5	939.	
		(Key)		211.					83MAU
[$C_4H_6N_2$] 4-Methylimidazole RN 822-36-6					216.6	906.	224.4	939.	
	600	(Key)		216.6					83MAU

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_4H_{10}N_2]$ Piperazine RN 110-85-0				216.4	905.	224.2	938.	
300	C	(6.3)	216.4					73AUE/WEB
$[C_6H_7N]$ 3-Methylpyridine RN 108-99-6				216.2	905.	224.1	938.	
320	A	(20.6)	216.2					TAFT
300	B	(9.3)	215.0*					76AUE/WEB
			215.0*					76AUE/WEB(2)
600	D	(4.2)	217.3					83MAU
$[C_8H_{18}O_4]$ $CH_3(OCH_2CH_2)_3OCH_3$ RN 112-49-2				210.8	882.	224.1	938.	
300	(Key)		~212					83MAU
300	A	(15.2)	210.8					84SHA/BLA
$[C_7ClH_{10}N]$ 3-Chloro-1-azabicyclo[2.2.2]-oct-2-ene RN xxxxx				216.2**	904.5**	224.0**	937.**	
			216.2**					79AUE/BOW
$[C_{10}H_{17}NO]$ cis-3-Amino-2-twistanol RN xxxxx				216.2	904.5	224.0	937.	
	(Key)		216.2					83HOU/RUF
$[C_8H_{15}NO]$ cis-3-Aminobicyclo[2.2.2]octan-2-ol RN 17997-65-8				216.1	904.	223.9	937.	
	(Key)		216.1					83HOU/RUF
$[C_3H_8Pb]$ $(CH_3)_2Pb=CH_2$ RN 82065-01-8				216.1	904.	223.9	937.	
320	A	(20.5)	216.1					82PIE/HEH
$[C_7H_9N]$ 3-Ethylpyridine RN 536-78-7				216.1*	904.*	223.9*	937.*	
			216.1*					76AUE/WEB(2)
$[C_{10}H_{10}N_2]$ 1,8-Diaminonaphthalene RN 479-27-6				216.2	904.5	223.8	936.	
600	A	(21.1)	216.2					78LAU/SAL
$[C_4H_5N_3O]$ Cytosine RN 71-30-7				216.0	904.	223.8	936.	
535	C	(5.9)	216.0					79MAU
	(br)		~215					75WIL/MCC
$[C_5H_6N_2]$ 2-Pyridinamine RN 504-29-0				216.0*	904.*	223.8*	936.*	
			216.0*					79AUE/BOW
$[C_{12}H_8N_2]$ Phenazine RN 92-82-0				216.6	906.	223.7	936.	
514	C	(6.5)	216.6					79MAU
$[C_{10}H_{20}O_5]$ 1,4,7,10,13-Pentaoxacyclopentadecane (15-Crown-5) RN 33100-27-5				212.5	889.	223.6	935.	
300	(Key)		212.					83MAU
300	A		212.5					84SHA/BLA
$[C_6H_7NO]$ 3-Methoxypyridine RN 7295-76-3				215.7	902.	223.6	935.	
320	A	(20.9)	216.5					TAFT
			214.7*					76AUE/WEB(2)
$[C_5H_5N_5]$ Adenine RN 73-24-5				215.7	902.	223.5	935.	
550	C	(5.6)	215.7					79MAU
	(br)		~215					75WIL/MCC

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[C_3H_7N] Azetidine RN 503-29-7					215.7	902.	223.5	935.	
	300	B	(9.1)	214.8					75AUE/WEB(2)
	300	B	(8.8)	214.5*					76AUE/WEB
	300	E	(-2.1)	215.3					71BOW/AUE
[$C_8H_{11}N$] $C_6H_5N(CH_3)_2$ RN 121-69-7					215.4	901.	223.4	935.	
	320	I	(0.0)	215.4					LIA/JAC
	320	A	(19.9)	215.5					75TAF-83TAF
		A	(19.8)	215.4					83MCI
	320	F	(12.5)	215.4					77POL/DEV
	600	A	(21.7)	216.8					73YAM/KEB-78LAU/SAL
[C_7H_7N] 2,3-Cyclobutenopyridine RN xxxxx					215.5**	902.**	223.3**	934.**	
	300			215.5**					79AUE/BOW
[C_3H_9NO] $CH_3OCH_2CH_2NH_2$ RN 109-85-3					212.3*	888.*	223.3*	934.*	
	300	C	(2.2)	212.3*					73AUE/WEB
[C_7H_7N] 4-Vinylpyridine RN 100-43-6					215.4**	901.**	223.2**	934.**	
				215.4**					79AUE/BOW
[$C_8H_6N_2$] Cinnoline RN 253-66-7					215.4	901.	223.2	934.	
	535	C	(5.3)	215.4					79MAU
[$C_{10}H_{10}Ni$] $Ni(C_5H_5)_2$ RN 1271-28-9					216.	904.	223.	933.	
	320	(Key)		216.					76COR/BEA
	320	A	(19.1)	214.7					81STE/BEA
[$C_5H_5N_5O$] Guanine RN 73-40-5					~215	~899	~223	~933	
		(br)		~215					75WIL/MCC
[$C_6H_6N_4$] 6-Methylpurine RN 2004-03-7					~215	~899	~223	~933	
		(br)		~215					75WIL/MCC
[C_3H_9N] $(CH_3)(C_2H_5)NH$ RN 624-78-2					215.1	900.	222.8	932.	
	320	A	(19.8)	215.3					TAFT
	320	A	(19.1)	214.7					75TAF-75ARN
	300	B	(9.1)	214.8*					76AUE/WEB
[C_4H_9N] $CH_3CH{=}NC_2H_5$ RN 1190-79-0					214.9	899.	222.7	932.	
	300	B	(9.2)	214.9					75AUE/WEB(2)
[$C_6H_8N_2$] 1,3-$C_6H_4(NH_2)_2$ RN 108-45-2					214.7	898.	222.4	930.5	
	600	F	(12.2)	214.7					81LAU/NIS
	600	A	(19.7)	214.8					78LAU/SAL
[$C_9H_{11}NO_3$] L-Tyrosine RN xxxxx					214.5	897.	222.3	930.	
		A	(18.9)	214.5					83MCI
[$C_5H_{13}N$] t-$C_5H_{11}NH_2$ RN 594-39-8					213.9*	895.*	222.3*	930.*	
	300	B	(8.2)	213.9*					76AUE/WEB

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_{10}H_{19}NO]$ 4-Aminodecahydro-3-naphthalenol RN xxxxx					214.3	897.	222.1	929.	
		(Key)		214.3					83HOU/RUF
$[C_6H_7NS]$ 2-(Methylthio)-pyridine RN 18438-38-5					214.2	896.	222.0	929.	
	300	B	(8.5)	214.2					79AUE/BET
				214.2*					76AUE/WEB(2)
$[C_7H_6O]$ 4-Methylene-2,5-cyclohexadiene-1-one RN 502-87-4							~222**	~929**	
		(br)							77DIT/NIB
$[C_7H_{11}NO]$ 1-Azabicyclo[2.2.2]octan-3-one RN 3731-38-2					214.1**	896.**	221.9**	928.**	
				214.1**					79AUE/BOW
$[C_6H_7NO]$ 2-Methoxypyridine RN 1628-89-3					214.1	896.	221.9	928.	
	320	A	(18.8)	214.4					76COO/KAT
	300	B	(7.8)	213.5					79AUE/BET
				213.5*					76AUE/WEB(2)
$[C_6H_{14}O_2]$ $CH_3O(CH_2)_4OCH_3$ RN 13179-96-9					209.0	874.	221.8	928.	
	300	A	(13.4)	209.0					84SHA/BLA
$[C_7H_{16}O_2]$ $CH_3O(CH_2)_5OCH_3$ RN 111-89-7					208.8	874.	221.8	928.	
	300	A	(13.2)	208.8					84SHA/BLA
$[C_8H_{11}N]$ $C_6H_5NHC_2H_5$ RN 103-69-5					214.0	895.	221.8	928.	
	600	A	(18.4)	214.0					73YAM/KEB-78LAU/SAL
	425	(Key)		218.8					81MCL/CAM
$[C_7F_2H_{11}N]$ 3,3-Difluoro-1-azabicyclo-[2.2.2]octane RN xxxxx					214.0**	895.**	221.8**	928.**	
				214.0**					79AUE/BOW
$[C_7H_{13}N]$ Bicyclo[2.2.1]heptan-2-amine, exo (2-Aminonorbornane) RN 7242-92-4					213.3**	892.**	221.7**	927.**	
				213.3**					79AUE/BOW
$[C_7H_{13}N]$ Bicyclo[2.2.1]heptan-2-amine, endo (2-Aminonorbornane) RN 31002-73-0					213.3**	892.**	221.7**	927.**	
				213.3**					79AUE/BOW
$[C_8H_{16}O_4]$ 1,4,7,10-Tetraoxa-cyclododecane (12-Crown-4) RN 294-93-9					211.3	884.	221.6	927.	
	300	(Key)		211.0					83MAU
	300	A		211.3					84SHA/BLA
$[C_3H_7N]$ N-Methylaziridine RN 1072-44-2					213.8	894.	221.6	927.	
	300	B	(8.1)	213.8					75AUE/WEB(2)
$[C_{10}H_{17}NO]$ trans-3-Amino-2-twistanol					213.7	894.	221.5	927.	
		(Key)		213.7					83HOU/RUF

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	kJ/mol	Proton affinity kcal/mol	kJ/mol	Reference
[$C_5H_{11}NO_2S$] L-Methionine RN 59-51-8				213.6	894.	221.4	926.	
	A	(18.0)	213.6					83MCI
[C_2H_7NO] $NH_2(CH_2)_2OH$ RN 141-43-5				213.4	893.	221.3	926.	
330	D	(0.3)	213.4					80MAU/HAM
[$C_6H_{13}N$] c-$C_6H_{11}NH_2$ RN 108-91-8				213.4	893.	221.2	925.5	
320	A	(17.5)	213.1					75TAF-75ARN-83TAF
300	B	(7.2)	212.9*					76AUE/WEB
600	A	(19.5)	214.6					73YAM/KEB
[$C_5H_6N_2$] 3-Aminopyridine RN 462-08-8				213.2*	892.*	221.0*	925.*	
			213.2*					76AUE/WEB(2)
[$C_6H_{14}OSi$] $CH_2{=}C(CH_3)OSi(CH_3)_3$ RN 1833-53-0				213.	891.	221.	925.	
	(br)		213.					82HEN/WEI
[$C_4H_{11}N$] t-$C_4H_9NH_2$ RN 75-64-9				213.0	891.	220.8	924.	
320	A	(17.1)	213.0					75TAF-75ARN
320	A	(17.6)	213.2					72HEN/TAA-72ARN/JON
	A	(17.8)	213.4					83MCI-83TAF
300	B	(7.2)	212.9*					76AUE/WEB
300	B	(7.0)	212.7					72AUE/WEB
514	C	(3.3)	213.4					79MAU
550	A	(16.9)	212.1					80MAU
[C_5H_5N] Pyridine RN 110-86-1				213.1	892.	220.8	924.	
425	D	(0.0)	213.1					83MAU/SIE
	D	(0.0)	213.1					80MAU/HAM
	D	(0.0)	213.1					83MAU
320	A	(17.7)	213.3					83TAF
320	A	(17.0)	212.6					75TAF-75ARN
300	B	(6.4)	212.1					75AUE/WEB(2)
300	B	(6.9)	212.6*					76AUE/WEB
520	C	(3.0)	213.1					79MAU
550	A	(17.3)	212.5					80MAU
600	A	(17.6)	212.7					78LAU/SAL
600	A	(18.6)	213.7					72BRI/YAM
[C_3H_7N] $(CH_3)_2C{=}NH$ RN 38697-07-3				212.9	891	220.7	923	
	(br)		212.9					81ELL/DIX
[$C_{10}H_{23}N$] n-$(C_{10}H_{21})NH_2$ RN 2016-57-1				212.3**	888.**	220.7**	923.**	
			212.3**					79AUE/BOW
[$C_3H_9O_3P$] $P(OCH_3)_3$ RN 121-45-9				213.0	891.	220.6	923.	
300	(Key)		213.0					80HOD/MCD
[$C_9H_{12}O_3$] 1,3,5-$C_6H_3(OCH_3)_3$ RN 621-23-8				213.1	892.	220.6	923.	
320	A	(17.5)	213.1					TAFT
[$C_8H_{15}NO$] trans-3-Aminobicyclo[2.2.2]-octan-2-ol RN 40335-14-6				212.8	890.	220.6	923.	
	(Key)		212.8					83HOU/RUF

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_2H_7N]$ $(CH_3)_2NH$ RN 124-40-3					212.8	890.	220.6	923.	
	320	A	(17.1)	212.7					83TAF
	320	A	(16.8)	212.4					75TAF-75ARN
	320	A	(16.8)	212.4					72HEN/TAA-72ARN/JON
		A	(16.8)	212.4					83MCI
	300	B	(6.8)	212.5					72AUE/WEB
	300	B	(6.5)	212.1					75AUE/WEB(2)
	300	B	(6.6)	212.3*					76AUE/WEB
	600	A	(18.3)	213.4					72BRI/YAM
		D	(0.1)	213.2					80MAU/HAM
$[C_4H_{11}N]$ sec-$C_4H_9NH_2$ RN 13952-84-6					211.7	886.	220.5	922.	
	300	B	(6.4)	212.1*					76AUE/WEB
	300	B	(6.0)	211.7					72AUE/WEB
$[C_8H_{19}N]$ n-$(C_8H_{17})NH_2$ RN 111-86-4					212.0**	887.**	220.4**	922.**	
				212.0**					79AUE/BOW
$[C_5H_5NO]$ Pyridine-N-oxide RN 694-59-7					213.3	892.	220.3	922.	
	550	C	(3.2)	213.3					79MAU
$[C_9H_9N]$ $(HCCCH_2)_3N$ RN 6921-29-5					212.4	889.	220.2	921.	
	320	A	(16.6)	212.2					TAFT
	320	A	(16.0)	211.6					75TAF-75ARN
$[C_6H_7NO]$ 1-Methyl-2-pyridinone RN 694-85-9					212.2	888.	220.2	921.	
	300	B	(6.5)	212.2					79AUE/BET
	320	D	(-1.0)	212.6					76COO/KAT
$[C_5H_9NO_2]$ c-C_4H_7NH(2-COOH) (L-Proline) RN 609-36-9					212.4	889.	220.2	921.	
	370	A	(20.1)	215.7					83MCI
	600	A	(11.0)	212.4					73YAM/KEB
$[C_{10}H_{17}NO]$ trans-3-Amino-2-twistanol RN xxxxx					212.2	888.	220.0	920.	
		(Key)		212.2					83HOU/RUF
$[C_{12}H_{21}NO]$ 3-Amino-tricyclo$[7.3.0.0^{4,8}]$ dodecan-2-ol RN xxxxx					212.2	888.	220.0	920.	
		(Key)		212.2					83HOU/RUF
$[C_{10}H_8]$ Azulene RN 275-51-4					212.5	889.	220.	921.	
	320	A	(23.7)	219.3					TAFT
	320	A	(22.6)	218.2					75WOL/HAR
	320	ZZ	(18.1)	218.1					77WOL/ABB
	550	A	(17.3)	212.5	(1983, value reconfirmed)				80MAU
$[C_2H_8N_2]$ $(CH_3)_2NNH_2$ RN 57-14-7					212.1	887.	219.9	920.	
	320	A	(16.8)	212.4					TAFT
	320	A	(16.2)	211.8					75TAF-75ARN
$[C_4H_8N_2O_3]$ L-Asparagine RN 3130-87-8					212.0	887.	219.8	920.	
		A	(16.4)	212.0					83MCI

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_3H_4N_2$] Imidazole RN 288-32-4					212.0	887.	219.8	920.	
	600	D	(-1.1)	212.0					83MAU
[$C_4H_9O_3P$] 2-Methoxy-1,3,2-dioxaphosphorinane RN 31121-06-9					211.7	886.	219.4	918.	
	320	(Key)		211.7					80HOD/HOU
[C_4H_9NO] Morpholine RN 110-91-8					211.6	885.	219.4	918.	
	300	C	(1.5)	211.6					73AUE/WEB
[$C_6H_{14}O_3$] $CH_3(OCH_2CH_2)_2OCH_3$ RN 111-96-6					207.4	868.	219.4	918.	
	300	(Key)		207.4					83MAU
	300	A	(10.9)	206.5					84SHA/BLA
[$C_5H_{13}N$] neo-$C_5H_{11}NH_2$ RN 5813-64-9					211.7	886.	219.3	917.5	
	320	A	(16.1)	211.6					TAFT
	300	B	(6.1)	211.8					76AUE/WEB
[$C_5H_4N_4$] Purine RN 120-73-0					211.5	885.	219.3	917.5	
	515	C	(+1.4)	211.5					79MAU
		(br)		~209					75WIL/MCC
[$C_6H_{11}NO$] c-C_5H_8N(2-O)1-CH_3 RN 931-20-4					211.5	885.	219.3	917.5	
	300	B	(5.8)	211.5					79AUE/BET
	320	A	(15.6)	211.2					76COO/KAT
				209.1**					79AUE/BOW
[C_3H_7N] 2-Methylaziridine RN 75-55-8					211.4**	884.**	219.2**	917.**	
				211.4**					79AUE/BOW
[C_2H_5N] CH_2=$CHNH_2$ RN 593-67-9					211.3	884.	219.1	917.	
		(Key)		211.3					81ELL/DIX
[$C_7H_{17}N$] n-$C_7H_{15}NH_2$ RN 111-68-2					211.2	884.	219.0	916.	
	300	C	(1.1)	211.2					73AUE/WEB
[C_6H_6N] C_6H_5NH radical RN xxxxx					211	883	219	916	
		(br)		211					82MAU
[C_6ClH_6N] 2-Chloro-6-methylpyridine RN 18368-63-3					211**	883*	219**	916**	
				211**					79AUE/BOW
[Mg_2] Mg_2 RN 29904-79-8							219±7	916.	
		(Key)							77PO/POR

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_7H_6O]$ 2,4,6-Cycloheptatriene-1-one (Tropone) RN 539-80-0				212	887	219	918	
	(br)					226**	945**	77DIT/NIB
	(br)		212					83CAS/FRE
$[C_5H_{13}N]$ n-$C_5H_{11}NH_2$ RN 110-58-7				211.1	883.	218.9	916.	
300	B	(5.6)	211.3					79AUE/BET
535	C	(+0.8)	210.9					79MAU
$[C_6H_{13}NO_2]$ L-Isoleucine RN 73-32-5				211.1	883.	218.9	916.	
	A	(15.6)	211.1					83MCI
$[C_6H_{15}N]$ n-$C_6H_{13}NH_2$ RN 111-26-2				211.1	883.	218.9	916.	
300	C	(1.0)	211.1					73AUE/WEB
			211.7**					79AUE/BOW
$[C_4H_{11}N]$ i-$C_4H_9NH_2$ RN 78-81-9				211.1*	883.*	218.8*	915.*	
300	B	(5.4)	211.1*					76AUE/WEB
300	B	(4.8)	210.5					72AUE/WEB
320	A	(17.1)	212.7					75ARN
$[C_3H_7NO_2]$ Sarcosine RN xxxxx				210.9	882.	218.7	915.	
	A	(15.3)	210.9					83MCI
$[C_3H_9N]$ i-$C_3H_7NH_2$ RN 75-31-0				211.0	883.	218.6	915.	
320	A	(15.4)	211.0					75TAF-72HEN/TAA-72ARN/JON-83TAF
300	B	(5.3)	211.0*					76AUE/WEB
300	B	(4.9)	210.6					72AUE/WEB
600	D	(-3.5)	209.6					83MAU
$[C_4H_9NO_3]$ L-Threonine RN xxxxx				210.8	882.	218.6	915.	
	A	(15.2)	210.8					83MCI
$[C_6ClH_6N]$ 2-Chloro-4-methylpyridine RN 3678-62-4				210.8**	882.**	218.6**	915.**	
			210.8**					79AUE/BOW
$[C_5H_{10}N_2O_3]$ L-Glutamine RN 585-21-7				210.6	881.	218.4	914.	
	A	(15.0)	210.6					83MCI
$[C_4H_{11}N]$ n-$C_4H_9NH_2$ RN 109-73-9				210.6	881.	218.4	914.	
320	A	(14.6)	210.2					83TAF
320	A	(14.5)	210.1					75TAF-75ARN
	A	(14.8)	210.4					83MCI
300	B	(4.9)	210.6*					76AUE/WEB
300	B	(4.5)	210.2					72AUE/WEB
515	C	(0.5)	210.6					79MAU
$[C_6H_9N]$ 2,5-Dimethylpyrrole RN 625-84-3				210.6	881.	218.4	914.	
600	D	(-2.5)	210.6					83MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[C_4H_9N] $CH_2=C(CH_3)CH_2NH_2$ RN 2878-14-0					209.6**	877.**	218.2**	913.**	
				209.6**					79AUE/BOW
[C_7H_9N] $C_6H_5NHCH_3$ RN 100-61-8					210.3	880.	218.1	912.5	
		A	(15.1)	210.3					72BRI/YAM-78LAU/SAL
[$C_6H_{13}NO_2$] $(CH_3)_2CHCH_2CH(NH_2)COOH$ (L-Leucine) RN 61-90-5					210.3	879.	218.1	912.5	
	500	F	(6.0)	208.5					79MAU/HUN
		A	(14.7)	210.3					83MCI
[$C_{10}H_{10}Ru$] $(C_5H_5)_2Ru$ RN 1287-13-4							218**	912**	
	320	A	(14±2)						81STE/BEA
[BrC_5H_4N] Pyridine,4-Br RN 1120-87-2					210.1*	879.*	217.9*	912.*	
				210.1*					76AUE/WEB(2)
[C_3H_9N] n-$C_3H_7NH_2$ RN 107-10-8					210.1	879.	217.9	912.	
	535	C	(0.0)	210.1					79MAU
	300	C	(0.0)	210.1					73AUE/WEB
	320	A	(14.1)	209.7					83TAF
	320	A	(13.9)	209.5					75TAF-75ARN
		A	(14.4)	210.0					83MCI
	300	B	(4.4)	210.1*					76AUE/WEB
	300	B	(3.9)	209.6					72AUE/WEB
[C_5ClH_4N] 4-Chloropyridine RN 626-61-9					210.0	879.	217.8	911.	
	320	A	(14.4)	210.0					TAFT
	320	A	(14.1)	209.7					75TAF-75ARN
				210.0*					76AUE/WEB(2)
[$C_{18}H_{12}$] Tetracene RN 92-24-0					210.4	880.	217.8	911.	
	550	A	(14.8)	210.4					80MAU
[C_3FH_8N] $FCH_2CH_2CH_2NH_2$ RN 462-41-9					210.3*	880.*	217.8*	911.*	
				210.3**					79AUE/BOW
[C_6ClH_6NO] 6-Chloro-1-methyl-2(1H)pyridinone RN 17228-63-6					210.0	879.	217.8	911.	
	300	B	(4.3)	210.0					79AUE/BET
[$C_5H_9NO_3$] $CH_3CONHCH_2COOCH_3$ RN xxxxx					205.8	861.	217.7	911.	
		(Key)		205.8					83MAU
[C_7H_9NO] 3-$CH_3OC_6H_4NH_2$ RN 536-90-3					209.8	878.	217.6	910.	
	600	F	(7.3)	209.8					81LAU/NIS
[$C_{10}H_{12}O$] 4-$CH_3OC_6H_4(CCH_3CH_2)$ RN 1712-69-2					209.6	877.	217.4	910.	
	320	A	(14.0)	209.6					TAFT
[C_7H_7NO] 1-(4-Pyridinyl)-ethanone RN 1122-54-9					209.6	877.	217.4	910.	
	320	A	(14.0)	209.6					TAFT
				209.6**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_7H_7NO] 1-(3-Pyridinyl)-ethanone RN 350-03-8				209.4	876.	217.2	909.	
320	A	(13.8)	209.4					TAFT
[$C_6H_{15}O_4P$] $OP(OC_2H_5)_3$ RN 78-40-0				~209.5	~877	~217	~910	
300	(Key)		~209.5					80HOD/MCD
[$C_5H_{11}NO_2$] $(CH_3)_2CHCH(NH_2)COOH$ (L-Valine) RN 72-18-4				209.2	875.	217.0	908.	
500	F	(5.4)	207.9					79MAU/HUN
	A	(13.6)	209.2					83MCI
[C_2H_7N] $C_2H_5NH_2$ RN 75-04-7				208.5	872.	217.0	908.	
320	A	(12.8)	208.4					72HEN/TAA-72ARN/JON
320	A	(12.7)	208.3					75TAF-75ARN-83TAF
	A	(12.7)	208.3					83MCI
300	B	(2.2)	207.9					72AUE/WEB
300	B	(2.7)	208.4					75AUE/WEB(2)
300	B	(3.0)	208.7*					76AUE/WEB
550	A	(12.0)	207.2					80MAU
320	G	(0.0)	208.5					74STA/BEA
535	G	(0.0)	207.6					79MAU
[$C_4H_4N_2S_2$] Dithiouracil RN 2001-93-6				~209	~874	~217	~907	
	(br)		~209					75WIL/MCC
[$C_5H_4N_4O$] Hypoxanthine RN 68-94-0				~209	~874	~217	~907	
	(br)		~209					75WIL/MCC
[$C_{10}H_9N$] 1-Naphthylenamine RN 134-32-7				209.1	875.	216.9	907.5	
600	A	(14.0)	209.1					78LAU/SAL
[C_4H_9NO] Dimethylacetamide RN 127-19-5				209.0	874.	216.8	907.	
320	A	(13.4)	209.0					75TAF
320	A	(12.8)	208.4					83TAF
[C_7H_9N] $C_6H_5CH_2NH_2$ RN 100-46-9				209.0	874.	216.8	907.	
320	A	(13.2)	208.8					TAFT
			211.3**					79AUE/BOW
[C_5H_9NO] 1-Methyl-2-pyrrolidinone RN 872-50-4				209.0	874.	216.8	907.	
300	B	(3.3)	209.0					79AUE/BET
[$C_3H_7NO_3$] L-Serine RN 302-84-1				209.0	874.	216.8	907.	
	A	(13.4)	209.0					83MCI
[$C_4H_7NO_4$] L-Aspartic Acid RN 617-45-8				208.9	874.	216.7	907.	
	A	(13.3)	208.9					83MCI
[C_5FH_4N] 4-Fluoropyridine RN 694-52-0				209.2	875.	216.6	906.	
320	A	(13.6)	209.2					75TAF-81TAA/SUM
			209.1**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	kJ/mol	Proton affinity kcal/mol	kJ/mol	Reference
[$C_9H_{11}NO_2$] $C_6H_5CH_2CH(NH_2)COOH$ (L-Phenylalanine) RN 150-30-1					208.7	873.	216.5	906.	
	500	F	(6.2)	208.7					79MAU/HUN
		A	(16.7)	212.3					83MCI
[C_8H_{12}] $(c\text{-}C_3H_5)_2C{=}CH_2$ RN 822-93-5					208.7	873.	216.5	906.	
	300	ZZ	(8.7)	208.7					77WOL/ABB
				209.5**					79AUE/BOW
[$C_5H_9NO_4$] L-Glutamic Acid RN 617-65-2					208.7	873.	216.5	906.	
		A	(13.1)	208.7					83MCI
[C_2H_7P] $(CH_3)_2PH$ RN 676-59-5					208.6	873.	216.3	905.	
	320	A	(12.9)	208.7					74STA/BEA
[C_6H_7N] $(HCCCH_2)_2NH$ RN 6921-28-4					208.3	872.	216.1	904.	
	320	A	(12.7)	208.3					TAFT
[$C_{10}H_{16}$] 1,5,5-Trimethyl-3-methylenecyclohexene RN 16609-28-2					207.7**	869.**	216.1**	904.**	
				207.7**					79AUE/BOW
[$C_6H_8N_2$] 1,4-$C_6H_4(NH_2)_2$ RN 106-50-3					208.1	870.	215.9	903.	
	600	F	(5.6)	208.1					81LAU/NIS
[C_6ClH_6NO] 2-Chloro-6-methoxypyridine RN 17228-64-7					208.1	870.	215.9	903.	
		B	(2.4)	208.1					79AUE/BET
[C_3H_7N] $H_2C{=}CHCH_2NH_2$ RN 107-11-9					207.9	870.	215.8	903.	
	320	A	(12.3)	207.9					TAFT
	320	A	(12.0)	207.6					75ARN
		B	(2.4)	208.1*					76AUE/WEB
[C_3H_8Sn] $(CH_3)_2Sn{=}CH_2$ RN 82065-00-7					207.4	868.	215.8	903.	
	320		(11.8)	207.4					82PIE/HEH
[C_8H_8] 1,4-$C_6H_4(=CH_2)_2$ RN xxxxx							215.7	902.	
		(br)							81POL/RAI
[C_2H_5N] Aziridine (Azirane) RN 151-56-4					207.5	868.	215.7	902.	
	320	A	(11.6)	207.1					TAFT
	320	A	(11.9)	207.4					75TAF-75ARN
	300	B	(1.7)	207.4					75AUE/WEB(2)
	300	B	(1.9)	207.6*					76AUE/WEB
	300	A	(11.9)	207.5					80AUE/WEB
[$C_4H_4N_2$] Pyridazine RN 289-80-5 (1,2-Diazine)					208.8	874.	215.6	902.	
	320	A	(13.6)	209.2					TAFT
	535	C	(-0.8)	208.4					79MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_{16}H_{16}$] (4-$CH_3C_6H_4$)$_2$C=CH_2 RN xxxxx					207.6	868.	215.4	901.	
		ZZ	(7.6)	207.6					77WOL/ABB
[C_6H_5NO] 4-Pyridinecarboxaldehyde RN 872-85-5				207.4**	207.4**	868.**	215.2**	900.**	79AUE/BOW
[BrC_5H_4N] 3-Bromopyridine RN 626-55-1					207.3	867	215.1	900.	
		B	(1.6)	207.3					79AUE/BET
				208.5*					76AUE/WEB(2)
[$C_4F_3H_8N$] $CF_3CH_2N(CH_3)_2$ RN 819-06-7					207.4	868.	215.0	900.	
	320	A	(11.8)	207.4					
				207.1**					79AUE/BOW
[C_3H_7N] c-$C_3H_5NH_2$ RN 765-30-0					206.6**	864.**	215.0**	899.**	
				206.6**					79AUE/BOW
[$C_4H_{10}N_2$] c-C(CH_3)(C_2H_5)NHNH RN 4901-75-1					207.1**	867.**	214.9**	899.**	
				207.1**					79AUE/BOW
[C_8H_8] 1,2-C_6H_4(=CH_2)$_2$ RN xxxxx					207.4	868.	214.8	899.	
	320	(br)		207.4					81POL/RAI
[C_5ClH_4N] 3-Chloropyridine RN 626-60-8					207.0	866.	214.8	899.	
	320	A	(11.5)	207.1					75TAF
		A	(11.5)	207.1					83MCI
	300	A	(12.3)	207.9*					76AUE/WEB(2)
	550	A	(11.5)	206.7					80MAU
[$C_3H_7NO_2$] L-Alanine RN 56-41-7					206.6	864.	214.8	899.	
		A	(11.0)	206.6					83MCI
	500	F	(6.2)	208.7					79MAU/HUN
[BrC_5H_4N] 2-Bromopyridine RN 109-04-6					207.1	866.5	214.7	898.	
		B	(2.1)	207.8					79AUE/BET
				207.8*					76AUE/WEB(2)
	320	A	(11.5)	207.1					TAFT
	320	A	(10.8)	206.5					75TAF-75ARN
[C_7H_9NO] 2-$CH_3OC_6H_4NH_2$ (o-Anisidine) RN 90-04-0					206.9	866.	214.7	898.	
	600	A	(15.1)	210.2					73YAM/KEB
	600	A	(11.8)	206.9					78LAU/SAL
[C_7H_9NS] 3-$CH_3SC_6H_4NH_2$ RN 1783-81-9					206.7	865.	214.5	897.	
	600	F	(4.7)	206.7					81LAU/NIS
[$C_3H_9O_3PS$] SP(OCH_3)$_3$ RN 29952-66-79					206.7	865.	214.5	897.	
	300	(Key)		206.7					80HOD/MCD
[C_5ClH_4N] 2-Chloropyridine RN 109-09-1					206.6	864.	214.4	897.	
	320	A	(11.0)	206.6					TAFT
	320	A	(10.8)	206.4					75TAF-75ARN
				207.0*					76AUE/WEB(2)
	500	A	(10.0)	205.1					84SHA/BLA
	546	G	(-1.0)	206.6					79MAU
	550	A	(11.0)	206.2					80MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_8H_6N_2]$ Quinoxaline RN 91-19-0					207.3	867.	214.4	897.	
	535	G	(-0.3)	207.3					79MAU
$[C_{13}H_{25}N]$ out-6H-1-Azabicyclo[4.4.4] tetradecane RN xxxxx					206.5	864.	214.3	897.	
	320	A	(10.9)	206.5					81ALD/ARR
$[C_4F_3H_8N]$ $CF_3(CH_2)_3NH_2$ RN 819-46-5					206.5	864.	214.3	897.	
	320	A	(10.9)	206.5					TAFT
	320	A	(10.7)	206.3					75TAF-75ARN
				206.9**					79AUE/BOW
$[C_7H_9NO]$ $4\text{-}CH_3OC_6H_4NH_2$ RN 104-94-9					206.5	864.	214.3	897.	
	320	A	(10.9)	206.5					77SUM/POL-81TAA/SUM
				206.6**					79AUE/BOW
$[C_5FH_4N]$ 3-Fluoropyridine RN 372-47-4					206.2	863.	214.3	897.	
	320	A	(10.6)	206.2					TAFT
				207.0*					76AUE/WEB(2)
$[C_3H_7NO_2S]$ L-Cysteine RN 3374-22-9					206.5	864.	214.3	897.	
		A	(10.9)	206.5					83MCI
$[C_6H_7NO]$ $2\text{-}(OH)C_6H_4NH_2$ RN xxxxx					206.4	864.	214.2	896.	
	600	F	(3.9)	206.4					81LAU/NIS
$[C_6H_7NO]$ $3\text{-}(OH)C_6H_4NH_2$ RN 591-27-5					206.4	864.	214.2	896.	
	600	F	(3.9)	206.4					81LAU/NIS
$[CH_5N]$ CH_3NH_2 RN 74-89-5					205.7	861.	214.1	896.	
	300	B	(0.0)	205.7					72AUE/WEB
	300	B	(0.0)	205.7					75AUE/WEB
	300	B	(0.0)	205.7*					76AUE/WEB
	320	B	(0.0)	205.7					75HOD/BEA
	320	A	(9.8)	205.4					75TAF-83TAF
	320	A	(10.1)	205.7					72HEN/TAA-72ARN/JON
	382	F	(2.65)	205.2					79LOC/HUN
		A	(9.8)	205.4					83MCI
	600	A	(10.0)	205.1					78LAU/SAL
	600	A	(10.8)	205.9					72BRI/YAM
$[CH_6N_2]$ CH_3NHNH_2 RN 60-34-4					206.3**	863**	214.1**	896.**	
				206.3**					79AUE/BOW
$[C_8H_{11}N]$ $3\text{-}C_2H_5C_6H_4NH_2$ RN 587-02-0					206.2	863.	214.0	895.	
	600	F	(3.7)	206.2					81LAU/NIS
$[C_6H_{10}]$ 1,3,3-Trimethylcyclopropene RN 3664-56-0					206.**	862.**	214.**	895**	
				206.**					79AUE/BOW
$[C_2H_5N]$ $CH_3CH\text{-}NH$ RN 20729-41-3					206.1	862.	213.9	895.	
		(br)		206.1					81ELL/DIX
		(br)		206.1					79ELL/EAD

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_{15}H_{12}$] 9-Methylanthracene RN 779-02-2				206.1	862.	213.9	895.	
550	A	(10.9)	206.1					80MAU
[$C_6H_9O_3P$] 2,8,9-Trioxa-1-phosphadamantane RN 281-33-4				206.0	862.	213.8	894.	
	(Key)		206.0					80HOD/HOU
[$C_5H_{12}O_2$] $CH_3O(CH_2)_3OCH_3$ RN 17081-21-9				204.8	857.	213.8	894.	
300	(Key)		204.8					83MAU
[$C_5H_{11}NO_2$] $(CH_3)_2NCOOC_2H_5$ RN 687-48-9				205.9	861.	213.7	894.	
320	A	(10.3)	205.9					TAFT
[C_7H_9N] 4-$CH_3C_6H_4NH_2$ RN 106-49-0				205.9	861.	213.7	894.	
320	A	(10.1)	205.7					77SUM/POL-81TAA/SUM
320	A	(10.7)	206.3					75ARN
[$C_8H_8O_2$] 4-$CH_3OC_6H_4CHO$ RN 123-11-5				205.7	861.	213.5	893.	
320	A	(9.9)	205.5					TAFT
320	A	(10.4)	206.0					
[C_7H_9N] 3-$CH_3C_6H_4NH_2$ RN 108-44-1				205.6	860.	213.4	893.	
320	A	(10.1)	205.7					75TAF-77SUM/POL
600	F	(3.0)	205.5					81LAU/NIS
[$C_9H_{13}N$] 3-$CH_3C_6H_4N(CH_3)_2$ RN 121-72-2				205.6	860.	213.4	893.	
320	F	(3.0)	205.9					77POL/DEV
	A	(10.0)	205.6					83MCI
[AsC_3H_9] $(CH_3)_3As$ RN 593-88-4				205.6	860.	213.4	893.	
320	B	(0.1)	205.6					75HOD/BEA
[C_3H_3NS] Thiazole RN 288-47-1				205.4	859.	213.2	892.	
600	(Key)		205.4					83MAU
[$C_6H_{10}O_2$] $CH_3COCH_2CH_2COCH_3$ RN 110-13-4				201.5	843.	213.2	892.	
300	(Key)		201.5					83MAU
[C_7H_{12}] $(CH_3)_2C=CHC(CH_3)=CH_2$ RN xxxxx				204.3**	855.	213.1**	892.	
			204.3**					79AUE/BOW
[C_6H_4] o-Benzyne RN xxxxx				205.7	861.	213.0	891.	
	(br)		205.7					80POL/HEH
[$C_6F_3H_4N$] 4-Trifluoromethylpyridine RN 3796-24-5				205.0	858.	212.8	890.	
320	D	(-11.7)	201.4					72TAA/HEN
320	A	(9.4)	205.0					83TAF
320	A	(9.3)	204.9					75TAF-75ARN
			205.2*					76AUE/WEB(2)

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	kJ/mol	Proton affinity kcal/mol	kJ/mol	Reference
[$C_6H_8N_2$] 1,2-$C_6H_4(NH_2)_2$ RN 95-54-5				206.4	864.	212.8	890.	
600	F	(3.9)	206.4					81LAU/NIS
[$C_8H_{18}S$] (t-$C_4H_9)_2S$ RN 107-47-1				205.0	858.	212.8	890.	
320	A	(9.9)	205.0					TAFT
[$C_3H_7O_3P$] 2-Methoxy-1,3,2-dioxaphospholane RN 3741-36-4				204.9	857.	212.7	890.	
320	(Key)			204.9				80HOD/HOU
[$C_6F_3H_4N$] 3-Trifluoromethylpyridine RN 3796-23-4				204.8	857.	212.6	889.	
320	A	(9.2)	204.8 205.0*					75TAF-75ARN 79AUE/BOW
[C_2FH_6N] $CH_2FCH_2NH_2$ RN 406-34-8				204.5	856.	212.3	888.	
320	A	(8.7)	204.3 204.6**					75TAF-75ARN 79AUE/BOW
[$C_3H_9O_4P$] $OP(OCH_3)_3$ RN 512-56-1				204.2	854.	212.0	887.	
300	(Key)		204.2 202.0			 213.5	 893.	80HOD/MCD ***82PIE/HEH
[$C_4H_{10}O_2$] $HO(CH_2)_4OH$ RN 110-63-4				198**	828**	212**	887**	
			198**					79AUE/BOW
[C_3H_5N] 1-Azabicyclo[1.1.0]butane RN 19540-05-7				204**	853**	212**	887**	
300	T	(24.0)	~202. 204**					75AUE/WEB(2) 79AUE/BOW
[C_6H_8] 1-Methyl-3-methylenecyclobutene RN 15082-13-0				204**	853**	212**	887**	
			204**					79AUE/BOW
[$C_7H_5O_2Rh$] $(C_5H_5)Rh(CO)_2$ RN 12192-97-1						212**	887.**	
320	A	(8±2)						81STE/BEA
[$C_{14}H_{12}$] $(C_6H_5)_2C{=}CH_2$ RN 530-48-3				204.1	854.	211.9	887.	
320	A	(8.2)	203.8					75TAF
320	A	(8.5)	204.0					75WOL/HAR
320	ZZ	(4.1)	204.1					77WOL/ABB
			204.0**					79AUE/BOW
[$C_6H_8O_2$] 1,3-Cyclohexanedione RN 504-02-9				204.5	856.	211.9	886.	
300	(Key)		204.5					83MAU
[$C_2H_5NO_2$] NH_2CH_2COOH (Glycine) RN 56-40-6				203.7	852.	211.6	885.	
382	F	(+1.2)	203.7					79LOC/HUN
	A	(8.2)	203.8					83MCI
500	F	(0.0)	202.5					79MAU/HUN

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	kJ/mol	Proton affinity kcal/mol	kJ/mol	Reference
$[C_6F_3H_4N]$ 2-Trifluoromethylpyridine RN 368-48-9					203.6	852.	211.5	885.	
	320	A	(8.0)	203.6					75TAF
$[C_{20}H_{12}]$ Perylene RN 198-55-0					204.3	855.	211.4	884.	
	550	A	(+9.1)	204.3					80MAU
$[C_3H_7NO]$ $(CH_3)_2NCHO$ RN 68-12-2					203.6	852.	211.4	884.	
	320	A	(8.0)	203.6					75TAF
				204.6**					79AUE/BOW
	382	F	(0.95)	203.6					79LOC/HUN
$[C_2H_6OS]$ $(CH_3)_2SO$ RN 67-68-5					203.5	851.	211.3	884.	
	320	A	(7.7)	203.3					75TAF-83TAF
		(br)		177.					77MCA
	600	A	(8.5)	203.6					79LAU
$[C_4H_8N_2]$ $NCCH_2N(CH_3)_2$ RN 926-64-7					203.3	851.	211.1	883.	
	320	A	(7.7)	203.3					TAFT-75ARN
$[C_{10}H_{12}]$ $4\text{-}CH_3C_6H_4C(CH_3)CH_2$ RN 1195-32-0					203.2	850.	211.0	883.	
	320	A	(7.6)	203.2					TAFT
$[C_{13}H_{10}O]$ $(C_6H_5)_2CO$ RN 119-61-9					203.1	850.	210.9	882.	
	320	A	(7.5)	203.1					83TAF
$[C_3H_5N]$ $HCCCH_2NH_2$ RN 2450-71-7					203.0	849.	210.8	882.	
	320	A	(7.4)	202.9					TAFT
				203.1**					79AUE/BOW
$[C_7H_{10}O]$ $(c\text{-}C_3H_5)_2CO$ RN 1121-37-5					202.9	849.	210.7	881.5	
	320	ZZ	(2.9)	202.9					83TAF
	320	U	(9.8)	198.7					81BRO/ABB
$[C_3F_3H_6N]$ $CF_3CH_2CH_2NH_2$ RN 460-39-9					202.8	849.	210.6	881.	
	320	A	(7.4)	202.9					TAFT
	320	A	(7.2)	202.7					75TAF-75ARN
				203.4**					79AUE/BOW
$[C_5FH_4N]$ 2-Fluoropyridine RN 372-48-5					202.8	849.	210.6	881.	
	320	A	(7.4)	202.9					TAFT
	320	A	(7.2)	202.7					75TAF-75ARN
		A	(7.3)	202.8					83MCI
				204.0					76AUE/WEB(2)
	382	F	(0.35)	202.8					79LOC/HUN
	500	A	(6.6)	201.7					84SHA/BLA
$[C_8H_{14}]$ $(CH_3)_2C{=}C(CH_3)C(CH_3){=}CH_2$ RN xxxxx					201.8**	844.**	210.6**	881.**	
				201.8**					79AUE/BOW
$[C_4H_4N_2]$ Pyrimidine (1,3-Diazine) RN 289-95-2					203.5	851.	210.5	881.	
	320	A	(8.0)	203.6					TAFT
	510	G	(-4.2)	203.4					79MAU
$[C_{15}H_{12}]$ 2-Methylanthracene RN 613-12-7					202.5	847.	210.3	880.	
	550	A	(+7.3)	202.5					80MAU

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
				kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_6H_4N_2]$ 4-Pyridinecarbonitrile RN 100-48-1				202.5	851.	210.3	880.	
320	A	(6.5)	202.1					75TAF-75ARN
			202.8*					76AUE/WEB(2)
$[C_5H_9O_3P]$ 4-Methyl-3,6,7-trioxa-1-phospha-bicyclo[2.2.2]-octane RN 1449-91-8				202.2	846.	210.0	879.	
320	(Key)		202.2					80HOD/HOU
$[C_4H_9NO]$ n-C_3H_7NHCHO RN 6281-94-3				202.2**	846.	210.0**	879.	
			202.2**					79AUE/BOW
$[C_{10}FeH_{10}]$ $(C_5H_5)_2Fe$ RN 102-54-5				~202	~845.	~210	~879.	
	(br)		~202					75FOS/BEA
$[C_3F_3H_6N]$ $CF_3CH_2NHCH_3$ RN 2730-67-8				202.2	846.	209.8	878.	
320	A	(6.3)	201.9					75TAF
			202.4**					79AUE/BOW
$[C_3H_4N_2]$ Pyrazole RN 288-13-1				202.0	845.	209.8	878.	
600	(Key)		202.0					83MAU
$[C_6H_{14}S]$ $(i\text{-}C_3H_7)_2S$ RN 625-80-9				201.8	844.	209.6	877.	
320	A	(6.2)	201.8					TAFT
			202.0**					79AUE/BOW
$[C_6H_7N]$ $C_6H_5NH_2$ RN 62-53-3				202.5	847.	209.5	876.	
320	F	(0.0)	202.8					77POL/DEV
382	F	(0.0)	202.5					79LOC/HUN
500	F	(0.0)	202.5					79MAU/HUN
600	F	(0.0)	202.5					81LAU/NIS
320	A	(7.2)	202.8					75TAF-75ARN
320	A	(6.9)	202.5					83TAF
550	G	(-5.2)	202.4					79MAU
550	A	(+5.8)	201.0					80MAU
600	A	(6.9)	202.0					78LAU/SAL
600	J	(25.6)	201.2					76LAU/KEB
600	A	(8.9)	203.5					72BRI/YAM
$[C_6H_4N_2]$ 3-Pyridinecarbonitrile RN 100-54-9				201.5	843.	209.3	876.	
320	A	(5.6)	201.2					TAFT
320	A	(5.9)	201.5					75TAF-75ARN
			201.7*					76AUE/WEB(2)
$[C_6H_8O]$ 2,5-Dimethylfuran RN 625-86-5				201.3	842.	209.1	875.	
600	(Key)		201.3					83MAU
$[C_4H_4N_2]$ Pyrazine (1,4-Diazine) RN 290-37-9				201.2	842.	209.0	874.	
320	A	(5.6)	201.2					TAFT
550	G	(-6.0)	201.2					79MAU
$[C_6H_{10}]$ c-$C_3H_5C(CH_3)=CH_2$ RN 4663-22-3				201.2	842.	209.0	874.	
320	A	(5.6)	201.2					TAFT
			200.9**					79AUE/BOW
$[C_8H_{18}O]$ (sec-$C_4H_9)_2O$ RN 6863-58-7				201.2	842.	209.0	874.	
335	XX	(6.7)	201.2					82MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_6H_6IN]$ 3-$IC_6H_4NH_2$ RN 626-01-7					201.1	841.	208.9	874.	
	600	F	(-0.9)	201.1					81LAU/NIS
$[C_5H_6N_2O_2]$ Thymine RN 65-71-4					201.0	841.	208.8	874.	
	550	G	(-6.6)	201.0					79MAU
		(br)		~200					75WIL/MCC
$[C_7H_{16}O]$ $(i-C_3H_7)O(t-C_4H_9)$ RN 17348-59-3					201.0**	841.**	208.8**	874.**	
				201.0**					79AUE/BOW
$[C_9H_{10}O]$ $(4-CH_3)C_6H_4COCH_3$ RN xxxxx					200.9	840.5	208.7	873.	
	320	A	(12.0)	200.9					81BRO/ABB
$[C_8H_{18}S]$ $(n-C_4H_9)_2S$ RN 544-40-1					200.9	840.5	208.7	873.	
	300	(Key)		200.9					83MAU
$[C_6ClH_6N]$ 4-$ClC_6H_4NH_2$ RN 106-47-8					201.0	841.	208.6	873.	
	320	A	(5.1)	200.7					TAFT
	320	A	(5.4)	201.0					75TAF-75ARN-77SUM/POL
$[C_5H_4N_2O_2]$ 4-Nitropyridine RN 1122-61-8					200.7	840.	208.5	872.	
	320	D	(-18.1)	194.9					72TAA/HEN
	320	A	(5.0)	200.6					TAFT
	320	A	(5.2)	200.8					75TAF-75ARN
				201.7**					79AUE/BOW
$[C_{22}H_{12}]$ 1,12-Benzoperylene RN 191-24-2					201.1	841.	208.5	872.	
	550	A	(5.9)	201.1					80MAU
$[C_3H_3NO]$ Oxazole RN 288-42-6					200.6	839.	208.4	872.	
	600	(Key)		199.2					83MAU
$[C_4H_8O]$ $C_2H_5OCH=CH_2$ RN 109-92-2					200.4	838.	208.2	871.	
	600	(Key)		200.4					83MAU
$[C_6H_4N_2]$ 2-Pyridinecarbonitrile RN 100-70-9					200.3	838.	208.1	871.	
	320	A	(4.3)	199.9					TAFT
				201.1*					76AUE/WEB(2)
	500	F	(-1.9)	200.6					79MAU/HUN
$[BrC_6H_6N]$ 3-$BrC_6H_4NH_2$ RN 591-19-5					200.3	838.	208.1	871.	
	600	F	(-2.2)	200.3					81LAU/NIS
$[C_6FH_6N]$ 4-$FC_6H_4NH_2$ RN 371-40-4					200.3	838.	208.1	871.	
	320	A	(4.6)	200.2					81TAA/SUM
	320	A	(5.0)	200.6					75TAF-75ARN
$[C_{10}H_{14}N_2O_5]$ Thymidine RN 50-89-5					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_9H_{12}N_2O_6]$ Uridine RN 58-96-8					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_9H_{14}N_2O_6]$ 5,6-Dihydrouridine RN 5627-05-4					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_{12}H_{16}N_2O_6]$ 2',3'-O-Isopropylideneuridine RN 362-43-6					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_4H_4N_2O]$ 2(1H)-Pyrimidinone RN 557-01-7					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_4H_4N_2O_2]$ Uracil RN 66-22-8					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_5H_3ClN_4]$ 6-Chloropurine RN 87-42-3					~200	~837	~208	~870	
		(br)		~200					75WIL/MCC
$[C_6H_{10}]$ $CH_3CH{=}CHC(CH_3){=}CH_2$ RN 1118-58-7					199.9**	836.**	207.9**	870.**	
				199.9**					79AUE/BOW
$[C_5H_8O_2]$ $CH_3COCH{=}C(OH)CH_3$ RN 123-54-6					199.3	834.	207.8	869.	
	320	A	(3.7)	199.3					TAFT
	300	(Key)		199.2					83MAU
				200.1**					79AUE/BOW
$[C_4H_5N]$ Pyrrole RN 109-97-7					200.3	838.	207.6	868.	
				201.6**					79AUE/BOW
	550	G	(-6.4)	200.8					79MAU
	600	A	(5.6)	200.3					79LAU
	600	A	(7.15)	201.8					73YAM/KEB
$[C_2F_2H_5N]$ $CF_2HCH_2NH_2$ RN 430-67-1					199.8	836.	207.5	868.	
	320	A	(4.0)	199.6					TAFT
	320	A	(4.2)	199.8					75TAF-75ARN
				200.0**					79AUE/BOW
$[C_3H_6O]$ $CH_2{=}CHOCH_3$ RN 107-25-5					199.6	835.	207.4	868.	
	600	(Key)		199.6					83MAU
$[C_{12}H_{18}]$ $(CH_3)_6C_6$ RN 87-85-4					200.0	837.	207.3	867.	
	320	ZZ	(0.0)	200.0					77WOL/ABB
	320	A	(4.2)	199.8					83TAF
	320	J	(25.1)	199.7					76WOL/DEV
	320	A	(4.8)	200.4					75WOL/HAR
$[C_6ClH_6N]$ 3-Chlorobenzeneamine RN 108-42-9					199.4	834.	207.2	867.	
	320	A	(4.5)	200.0					75ARN
	320	A	(4.0)	199.6					77SUM/POL
	600	A	(3.6)	198.8					79LAU
	600	F	(-3.1)	199.4					81LAU/NIS
$[C_2H_7O_3P]$ $(CH_3O)_2PHO$ RN 868-85-9							207.2	867.	
		(br)	(PA associated with P-protonation: 213.5 kcal/mol)						82PIE/HEH(2)
$[C_4F_2H_7NO]$ $CF_2HCON(CH_3)_2$ RN 667-50-5							207.2	867.	
									**82PIE/HEH(2)
$[C_4H_7O_3P]$ 2,6,7-Trioxa-1-phosphabicyclo-[2.2.2]octane RN 280-45-5					200.0	837.	207.1	866.5	
	320	(Key)		200.0					80HOD/HOU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_8H_{12}]$ 2-Methylenebicyclo[2.2.1]heptane RN 497-35-8					199**	833**	207**	866**	
				199**					79AUE/BOW
$[C_{14}H_{10}]$ Anthracene RN 120-12-7					199.9	836.	207.0	866.	
	550	A	(4.7)	199.9					80MAU
$[B_4C_2H_6]$ 1,6-$C_2B_4H_6$ RN 20693-67-8					199.	833.	207.	866.	
		(br)		199.					80DIX
$[C_6FH_6N]$ 3-Fluorobenzenamine RN 372-19-0					199.2	833.	207.0	866.	
	320	A	(3.5)	199.1					77SUM/POL
	600	F	(-3.2)	199.3					81LAU/NIS
$[C_9H_{10}]$ $C_6H_5C(CH_3)=CH_2$ RN 98-83-9					199.2	833.	207.0	866.	
	320	A	(3.6)	199.2					75TAF-75WOL/HAR-78TAF/WOL
	320	ZZ	(-1.0)	199.0					77WOL/ABB
$[C_3H_6N_2]$ $H_2N(CH_2)_2CN$ RN 151-18-8					198.1	829.	207.0	866.	
	320	A	(2.6)	198.2					TAFT
	320	A	(3.2)	198.7					75ARN
	550	G	(-9.6)	198.0					79MAU
	550	A	(+2.4)	197.6					80MAU
$[C_2H_6N_2]$ (E)-$CH_3N=NCH_3$ RN 4143-41-3					199.1	833.	206.9	866.	
		(Key)		199.1					74FOS/WIL
		(br)		200					72FOS/BEA
$[C_9FH_9]$ 4-$FC_6H_4C(CH_3)=CH_2$ RN 350-40-3					199.0	833.	206.7	865.	
	320	A	(3.4)	199.0					TAFT
$[C_6H_{14}S]$ $(n-C_3H_7)_2S$ RN 111-47-7					198.7	831.	206.5	864.	
	320	A	(3.1)	198.7					TAFT
$[C_9H_{18}O]$ $(tert-C_4H_9)_2CO$ RN 815-24-7							206.5	864.	
									*82PIE/HEH(2)
$[C_2H_5NO]$ CH_3CONH_2 RN 60-35-5					198.4	830.	206.2	863.	
	320	A	(3.3)	198.4					73YAM/KEB
$[C_{16}H_{10}]$ Pyrene RN 129-00-0					199.8	836.	206.1	862.	
	550	A	(4.6)	199.8					80MAU
$[C_3H_6N_2]$ CH_3NHCH_2CN RN 5616-32-0					198.2	829.	206.0	862.	
	320	A	(2.6)	198.2					TAFT
$[C_6H_{14}O]$ $(i-C_3H_7)_2O$ RN 108-20-3					198.4	830.	206.0	862.	
	320	U	(9.7)	198.6					81BRO/ABB
	335	XX	(3.9)	198.4					82MAU
	340	H	(10.9)	198.0					80LIA/SHO
				198.7**					79AUE/BOW
$[C_8H_{12}]$ 2-Methylbicyclo[2.2.1]hept-2-ene RN xxxxx							206.	862.	
		(Key)							76SOL/FIE

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_4H_6]$ 1-Methylcyclopropene RN 3100-04-7					198**	828**	206**	862**	
				198**					79AUE/BOW
$[C_6H_{10}]$ $CH_2{=}CH(CH_3)C(CH_2)_2$ RN 16906-27-7					198*	828*	206*	862*	
				198*					79AUE/BOW
$[C_9CrH_8O_3]$ $(C_5H_5)Cr(CO)_3CH_3$ RN 41311-89-1							206**	862**	
	320	A	(2.0±2.0)						81STE/BEA
$[C_2H_5NO]$ $HCONHCH_3$ RN 123-39-7					198.0	828.	205.8	861.	
	320	U	(9.1)	198.0					81BRO/ABB
$[C_4H_9NO_2]$ t-C_4H_9ONO RN 540-80-7					197.9	828.	205.7	861.	
		(br)		197.9					78FAR/MCM
$[C_5H_6S]$ 2-Methylthiophene RN 554-14-3					197.9	828.	205.7	861.	
	600	(Key)		197.9					83MAU
$[C_6H_{10}]$ $CH_3CH{=}C(CH_3)CH{=}CH_2$ RN 4549-74-0					197.3**	825.5**	205.7**	861.	
				197.3**					79AUE/BOW
$[C_5H_6O]$ 2-Methylfuran RN 534-22-5					197.8	828.	205.6	860.	
	600	(Key)		197.8					83MAU
$[C_8H_8O]$ $C_6H_5COCH_3$ RN 98-86-2					197.4	826.	205.4	859.	
	320	A	(1.7)	197.3					83TAF
	320	U	(8.9)	197.8					81BRO/ABB
	600	A	(2.0)	197.1					79LAU
	600	F	(-4.7)	197.8					81LAU/NIS
$[C_6H_{12}O]$ 2,2-Dimethyltetrahydrofuran RN xxxx					197.6	827.	205.4	859.	
	320	U	(8.7)	197.6					81BRO/ABB
$[C_6H_{14}O]$ $C_2H_5O(t\text{-}C_4H_9)$ RN 637-92-3					197.5	826.	205.3	859.	
	320	A	(1.9)	197.5					TAFT
$[C_{10}H_{22}O]$ $(n\text{-}C_5H_{11})_2O$ RN 693-65-2					197.9**	828.**	205.2**	859.**	
				197.9**					79AUE/BOW
$[C_5H_8O]$ c-$C_3H_5COCH_3$ RN 765-43-5					197.3	826.	205.1	858.	
	320	A	(0.7)	196.3					83TAF
	320	U	(8.4)	197.3					
$[C_4H_{10}S]$ $(C_2H_5)_2S$ RN 352-93-2					197.2	825.	205.0	858.	
	320	A	(1.6)	197.2					TAFT
				198.3**					79AUE/BOW
$[C_9ClH_9]$ 4-$ClC_6H_4C(CH_3){=}CH_2$ RN 1712-70-5					197.2	825.	205.0	858.	
	320	A	(1.6)	197.2					TAFT
$[C_{24}H_{12}]$ Coronene RN 191-07-1					199.9	836.	205.0	858.	
	550	A	(4.3)	199.9					80MAU
$[CH_2N_2]$ CH_2N_2 RN 334-88-3					197.	824.	205.	858.	
		(br)		197.					72FOS/BEA

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_{10}CrH_7O_3$] ($C_6H_5CH_2$)Cr(CO)$_3$ RN 32984-97-7						205**	858**	
320	A	(1±2)						81STE/BEA
[C_3GeH_8] $(CH_3)_2Ge{=}CH_2$ RN 82064-99-1				195.6	818.	204.9	857.	
320	A	(0.9)	196.5					82PIE/HEH
[$C_4H_{10}O_2$] $CH_3OCH_2CH_2OCH_3$ RN 110-71-4				195.8	819.	204.9	857.	
300	(Key)		195.8					83MAU
300	A	(0.2)	195.3					84SHA/BLA
[$C_7H_{14}O$] $(i\text{-}C_3H_7)_2CO$ RN 565-80-0				197.0	824.	204.9	857.	
320	ZZ	(-3.9)	196.1					83TAF
320	U	(8.1)	197.0					81BRO/ABB
[$C_6H_8O_2$] 1,2-Cyclohexanedione RN 765-87-7				197.4	825.	204.8	857.	
300	(Key)		197.4					83MAU
[C_6H_5NO] Nitrosobenzene RN 586-96-9				197.0	824.	204.8	857.	
	(br)		197.0					80REE/FRE
[H_4N_2] H_2NNH_2 RN 302-01-2				196.7	823.	204.7	856.	
320	A	(4.0)	199.6					75ARN
600	(Key)		196.7					83MAU
[$C_{14}H_{18}$] 1,2,3,4,5,6,7,8-Octahydrophenanthrene RN 5325-97-3				195.1	816.	204.7	856.	
550	A	(-0.1)	195.1					80MAU
[$C_7F_3H_6N$] $3\text{-}CF_3C_6H_4NH_2$ RN 98-16-8				196.4	822.	204.2	854.	
600	F	(-6.1)	196.4					81LAU/NIS
[CH_5P] CH_3PH_2 RN 593-54-4				196.3	821.	204.1	854.	
320	A	(-0.3)	195.3					74STA/BEA
320	H		196.3					
[C_6H_5O] C_6H_5O radical RN xxxxx				~196	~820	~204	~853	
	(br)		~196					80DEF/MCI
[H_3N] NH_3 RN 7664-41-7				195.6	818.	204.0	853.5	
Threshold Value						203.6		79CEY/TIE
320	A	(0.0)	195.6					TAFT
320	A	(0.0)	195.6					83TAF
320	A	(0.0)	195.6					77WOL/STA
320	A	(0.0)	195.6					75TAF
320	A	(0.0)	195.6					72HEN/TAA
320	A	(0.0)	195.6					72ARN/JON
320	A	(0.0)	195.6					82PIE/HEH
	A	(0.0)	195.6					83MCI
550	A	(0.0)	195.2					80MAU
600	A	(0.0)	195.1					79LAU
600	A	(0.0)	195.1					73YAM/KEB
600	A	(0.0)	195.1					78LAU/SAL
340	H	(8.3)	195.6					80LIA/SHO
320	H		196.6					77WOL/STA
[$C_7CoH_5O_2$] $(C_5H_5)Co(CO)_2$ RN 12078-25-0						~204**	853**	
320	A	(0±2)						81STE/BEA

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
		kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[$C_8H_{18}O$] $(n\text{-}C_4H_9)_2O$ RN 142-96-1				195.9	820.	203.7	852.	
			196.6**					79AUE/BOW
335	XX	(1.4)	195.9					82MAU
[C_8H_8O] 4-$(CH_3)C_6H_4CHO$ RN 104-87-0				195.9	820.	203.7	852.	
320	A	(0.3)	195.9					TAFT
[$C_8H_{14}O_2$] c-$C_6H_{11}COOCH_3$ RN 4630-82-4				195.9	820.	203.7	852.	
320	A	(-0.7)	194.9					83TAF
320	H		195.9					
[$C_8H_8O_2$] $C_6H_5CO_2CH_3$ RN 95-58-3				195.9	820.	203.7	852.	
320	U	(7.1)	196.0					81BRO/ABB
320	H		195.9					
[$C_6F_3H_{10}NO$] $CF_3CONH(n\text{-}C_4H_9)$ RN 400-59-9				195.8	819.	203.6	852.	
320	A	(0.2)	195.8					TAFT
[$C_5H_{10}O$] c-$C_4H_7O(2\text{-}CH_3)$ RN 96-47-9				195.8	819.	203.6	852.	
320	U	(6.9)	195.8					81BRO/ABB
[$C_{12}H_{10}$] Acenaphthene RN 83-32-9				196.4	822.	203.5	851.	
550	A	(1.2)	196.4					80MAU
[C_3H_8S] $CH_3SC_2H_5$ RN 624-89-5				195.7	819.	203.5	851.	
320	A	(-0.9)	194.7					TAFT
320	H		195.7					
			195.8**					79AUE/BOW
[$C_5H_{12}O$] $C_2H_5O(i\text{-}C_3H_7)$ RN 625-54-7				195.7	819.	203.5	851.	
320	A	(-0.9)	194.7					77WOL/STA
320	H		195.7					
320	U	(7.3)	196.2					81BRO/ABB
[$C_{22}H_{14}$] Picene RN 213-46-7				196.3	821.	203.4	851.	
550	A	(1.1)	196.3					80MAU
[$C_{12}H_8$] Biphenylene RN 259-79-0				196.3	821.	203.4	851.	
550	A	(1.1)	196.3					80MAU
[$C_6H_{18}OSi_2$] $((CH_3)_3Si)_2O$ RN 107-46-0				~195	~816	~203	~849	
	(br)		~195±3					75PIT/BUR
[$C_4H_{14}OSi_2$] $((CH_3)_2SiH)_2O$ RN 3277-26-7				~195	~816	~203	~849	
	(br)		~195±3					75PIT/BUR
[$C_4H_{12}OSi$] $(CH_3)_3SiOCH_3$ RN 1825-61-2				~195	~816	~203	~849	
	(br)		~195±3					75PIT/BUR
[C_5H_8] 3,3-Dimethylcyclopropene RN 3907-06-0				196*	820.	203*	849*	
			196*					76AUE/DAV

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_5H_8O_2$] c-$C_3H_5COOCH_3$ RN 2868-37-3				195.1	816.	202.9	849.	
320	A	(-1.5)	194.1					83TAF
320	H		195.1					
320	U	(6.2)	195.1					81BRO/ABB
[$C_6H_{12}O_2$] t-$C_4H_9COOCH_3$ RN 598-98-1				195.0	816.	202.8	848.5	
320	A	(-1.6)	194.0					83TAF
320	H		195.0					
[$C_4H_8O_3$] $C_2H_5OCOOCH_3$ RN 623-53-0				194.9	815.	202.7	848.	
320	A	(-1.7)	193.9					TAFT
320	H		194.9					
[$C_{14}H_{18}$] 1,2,3,4,5,6,7,8-Octahydroanthracene RN 1079-71-6				194.8	815.	202.5	847.	
550	A	(-0.4)	194.8					80MAU
[$C_2F_3H_4N$] $CF_3CH_2NH_2$ RN 753-90-2				194.7	815.	202.5	847.	
320	A	(-1.9)	193.7					77STA/TAA-83TAF
320	H		194.7					
320	A	(-1.5)	194.1					75TAF-75ARN
320	H		195.1					
			194.9**					79AUE/BOW
[C_9H_{11}] $C_6H_5C(CH_3)_2$ radical RN xxxxx				194.6	814.	202.4	847.	
	(br)		194.6					82MAU
[$C_8H_{14}O$] c-$C_6H_{11}COCH_3$ RN 823-76-7				194.6	814.	202.4	847.	
320	A	(-2.0)	193.6					83TAF
320	H		194.6					
320	U	(6.4)	195.1					81BRO/ABB
[C_3H_3NO] Isooxazole RN 288-14-2				194.5	814.	202.3	846.	
600	(Key)		194.5					83MAU
[$C_6H_{12}O$] t-$C_4H_9COCH_3$ RN 75-97-8				194.5	814.	202.3	846.	
320	A	(-2.1)	193.5					83TAF
320	H		194.5					
320	U	(5.8)	194.7					81BRO/ABB
[$C_6H_{14}O$] $(n-C_3H_7)_2O$ RN 111-43-3				194.5	814.	202.3	846.	
335	XX	(0.0)	194.5					82MAU
320	U	(5.5)	194.4					81BRO/ABB
320	H		194.7					
340	H	(+7.0)	194.3					80LIA/SHO
			195.6**					79AUE/BOW
[$C_5H_{12}O$] t-$C_4H_9OCH_3$ RN 1634-04-4				194.4	813.	202.2	846.	
320	A	(-2.2)	193.4					TAFT
320	H		194.4					
335	XX	(+0.2)	194.7					82MAU
			196.0**					79AUE/BOW
	(br)		$\sim 195 \pm 3$					75PIT/BUR
[C_6H_{10}] $CH_2=C(CH_3)C(CH_3)=CH_2$ RN 513-81-5				194.1**	812.**	202.1**	846.**	
			194.1**					79AUE/BOW
[C_9H_{11}] $C_6H_5(CHC_2H_5)$ radical RN xxxxx				$\sim$194	$\sim$812	$\sim$202	$\sim$845	
	(br)		$\sim$194					82MAU

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_8H_8] $C_6H_5CH{=}CH_2$ RN 100-42-5				194.2	812.5	202.0	845.	
320	A	(-2.4)	193.2					75WOL/HAR
320	H		194.2					
[$C_6H_{12}O$] c-$C_6H_{12}O$ (Oxepane) RN 592-90-5				195	816	202	845	
300	(Key)		195					83MAU
[C_5FeO_5] $(CO)_5Fe$ RN 13463-40-6				~194	~812	~202	~845	
320	A	(-3±3)	192.4					75FOS/BEA(2)
	(br)		194					75FOS/BEA(3)
[$C_3H_7NO_2$] i-C_3H_7ONO RN 541-42-4				194.1	812.	201.9	845.	
	(br)		194.1					78FAR/MCM
[C_5H_8] (E)-1,3-Pentadiene RN 2004-70-8				193.4**	809.**	201.8**	844.**	
			193.4**					79AUE/BOW
[$C_{18}H_{12}$] Chrysene RN 218-01-9				193.8	811.	201.6	843.	
550	A	(-1.4)	193.8					80MAU
[$C_5H_{10}O_2$] i-$C_3H_7COOCH_3$ RN 547-63-7				193.8	811.	201.6	843.	
320	A	(-2.8)	192.8					83TAF
320	H		193.8					
[$C_5H_{10}O$] $(C_2H_5)_2CO$ RN 96-22-0				193.5	810.	201.4	843.	
320	A	(-2.8)	192.8					TAFT
320	H		193.8					
340	H	(+6.0)	193.3					80LIA/SHO
[$C_6H_{10}O$] Cyclohexanone RN 108-94-1				194.0	812.	201.4	843.	
300	(Key)		196.4					83MAU
320	U	(4.8)	193.7					
560	(Key)		194.4					79SAL/KEB
[C_3H_6S] Thietane RN 287-27-4				194.0**	812.**	201.3**	842.**	
			194.0**					79AUE/BOW
[$C_5H_{10}O$] (i-C_3H_7)$COCH_3$ RN 563-80-4				193.3	809.	201.1	841.	
320	A	(-3.1)	192.3					83TAF
320	H		193.3					
[$C_3H_3N_3$] 1,3,5-Triazine RN 290-87-9				194.5	814.	201.1	841.	
550	G	(-13.0)	194.5					79MAU
[$C_4H_8O_2S$] $C_2H_5S(OCH_3)CO$ RN 38103-96-7				193.2	808.	201.0	841.	
320	A	(-3.4)	192.2					TAFT
320	H		193.2					
[C_8H_9] $C_6H_5CHCH_3$ radical RN xxxxx				~193	~807	~201	~841	
	(br)		~193					82MAU
[C_6H_{10}] 1,2-Dimethylcyclobutene RN 1501-58-2				194*	812*	201*	841*	
			194*					76AUE/DAV
[C_5H_8] 1-Methylcyclobutene RN xxxxx				194*	812*	201*	841*	
			194*					76AUE/DAV

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[C_5HMnO_5] $(CO)_5MnH$ RN 16972-33-1							201**	841**	
	320	A	(-3.8)						81STE/BEA
[C_6H_{10}] c-C_5H_8=CH_2 RN 1528-30-9					193.4	809.	200.8	840.	
	320	A	(-3.2)	192.4					77POL/WOL
	320	H		193.4					
[C_9H_{12}] Mesitylene RN 108-67-8					193.6	810.	200.7	840.	
	320	J	(18.0)	192.6					76DEV/WOL
	550	A	(-1.4)	194.6					80MAU
[$C_7H_6N_2$] m-$NCC_6H_4NH_2$ RN 2237-30-1					192.9	807.	200.7	840.	
	600	F	(-9.6)	192.9					81LAU/NIS
[$C_{11}H_{10}$] 1-Methylnaphthalene RN 90-12-0					192.9	807.	200.7	840.	
	550	A	(-2.3)	192.9					80MAU
[$C_4H_8O_2$] $CH_3COOC_2H_5$ RN 141-78-6					192.9	807	200.7	840.	
	373	X	(0.0)	192.9					79VAJ/HAR
	600	X	(0.0)	192.9					76KEB/YAM
	320	A	(-3.7)	191.9					77WOL/STA
	320	H		192.9					
	320	U	(+4.3)	193.0					81BRO/ABB
				193.5**					79AUE/BOW
	340	H	(+5.3)	192.6					80LIA/SHO
	370	U	(+2.0)	190.7					76HAR/LIN
	600	A	(-2.7)	192.5					76YAM/KEB
[C_2H_6S] $(CH_3)_2S$ RN 75-18-3					192.8	807.	200.6	839.	
	320	A	(-3.7)	191.9					77WOL/STA-83TAF
	320	H		192.8					
				193.4**					79AUE/BOW
[C_3H_6S] 2-Methylthiirane RN 1072-43-1					192.8**	807.**	200.6**	839.**	
				192.8**					79AUE/BOW
[$C_9H_7MnO_3$] $(CH_3C_5H_4)Mn(CO)_3$ RN 12108-13-3							200.6**	839.**	
	320	A	(-4.2)						81STE/BEA
[$C_5H_{10}O_2$] $CH_3COOC_3H_7$ RN 109-60-4					192.8	807.	200.6	839.	
	550	A	(-2.3)	192.8					80MAU
	600	A	(-2.3)	192.8					79LAU
[C_7H_{10}] Bicyclo[2.2.1]hept-2-ene (Norbornene) RN 498-66-8					193.1	808.	200.4	838.	
	320	P	(0.5)	193.1					77STA/WIE
		(Key)		191.2			198.5	830.5	76SOL/FIE
				193.8**					79AUE/BOW
	560	(Key)		192.6					79SAL/KEB
[$C_6H_{10}O$] $(CH_2$=$CHCH_2)_2O$ RN 557-40-4					192.6	806.	200.4	838.	
	320	A	(-4.0)	191.6					TAFT
	320	H		192.6					

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_5H_8] CH_2=CHC(CH_3)=CH_2 RN 78-79-5				192.0**	803.**	200.4**	838.**	
			192.0**					79AUE/BOW
[C_7H_8O] $C_6H_5OCH_3$ RN 100-66-3				192.5	806.	200.3	838.	
500	A	(-3.1)	192.0					84SHA/BLA
600	J	(+15.7)	191.3					76LAU/KEB
600	F	(-9.8)	192.7					81LAU/NIS
600	A	(-2.7)	192.4					79LAU
[$C_4H_{10}O$] $(C_2H_5)_2O$ RN 60-29-7				192.4	805.	200.2	838.	
320	P	(0.0)	192.6					77STA/WIE
320	A	(-3.9)	191.7					77WOL/STA-83TAF
320	H		192.6					
320	U	(+3.5)	192.4					81BRO/ABB
			193.1**					79AUE/BOW
340	H	(+4.9)	192.2					80LIA/SHO
370	U	(+2.2)	190.9					76HAR/LIN
500	A	(-3.7)	191.4					84SHA/BLA
600	A	(-2.8)	192.3					78DAV/LAU
600	F	(-10.1)	192.4					81LAU/NIS
[C_7H_6O] C_6H_5CHO RN 100-52-7				192.4	805.	200.2	838.	
320	A	(-3.5)	192.0					83TAF
320	H		193.0					
320	U	(+4.2)	193.1					81BRO/ABB
550	A	(-3.2)	192.0					80MAU
600	J	(+15.4)	191.0					76LAU/KEB
600	A	(-3.0)	192.1					79LAU
[$C_3H_6O_3$] $(CH_3O)_2CO$ RN 616-38-6				192.4	805.	200.2	838.	
320	A	(-4.2)	191.4					77WOL/STA
320	H		192.4					
[$C_4H_8O_2$] $C_2H_5COOCH_3$ RN 554-12-1				192.4	805.	200.2	838.	
320	A	(-4.2)	191.4					83TAF
320	H		192.4					
[C_7ClH_5O] 4-ClC_6H_4CHO RN 104-88-1				192.4	805.	200.2	838.	
320	A	(-4.2)	191.4					TAFT
320	H		192.4					
[C_4H_6O] CH_2=$CHCOCH_3$ RN 78-94-4				192.4	805.	200.2	838.	
373	X	(-0.5)	192.4					79VAJ/HAR
[$C_5H_{10}O_2$] $C_3H_7COOCH_3$ RN 623-42-7				192.6	806.	200.1	837.	
550	G	(-15.3)	192.3					79MAU
550	A	(-2.3)	192.9					80MAU
[C_5H_5NNiO] $(C_5H_5)NiNO$ RN 12071-73-7						200.1**	837.**	
320	A	(-4.8)						81STE/BEA
[$C_{13}H_{10}$] Fluorene RN 86-73-7				192.9	807.	200.0	837.	
550	A	(-2.3)	192.9					80MAU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_{11}H_{10}$] 2-Methylnaphthalene RN 91-57-6					192.2	804.	200.0	837.	
	550	A	(-3.0)	192.2					80MAU
[CCl_2] CCl_2 RN 1605-72-7					~192.2	~804.	~200.0	~837.	
		(br)		~192.2					78AUS/LIA(2)
[C_7FH_6] 3-$FC_6H_4CH_2$ radical RN xxxxx					~192	~803	~200	~837	
		(br)		~192					82MAU
[C_4H_8O] $CH_3COC_2H_5$ RN 78-93-3					192.0	803.	199.8	836.	
	320	A	(-4.7)	190.7					83TAF
	320	H		191.7					
	340	H	(+4.4)	191.6					80LIA/SHO
	600	X	(-0.1)	192.8					76KEB/YAM
[$C_5H_{10}O$] c-$C_5H_{10}O$ RN 142-68-7					191.9	803.	199.7	835.5	
	320	A	(-4.2)	191.4					77WOL/STA
	320	H		192.4					
	320	U	(+3.4)	192.3					81BRO/ABB
	600	U	(+2.8)	191.5					83MAU
[C_4H_6O] CH_3CH=CHCHO RN 4170-30-3					191.9	803.	199.7	835.5	
	373	(Key)		191.9					79VAJ/HAR
[$C_{10}F_3H_9$] 4-$CF_3C_6H_4C(CH_3)CH_2$ RN 55186-75-9					191.9	803.	199.7	835.5	
	320	A	(-4.7)	190.9					TAFT
	320	H		191.9					
[C_5H_6] c-C_5H_6 RN 542-92-7					192.5	805.	199.6	835.	
		(br)		182.8					81HOU/SCH
	550	A	(-2.7)	192.5					80MAU
				192.2**					79AUE/BOW
	Threshold Value						197.8	828.	75LOS/TRA
[C_7H_7] c-C_7H_7 radical RN 3551-27-7					192.4	805.	199.4	834.	
		(br)		192.4					80DEF/MCI
[C_3H_4O] CH_3CH=CO RN 6004-44-0					191.6	802.	199.4	834.	
	320	V	(+1.6)	191.6					80ARM/HIG
[$C_{16}H_{10}$] Fluoranthene RN 206-44-0							199.3	834.	
	550	A	(-3.0)	192.2					80MAU
[C_7FH_5O] 4-FC_6H_4CHO RN 459-57-4					191.4	801.	199.2	833.	
	320	A	(-5.1)	190.5					TAFT
	320	H		191.5					
[C_7H_7] $C_6H_5CH_2$ RN 2154-56-5					191.7	802.	199.1	833.	
		(br)		192.9					82MAU
		(br)		191.7					80DEF/MCI
	Threshold Value			191.3			198.7	832.	78HOU/BEA

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[CH_4N] CH_2NH_2 RN 54088-53-8					191	799	199	833	
		(br)		191					81MCA/NIC
[C_6H_{12}] $(CH_3)_2C=C(CH_3)_2$ RN 563-79-1							199.0	833.	
		(Key)							76GOR/MUN-75SOL/FIE
[C_5H_5] c-C_5H_5 radical RN xxxxx					~191	~799	~199	~833	
		(br)		~191					80DEF/MCI
[$C_4H_8O_2$] 1,3-Dioxane RN 505-22-6					191.2	800.	198.8	832.	
		(Key)		191.2					83MAU
[C_4H_8O] c-C_4H_8O (Tetrahydrofuran) RN 109-99-9					191.4	801.	198.8	831.	
	320	A	(-4.9)	190.7					77WOL/STA-83TAF
	320	H		191.6					
	320	U	(+2.7)	191.6					81BRO/ABB
	340	H	(+4.0)	191.3					80LIA/SHO
				192.3**					79AUE/BOW
	500	A	(-4.7)	190.4					84SHA/BLA
[C_5H_8O] Cyclopentanone RN 120-92-3					191.5	801.	198.8	832.	
	320	U	(+2.6)	191.5					81BRO/ABB
				192.5**					79AUE/BOW
[C_7H_{12}] 1-Methylcyclohexene RN 591-49-1					191.0	799.	198.8	832.	
	320	A	(-5.6)	190.0					77POL/WOL
	320	H		191.0					
[C_7H_{12}] c-C_5H_6-1,2-$(CH_3)_2$ RN 765-47-9					191.0	799.	198.8	832.	
	320	A	(-5.8)	190.0					77POL/WOL
	320	H		191.0					
[$C_{14}H_{10}$] Phenanthrene RN 85-01-8					191.6	802.	198.7	831.	
	550	A	(-3.6)	191.6					80MAU
[$C_{18}H_{12}$] Triphenylene RN 217-59-4					191.4	801.	198.5	830.5	
	550	A	(-3.8)	191.4					80MAU
[CH_3NO] $HCONH_2$ RN 75-12-7					190.6	797.	198.4	830.	
	600	U	(1.9)	190.6					83MAU
[C_6H_{12}] $CH_3CH=C(CH_3)C_2H_5$ RN 922-61-2							198.2	829.	
		(Key)							76GOR/MUN-75SOL/FIE
[$C_7H_6O_2$] C_6H_5COOH RN 65-85-0					189.6	793.	198.2	829.	
	600	A	(-5.5)	189.6					79LAU
[$C_4H_7O_3P$] Methyltrioxaphosphabicycloheptane RN 61580-09-4					190.3	796.	198.1	829.	
	325	(Key)		190.3					80HOD/HOU

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_5H_8] $(CH_3)_2CHCCH$ RN 598-23-2					190**	795**	198**	828**	
				190**					79AUE/BOW
[C_2H_2O] $CH_2C=O$ RN 463-51-4					189.5	793.	198.0	828.	
		(Key)		189.7					79LIA
	600	A	(-6.3)	189.3					78DAV/LAU
	Threshold Value			189.0			197.3		82TRA/MCL
[C_3H_4] Cyclopropene RN 2781-85-3					190*	795*	198*	828*	
				190*					76AUE/DAV
[C_6H_{12}] $(CH_3)_2C=CHCH_2CH_3$ RN 625-27-4					190.1	795.	197.9	828.	
	340	H	(+2.8)	190.1					78AUS/LIA
		(Key)					197.4		75SOL/FIE
		(Key)					198.0		76GOR/MUN
[$C_3H_6O_2$] CH_3COOCH_3 RN 79-20-9					190.0	795.	197.8	828.	
	320	V	(0.0)	190.0					80ARM/HIG
	320	A	(-6.4)	189.2					77WOL/STA-83TAF
	320	H		190.2					
	320	U	(+1.2)	190.1					81BRO/ABB
				190.5**					79AUE/BOW
	340	H	(+2.7)	190.0					80LIA/SHO
	340	H	(+2.7)	190.0					78AUS/LIA
	370	U	(+0.2)	188.9					76HAR/LIN
	600	A	(-5.7)	189.4					79LAU
	600	X	(-2.9)	190.0					76KEB/YAM
[C_5H_8] $c\text{-}C_3H_5CH=CH_2$ RN 693-86-7					189.9	794.5	197.7	827.	
	320	A	(-6.7)	188.9					77WOL/STA
	320	H		189.9					
[$C_2H_4N_2$] $NCCH_2NH_2$ RN xxxxx					189.6	793.	197.4	826.	
	320	G	(-18.9)	189.6					83TAF
[$C_2H_5NO_2$] C_2H_5ONO RN 109-95-5					189.5	793.	197.3	825.5	
		(br)		189.5					78FAR/MCM
[C_6H_{10}] 1-Methylcyclopentene RN 693-89-0					189.2	792.	197.0	824.	
	320	A	(-7.6)	188.2					77POL/WOL
	320	H		189.2					
				190.4**					79AUE/BOW
[$C_4H_{10}S$] $t\text{-}C_4H_9SH$ RN 75-66-1					189.2	792.	197.0	824.	
	320	A	(-7.6)	188.2					TAFT
	320	H		189.2					
[C_3H_6O] $c\text{-}C_3H_6O$ (Oxetane) RN 503-30-0					189.6*	793.*	196.9*	824.*	
				189.6*					79AUE/BOW
[$C_7CrH_5NO_3$] $(C_5H_5)Cr(CO)_2NO$ RN 36312-04-6							196.9**	824.**	
	320	A	(-7.7)						81STE/BEA

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_3H_6O] $(CH_3)_2CO$ RN 67-64-1				188.9	790.	196.7	823.	
320	U	(0.0)	188.9					81BRO/ABB
600	U	(0.0)	188.9					83MAU
370	U	(0.0)	188.9					76HAR/LIN
320	A	(-7.9)	187.9					77WOL/STA
320	H		188.9					
			189.9**					79AUE/BOW
340	H	(+1.6)	188.9					80LIA/SHO
340	H	(+1.5)	188.8					78AUS/LIA
550	A	(-6.9)	188.3					80MAU
600	A	(-6.5)	188.6					78DAV/LAU
600	X	(-3.5)	189.4					76KEB/YAM
[C_4H_4S] c-C_4H_4S Thiophene RN 110-02-1				189.5	793.	196.5	822.	
320	A		189.5					TAFT
	(br)		183					81HOU/SCH
600	(Key)		185.0					83MAU
[C_7FH_5O] 3-FC_6H_4CHO RN 456-48-4				188.7	788.	196.5	822.	
320	A	(-8.1)	187.7					TAFT
320	H		188.7					
[C_5H_{10}] $(CH_3)_2C=CHCH_3$ RN 513-35-9				188.6	789.	196.4	822.	
340	H	(+1.3)	188.6					78AUS/LIA
			189.5**					79AUE/BOW
	(Key)					197.8		76GOR/MUN
	(Key)					198.3		75SOL/FIE
[C_3H_8O] $CH_3OC_2H_5$ RN 540-67-0				188.6	789.	196.4	822.	
320	A	(-8.2)	187.6					77WOL/STA
320	H		188.6					
			189.2**					79AUE/BOW
[C_6H_6O] C_6H_5OH RN 108-95-2				188.5	789.	196.3	821.	
550	A	(-6.3)	188.9					80MAU
600	J	(+11.3)	186.9					76LAU/KEB
600	A	(-7.1)	188.1					79LAU
For protonation on O atom: PA -175±4 kcal/mol (754 kJ/mol)								77DEF/MCI
[$C_{12}H_{10}$] Biphenyl RN 92-52-4				188.3	788.	196.1	820.	
550	A	(-6.9)	188.3					80MAU
[C_7H_{14}] $(CH_3)_2C=CHCH(CH_3)_2$ RN xxxxx						196.1	820.	
	(Key)							76MAU/SOL
[$C_4H_8O_2$] $HCOOCH(CH_3)_2$ RN 625-55-8				188.2	787.	196.0	820.	
370	U	(-0.5)	188.2					76HAR/LIN
[$C_2H_6S_2$] CH_3SSCH_3 RN 624-92-0				~188	~787	~196	~820	
	(br)		~188					81KIM/BON
[C_5H_8] $C_2H_5CCCH_3$ RN 627-21-4				188**	787**	196**	820**	
			188**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_2H_3NS] CH_3SCN RN 556-64-9				188.1	787.	195.9	820.	
	(br)		188.1					74MCA
[C_2H_3NS] CH_3NCS RN 556-61-6				188.1	787.	195.9	820.	
	(br)		188.1					74MCA
[C_4H_8] $(CH_3)_2C{=}CH_2$ RN 115-11-7				187.3	784.	195.9	820.	
Threshold Value			187.3					
320	H	(0.0)	187.3					77WOL/STA
340	H	(0.0)	187.3					80LIA/SHO
			188.3**					79AUE/BOW
320	A	(-9.2)	186.4					77WOL/STA
600	A	(-8.1)	187.0					78DAV/LAU
600	X	(-5.1)	187.8					76KEB/YAM
[C_7H_5N] C_6H_5CN RN 100-47-0				188.1	787.	195.9	820.	
600	J	(+11.4)	187.0					76LAU/KEB
600	A	(-7.0)	188.1					79LAU
[$C_{16}H_{18}$] $C_6H_5(CH_2)_4C_6H_5$ RN 1083-56-3				188.1	787.	195.9	820.	
350	R	(1.8)	188.1					80MAU/HUN
[C_8H_{10}] m-Xylene RN 108-38-3				188.1	787.	195.9	820.	
320	J	(13.5)	188.1					76DEV/WOL
	(Key)		184.2					72CHO/FRA(2)
[C_4H_5N] c-C_3H_5CN RN 5500-21-0				187.6	785.	195.4	817.5	
320	A	(-8.9)	186.5					76STA/KLE
320	H		187.6					
320	U	(-1.2)	187.7					81BRO/ABB
[C_4H_6O] $CH_2{=}C(CH_3)CHO$ RN 78-85-3				187.4	784.	195.2	817.	
373	(Key)		187.4					79VAJ/HAR
[$C_5H_{10}O_2$] $HCO_2(n\text{-}C_4H_9)$ RN 592-84-7				186.9	824.	194.8	815.	
320	A	(-9.6)	185.9					77WOL/STA
320	H		187.0					
340	H	(-0.4)	186.9					80LIA/SHO
			188.0**					79AUE/BOW
[$C_4H_6O_2$] $CH_3COCOCH_3$ RN 431-03-8				186.2	779.	194.8	815.	
300	U	(-2.7)	186.2					83MAU
[$C_{10}H_{12}$] 1,2,3,4-Tetrahydronaphthalene RN 119-64-2				187.7	785.	194.7	815.	
550	A	(-7.5)	187.7					80MAU
[$C_{10}H_8$] Naphthalene RN 91-20-3				187.8	785.5	194.7	815.	
550	A	(-7.6)	187.6					80MAU
600	A	(-7.2)	187.9					78LAU/SAL
[C_3H_6O] 2-Methyloxirane RN 75-56-9				186.9	782.	194.7	815.	
			186.9**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_{14}H_{14}]$ $C_6H_5(CH_2)_2C_6H_5$ RN 103-29-7					187.3	784.	194.6	814.	
	350	R	(+0.9)	187.3					80MAU/HUN
$[C_2H_4S]$ c-C_2H_4S (Thiirane) RN 420-12-2					187.3	784.	194.6	814.	
		(Key)		187.3					80AUE/WEB
				188.5**					79AUE/BOW
$[C_6O_6V]$ $(CO)_6V$ RN 20644-87-5							194.5**	814.**	
	320	A	(-10.3)						81STE/BEA
$[C_4H_7N]$ i-C_3H_7CN RN 78-82-0					186.4	780.	194.3	813.	
	320	A	(-9.8)	185.7					77WOL/STA
	320	H		186.5					
	320	Q	(+1.0)	186.3					76STA/KLE
$[C_4H_8O_2]$ $HCO_2(n-C_3H_7)$ RN 110-74-7					186.4	780.	194.2	812.5	
				187.4**					79AUE/BOW
	320	A	(-9.8)	185.9					77WOL/STA
	320	H		186.7					
	340	H	(-0.6)	186.7					80LIA/SHO
	370	U	(-2.0)	186.8					76HAR/LIN
	600	A	(-9.5)	185.6					79LAU
	600	X	(-6.6)	186.3					76KEB/YAM
$[C_3H_8S]$ i-C_3H_7SH RN 75-33-2					186.3	779.	194.1	812.	
	320	A	(-10.1)	185.5					TAFT
	320	H		186.3					
$[B_3H_6N_3]$ Borazine RN 6569-51-3					186.3	779.	194.1	812.	
	298	(Key)		186.3					79DOI/GRE
$[C_5H_9N]$ n-C_4H_9CN RN 110-59-8					186.2	779.	194.0	812.	
	320	A	(-10.2)	185.4					76STA/KLE
	320	H		186.2					
$[C_3H_5O_3P]$ 2,6,7-Trioxa-1-phosphabicyclo[2.2.1]heptane RN 279-53-8					186.1	779.	194.0	812.	
	320	(Key)		186.1					80HOD/HOU
$[C_3H_4O]$ CH_2=CHCHO RN 107-02-8					186.1	779.	193.9	811.	
	373	Q	(+0.8)	186.1					79VAJ/HAR
$[C_4H_6O]$ C-C_4H_6(=O) RN xxxxx					186.4	780.	193.8	811.	
	320	U	(-2.5)	186.4					81BRO/ABB
$[C_4H_8O_2]$ 1,4-Dioxane RN 123-91-1					186.0	778.	193.8	811.	
	320	A	(-10.4)	184.8					77WOL/STA
	320	H		186.0					
	320	U	(-2.8)	186.1					81BRO/ABB
	500	A	(-10.5)	184.6					84SHA/BLA
$[C_3F_3H_6N]$ $CF_3N(CH_3)_2$ RN 677-41-8					186.	778.	193.8	811.	
	320	A	(~-10.4)	185.2					77STA/TAA
	320	H		186.0					
				187.0**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_4H_7O_2]$ 1,4-Dioxyl radical RN 4598-47-4					186.0	778.	193.8	811.	
	340	(Key)		186.0					83AUS/LUT
$[C_4H_{10}O]$ t-C_4H_9OH RN 75-65-0					185.9	778.	193.7	810.	
				187**					76AUE/BOW
	600	A	(-9.2)	185.9					79LAU
		(Key)		183.2					77HIR/KEB
$[C_4H_7N]$ n-C_3H_7CN RN 109-74-0					185.7	777.	193.7	810.	
	320	A	(-10.7)	184.9					76STA/KLE
	320	H		185.7					
				186.0**					79AUE/BOW
$[B_3H_5N_3]$ B-Borazinyl radical RN xxxxx					185.8	777.	193.6	810.	
		(br)		185.8					76DES/POR
$[C_6H_5NO_2]$ $C_6H_5NO_2$ RN 98-95-3					185.6	776.5	193.4	809.	
	600	J	(+8.9)	184.5					76LAU/KEB
	600	A	(-9.5)	185.6					79LAU
$[C_8H_{10}]$ o-Xylene RN 95-47-6					186.1	779.	193.3	809.	
	350	R	(0.0)	186.4					80MAU/HUN
	320	A	(-10.6)	185.0					74HEH/MCI
	320	H		185.8					
	320	J	(9.6)	184.2					76DEV/WOL
				184.2					72CHO/FRA(2)
	550	A	(-8.8)	186.4					80MAU
$[C_3H_6O_2]$ $HCO_2C_2H_5$ RN 109-94-4					185.3	775.	193.1	808.	
	320	Q	(0.0)	185.3					76STA/KLE
				186.4**					79AUE/BOW
	320	A	(-11.0)	184.6					77WOL/STA
	320	H		185.4					
	320	U	(-3.3)	185.6					81BRO/ABB
	340	H	(-2.4)	184.9					80LIA/SHO
	370	U	(-2.0)	186.7					76HAR/LIN
	600	A	(-10.0)	185.6					78DAV/LAU
$[C_4H_6]$ $CH_2=CHCH=CH_2$ RN 106-99-0					185**	774**	193**	807.5**	
				185**					79AUE/BOW
$[C_{10}H_{14}]$ t-$C_4H_9C_6H_5$ RN 98-06-6					185.2	775.	193.0	807.	
	320	A	(-11.2)	184.4					74HEH/MCI
	320	H		185.2					
$[C_3H_5N]$ C_2H_5CN RN 107-12-0					184.1	770.	192.6	806.	
	320	A	(-12.0)	183.6					76STA/KLE
	320	H		184.4					
	340	H	(-3.4)	183.9					80LIA/SHO
				185.0**					79AUE/BOW
$[C_4H_8O]$ i-C_3H_7CHO RN 78-84-2					184.8	773.	192.6	806.	
	320	A	(-11.6)	184.0					77WOL/STA
	320	H		184.8					
				185.5**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_5H_{10}O$] n-C_4H_9CHO RN 110-62-3				184.8	773.	192.6	806.	
320	A	(-11.6)	184.0					77WOL/STA
320	H		184.8					
			185.5**					79AUE/BOW
[CH_3NO_2] CH_3ONO RN 624-91-9				184.7	773.	192.5	805.	
	(br)		184.7					78FAR/MCM
	(br)		184.7					76MCA/PIT
[C_9H_{12}] n-$C_3H_7C_6H_5$ RN 103-65-1				184.6	772.	192.4	805.	
320	A	(-11.8)	183.8					74HEH/MCI
320	H		184.6					
600	J	(+7.5)	183.1					76YAM/KEB
[C_4H_4O] Furan RN 110-00-9				185.0	774.0	192.2	804.	
600	(Key)		185.0					83MAU
	(br)		183					81HOU/SCH
[C_9H_{12}] i-$C_3H_7C_6H_5$ RN 98-82-8				184.3	771.	192.1	804.	
320	A	(-11.3)	184.3					74HEH/MCI
320	H		185.1					
600	J	(+7.9)	183.5					76YAM/KEB
[$C_{10}H_{14}$] n-$C_4H_9C_6H_5$ RN 104-51-8				184.3	771.	192.1	804.	
320	A	(-11.4)	184.2					74HEH/MCI
320	H		185.0					
600	J	(+7.9)	183.5					76YAM/KEB
[C_2H_6O] $(CH_3)_2O$ RN 115-10-6				184.3	771.	192.1	804.	
320	A	(-11.7)	183.9					77WOL/STA-83TAF
320	H		184.7					
320	U	(-4.0)	184.9					81BRO/ABB
340	H	(-3.2)	184.1					80LIA/SHO
370	T	(+4.4)	182.8					76HAR/LIN
373	T	(+4.5)	183.1					75SOL/HAR
500	A	(-11.0)	184.1					84SHA/BLA
600	A	(-11.1)	184.0					76YAM/KEB
600	X	(-7.7)	185.2					76KEB/YAM
			185.8**					79AUE/BOW
[C_3FH_5O] CH_3COCH_2F RN 430-51-3				184.2	771.	192.0	803.	
298	(Key)		184.2					82DRU/MCM
[C_8H_{10}] p-Xylene RN 106-42-3				184.6	772.	192.0	803.	
320	A	(-11.3)	184.3					74HEH/MCI
320	H		185.1					
320	J	(+8.9)	184.5					76DEV/WOL
	(Key)		184.1					72CHO/FRA(2)
[$C_3H_6O_2$] C_2H_5COOH RN 79-09-4				184.0	770.	191.8	802.	
600	A	(-11.8)	183.3					76YAM/KEB
600	X	(-8.2)	184.7					76KEB/YAM
[C_3H_8S] n-C_3H_7SH RN 107-03-9				183.8	769.	191.6	802.	
320	A	(-12.6)	183.0					TAFT
320	H		183.8					

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_8H_{10}] $C_2H_5C_6H_5$ RN 100-41-4				183.8	769.	191.6	802.	
320	A	(-12.7)	182.9					77WOL/STA,74HEH/MCI
320	H		183.7					
600	J	(+7.3)	182.9					76LAU/KEB
600	A	(-11.1)	184.0					79LAU
[$C_4F_9H_2N$] $(CF_3)_3CNH_2$ RN 2809-92-9				183.1**	766.**	191.5**	801.**	
			183.1**					79AUE/BOW
[C_4H_8O] n-C_3H_7CHO RN 123-72-8				183.7	769.	191.5	801.	
320	A	(-12.6)	183.0					77WOL/STA
320	H		183.8					
340	H	(-3.7)	183.6					80LIA/SHO
			185.8**					79AUE/BOW
[C_2H_5P] c-C_2H_4PH (Phosphirane) RN 6569-82-0				184.2	771.	191.4	801.	
	(Key)		184.2					80AUE/WEB
			187.6**					79AUE/BOW
[C_3H_8O] i-C_3H_7OH RN 67-63-0				183.4	767.	191.2	800.	
600	A	(-11.7)	183.4					79LAU
[$C_4H_{10}O$] n-C_4H_9OH RN 71-36-3				183.3	767.	191.1	799.5	
320	A	(-13.1)	182.5					TAFT
320	H		183.3					
[$C_8F_3H_5O$] p-$CF_3C_6H_4$CHO RN 455-19-6				183.2	766.5	191.0	799.	
320	A	(-13.2)	182.4					TAFT
320	H		183.2					
[C_4H_6] Cyclobutene RN 822-35-5				183**	766**	191**	799**	
			183**					79AUE/BOW
[C_2H_6S] C_2H_5SH RN 75-08-1				182.9	765.	190.8	798.	
320	A	(-13.8)	181.8					TAFT
320	H		182.6					
340	H	(-4.0)	183.3					80LIA/SHO
[C_6H_6O] $(HCCCH_2)_2O$ RN 6921-27-3				183.0	766.	190.8	798.	
320	A	(-13.4)	182.2					TAFT
320	H		183.0					
[C_3H_8O] n-C_3H_7OH RN 71-23-8				183.0	766.	190.8	798.	
320	U	(-5.9)	183.0					81BRO/ABB
			183.6**					79AUE/BOW
[C_2D_6O] $(CD_3)_2O$ RN 17222-37-6				182.8	765.	190.6	797.	
370	T	(14.2)	182.8					76HAR/LIN
[$C_8FeH_8O_2$] $(C_5H_5)Fe(CO)_2CH_3$ RN 12080-06-7						190.6**	797.**	
320	A	(-14.2)						81STE/BEA
[CHN] HNC RN xxxxx				182.4	763.	190.2	796.	
	(br)		182.4					82PAU/HEH

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[C_2H_4O_2]$ CH_3COOH RN 64-19-7				181.7	760.	190.2	796.	
320	A	(-14.8)	180.8					77WOL/STA
320	H		181.6					
600	A	(-13.3)	181.8					76YAM/KEB
$[C_7H_8]$ $C_6H_5CH_3$ RN 108-88-3				182.0	761.	189.8	794.	
320	A	(-13.7)	181.9					74HEH/MCI
320	H		182.7					
320	J	(+6.6)	181.2					76DEV/WOL
340	(Key)		182.1					77AUS/LIA
	(Key)		184.1					72CHO/FRA(2)
478	W	(0.0)	182.0					82STO/SPL
550	A	(-11.0)	184.2					80MAU
600	J	(+6.3)	181.9					76LAU/KEB
600	A	(-12.1)	183.0					79LAU
$[C_7D_3H_5]$ $C_6H_5CD_3$ RN 1124-18-1				182.0	761.	189.8	794.	
340	(Key)		182.1					77AUS/LIA
$[C_3H_3N]$ CH_2=CHCN RN 107-13-1				181.9	761.	189.7	794.	
320	A	(-14.5)	181.1					76STA/KLE
320	H		181.9					
$[C_3H_6O]$ C_2H_5CHO RN 123-38-6				181.8	761.	189.6	793.	
320	A	(-14.4)	181.2					77WOL/STA
320	H		182.0					
300			183.6**					79AUE/BOW
340	H	(-5.6)	181.7					80LIA/SHO
370	T	(+2.5)	181.1					75SOL/HAR
600	A	(-13.4)	181.7					76YAM/KEB
$[C_7FH_7]$ 3-$FC_6H_4CH_3$ RN 352-70-5				181.8	761.	189.3	792.	
478	W	(-0.2)	181.8					82STO/SPL
$[C_6H_{10}]$ c-C_6H_{10} RN 110-83-8				181.5	759.	189.3	792.	
340	H	(-5.8)	181.5					80LIA/SHO
$[C_2H_4O_2]$ HCO_2CH_3 RN 107-31-3				181.0	757.	188.9	790.	
320	A	(-14.7)	180.9					77WOL/STA
320	H		181.7					
340	H	(-6.0)	181.2					80LIA/SHO
370	T	(+2.0)	180.6					76HAR/LIN
478	W	(-1.3)	180.2					82STO/SPL
600	A	(-13.5)	181.6					79LAU
$[H_3P]$ PH_3 RN 7803-51-2				180.2	754.	188.6	789.	
320	A	(-15.8)	179.8					77WOL/STA-83TAF
320	H		180.5					
340	H	(-7.4)	179.9					80LIA/SHO
			182.5**					79AUE/BOW
$[C_2H_3N]$ CH_3CN RN 75-05-8				180.6	756.	188.4	788.	
320	A	(-15.5)	180.1					77WOL/STA
320	H		180.9					
340	H	(-6.9)	180.4					80LIA/SHO
600	A	(-14.5)	180.6					79LAU
			183.1**					79AUE/BOW

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[C_2H_6O]$ C_2H_5OH RN 64-17-5					180.2	754.	188.3	788.	
	320	A	(-15.8)	179.8					77WOL/STA-83TAF
	320	H		180.6					
	370	T	(+1.3)	179.9					76HAR/LIN
	600	A	(-14.7)	180.4					79LAU
				182.5**					79AUE/BOW
$[C_3H_5]$ c-C_3H_5 radical RN xxxxx					179.	749.	188.	787.	
		(br)		179.					80DEF/MCI
$[B_4H_8]$ B_4H_8 RN 12007-71-5					180	753	188	787	
		(br)		180					72SOL/POR
$[C_2H_4O]$ c-C_2H_4O (Oxirane) RN 75-21-8					180.6	756.	187.9	786.	
		(Key)		180.6					80AUE/WEB
				182.3**					79AUE/BOW
$[C_3ClH_4N]$ $Cl(CH_2)_2CN$ RN 542-76-7					179.9	752.	187.5	784.5	
	320	A	(-16.4)	179.2					76STA/KLE
	320	H		179.9					
$[CH_4S]$ CH_3SH RN 74-93-1					179.2	750.	187.4	784.	
	320	A	(-16.6)	179.0					77WOL/STA
	320	H		179.7					
	340	H	(-7.9)	179.4					80LIA/SHO
	370	T	(+0.4)	178.7					76HAR/LIN
	370	(Key)		179.1					75SOL/HAR
$[H_2N]$ NH_2 RN 15194-15-7					179	749	187	782	
		(br)		179.					82DEF/HEH
$[C_4H_6]$ CH_3CCCH_3 RN 503-17-3					179**	749**	187**	782**	
				179**					79AUE/BOW
$[C_8H_5NO]$ 4-CNC_6H_4CHO RN 105-07-7					179.2	750.	187.0	782.	
	320	A	(-17.1)	178.5					TAFT
	320	H		179.2					
$[C_3F_2H_4O]$ CFH_2COCFH_2 RN 453-14-5					179	749	187	782	
	298	(Key)		179					82DRU/MCM
$[C_6H_3O_5Re]$ $(CO)_5ReCH_3$ RN 14524-92-6							187**	782**	
	320	A	(-17.4)						81STE/BEA
$[C_7FH_7]$ 2-$FC_6H_4CH_3$ RN 95-52-3					178.8	748.	186.6	781.	
	478	W	(-3.2)	178.8					82STO/SPL
$[C_2H_4O]$ CH_3CHO RN 75-07-0					178.6	747.	186.6	781.	
	Threshold Value						184.6	772.	68REF/CHU
	370	T	(0.0)	178.6					76HAR/LIN
	370	T	(0.0)	178.6					75SOL/HAR
	320	A	(-17.6)	178.0					77WOL/STA
	320	H		178.7					
	300			181.1**					79AUE/BOW
	340	H	(-8.8)	178.5					80LIA/SHO
	600	A	(-16.1)	179.0					79LAU
	600	N		177.4					

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_4F_3H_7O$] $C_2H_5OCH_2CF_3$ RN 461-24-5					178.6	747.	186.4	780.	
	320	A	(-17.7)	177.9					TAFT
	320	H		178.6					
[C_3H_4] $H_2C{=}C{=}CH_2$ RN 463-49-0					179.	749.	186.3	779.	
	Threshold Value						185.3	775.	77ROS/DRA
		(br)		179.					AUS/LIA
[CH_2S] CH_2S RN 865-36-1					178.	745.	186.	778.	
		(br)		178					82ROY/MCM
[C_2H_6Hg] CH_3HgCH_3 RN 593-74-8					~178	~744	~186	~778	
		(br)		~178					80STO/CAM
[C_7FH_7] 4-$FC_6H_4CH_3$ RN 352-32-9					178.0	745.	185.8	777.	
	478	W	(-4.0)	178.0					82STO/SPL
[$C_6F_3H_9O_2$] $CF_3CO_2(n\text{-}C_4H_9)$ RN 367-64-6					178.0	745.	185.8	777.	
	320	A	(-18.2)	177.3					77WOL/STA
	320	H		178.0					
[$C_5F_3H_7O_2$] $CF_3CO_2(n\text{-}C_3H_7)$ RN 383-66-4					177.9	744.	185.7	777.	
	320	A	(-18.4)	177.2					77WOL/STA
	320	H		177.9					
[C_3] C_3 RN 12075-35-3					~177	~742	~185	~775	
		(br)		~177					83RAK/BOH
[C_6MoO_6] $(CO)_6Mo$ RN 13939-06-5							185**	774**	
	320	A	(-19.2)						81STE/BEA
[$C_2H_5NO_2$] $C_2H_5NO_2$ RN 79-24-3					177.0	740.	184.8	773.	
	340	H	(-10.3)	177.0					80LIA/SHO
[$C_4F_3H_5O_2$] $CF_3CO_2C_2H_5$ RN 383-63-1					176.8	740.	184.6	772.	
	320	A	(-19.5)	176.1					77WOL/STA
	320	H		176.8					
[C_3HN] HCCCN RN xxxxx					176.	737.	184.	770.	
		(br)		176.					84RAK/BOH
[B_5H_8] B_5H_8 RN 65930-58-7					177.	740.	184.	770.	
		(br)		177.					78WAN/DES
[C_6O_6W] $(CO)_6W$ RN 14040-11-0							184**	770**	
	320	A	(-20.3)						81STE/BEA
[$C_2FH_3O_2$] CH_2FCOOH RN 144-49-0					175.7	735.1	183.5	768.	
	600	A	(-19.4)	175.7					76YAM/KEB
[$C_2Cl_3HO_2$] CCl_3COOH RN 76-03-9					175.7	735.	183.5	768.	
	600	A	(-18.3)	176.8					76YAM/KEB
		N		175.7					
[C_5H_8] c-C_5H_8 RN 142-29-0							183.4	767.5	
	Threshold Value						183.6	768.	HOU/BEA
		(br)		178.2			186.0	778.	80LIA/SHO
		(Key)					183.3	767.	76SOL/FIE

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_6H_3MnO_5$] $(CO)_5MnCH_3$ RN 13601-24-6					175	732	183	766	
	320	A	(-19.9)				185**		81STE/BEA
		(br)		175.					79STE/BEA
[C_6FH_5] Fluorobenzene RN 462-06-6					174.8	731.4	182.6	764.	
	334	J	(+0.2)	174.8					81BOH/STO
	400	J	(-0.2)	174.6					78HAR/LIA
	600	J	(-0.8)	174.8					76LAU/KEB
	600	A	(-19.2)	175.9					79LAU
	600	N		174.8					
[BrC_6H_5] Bromobenzene RN 108-86-1					174.6	730.5	182.4	763.	
	334	J	(0.0)	174.6					81BOH/STO
[$C_2ClH_3O_2$] $CH_2ClCOOH$ RN 79-11-8					174.6	730.5	182.4	763.	
	600	A	(-19.4)	175.7					76YAM/KEB
		N		174.6					
[C_3H_4] CH_3CCH RN 74-99-7					174*	728*	182*	761*	
				174*					76AUE/DAV
[CH_4O] CH_3OH RN 67-56-1					174.1	728.	181.9	761.	
	320	A	(-20.6)	175.0					77WOL/STA-83TAF
	320	L		173.7					
	340	H	(-12.9)	174.4					80LIA/SHO
	600	A	(-19.7)	175.4					79LAU
	600	N		174.3					
[$C_6F_2H_4$] 1,2-Difluorobenzene RN 367-11-3					174.4	729.7	181.8	761.	
	400	J	(-0.4)	174.4					78HAR/LIA
[C_6ClH_5] Chlorobenzene RN 108-90-7					174.4	730.	181.7	760.	
	334	J	(-0.2)	174.4					81BOH/STO
	400	J	(-0.5)	174.3					78HAR/LIA
	600	J	(-1.0)	174.1					76LAU/KEB
	600	A	(-19.4)	175.7					79LAU
	600	N		174.6					
[$C_6F_2H_4$] 1,3-Difluorobenzene RN 372-18-9					174.1	728.	181.5	759.	
	400	J	(-0.3)	174.5					78HAR/LIA
	600	A	(-20.3)	175.3					76YAM/KEB
		N		173.7					
[$C_6F_3H_3$] 1,2,4-$C_6H_3F_3$ RN 367-23-7					173.6	726.	181.4	759.	
	400	J	(-1.2)	173.6					78HAR/LIA
[C_6H_6] Benzene RN 71-43-2					174.6	730.5	181.3	758.5	
	320	J	(0.0)		174.6	730.5			76DEV/WOL
	334	J	(0.0)		174.6	730.5			81BOH/STO
	400	J	(0.0)		174.8	731.4			78HAR/LIA
	600	J	(0.0)		175.6	734.7			76LAU/KEB
	320	A	(-20.3)	175.3					77WOL/STA
	320	H		176.0					
	340	H	(-12.1)	175.2					80LIA/SHO
	550	A	(-18.9)	176.7					80MAU
	600	A	(-18.4)	177.2					78LAU/SAL
	600	N		175.6					

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[$C_6F_2H_4$] 1,4-$C_6H_4F_2$ RN 540-36-3					173.8	727.	181.2	758.	
	400	J	(-1.0)	173.8					78HAR/LIA
[$C_6F_4H_2$] 1,2,3,4-$C_6H_2F_4$ RN 551-62-2					173.3	725.	181.1	758.	
	400	J	(-1.5)	173.3					78HAR/LIA
[$C_6F_3H_3$] 1,3,5-$C_6H_3F_3$ RN 372-38-3					173.7	727.	181.	757.	
	400	J	(-0.7)	174.1					78HAR/LIA
	600	A	(-20.7)	174.4					79LAU
	600	N		173.3					
[C_2H_3] C_2H_3 radical RN 2669-89-8					~172	~720	~181	~757	
		(br)		~172					80DEF/MCI
[$C_6F_4H_2$] 1,2,3,5-$C_6H_2F_4$ RN 2367-82-0					173.2	725.	180.6	756.	
	400	J	(-1.6)	173.2					78HAR/LIA
[C_4NiO_4] $(CO)_4Ni$ RN 13463-39-3							180**	753**	
	320	A	(-24.5)						81STE/BEA
[C_6CrO_6] $(CO)_6Cr$ RN 13007-92-6							180**	753**	
	320	A	(-24.8)						81STE/BEA
[C_6F_5H] C_6HF_5 RN 363-72-4					172.5	722.	179.9	753.	
	400	J	(-2.3)	172.5					78HAR/LIA
[C_3H_6] c-C_3H_6 RN 75-19-4					172.0	720.	179.8	752.	
	340	(Key)		173.7					72CHO/FRA
[$C_6F_4H_2$] 1,2,4,5-$C_6H_2F_4$ RN 327-54-8					173.0	724.	179.7	752.	
	400	J	(-1.8)	173.0					78HAR/LIA
[C_3H_6] $CH_3CH=CH_2$ RN 115-07-1					171.7	718.	179.5	751.	
	Threshold Value			171.7			179.5		82ROS/BUF
	340	H	(-14.0)	173.3					80LIA/SHO
	340	AA	(0.0)	171.7					
	340	(Key)		173.4					72CHO/FRA
	600	A	(-20.7)	174.9					76YAM/KEB
	600	N		173.3					
[$C_4H_5NO_2$] $NCCOOC_2H_5$ RN 623-49-4					171.7	718	179.5	751.	
	320	A	(-22.0)	174.6					77WOL/STA
	320	L		171.7					
[C_2ClH_2N] $ClCH_2CN$ RN 107-14-2					171.7	718.	179.5	751.	
	320	A	(-22.0)	174.6					77WOL/STA
	320	L		171.7					
[C_4H_8] (E)-$CH_3CH=CHCH_3$ RN 624-64-6					171.6	718.	179.4	751.	
	Threshold Value								81TRA
	340	H	(-14.1)	173.2					80LIA/SHO
	340	AA		171.6					

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[$C_3F_3H_3O_2$] $HCOOCH_2CF_3$ RN 32042-38-9					171.6	718.	179.4	751.	
	320	A	(-22.1)	174.5					77WOL/STA
	320	L		171.6					
[CH_3NO_2] CH_3NO_2 RN 75-52-5					171.7	718.	179.2	750.	
	298	(Key)		172.1					78MAC/BOH
	340	H	(-14.1)	173.2					80LIA/SHO
	340	AA		171.4					
		(Key)		~173					76MCA/PIT
[AsH_3] AsH_3 RN 7784-42-1					170.8	715.	179.2	750.	
	320	A	(-22.8)	173.8					77WOL/STA
	320	L		170.8					
	340	H	(-15.1)	172.2					80LIA/SHO
	340	AA		170.8					
[$C_3F_3H_3O_2$] CF_3COOCH_3 RN 431-47-0					171.0	715.	178.8	748.	
	320	A	(-22.6)	174.0					77WOL/STA
	320	L		171.0					
[CH_2O_2] HCOOH RN 64-18-6					170.4	713.	178.8	748.	
	320	A	(-23.2)	173.4					78WOL/STA
	320	L		170.4					
	340	H	(-15.4)	171.9					80LIA/SHO
	340	AA		170.3					
	600	A	(-23.6)	172.0					79LAU
	600	N		170.4					
[$C_4F_4H_4O_2$] $CF_3COOCH_2CH_2F$ RN 1683-88-1					170.8	715.	178.6	747.	
	320	A	(-22.8)	173.8					77WOL/STA
	320	L		170.8					
[BrCN] BrCN RN 506-68-3					170.5	713.	178.3	746.	
	320	A	(-23.1)	173.5					76STA/KLE
	320	L		170.5					
[C_6F_6] C_6F_6 RN 392-56-3					171.3	717.	177.7	743.	
	400	J	(-3.5)	171.3					78HAR/LIA
[$C_2Cl_3H_3O$] Cl_3CCH_2OH RN 115-20-8					169.6	710.	177.4	742.	
	320	A	(-24.0)	172.6					77WOL/STA
	320	L		169.6					
[$C_2F_2H_4O$] CF_2HCH_2OH RN 359-13-7					168.4	704.5	176.2	737.	
	320	A	(-25.2)	171.3					77WOL/STA
	320	L		168.4					
[$C_2F_2H_2$] CH_2CF_2 RN 75-38-7					168	703	176	736	
		(br)		~172					75RID
		(Key)		168					76WIL/LEB
[C_2H_5I] C_2H_5I RN 75-03-6					~168	~703	~176	~736	
		(br)	~168						72BEA/HOL

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	kJ/mol	Proton affinity kcal/mol	kJ/mol	Reference
$[C_2Cl_3N]$ CCl_3CN RN 545-06-2				168.0	703.	175.8	735.5	
320	A	(-25.6)	171.0					77WOL/STA
320	L		168.0					
$[C_3H_3]$ c-C_3H_3 radical RN xxxxx				168.7	706.	175.8	735.	
	(br)		168.7					80DEF/MCI
$[C_3H_5]$ CH_2=$CHCH_2$ radical RN xxxxx				168.7	706.	175.8	735.	
	(br)		168.7					80DEF/MCI
[CClN] ClCN RN 506-77-4				167.9	702.	175.7	735.	
320	A	(-25.7)	170.9					76STA/KLE
320	L		167.9					
$[C_3H_2N_2]$ $CH_2(CN)_2$ RN 109-77-3				167.4	700.	175.6	735.	
298	L	(0.0)	167.4					81DOI/MCM
298	L	(0.0)	167.4					82DRU/MCM
320	A	(-25.8)	170.8					77WOL/STA
320	L		167.4					
600	A	(-26.1)	169.0					79LAU
600	N		167.9					
$[C_2FH_3]$ C_2H_3F RN 75-02-5				167.	699.	175.	732.	
	(br)		~163					75RID
	(Key)		167.					76WIL/LEB
[CS] CS RN 2944-05-0				167	699	175	732	
	(br)		167					78MCA
$[C_3F_3H_3O]$ CH_3COCF_3 RN 421-50-1				166.4	696.	174.2	729.	
298	L	(-0.6)	166.8					81DOI/MCM
298	L	(-1.0)	166.4					82DRU/MCM
[CHNO] HNCO RN 75-13-8				165.5	692.	173.3	725.	
320	M	(+1.2)	165.5					80WIG/BEA
$[CF_2]$ CF_2 RN 2154-59-8				164.0	686.	171.9	719.	
	(br)		164.0					77LIA/AUS
$[CH_2O]$ H_2CO RN 50-00-0				164.3	687.	171.7	718.	
320	M	(0.0)	164.3					80WIG/BEA
298	N	(5.2)	164.2					78TAN/MAC
300	Y	(1.2)	160.2					78FRE/HAR
320	A	(-28.3)	168.3					77WOL/STA
320	N		164.3					
[CHN] HCN RN 74-90-8				163.8	685.	171.4	717.	
298	N	(4.9)	163.9					78TAN/MAC
320	A	(-28.8)	167.7					77WOL/STA
320	N		163.8					
340	Y	(1.0)	163.8					78FRE/HAR(2)

Table 1. Gas phase basicities and proton affinities--Continued

T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[H_2Se] H_2Se RN 7783-07-5				163.8	685.	171.3	717.	
320	A	(-28.8)	167.7					77WOL/STA
320	N		163.8					
			169.4**					79AUE/BOW
[CH_3I] CH_3I RN 74-88-4				~163	682	~171	~715	
	(br)		~163					72BEA/HOL
[C_2BrH_5] C_2H_5Br RN 74-96-4				~163	~682	~171	~715	
	(br)		~163					72BEA/HOL
[H_2S] H_2S RN 7783-06-4				162.8	681.	170.2	712.	
340	Y	(0.0)	162.8					78FRE/HAR(2)
296	N	(4.6)	163.6					73HOP/BON
298	N	(3.8)	162.8					78TAN/MAC
320	A	(-29.6)	167.0					77WOL/STA
320	N		162.9					
550	N	(3.9)	162.7					77MAU/FIE
600	A	(-31.8)	163.8					79LAU
600	N		162.2					
Threshold Value						168.4	705.	83PRE/TZE
[$C_3F_4H_2O$] CF_2HCOCF_2H RN 360-52-1				162.	678.	170.	711.	
	(br)		162.					82DRU/MCM
[CF_3NO] CF_3NO RN 334-99-6				161	674	169	707	
	(br)		161.					79FRE/HAR
[H_2O_4S] H_2SO_4 RN 7664-93-9				~161	~674.	~169	~707	
	(br)		~161					78SMI/MUN
[CF_3HO_3S] CF_3SO_3H RN 1493-13-6				~161	~674	~169	~707	
	(br)		~161					78SMI/MUN
[$C_2F_3H_3O$] CF_3CH_2OH RN 75-89-8				161.2	674.	169.0	707.	
298	K	(5.6)	161.2					83COL/MCM
320	A	(-31.2)	165.4					77WOL/STA
	N		161.3					
600	A	(-32.7)	162.9					79LAU
	N		161.2					
[C_2F_3H] C_2F_3H RN 359-11-5				~161	~674	~169	~707	
	(br)		~161					75RID
[C_6H_{12}] c-C_6H_{12} RN 110-82-7				~161	~674	~169	~707	
	(br)		~161					82AUS/REB
[$C_2F_3HO_2$] CF_3COOH RN 76-05-1				161.1	674.	169.0	707.	
298	(Key)		161.0					82DRU/MCM
320	A	(-30.5)	165.4					77WOL/STA
	N		162.0					
600	A	(-32.9)	162.7					79LAU
	N		161.1					

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[B_5H_9]$ B_5H_9 RN 19624-22-7					161.	674.	169.	707.	
		(br)		161.					72SOL/POR
$[C_2ClH_5]$ C_2H_5Cl RN 75-00-3					161.	674.	169.	707.	
		(br)		161.					72BEA/HOL
$[B_5C_2H_7]$ 2,4-$C_2B_5H_7$ RN 20693-69-0					160.	669.	168.	703.	
		(br)		160.					80DIX
$[F_3OP]$ OPF_3 RN 13478-20-1					160.0	669.	167.8	702.	
	298	K	(4.4)	160.0					83COL/MCM
$[C_4F_7N]$ C_3F_7CN RN 375-00-8					159.6	668.	167.4	700.	
	298	K	(4.0)	159.6					83COL/MCM
$[CS_2]$ CS_2 RN 75-15-0					160.7	672.	167.1	699.	
	550	N	(1.9)	160.7					77MAU/FIE
$[C_3F_5N]$ C_2F_5CN RN 422-04-8					159.3	666.5	167.1	699.	
	298	K	(3.7)	159.3					83COL/MCM
$[C_4F_6H_4O]$ $(CF_3)_2C(CH_3)OH$ RN 1515-14-6					159.2	666.	167.0	699.	
	298	K	(3.6)	159.2					83COL/MCM
$[H_2O]$ H_2O RN 7732-18-5					159.0	665.	166.5	697.	
	298	K	(3.4)	159.0					83COL/MCM
	298	K	(1.8)	157.4					81BOH/MAC
	320	A	(-33.5)	163.1					77WOL/STA
	320	N	(0.0)	159.0					
	600	A	(-34.7)	160.9					79LAU
		N	(0.0)	159.3					
	296	N	(0.0)	159.0					73HOP/BON
	298	N	(0.0)	159.0					78TAN/MAC
	550	N	(0.0)	159.3					77MAU/FIE
	Threshold Value			160.3			167.8		77NG/TRE
	Threshold Value			157.4			164.9		69HAN/FRA
$[C_2F_3N]$ CF_3CN RN 353-85-5					158.4	663.	166.1	695.	
	298	K	(2.8)	158.4					83COL/MCM
	320	A	(-37.1)	158.5					78COR/BEA
$[C_2F_2H_2]$ (E)-CHFCHF RN 1630-78-0					158	661	166	694	
		(br)		158					75RID
$[BrCH_3]$ CH_3Br RN 74-83-9					157.9	661.	165.7	693.	
		(br)		157.					72BEA/HOL
	298	K	(2.3)	157.9					83COL/MCM
$[C_2F_3HO]$ CF_3CHO RN 75-90-1					157.3	658.	165.1	691.	
	298	K	(1.6)	157.2					83COL/MCM
	320	A	(-38.2)	157.4					78COR/BEA

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[C_2FH_5] C_2H_5F RN 353-36-6					157.	657.	165.	690.	
		(br)		157.					72BEA/HOL
[$C_3F_6H_2O$] $(CF_3)_2CHOH$ RN 920-66-1					157.2	658	165.0	690.	
	298	K	(1.6)	157.2					83COL/MCM
[C_4H_{10}] iso-C_4H_{10} RN 75-28-5					155.5	651.	163.3	683.	
	100	(Key)		156.0			163.8		76HIR/KEB
		(Key)		162.7			162.7		78HIR
[F_3P] PF_3 RN 7783-55-3					154.9	648.	163.3	683.	
	298	K	(3.1)	158.7					83COL/MCM
		(br)		154.9					80DOI/MCM
		(br)		155.2					78COR/BEA-72BEA/HOL
[C_4F_9HO] $(CF_3)_3COH$ RN 2378-02-1					155.3	650.	163.1	682.	
	298	K	(-0.3)	155.3					83COL/MCM
[$CClH_3$] CH_3Cl RN 74-87-3					155	648	163	682	
	320	(Key)		155					78COR/BEA
		(br)		152					72BEA/HOL
[C_2H_4] C_2H_4 RN 74-85-1					155.6	651.	162.6	680.	
	298	K	(0.0)	155.6					81DOI/MCM
	298	K	(0.0)	155.6					83COL/MCM
	298	K	(0.0)	155.6					81BOH/MAC
	Threshold Value			155.6			162.6		81TRA/MCL
[C_2N_2] NCCN RN xxxxx					155.	648.	162.	679.	
		(br)		155.					84RAK/BOH
[H_2O_2] H_2O_2 RN 7722-84-1							162.	678.	
		(br)							75LIN/ALB
[O_2S] SO_2 RN 7446-09-5					154.2	645.	161.6	676.	
	298	K	(-~2)	153.6					81DOI/MCM
			(-1.4)	154.2					83COL/MCM
[C_3F_6O] $(CF_3)_2CO$ RN 684-16-2					153.4	642.	161.5	676.	
	298	K	(-2.7)	152.9					81DOI/MCM
	298		(-2.2)	153.4					83COL/MCM
	298	(Key)		153.4					82DRU/MCM
	320	A	(-39.3)	156.3					78COR/BEA
[CF_2O] F_2CO RN 353-50-4					152.9	640.	160.5	671.5	
	298	K	(-3.2)	152.4					81DOI/MCM
	298	K	(-2.7)	152.9					83COL/MCM
[C_2F_4O] CF_3CFO RN 354-34-7					152.4	638.	160.2	670.	
	298	K	(-3.6)	152.0					81DOI/MCM
	298	K	(-3.2)	152.4					83COL/MCM
[C_3H_7] i-C_3H_7 RN 19252-53-0							159.8	669.	
	Threshold Value								79HOU/BEA

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
$[F_2O_2S]$ F_2SO_2 RN 2699-79-8					151.6	634.	159.0	665.	
	298	K	(-3.8)	151.6					81DOI/MCM
	298	K	(-3.6)	152.0					80DOI/MCM
[S] S RN 7704-34-9					152.3	637.	158.3	662.	
	Threshold Value			152.3			158.3	662.	81SMI/ADA
$[HO_2]$ HO_2 RN 3170-83-0							~158.	~661.	
	Threshold Value								75BRO
[Zn] Zn RN 7440-66-6							156	653	
		(br)							78PO/RAD
$[H_4Si]$ SiH_4 RN 7803-62-5					~147	~615	~155	~648	
		(br)		~147					73CHE/LAM
$[AsF_3]$ AsF_3 RN 7784-35-2					147.	615.	155.	648.	
		(br)		147					80DOI/MCM
$[C_2H_2]$ C_2H_2 RN 74-86-2					146.1	611.	153.3	641.	
	Threshold Value			146.1					84LIA/LIE
[CHO] HCO RN 17030-74-9							152.	636.	
	Threshold Value						152.		74WAR
[COS] COS RN 463-58-1					143.	598.	151.	632.	
		(br)		143					81SMI/ADA
[HI] HI RN 10034-85-2					143.	598.	150.	628.	
		(br)		143					78POL/MUN
$[C_3H_8]$ C_3H_8 RN 74-98-6					142.	594.	150.	628.	
		(Key)		142					76HIR/KEB-75HIR/KEB
$[CFH_3]$ CH_3F RN 593-53-3					142.	594.	150.	628.	
		(br)		142					72BEA/HOL
$[CF_2H_2]$ CH_2F_2 RN 75-10-5					139.	581.5	147.	615.	
		(br)		139.					74BLI/MCM
$[CF_3H]$ CHF_3 RN 75-46-7					139.	581.5	147.	615.	
		(br)		139.					74BLI/MCM
$[B_2H_6]$ B_2H_6 RN 19287-45-7							~146	~611	
		(br)							73PIE/POR
[I] I RN 14362-44-8					140.4	587.	145.4	608.	
	Threshold Value			140.4					78POL/MUN
$[F_3N]$ NF_3 RN 7783-54-2					136	569	144	604	
		(br)		136					80DOI/MCM

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity	Gas basicity	Selected gas basicity		Proton affinity		Reference
			kcal/mol	kcal/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	
$[B_4H_{10}]$ B_4H_{10} RN 18283-93-7							~144	~602	
		(Key)							73PIE/POR
$[C_2H_6]$ C_2H_6 RN 74-84-0					135.8	568.	143.6	601.	
	298	O	(22.3)	133.0					81MAC/SCH
	298	Z	(1.4)	135.8					81BOH/MAC
	~200	(Key)		133.5A					76HIR/KEB
	~400	(Key)		141.3B					76HIR/KEB
[CO] CO RN 630-08-0					134.4	562.	141.9	593.	
	298	Z	(0.0)	134.4					81BOH/MAC
	298	Z	(0.0)	134.4					73HEM/RUN
	Threshold Value			136.7			144.4		76GUY/CHU
	Threshold Value			134.3			141.9		80DYK/JON
	Threshold Value			134.5			142.1		69MAT/WAR
	298	O	(20.9)	131.6					80BOH/MAC
	298	S	(11.0)	135.4					
$[O_3S]$ SO_3 RN 7446-11-9					~130	~544	~138	~577	
		(br)		~131					77MUN/SMI
$[N_2O]$ N_2O RN 10024-97-2					131.4	550.	136.5	571.	
	298	O	(18.0)	128.7					80BOH/MAC
	298	S	(8.1)	132.5					
	298	Z	(-3.0)	131.4					73HEM/RUN
[BrH] HBr RN 10035-10-6					131	548	136	569	
		(br)		131					78POL/MUN
	Threshold Value						132.9		79TIE/AND
[ClH] HCl RN 7647-01-0					127.	531.	134.8	564.	
	Threshold Value			127.					79TIE/AND
		(br)		129					78POL/MUN
		(Key)		>124					74FEH/FER
[Br] Br RN 10097-32-2					126.4	529.	132.0	552.	
	Threshold Value			126.4					78POL/MUN
$[CH_4]$ CH_4 RN 74-82-8					126.0	527.	132.0	552.	
	298	O	(11.8)	122.5					80BOH/MAC
	320	S	(2.1)	126.5					75STA/BEA
	340	S	(1.4)	125.8					75KAS/FRA
	340	S	(1.7)	126.1					LIA/AUS
	550	S	(1.3)	126.7					77MAU/FIE
	300	S	(1.5)	125.9					73HEM/RUN
	300	S	(1.9)	126.3					73BOH/HEM
	Threshold Value			120.5			126.5		71CHU/BER
$[CO_2]$ CO_2 RN 124-38-9					124.4	520.	130.9	548.	
	Threshold Value			124.4			130.9		74WAR
	798	S	(0.0)	126.7					76FEH/LIN
	320	S	(0.0)	124.4					75STA/BEA
	340	S	(0.0)	124.4					75KAS/FRA
	550	S	(0.0)	125.4					77MAU/FIE
	298	S	(0.0)	124.4					73HEM/RUN
	298	S	(0.0)	124.4					73BOH/HEM
	298	S	(0.0)	124.4					76MEI/MIT
	298	O	(+9.9)	120.8					80BOH/MAC

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity kcal/mol	Selected gas basicity kJ/mol	Proton affinity kcal/mol	Proton affinity kJ/mol	Reference
[NO] NO RN 10102-43-9					~119	~498	~127	~531	
		(br)		~119					71ROC/SUT
[CF_4] CF_4 RN 75-73-0					~119	~498	~126	~527	
		(br)		~119					71ROC/SUT
[Cl] Cl RN 22537-15-1					116.8	489.	123.0	515.	
	Threshold Value			116.8					78POL/MUN
[Xe] Xe RN 7440-63-3					113.4	474.	118.6	496.	
	298	O	(+2.7)	113.4					80BOH/MAC-76FEH/LIN
	298	S	(-7.2)	117.2					
[N_2] N_2 RN 7727-37-9					111.0	464.	118.2	494.5	
	298	O	(0.3)	111.0					80BOH/MAC-76FEH/LIN
		S	(-9.6)	114.8					
	Threshold Value						118.1		79WIB/FIS
	Threshold Value						114.3		78FON/HUD
	Threshold Value						112.2		76WIL/LOS
[O] O RN 17778-80-2					110.7	463.	116.3	487.	
	298	O	(0.0)	110.7					80BOH/MAC
	Threshold Value						116.3		76MCC
[Kr] Kr RN 7439-90-9					96.1	402.	101.6	425.	
	298	O	(-10.3)	100.4					80BOH/MAC
		O'	(+1.1)	96.1					
		BB	(+1.7)	96.4					75PAY/SCH
	Threshold Value						100.3		79HUB/HER
[H_2] H_2 RN 1333-74-0					94.6	396.	101.3	424.	
	298	O	(-11.8)	98.9					80BOH/MAC-73FEN/HEM
		O'	(-0.4)	94.6					
		O'	(-0.3)	94.7					75FEH/LIN
	296	BB	(0.0)	94.7					75PAY/SCH
		(Key)					101.		78PO/RAD
	Threshold Value			94.7			101.3		72COT/ROZ
[O_2] O_2 RN 7782-44-7					95.0	397.	100.9	422.	
	298	O	(-11.4)	99.3					80BOH/MAC-73FEN/HEM
		O'	(0.0)	95.0					
		O'	(0.0)	95.0					75FEH/LIN
	Threshold Value			94.6			100.5		81DYK/JON
	Threshold Value			95.0			100.9		77MCC
[FH] HF RN 7664-39-3									
	Threshold Value			87.3			95		79TIE/AND
	320	(Key)		109.4			117		75FOS/BEA
[F] F RN 14762-94-8					75.4	315.	81.0	339.	
	Threshold Value			75.4					
[Ar] Ar RN 7440-37-1							88.6	371.	
	Threshold Value						>61	>255	79HUB/HER
		BB					88.6	371.	82VIL/FUT

Table 1. Gas phase basicities and proton affinities--Continued

	T K	Reference base	Relative gas basicity kcal/mol	Gas basicity kcal/mol	Selected gas basicity		Proton affinity		Reference
					kcal/mol	kJ/mol	kcal/mol	kJ/mol	
[Ne] Ne		RN 7440-01-9					48.1	201.	
		Threshold Value					48.1		68CHU/RUS
		Threshold Value					48.0		79HUB/HER
[He] He		RN 7440-59-7					42.5	178.	
		Threshold Value					42.5		79HUB/HER

Annotated References to Table 1

81ALD/ARR R. W. Alder, R. J. Arrowsmith, A. Casson, R. B. Sessions, E. Heilbronner, B. Kovac, H. Huber, and M. Taagepera, "Proton Affinities and Ionization Energies of Bicyclic Amines and Diamines. The Effects of Ring Strain and of 3-Electron Sigma Bonding", J. Am. Chem. Soc. **103**, 6137 (1981).

ICR. Data related to TAFT scale corrected to 320 K.

80ARM/HIG M. A. Armitage, M. J. Higgins, E. G. Lewars, and R. E. March, "Methylketene. Ion Chemistry and Proton Affinity", J. Am. Chem. Soc. **102**, 5064 (1980).

Time-resolved quadrupole ion store (quistor)

75ARN E. M. Arnett, "Proton Transfer and the Solvation of Ammonium Ions", in *Proton Transfer Reactions*, E. F. Caldin and V. Gold, Editors, pp.79-101, Chapman and Hall, London (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.

72ARN/JON E. M. Arnett, F. M. Jones, III, M. Taagepera, W. G. Henderson, J. L. Beauchamp, D. Holtz, and R. W. Taft, "A Complete Thermodynamic Analysis of the 'Anomalous Order' of Amine Basicities in Solution", J. Am. Chem. Soc. **94**, 4724 (1972).

ICR. Data corrected from originally-reported temperature of 300 K to 320 K.

79AUE/BET D. H. Aue, L. D. Betowski, W. R. Davidson, M. T. Bowers, P. Beak, and J. Lee, "Gas-Phase Basicities of Amides and Imidates. Estimation of Protomeric Equilibrium Constants by the Basicity Method in the Gas Phase", J. Am. Chem. Soc. **101**, 1361 (1979).

ICR. Data relative to CH_3NH_2.

79AUE/BOW D. H. Aue, and M. T. Bowers in "Gas Phase Ion Chemistry" (M. T. Bowers, editor), 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 from earlier Aue et al papers, re-evaluated in 79AUE/BOW.

**Unpublished data from laboratory of authors

76AUE/DAV D. H. Aue, W. R. Davidson, and M. T. Bowers, "Heats of Formation of $C_3H_5^+$ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas Phase Proton Transfer Reactions", J. Am. Chem. Soc. **98**, 6700 (1976).

ICR.

72AUE/WEB D. H. Aue, H. M. Webb, and M. T. Bowers, "Quantitative Relative Gas Phase Basicities of Alkylamines. Correlations with Solution Basicity", J. Am. Chem. Soc. **94**, 4726 (1972).

ICR.

73AUE/WEB D. H. Aue, H. M. Webb, and M. T. Bowers, "Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase", J. Am. Chem. Soc. **95**, 2699 (1973).

ICR.

75AUE/WEB D. H. Aue, H. M. Webb, and M. T. Bowers, "Photoelectron Spectrum and Gas-Phase Basicity of Manxine. Evidence for a Planar Bridgehead Nitrogen", J. Am. Chem. Soc. **97**, 4136 (1975).

ICR.

75AUE/WEB(2) D. H. Aue, H. M. Webb, and M. T. Bowers, "Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects", J. Am. Chem. Soc. **97**, 4137 (1975).

ICR. Data relative to $(CH_3)NH_2$ included here; other data relative to CH_3CHO omitted because the "semiquantitative" values have been superseded by more recent equilibrium measurements.

76AUE/WEB D. H. Aue, H. M. Webb, and M. T. Bowers, "Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines", J. Am. Chem. Soc. **98**, 311 (1976).

ICR.

76AUE/WEB(2) D. H. Aue, H. M. Webb, M. T. Bowers, C. L. Liotta, C. J. Alexander, and H. P. Hopkins, Jr., "A Quantitative Comparison of Gas- and Solution Phase Basicities of Substituted Pyridines", J. Am. Chem. Soc. **98**, 854 (1976).

ICR. Data given in graphic form, difficult to read: Values cited are from 79AUE/BOW review.

80AUE/WEB D. H. Aue, H. M. Webb, W. R. Davidson, M. Vidal, M. T. Bowers, H. Goldwhite, L. E. Vertal, J. E. Douglas, P. A. Kollman, and G. L. Kenyon, "Proton Affinities and Photoelectron Spectra of Three Membered Ring Heterocycles", J. Am. Chem. Soc. **102**, 5151 (1980).

Aziridine: Related to earlier results from Aue et al, which were related to NH_3

Oxirane: Related to CH_3CN, C_2H_5OH. Gas basicity values chosen by authors appeared to be associated with a contracted scale. Results cited related to basicity values of 80LIA/SHO.

Thiirane: Related to CH_3COOCH_3, i-C_4H_8, HCOO(n-C_4H_9). Results cited related to gas basicity values of 80LIA/SHO.

Phosphirane: Related to HCOO(n-C_3H_7), $(CH_3)_2O$, Dioxane. Results cited related to corrected TAFT scale and 80LIA/SHO.

ICR.

77AUS/LIA P. Ausloos and S. G. Lias, "Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes", J. Am. Chem. Soc. **99**, 4198 (1977).

ICR. Toluene relative to propionaldehyde and methyl formate.

78AUS/LIA P. Ausloos and S. G. Lias, "Entropy Changes for the Protonation of Alkenes", J. Am. Chem. Soc. **100**, 1953 (1978).

ICR. Entropy changes determined.

78AUS/LIA(2) P. Ausloos and S. G. Lias, "Proton Affinity of Dichlorocarbene", J. Am. Chem. Soc. **100**, 4594 (1978).

ICR. Bracketing: $CCl_2 \leq C_2H_5OC_2H_5$

AUS/LIA P. Ausloos and S. G. Lias, unpublished results.

ICR. Bracketing: $CH_3CHO < CH_2{=}C{=}CH_2 < CH_3SH$

83AUS/LUT P. Ausloos, C. Lutz, F. Schwarz, and S. G. Lias, "Radiation-Induced Ionization and Excitation in Liquid p-Dioxane," 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 1 kcal/mol of that of p-dioxane.

82AUS/REB P. Ausloos, R. E. Rebbert, F. P. Schwarz, and S. G. Lias, "Pulse- and Gamma Radiolysis of Cyclohexane: Ion Recombination Mechanisms", Radiat. Phys. Chem. **19**, 27 (1982).

ICR. Bracketing: $H_2O < c\text{-}C_6H_{12} < H_2S$.

72BEA/HOL J. L. Beauchamp, D. Holtz, S. D. Woodgate, and S. L. Patt, "Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy", J. Am. Chem. Soc. **94**, 2798 (1972).

ICR. Bracketing:

$H_2S < C_2H_5I < C_3H_6$
$CH_3I \sim C_2H_5Br \sim H_2S$
$H_2O < C_2H_5Cl < H_2S$
$C_2H_4 < CH_3Br \sim C_2H_5F < H_2O$
$C_2H_2 < CH_3Cl < C_2H_4$
$CO < CH_3F < C_2H_2$

74BLI/MCM R. J. Blint, T. B. McMahon, and J. L. Beauchamp, "Gas Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities", J. Am. Chem. Soc. **96**, 1269 (1974).

ICR. Bracketing:
$C_2H_2 > CH_3F > CH_2F_2 = CHF_3 > CO > HCl > CH_4 > CF_4 > N_2$

73BOH/HEM D. K. Bohme, R. S. Hemsworth, H. W. Rundle, and H. I. Schiff, "Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. II. Kinetic Analysis of the Approach to the Attainment of Equilibrium", J. Chem. Phys. **58**, 3504 (1973).

Flowing afterglow. Equilibrium constant determinations through measurements of forward and reverse rate constants.

80BOH/MAC D. K. Bohme, G. I. Mackay, and H. I. Schiff, "Determination of Proton Affinities from the Kinetics of Proton Transfer Reactions. VII. The Proton Affinities of O_2, H_2, Kr, O, N_2, Xe, CO_2, CH_4, N_2O, and CO", J. Chem. Phys. **73**, 4976 (1980).

Flowing afterglow. Values first reported in 75SCH/BOH.

81BOH/MAC D. K. Bohme and G. I. Mackay, "Gas Phase Proton Affinities for H_2O, C_2H_4, and C_2H_6", J. Am. Chem. Soc. **103**, 2173 (1981).

Flowing afterglow.

81BOH/STO D. K. Bohme, J. A. Stone, R. S. Mason, R. S. Stradling, and K. R. Jennings, "A Determination of Proton-Transfer Equilibrium Constants in Benzene/Halobenzene Mixtures at Various Temperatures Using a High Pressure Ion Source", Int. J. Mass Spectrom. Ion Phys. **37**, 283 (1981).

High pressure mass spectrometer. Entropy change determinations made.

71BOW/AUE M. T. Bowers, D. H. Aue, H. M. Webb, and R. T. McIver, "Equilibrium Constants for Gas Phase Ionic Reactions. Accurate Determination of Relative Proton Affinity," J. Am. Chem. Soc. **93**, 4314 (1971).

ICR.

72BRI/YAM J. P. Briggs, R. Yamdagni, and P. Kebarle, "Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton-Exchange Equilibria", J. Am. Chem. Soc. **94**, 5128 (1972).

High pressure mass spectrometer.

81BRO/ABB J. Bromilow, J. L. M. Abboud, C. B. Lebrilla, R. W. Taft, G. Scorrano, and V. Lucchini, "Oxonium Ions. Solvation by Single Acetonitrile Molecules in the Gas Phase and by Bulk Solvents", J. Am. Chem. Soc. **103**, 5448 (1981).

ICR. Values of ΔG 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).

83CAS/FRE C. J. Cassady, B. S. Freiser, and D. H. Russell, "Structural Determination of $[C_7H_7O]^+$ Ions in the Gas Phase by Ion Cyclotron Resonance Spectrometry", Org. Mass Spectrom. **18**, 378 (1983).

79CEY/TIE S. T. Ceyer, P. W. Tiedemann, B. H. Mahan, and Y. T. Lee, "Energetics of Gas Phase Proton Solvation by NH_3", J. Chem. Phys. **70**, 14 (1979).

Absolute determination of the proton affinity of NH_3 from appearance potential of NH_4^+ from $(NH_3)_2$; entropy change of the half reaction ($NH_3 \rightarrow NH_4^+$) taken as -1.8 cal/mol K.

73CHE/LAM T. M. H. Cheng and F. W. Lampe, "SiH_5^+ and the Proton Affinity of Monosilane", Chem. Phys. Lett. **19**, 532 (1973).

Bracketing: C_2H_2, $C_2H_5 < SiH_4 < C_3H_7$

72CHO/FRA S.-L. Chong and J. L. Franklin, "Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane", J. Am. Chem. Soc. **94**, 6347 (1972).

High pressure mass spectrometer; equilibria relative to CH_3OH.

72CHO/FRA(2) S.-L. Chong and J. L. Franklin, "Proton Affinities of Benzene, Toluene, and the Xylenes", J. Chem. Soc. **94**, 6630 (1972).

High pressure mass spectrometer; equilibria relative to $(CH_3)_2O$.

71CHU/BER W. A. Chupka and J. Berkowitz, "Photoionization of Methane: Ionization Potential and Proton Affinity of CH_4", J. Chem. Phys. **54**, 4256 (1971).

Threshold for photoionization efficiency curve of CH_5^+ in methane.

83COL/MCM S. M. Collyer and T. B. McMahon, "The Proton Affinity of Water. A Scale of Gas Phase Basicities Including Ethylene and Water from Ion Cyclotron Resonance Proton Transfer Equilibria Measurements", 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 M. J. Cook, A. R. Katrisky, M. Taagepera, T. D. Singh, and R. W. Taft, "Application of Ion Cyclotron Resonance Spectroscopic Gas Phase Basicities to the Study of Tautomeric Equilibria" J. Am. Chem. Soc. **98**, 6048 (1976).

ICR. Data related to TAFT scale, corrected to 320 K.

77COO/KRU R. G. Cooks and T. L. Kruger, "Intrinsic Basicity Determination Using Metastable Ions", J. Am. Chem. Soc. **99**, 1279 (1977).

Dissociation of proton bound dimers indicates $C_4H_9NH_2 < C_5H_{11}NH_2$; $C_6H_5NH_2 < 3\text{-}CH_3C_6H_4NH_2$; $n\text{-}C_4H_9NH_2 < c\text{-}C_5H_5N$: Results not included.

76COR/BEA R. R. Corderman and J. L. Beauchamp, "Ion Chemistry and Gas Phase Basicity of Nickelocene by Ion Cyclotron Resonance Spectroscopy", Inorg. Chem. **15**, 665 (1976).

ICR. Data relative to $(CH_3)_3N$ and $(C_2H_5)_2NH$; both related to TAFT scale, $T = 320$ assumed.

78COR/BEA R. R. Corderman and J. L. Beauchamp, "Properties of Phosphorus Trifluoride in the Gas Phase by Ion Cyclotron Resonance Spectroscopy. Energetics of Formation of PF_2^+, PF_4^+, HPF_3^+, and $CH_3PF_3^+$", 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 R. J. Cotter, R. W. Rozett, and W. S. Koski, "Reactions of H_2O^+ and D_2O^+ with Molecular Hydrogen. I. Proton Affinity of Hydrogen", J. Chem. Phys. **57**, 4100 (1972).

Observed onset of reaction: ($H_2O^+ + H_2 \rightarrow H_3^+ + OH$) as a

function of energy.

78DAV/LAU W. R. Davidson, Y. K. Lau, and P. Kebarle, "Gas Phase Dissociation of Protonated Acetic Acid to the Acyl Cation and Water. Heat of Formation of CH_3CO^+ and the Proton Affinity of Ketene", Can. J. Chem. **56**, 1016 (1978).

High pressure mass spectrometer.

82DEF/HEH D. J. DeFrees, W. J. Hehre, R. T. McIver, Jr., and D. H. McDaniel, "Heat of Formation and Adiabatic Electron Affinity of NH_2", J. Phys. Chem. **83**, 232 (1979).

ICR. Bracketing: $NH_2 \sim CH_3SH$

77DEF/MCI D. J. DeFrees, R. T. McIver, Jr., and W. J. Hehre, "The Proton Affinities of Phenol," J. Am. Chem. Soc. **99**, 3853 (1977).

ICR. Bracketing. D^+ transfer from $C_6H_5OHD^+$ observed with propylene, not with HCN.

80DEF/MCI D. J. DeFrees, R. T. McIver, Jr., and W. J. Hehre, "Heats of Formation of Gaseous Free Radicals via Ion Cyclotron Double Resonance Spectroscopy", J. Am. Chem. Soc. **102**, 3334 (1980).

ICR. Bracketing:

$(C_2H_5)_2S < C_6H_5O < i\text{-}C_3H_7OC_2H_5$
$CH_3COOCH_3 < C_6H_5CH_2 < c\text{-}C_4H_8O$
$CH_3COC_2H_5 < c\text{-}C_7H_7 < i\text{-}C_3H_7COCH_3$
$C_5H_5 < C_2H_5OC_2H_5$
$NCCH_2CN < c\text{-}C_3H_3 < CF_3COOCH_3$
$NCCH_2CN < C_3H_5 < CF_3COOCH_3$
$CH_3CHO < c\text{-}C_3H_5 < C_2H_5OH$
$CF_3COOCH_3 < C_2H_3 < CH_3OH$

76DES/POR A. J. DeStefano and R. F. Porter, "Ion–Molecule Reactions of Cyclic Borazine Cations. Thermodynamic and Kinetic Considerations", 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 J. L. Devlin, III, J. F. Wolf, R. W. Taft, and W. J. Hehre, "The Proton Affinity of Toluene," J. Am. Chem. Soc. **98**, 1990 (1976).

ICR. Results related to TAFT scale. Temperature assumed to be 320 K.

77DIT/NIB H. Dits, N. M. M. Nibbering, and J. W. Verhoeven, "A MINDO/3 and Ion Cyclotron Resonance Study of Some $C_7H_7O^+$ Ions," Chem. Phys. Lett. **51**, 95 (1977).

ICR. Bracketing. Details not given.

80DIX D. A. Dixon, "Relative Proton Affinities of 1,6-$C_2B_4H_6$ and 2,4-$C_2B_5H_7$", Inorg. Chem. **19**, 593 (1980).

ICR. Bracketing:

$NH_3 < C_2B_4H_6 < C_6H_5NH_2$
$H_2O < C_2B_5H_7 < CF_3CH_2OH$

79DOI/GRE C. E. Doiron, F. Grein, T. B. McMahon, and K. Vasudevan, "An ab initio and Ion Cyclotron Resonance Study of the Protonation of Borazine," Can. J. Chem. **57**, 1751 (1979).

ICR. Borazine vs. $HCOOC_2H_5$, $c\text{-}C_4H_8O_2$

80DOI/MCM C. E. Doiron and T. B. McMahon, "Nucleophilic Addition–Elimination Reactions of Weak Bases with the Trifluoroarsonium Ion in the Gas Phase by Ion Cyclotron Resonance Spectroscopy", Inorg. Chem. **19**, 3037 (1980).

ICR. Bracketing:

$CH_3F < AsF_3 < CF_2O$
$CO < NF_3 < CH_3F$
$SO_2 < PF_3 < C_2H_4$

81DOI/MCM C. E. Doiron and T. B. McMahon, "Gas Phase Basicities of Fluorocarbonyl Compounds. An Ion Cyclotron Resonance Investigation of the Effects of Fluorine and Trifluoromethyl Substituents on Hydroxy Carbonium Ion Stabilities", Can. J. Chem. **59**, 2689 (1981).

ICR. Data relative to ethylene and $CH_2(CN)_2$.

82DRU/MCM D. F. Drummond and T. B. McMahon, "Gas Phase Ion Chemistry and Basicities of Fluorinated Acetones: An Ion Cyclotron Resonance Study of the Effects of Multiple Fluorine Substitution on Reactivities of Fluoroketones and Stabilities of Protonated Carbonyl Compounds", Int. J. Mass Spectrom. Ion Phys. **42**, 265 (1982).

ICR:

CH_2FCOCH_3 vs. $HCOOC_2H_5$, $(CH_3)_2O$
CH_2FCOCH_2F vs. CH_3CHO, CH_3SH
CF_3COCH_3 vs. HCOOH, $CH_2(CN)_2$, H_2S
CHF_2COCHF_2 vs. H_2S
CF_3COOH vs. CHF_2COCHF_2
CF_3COCF_3 vs. SO_2, CF_2O

81DYK/JON J. M. Dyke, N. B. H. Jonathan, A. Morris, and M. J. Winter, "Vacuum Ultraviolet Photoelectron Spectroscopy of Transient Species. Part 13. Observation of the X^3A'' State of HO_2^+," Molecular Physics **44**, 1059 (1981).

Photoelectron spectroscopy. First adiabatic IP of $HO_2 = 11.35 \pm 0.01$ eV.

81ELL/DIX M. R. Ellenberger, D. A. Dixon, and W. E. Farneth, "Proton Affinities and the Site of Protonation of Enamines in the Gas Phase", J. Am. Chem. Soc. **103**, 5377 (1981).

ICR. Bracketing:

$(CH_2{=}CHCH_2CH_2)_3N > CH_3CH{=}CHN(CH_3)_2 \sim (CH_3)_2C{=}CHN(CH_3)_2$
$\sim c\text{-}C_5H_{10}N(CH_3) > 1,3\text{-}c\text{-}C_3H_3N_2(CH_3)$
$(C_2H_5)_3N < CH_3CH{=}C(C_2H_5)N(CH_3)_2 = (CH_3)_2NCH_2CH_2N(CH_3)_2$
$CH_33CH{=}C(CH_3)N(CH_3)_2 > (CH_3)_2NCH_2CH_2N(CH_3)_2$
$< CH_3CH{=}C(C_2H_5)N(CH_3)_2$
$(n\text{-}C_3H_7)_2NH < c\text{-}C_3H_3N_3(CH_3) < (CH_3)_2C{=}CHN(CH_3)_2 < (i\text{-}C_2H_7)_2NH$
$(CH_3)_2N(CH_2)_3NH_2 < CH_3CH{=}C(CH_3)N(CH_3)_2$
$< (CH_3)_2NCH_2CH_2N(CH_3)_2$
$c\text{-}C_5H_{10}NH < CH_2{=}CHN(CH_3)_2 < c\text{-}C_3H_3N_3(CH_3)$
$1,3\text{-}C_6H_4(CH_3)(NH_2) < CH_3CH{=}NH < 2\text{-}ClC_5H_4N$

79ELL/EAD M. R. Ellenberger, R. A. Eades, M. W. Thomsen, W. E. Farneth, and D. A. Dixon, "Proton Affinities of Ethylidenimine and Vinylamine", J. Am. Chem. Soc. **101**, 7151 (1979).

ICR. Bracketing:

$3\text{-}CH_3C_6H_4NH_2 < C_2H_5N < 2\text{-}ClC_5H_4N$

81FAH/FEH D. W. Fahey, F. C. Fehsenfeld, and E. E. Ferguson, "Reactions of Si^+ with H_2O and O_2 and SiO^+ with H_2 and D_2", J. Chem. Phys. **75**, 669 (1981).

Flowing afterglow. Observation of: $Si^+ + H_2O \rightarrow SiOH^+ + H$ gives Δ_fH of $SiOH^+ < 185.9$ kcal/mol or $PA(SiO) > 156$ kcal. $SiOH^+$ 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 R. Farid and T. B. McMahon, "Gas Phase Ion–Molecule Reactions of Alkyl Nitrites by Ion Cyclotron Resonance Spectroscopy", Int. J. Mass Spectrom. Ion Phys. **27**, 163 (1978).

ICR. Bracketing:

$(CH_3)_2O < CH_3ONO < HCOOC_2H_5$
$(CH_3)_2CO < C_2H_5ONO < CH_3COOCH_3$
$(C_2H_5)_2O < i\text{-}C_3H_7ONO < NH_3$
$NH_3 < t\text{-}C_4H_9ONO <$ Pyrrole

74FEH/FER F. C. Fehsenfeld and E. E. Ferguson, "Rate Constants for the Reactions $Cl^+ + H_2 \rightarrow HCl^+ + H$ and $ClH^+ + H_2 \rightarrow ClH_2^+ + H$", J. Chem. Phys. **60** 5132 (1974).

Flowing afterglow.

75FEH/HOW F. C. Fehsenfeld, C. J. Howard, and A. L. Schmeltekopf, "Gas Phase Ion Chemistry of HNO_3", 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 F. C. Fehsenfeld, W. Lindinger, and D. L. Albritton, "A Study of the Isoenergetic Reaction $H_3^+ + O_2 \rightleftharpoons O_2H^+ + H_2$", J. Chem. Phys. **63**, 443 (1975).

Flowing afterglow.

76FEH/LIN F. C. Fehsenfeld, W. L. Lindinger, H. I. Schiff, R. S. Hemsworth, and D. K. Bohme, "Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. VI. The Relative Proton Affinities of N_2, Xe, and CO_2", J. Chem. Phys. **64**, 4887 (1976).

Flowing afterglow. Entropy change determination.

73FEN/HEM P. F. Fennelly, R. S. Hemsworth, H. I. Schiff, and D. K. Bohme, "Determination of the Proton Affinity from the

Kinetics of Proton Transfer Reactions. IV. The Equilibrium $O_2H^+ + H_2 \rightleftharpoons H_3^+ + O_2$ and the Relative Proton Affinity of O_2 and H_2", J. Chem. Phys. **59**, 6405 (1973).

Flowing afterglow.

78FON/HUD S. N. Foner and R. L. Hudson, "Determination of the Proton Affinity of N_2 from Ionization Data on trans-Diimide", J. Chem. Phys. **68**, 3169 (1978).

72FOS/BEA M. S. Foster and J. L. Beauchamp, "Gas Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance Spectroscopy", J. Am. Chem. Soc. **94**, 2425 (1972).

ICR. Bracketing:

$NH_3 < CH_3N{=}NCH_3 < CH_3NH_2$

$NH_3 < CH_2N_2 < CH_3N{=}NCH_3$

75FOS/BEA M. S. Foster and J. L. Beauchamp, "Proton Affinity and Gas Phase Ion Chemistry of Hydrogen Fluoride," Inorg. Chem. **14**, 1229 (1975).

ICR. Equilibrium observed between HF and N_2.

75FOS/BEA(2) M. S. Foster and J. L. Beauchamp, "Ion-Molecule Reactions and Gas Phase Basicity of Ferrocene", J. Am. Chem. Soc. **97**, 4814 (1975).

ICR. Bracketing:

$CH_3N{=}NCH_3 < (C_5H_5)_2Fe < CH_3NH_2$.

75FOS/BEA(3) M. S. Foster and J. L. Beauchamp, "Gas Phase Ion Chemistry of Iron Pentacarbonyl by Ion Cyclotron Resonance Spectroscopy. New Insights into the Properties and Reactions of Transition Metal Complexes in the Absence of Complicating Solvation Phenomena", J. Am. Chem. Soc. **97**, 4808 (1975).

ICR. Bracketing:

$((CH_3O)_2CO < Fe(CO)_5 < NH_3$

74FOS/WIL M. S. Foster, A. D. Williamson, and J. L. Beauchamp, "Photoionization Mass Spectrometry of trans-Azomethane", Int. J. Mass Spectrom. Ion Phys. **15**, 429 (1974).

Equilibrium vs. $CF_2HCH_2NH_2$; related to TAFT scale; Temperature of 320 K assumed.

78FRE/HAR C. G. Freeman, P. W. Harland, and M. J. McEwan, "The Equilibrium Systems H_3CO^+ (HCN, HCHO) H_2CN^+, H_3CO^+ (H_2S, HCHO) H_3S^+ and the Relative Proton Affinities of HCHO, HCN, and H_2S", Int. J. Mass Spectrom. Ion Phys. **28**, 19 (1978).

Flowing afterglow.

78FRE/HAR(2) C. G. Freeman, P. W. Harland, and M. J. McEwan, "The Equilibrium $H_3S^+ + HCN = H_2CN^+ + H_2S$ and the Relative Proton Affinities of HCN and H_2S", Int. J. Mass Spectrom. Ion Phys. **27**, 77 (1978).

Flowing afterglow.

79FRE/HAR C. G. Freeman, P. W. Harland, and M. J. McEwan, "The Positive Ion Chemistry of Trifluoronitrosomethane, CF_3NO", Int. J. Mass Spectrom. Ion Phys. **30**, 285 (1979).

Flowing afterglow. Bracketing:

$H_2O < CF_3NO < HCN$

75FRE/KEB M. French and P. Kebarle, "Protolysis of $C_2H_7^+$ and Other Ion-Molecule Reactions in Methane Containing Traces of Ethane", Can. J. Chem. **53**, 2668 (1975).

High pressure mass spectrometer. Determination of equilibrium constant of $(C_2H_7^+ + CH_4 \rightleftharpoons CH_5^+ + C_2H_6)$.

76GOR/MUN A. Goren and B. Munson, "Thermochemistry of Alkyl Ions", 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 $t\text{-}C_4H_9^+ = 165.8$ kcal/mol.

76GUY/CHU P. M. Guyon, W. A. Chupka and J Berkowitz, "Photoionization Mass Spectrometric Study of Formaldehyde H_2CO, HDCO, and D_2CO", J. Chem. Phys. **64** 1419 (1976).

69HAN/FRA M. A. Haney and J. L. Franklin, "Heats of Formation of H_3O^+, H_3S^+, and NH_4^+ by Electron Impact", J. Chem. Phys. **50**, 2028 (1969).

73HAR/CRO H. H. Harris, M. G. Crowley, T. R. Grossheim, P. J. Woessner, and J. J. Leventhal, "Binding Energy of H_3^+", J. Chem. Phys. **59**, 6181 (1973).

Measured onset of $H_3^+ + He \rightarrow H^+ + H_2 + He$

78HAR/LIA K. G. Hartman and S. G. Lias, "Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities", Int. J. Mass Spectrom. Ion Phys. **28**, 213 (1978).

ICR. Entropy change determinations included.

76HAR/LIN A. G. Harrison, P.-H. Lin, and C. W. Tsang, "Proton Transfer Reactions by Trapped Ion Mass Spectrometry", Int. J. Mass Spectrom. Ion Phys. **19**, 23 (1976).

Trapped ion mass spectrometry.

74HEH/MCI W. J. Hehre, R. T. McIver, Jr., J. A. Pople, and P. v. R. Schleyer, "Alkyl Substituent Effects on the Stability of Protonated Benzene," J. Am. Chem. Soc. **96**, 7162 (1974).

ICR. Data related to TAFT scale; temperature assumed to be 320 K.

73HEM/RUN R. S. Hemsworth, H. W. Rundle, D. K. Bohme, H. I. Schiff, D. B. Dunkin, and F. C. Fehsenfeld, "Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. III. The Measurement of the Equilibrium Constant at Various Temperatures", J. Chem. Phys. **59**, 61 (1973).

ΔH and ΔS measurements for CO_2-CH_4 and N_2O-CO systems. Flowing afterglow. [196 to 553 K].

83HEN/FRE M. L. Hendewerk, R. Frey, and D. A. Dixon, "Effect of Substituting Silicon for Carbon on Molecular Proton Affinities," J. Phys. Chem. **87**, 2026 (1983).

ICR. Bracketing:

$(CH_3)_3N < (CH_3)_3SiN(CH_3)_2 \sim (C_2H_5)_2NH <$ $(iso\text{-}C_3H_7)(CH_3)N$

72HEN/TAA W. G. Henderson, M. Taagepera, D. Holtz, R. T. McIver, Jr., J. L. Beauchamp, and R. W. Taft, "Methyl Substituent Effects in Protonated Aliphatic Amines and Their Radical Cations", J. Am. Chem. Soc. **94**, 4728 (1972).

ICR. Related to TAFT scale; temperature assumed to be 320 K.

82HEN/WEI M. L. Hendewerk, D. A. Weil, T. L. Stone, M. R. Ellenberger, W. E. Farneth, and D. A. Dixon, "Proton Affinity and Ion-Molecule Reactions of a Simple Silyl Enol Ether", J. Am. Chem. Soc. **104**, 1794 (1982).

ICR. Bracketing:

$(CH_3)_2NH < CH_2{=}C(CH_3)OSi(CH_3)_3 < t\text{-}C_4H_9NH_2$

78HIR K. Hiraoka, "Endothermic Ion-Molecule Reactions: The Reactions of H_3O^+ and H_3S^+ with Isobutane", Int. J. Mass Spectrom. Ion Phys. **27**, 139 (1978).

High pressure mass spectrometer. Arrhenius plots of k_{Rn} for $H_3O^+ + i\text{-}C_4H_8$ and $H_3S^+ + i\text{-}C_4H_8$.

75HIR/KEB K. Hiraoka and P. Kebarle, "Information on the Proton Affinity and Protolysis of Propane from Measurement of the Ion Cluster Equilibrium: $C_2H_5^+ + CH_4 = C_3H_9^+$", Can. J. Chem. **53**, 970 (1975).

High pressure mass spectrometer. $\Delta H[C_2H_5^+ + CH_4 \rightleftharpoons C_3H_9^+] = -6.6$ kcal/mol

76HIR/KEB K. Hiraoka and P. Kebarle, "Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric $C_2H_7^+$ Ions and Some Higher Analogues: $C_3H_9^+$ and $C_4H_{11}^+$", J. Am. Chem. Soc. **98**, 6119 (1976).

High pressure mass spectrometer. A and B: The heat of formation of $C_2H_7^+$ was determined from the equilibrium constant for the process: $C_2H_5^+ + H_2 \rightarrow C_2H_7^+$. Different values were obtained at low and at high temperature regimes. The authors interpret this as evidence for two $C_2H_7^+$ structures.

The heat of formation of $C_3H_9^+$ was determined from the equilibrium constant for the process: $C_2H_5^+ + CH_4 \rightleftharpoons C_3H_9^+$ and that of $C_4H_{11}^+$, from the equilibrium constant for the process: $sec\text{-}C_3H_7^+ + CH_4 \rightleftharpoons C_4H_{11}^+$. Values reported in the paper have been modified slightly to take into account more recent values for heats of formation of relevant ions.

77HIR/KEB K. Hiroaka and P. Kebarle, "Condensation Reactions Involving Carbonium Ions and Lewis Bases in the Gas Phase. Hydration of the tert-Butyl Cation", J. Am. Chem. Soc. **99**, 360 (1977).

Heat of formation of $t\text{-}C_4H_90H_2^+$ determined from equilibrium constant for the process: $t\text{-}C_4H_9^+ + H_2O \rightleftharpoons C_4H_9OH_2^+$.

75HOD/BEA R. V. Hodges and J. L. Beauchamp, "Basicity and Ion-Molecule Reactions of Trimethylarsine in the Gas Phase Determined by Ion Cyclotron Resonance Spectroscopy", Inorg. Chem. **14**, 2887 (1975).

ICR. Data related to TAFT scale.

80HOD/HOU R. V. Hodges, F. A. Houle, J. L. Beauchamp, R. A. Montag, and J. G. Verkade, "Effects of Molecular Structure on Basicity. Gas Phase Proton Affinities of Cyclic Phosphites", J. Am. Chem. Soc. **102**, 932 (1980).

$C_3H_5O_3P$ vs. c-C_3H_5CN, n-C_3H_7CN
$C_4H_7O_3P$ vs. c-$C_5H_{10}O$, CH_3COOCH_3
$C_4H_7O_3P$ vs. $CH_3COCH_2COCH_3$, $(CH_3)_6C_6$
$C_5H_9O_3P$ vs. $HCON(CH_3)_2$
$C_6H_9O_3P$ vs. 2-Cl-pyridine, (t-$C_4H_9)_2S$
$C_3H_7O_3P$ vs. 2-Cl-pyridine, (t-$C_4H_9)_2S$
$C_4H_9O_3P$ vs. pyridine
trans-2-methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane vs.
3-CH_3-pyridine, $(C_2H_5)_2NH$, 2-CH_3-pyridine
cis,cis-2-methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane vs.
4-CH_3pyridine, c-$C_5H_{10}NH$

80HOD/MCD R. V. Hodges, T. J. McDonnell, and J. L. Beauchamp, "Properties and Reactions of Trimethyl Phosphite, Trimethyl Phosphate, Triethyl Phosphate, and Trimethyl Phosphorothionate by Ion Cyclotron Resonance Spectroscopy", J. Am. Chem. Soc. **102**, 1327 (1980).

$P(OCH_3)_3$: Equilibrium with C_5H_5N, c-$C_6H_{11}NH_2$
$OP(OCH_3)_3$: Equilibrium with $C_6H_5NH_2$, $(C_6H_5)_2C=CH_2$
$OP(OC_2H_5)_3$: Close to 3-$(CH_3CO)C_5H_4N$ and pyridazine ($C_4H_4N_2$)
$SP(OCH_3)_3$: Equilibrium with 4-$CH_3OC_6H_4CHO$

73HOP/BON J. M. Hopkins and L. I. Bone, "Relative Proton Affinities of Hydrogen Sulfide and Water", J. Chem. Phys. **58**, 1473 (1973).

High pressure mass spectrometer.

78HOU/BEA F. A. Houle and J. L. Beauchamp, "Detection and Investigation of Allyl and Benzyl Radicals by Photoelectron Spectroscopy", J. Am. Chem. Soc. **100**, 3290 (1978).

Determination of ionization potentials of allyl and benzyl radicals.

79HOU/BEA F. A. Houle and J. L. Beauchamp, "Photoelectron Spectroscopy of Methyl, Ethyl, Isopropyl, and tert-Butyl Radicals. Implications for the Thermochemistry and Structures of the Radicals and Their Corresponding Carbonium Ions," J. Am. Chem. Soc., **101**, 4067 (1979).

Determination of ionization potentials of ethyl, isopropyl, and tert-butyl radicals.

83HOU/RUF R. Houriet, H. Rufenacht, P.-A. Carrupt, P. Vogel, and M. Tichu, "Site of Protonation and Conformational Effects on Gas Phase Basicity in Beta-Amino Alcohols. The Nature of Internal H-Bonding in Beta-Hydroxy Ammonium Ions", J. Am. Chem. Soc. **105**, 3417 (1983).

ICR. Bicyclo[2.2.2]octane, 2-OH, 3-NH_2 (cis): gas basicity 0.2 kcal/mol above 4-methylpyridine. cis-3-Amino-2-twistanol: gas basicity 0.3 kcal/mol above 4-Methyl-pyridine. Decalin, 3-OH, 4-NH_2: gas basicity 0.7 kcal/mol below 3-Methylpyridine. trans-3-Amino-2-twistanol: gas basicity 1.3 kcal/mol below 3-Methyl-pyridine. Bicyclo[2.2.2]octane, 2-OH, 3-NH_2 (trans): gas basicity 0.1 kcal/mol below cyclohexylamine. trans-3-Amino-2-twistanol: gas basicity 0.9 kcal/mol below cyclohexylamine and pyridine. 4-Aminodecahydro-3-naphthalenol: gas basicity 0.9 kcal/mol below cyclohexylamine; 0.5 kcal/mol below pyridine; 0.2 kcal/mol below sec-butylamine.

81HOU/SCH R. Houriet, H. Schwarz, W. Zummack, J. G. Andrade, and P. v. R. Schleyer, "Alpha vs. Beta Protonation of Pyrrole, Furan, Thiophene, and Cyclopentadiene. Gas Phase Proton and Hydrogen Affinities. The Bishomocyclopropenyl Cation," Nouv. J. Chim. **5**, 505 (1981).

ICR. Bracketing. All gas basicities lay between dimethyl ether and n-propanol.

80HOU/VOG R. Houriet, J. Vogt, and E. Haselbach, "Gas Phase Protonation of Enamines," Chimia **34**, 277 (1980).

ICR. Details not given.

79HUB/HER K. P. Huber and G. Herzberg, "Molecular Spectra and Molecular Structure Constants of Diatomic Molecules," Van Nostrand Reinhold Co., New York (1979).

82IKU/KEB S. Ikuta, P. Kebarle, G. M. Bancroft, T. Chan, and R. J. Puddephatt, "Basicities of Methyl-, Methylphenyl-, and Phenylphosphines in the Gas Phase", J. Am. Chem. Soc. **104**, 5899 (1982).

High pressure mass spectrometer. Equilibria at 320 and 348 K: Entropy change assumed equal to zero.

81JON/BIR J. D. C. Jones, K. Birkinshaw, and N. D. Twiddy, "Rate Coefficients and Product Ion Distributions for the Reactions of OH^+ and H_2O^+ with N_2, O_2, N_2O, Xe, CO, CO_2, H_2S, and H_2 at 300 K", Chem. Phys. Lett. **77**, 484 (1981).

SIFT. $PA(N_2) \sim PA(O)$

72KAS/FRA S. F. Kaspar and J. L. Franklin, "Ion-Molecule Reactions in the System CO_2-CH_4", J. Chem. Phys. **56**, 1156 (1972).

High pressure mass spectrometer.

76KEB/YAM P. Kebarle, R. Yamdagni, K. Hiroaka, and T. B. McMahon, "Ion Molecule Reactions at High Pressure: Recent Proton Affinities, Gas Phase Acidities and Hydrocarbon Clustering Results", Int. J. Mass Spectrom. Ion Phys. **19**, 71 (1976).

High pressure mass spectrometer. 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.

81KIM/BON J. K. Kim, J. Bonicamp, and M. C. Caserio, "Thiosulfonium Ions by Gas-Phase Methylation and Thiomethylation of Sulfur Nucleophiles. 1. Methoxymethyl Cations", J. Org. Chem. **46**, 4230 (1981).

ICR. Bracketing:
$(CH_3)_2O < CH_3SSCH_3 < (CH_3)_2S$

LAU/KEB Y. K. Lau, Ph. D. Thesis, University of Alberta (1979).

High pressure mass spectrometer. Some entropy change determinations.

76LAU/KEB Y. K. Lau and P. Kebarle, "Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes", J. Am. Chem. Soc. **98**, 7452 (1976).

High pressure mass spectrometer. Some entropy change determinations.

81LAU/NIS Y. K. Lau, K. Nishizawa, A. Tse, R. S. Brown, and P. Kebarle, "Protonation and Site of Protonation of Anilines. Hydration and Site of Protonation after Hydration", J. Am. Chem. Soc. **103**, 6291 (1981).

Data related to aniline. High pressure mass spectrometer.

78LAU/SAL Y. K. Lau, P. P. S. Saluja, P. Kebarle, and R. W. Alder, "Gas Phase Basicities of N-Methyl Substituted 1,8-Diaminonaphthalenes and Related Compounds", J. Am. Chem. Soc. **100**, 7328 (1978).

High pressure mass spectrometer.

79LIA S. Lias in "Kinetics of Ion-Molecule Reactions" (P. Ausloos, Editor), "Thermochemistry of Polyatomic Cations", p. 223 (1979).

ICR. Proton transfer equilibria of ketene with acetone and methyl acetate measured as a function of temperature.

LIA/JAC S. G. Lias, J.-A. A. Jackson, H. Argentar and J. F. Liebman, "Substituted Dialkyl Anilines: Relative Ionization Energies and Proton Affinities through Determination of Ion-Molecule Reaction Equilibrium Constants", J. Org. Chem., in press.

ICR.

84LIA/LIE S. G. Lias, J. F. Liebman, J. L. Holmes, J. E. Bartmess, R. D. Levin, and M. Motevalli-Aliabadi, Phys. Chem. Ref. Data, to be published.

An evaluated compilation of heats of formation of ions now in preparation.

80LIA/SHO S. G. Lias, D. M. Shold, and P. Ausloos, "Proton-Transfer Reactions Involving Alkyl Ions and Alkenes. Rate Constants, Isomerization Processes, and the Derivation of

Thermochemical Data", J. Am. Chem. Soc. **102**, 2540 (1980).
ICR. Data relative to i-C_4H_8. Trans-2-C_4H_8 and c-C_6H_{10} by bracketing. 2-C_4H_8~CH_3NO_2; c-C_6H_{10}~$HCOOCH_3$.

75LIN/ALB W. Lindinger, D. L. Albritton, C. J. Howard, F. C. Fehsenfeld, and E. E. Ferguson, "Flow-drift Tube Measurements of $H_2O_2^+$ Reactions with H_2O, NH_3, NO and CO and Charge Transfer of O_2^+ with H_2O_2", J. Chem. Phys. **63**, 5220 (1975).
Flowing afterglow.

79LOC/HUN M. J. Locke, R. L. Hunter, and R. T. McIver, Jr., "Experimental Determination of the Acidity and Basicity of Glycine in the Gas Phase", J. Am. Chem. Soc. **101**, 272 (1979).
ICR. [382 K].

83LOC/HUN See 83MCI

75LOS/TRA F. P. Lossing and J. C. Traeger, "Stabilization in Cyclopentadienyl, Cyclopentenyl, and Cyclopentyl Cations", J. Am. Chem. Soc. **97**, 1579 (1975).
Appearance potential of $C_5H_7^+$ from cyclopentene.

78MAC/BOH G. I. Mackay and D. K. Bohme, "Proton Transfer Reactions in Nitromethane at 297 K", Int. J. Mass Spectrom. Ion Phys. **26**, 327 (1978).
Flowing afterglow.
CH_3NO_2 related to CH_3OH and $CH_3CH{=}CH_2$; absolute scale related to LIA/SHO.

81MAC/SCH G. I. Mackay, H. I. Schiff, and D. K. Bohme, "A Room-Temperature Study of the Kinetics and Energetics for the Protonation of Ethane", Can. J. Chem. **59**, 1771 (1981).
Flowing afterglow.

79MAU M. Meot-Ner (Mautner), "Ion Thermochemistry of Low Volatility Compounds in the Gas Phase. 2. Intrinsic Basicities and Hydrogen-Bonded Dimers of Nitrogen Heterocyclics and Nucleic Bases", J. Am. Chem. Soc. **101**, 2396 (1979).
High pressure mass spectrometer [500–600 K].

80MAU M. Meot-Ner (Mautner), "Ion Thermochemistry of Low Volatility Compounds in the Gas Phase. 3. Polycyclic Aromatics: Ionization Energies, Proton and Hydrogen Affinities. Extrapolations to Graphite", J. Phys. Chem. **84**, 2716 (1980).
High pressure mass spectrometer. [550 K]

82MAU M. Meot-Ner (Mautner), "Carbon-Hydrogen Bond Dissociation Energies in Alkylbenzenes. Proton Affinities of the Radicals and the Absolute Proton Affinity Scale", 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 M. Meot-Ner (Mautner), "The Ionic Hydrogen Bond. 2. Intramolecular and Partial Bonds. Protonation of Polyethers, Crown Ethers, and Diketones," J. Am. Chem. Soc. **105**, 4906 (1983); M Meot-Ner (Mautner), S. F. Nelsen, M. F. Willi, and T. B. Frigo, J. Am. Chem. Soc., in press; and other papers, to be published. (All data made available to this compilation before publication).
High pressure mass spectrometer. Enthalpy and entropy changes determined for most reactions; assumed entropy changes indicated here by parentheses. Gas basicity values cited for 300 K in Table 1.

	ΔH kcal/mol	ΔS cal/K mol
THF:Oxepane	-2.7	(0)
$C_2H_5SCH_3$:Oxepane	+0.5	(1.4)
THF:1,3-Dioxane	+0.2	(0)
$(C_2H_5)_2O$:1,3-Dioxane	+1.4	(0)
n-$(C_3H_7)_2O$:$CH_3OCH_2CH_2OCH_3$	-2.2	-5.0
$(C_2H_5)SCH_3$*$CH_3OCH_2CH_2OCH_3$	-1.8	-3.6
n-Bu_2S:$CH_3O(CH_2)_3OCH_3$	-5.2	-5.4
2-FPyr:$CH_3O(CH_2)_3OCH_3$	-3.6	-5.5
3-FPyr:$CH_3O(CH_2)_3OCH_3$	+0.8	-7.0
2-FPyr:$CH_3(OCH_2CH_2)_2OCH_3$	-8.5	-13.2
3-FPyr:$CH_3(OCH_2CH_2)_2OCH_3$	-5.7	-15.7
1.2-Diazine: "	-1.4	-11.7
1,2-Diaz:$CH_3(OCH_2CH_2)_3OCH_3$	-9.1	-17.7
1,2-Diaz:12-Crown-4	-3.3	-3.1
Pyr:12-Crown-4	+1.2	-2.6
1,2-Diaz:15-Crown-5	-3.6	(-3)
Pyr:15-Crown-5	+0.1	(-3)
1,2-Diaz:18-Crown-6	-2.7	(-3)
Pyr:18-Crown-6	+0.9	(-3)
HCOOn-C_4H_9:$CH_3COCOCH_3$	-1.7	(1.4)
$(CH_3)_2CO$:$CH_3COCOCH_3$	+1.9	2.6
$CH_3COC_2H_5$: "	+3.7	(1.4)
$(n\text{-}C_3H_7)_2S$:$CH_3COCH_2COCH_3$	-1.2	-3.0
Pyrrole:$CH_3COCH_2COCH_3$	+0.1	-4.1
Pyrrole:$CH_3COCH_2CH_2COCH_3$	-3.9	-8.5
2-FPyr:$CH_3COCH_2CH_2COCH_3$	-2.6	-5.6
$(C_2H_5)_2CO$:Cyclohexanone	-2.5	(0)
$C_2H_5SCH_3$:Cyclohexanone	-1.0	(0)
$C_2H_5SCH_3$:1,2-Cyclohexanedione	-1.7	(1.4)
$(n\text{-}C_3H_7)_2S$:1,2-Cyclohexanedione	+3.8	(0)
Pyrrole:1,3-Cyclohexanedione	-2.7	(1.4)
2-FPyr:1,3-Cyclohexanedione	-1.0	(1.4)
2-FPyr:$CH_3CONHCH_2COOCH_3$	-7.0	-13.4
2-FPyr:$CH_3CONHCNCH_3COOCH_3$	-12.3	-14.7
3-FPyr:$CH_3CONHCNCH_3COOCH_3$	-9.6	-15.7

H_2NNH_2: $\Delta G = -4.7$ kcal/mol to pyrrole; -0.1 kcal/mol to cyclopropylmethylketone, +2.1 kcal/mol to n-propylether at 600 K.
Isooxazole: $\Delta G = +2.7$ kcal/mol to $(C_2H_5)_2O$ at 600 K.
Oxazole: $\Delta G = 0.3$ kcal/mol to pyrrole at 600 K.
Furan: $\Delta G = +3.2$ kcal/mol to toluene; -0.6 kcal/mol to ethylformate at 600 K.
2,5-Dimethylfuran: $\Delta G = 2.4$ kcal/mol to pyrrole at 600 K.
2-Methylfuran: $\Delta G = -1.8$ kcal/mol to pyrrole at 600 K.
Thiophene: $\Delta G = 1.5$ kcal/mol to 1,4-dioxane; -2.5 kcal/mol to $CH_3COC_2H_5$ at 600 K.
2-Methylthiophene: $\Delta G = 0.7$ kcal/mol to c-$C_3H_5COCH_3$ at 600 K.
N-Methylimidazole: $\Delta G = 4.7$ kcal/mol to 3-methylpyridine; -5.5 kcal/mol to $(C_2H_5)_3N$ at 600 K.
4-Methylimidazole: $\Delta G = 0.4$ kcal/mol to 3-ethylpyridine at 600 K.
Imidazole: $\Delta G = 2.6$ kcal/mol to iso-$C_3H_7NH_2$ at 600 K.
2,5-Dimethylpyrrole: $\Delta G = 1.0$ kcal/mol to iso-$C_3H_7NH_2$ at 600 K.
Thiazole: $\Delta G = -0.8$ kcal/mol to 3-fluoropyridine at 600 K.
Pyrazole: $\Delta G = 0.8$ kcal/mol to 2-fluoropyridine at 600 K.
$CH_2{=}CHOCH_3$: $\Delta G = -0.7$ kcal/mol to pyrrole at 600 K.
$C_2H_5OCH{=}CH_2$: $\Delta G = 1.0$ kcal/mol to pyrrole; 2.6 kcal/mol to 2-fluoropyridine at 600 K.

77MAU/FIE M. Meot-Ner (Mautner) and F. H. Field, "Proton Affinities and Cluster Ion Stabilities in CO_2 and CS_2. Applications in Martian Ionospheric Chemistry," J. Chem. Phys. **66**, 4527 (1977).
High pressure mass spectrometer.

80MAU/HAM M. Meot-Ner (Mautner), P. Hamlet, E. P. Hunter, and F. H. Field, "Internal and External Solvation of Polyfunctional Ions", J. Am. Chem. Soc. **102**, 6393 (1980).
High pressure mass spectrometer.

79MAU/HUN M. Meot-Ner (Mautner), E. P. Hunter, and F. H. Field, "Ion Thermochemistry of Low Volatility Compounds in the Gas Phase. 1. Intrinsic Basicities of a-Amino Acids", J. Am. Chem. Soc. **101**, 686 (1979).
High pressure mass spectrometer.

80MAU/HUN M. Meot-Ner (Mautner), E. P. Hunter, P. Hamlet, and F. H. Field, "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 (1980), p.233.
High pressure mass spectrometer.

83MAU/SIE M. Mautner and L. W. Sieck, "Structure Effects on Ion

Thermochemistry. 1. Steric Hindrance of the Hydrogen Bond: Solvation and Clustering of Protonated Amines and Pyridines", J. Am. Chem. Soc. **105**, 2956 (1983).

High pressure mass spectrometer. Includes entropy change measurements.

76MAU/SOL M. Mautner (Meot-Ner), J. J. Solomon, and F. H. Field, "Stability of Some C_7 Tertiary Carbonium Ions", J. Am. Chem. Soc. **98**, 1025 (1976).

High pressure mass spectrometer. Heats of formation of alkyl ions from hydride transfer equilibrium constant measurements; values calculated relative to a value of 165.8 kcal/mol for $t\text{-}C_4H_9^+$.

74MCA T. McAllister, "Ion-Molecule Reactions and Proton Affinities of Methyl Thio- and Isothiocyanate", Int. J. Mass Spectrom. Ion Phys. **15**, 303 (1974).

ICR. Bracketing:

$i\text{-}C_4H_8 < C_2H_3NS < CH_3COCH_3$

77MCA T. McAllister, "Ion Cyclotron Resonance Mass Spectroscopy of Dimethyl Sulfoxide", Int. J. Mass Spectrom. Ion Phys. **25**, 353 (1977).

ICR. Bracketing: $CH_3OH < (CH_3)_2SO < C_2H_5OH$. Disagrees with equilibrium results.

78MCA T. McAllister, "The Formation of Interstellar HCS", Astrophys. J. **222**, 857 (1978).

ICR. Bracketing.

81MCA/NIC T. McAllister, J. C. Nicholson, and J. D. Scott, "Ionization of Nitromethane in the Flame Ionization Detector", Can. J. Chem. **59**, 1819 (1981).

76MCA/PIT T. McAllister and P. Pitman, "Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane", Int. J. Mass Spectrom. Ion Phys. **19**, 241 (1976).

ICR. Bracketing:

$C_2H_5OH < CH_3ONO < CH_3COCH_3$

$CH_3NO_2 \sim CH_3OH$

76MCC K. E. McCulloh, "Energetics and Mechanisms of Fragment Ion Formation in the Photoionization of Normal and Deuterated Water and Ammonia", Int. J. Mass Spectrom. Ion Phys. **21**, 333 (1976).

Appearance potential of OH^+ from H_2O.

77MCC K. E. McCulloh, "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.

83MCI R. T. McIver, Jr., Table from work in press provided for this compilation. Complete reference: M. J. Locke and R. T. McIver, Jr., "Effect of Solvation on the Acid/Base Properties of Glycine," J. Am. Chem. Soc. **105**, 4226 (1983).

ICR. 382 K.

81MCL/CAM S. A. McLuckey, D. Cameron, and R. G. Cooks, "Proton Affinities from Dissociations of Proton Bound Dimers", J. Am. Chem. Soc. **103**, 1313 (1981).

Proton affinity(Quinoline) 0.4 kcal/mol less than that for 3,4-$(CH_3)_2C_5H_3N$.

$PA(C_6H_5NHC_2H_5)$ 0.7 kcal/mol less than that of $n\text{-}C_6H_{13}NH_2$ and 1.1 kcal/mol less than that of $sec\text{-}C_4H_9NH_2$.

76MEI/MIT G. G. Meisels, R. K. Mitchum, and J. P. Freeman, "Arrival Time Distributions in High Presesure Mass Spectrometry. 5. Effect of E/P on Measured Apparent Heats and Entropies of Reaction", J. Phys. Chem. **80**, 2845 (1976).

High pressure mass spectrometer. Entropy change measurement for $CO_2:CH_4 = 7.1$ J/mol s (1.7 cal/K mol).

77MUN/SMI B. Munson, D. Smith, and C. Polley, "The Mass Spectrum, Proton Affinity and Ion-Molecule Reactions of SO_3", Int. J. Mass Spectrom. Ion Phys. **25**, 323 (1977).

High pressure mass spectrometer. Bracketing: $HBr < SO_3 < CO$

77NG/TRE C. Y. Ng, D. J. Trevor, P. W. Tiedemann, S. T. Ceyer, P. L. Kronebusch, B. H. Mahan, and Y. T. Lee, "Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H_2O and HF", J. Chem. Phys. **67**, 4235 (1977).

Determination of proton affinities of H_2O and HF through appearance potential measurements on neutral dimers.

82PAU/HEH C.-F. Pau and W. J. Hehre, "Heat of Formation of Hydrogen Isocyanide by Ion Cyclotron Double Resonance Spectroscopy", J. Phys. Chem. **86**, 321 (1982).

ICR. Bracketing of deuteron transfer from protonated DCN: $C_2H_5CHO < HNC < C_2H_5SH$.

82PAU/HEH(2) C.-F. Pau and W. J. Hehre, "Relative Thermochemical Stabilities of Hydroxymethylene and Formaldehyde by Ion Cyclotron Double Resonance Spectroscopy", 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

75PAY/SCH J. D. Payzant, H. I. Schiff, and D. K. Bohme, "Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. V. The Equilibrium $H_3^+ + Kr \rightleftharpoons KrH^+ + H_2$ and the Relative Proton Affinity of Kr and H_2", J. Chem. Phys. **63**, 149 (1975).

Flowing afterglow.

82PIE/HEH W. J. Pietro and W. J. Hehre, "Thermochemistry of Group 4A Isobutene Analogues by Pulsed Ion Cyclotron Double Resonance Spectroscopy", J. Am. Chem. Soc. **104**, 4329 (1982).

ICR. Bracketing: Identities of reference bases not specified; temperature correction of TAFT scale made by authors.

82PIE/HEH(2) W. J. Pietro and W. J. Hehre, "Tautomerization of Dimethyl Phosphonate," 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."

73PIE/POR R. C. Pierce and R. F. Porter, "Low Temperature Chemical Ionization Mass Spectrometry of Boron Hydrides. The Proton Affinities of Diborane and Tetraborane", J. Am. Chem. Soc. **95**, 3849 (1973).

High pressure mass spectrometer.

79PIE/POL W. J. Pietro, S. K. Pollack, and W. J. Hehre, "Heat of Formation of 1,1-Dimethylsilaethylene by Ion Cyclotron Resonance Spectroscopy", J. Am. Chem. Soc. **101**, 7126 (1979).

ICR. Bracketing:

Piperidine $< (CH_3)_2Si{=}CH_2 < i\text{-}C_3H_7NHC_2H_5$

75PIT/BUR C. G. Pitt, M. M. Bursey, and D. A. Chatfield, "The Relative Gas Phase Proton Affinities and Polarisabilities of Alkyl and Silyl Ethers", J. C. S. Perkin II, 434 (1975).

High pressure mass spectrometer. Ordering, with brackets at ends of scale:
$(i\text{-}C_3H_7)_2O\{GB = 198.0\} > t\text{-}C_4H_9OCH_3 > ((CH_3)_3Si)_2O >$
$((CH_3)_2HSi)_2O > (CH_3)_3SiOCH_3 > (C_2H_5)_2O\{GB = 192$
kcal/mol$\}$.

Also given, but not included here for lack of brackets:
$(t\text{-}C_4H_9)_2O > t\text{-}C_4H_9O(i\text{-}C_3H_7)$ and
$((CH_3)_2HSi)_2O > ((CH_3)_3SiCH_2)_2O$ and
$(CH_3)_3SiOCH_3 > (CH_3)_3SiOH$

77PO/POR P. L. Po and R. F. Porter, "High Temperature Ion–Molecule Chemistry. A Kinetic Study of Gas Phase Reactions of Magnesium Atoms with D_3^+, Methanium, Ammonium, and tert-$C_4H_9^+$ Ions", J. Am. Chem. Soc. **99**, 4922 (1977).

High pressure mass spectrometer. Proton affinity $(Mg) > 193$ kcal/mol. (Not included in Table)

78PO/POR P. L. Po and R. F. Porter, "A Thermodynamic Study of the Reactions of $Mg^+(g)$ and $MgH^+(g)$ with Magnesium", J. Phys. Chem. **81**, 2233 (1977).

High pressure mass spectrometer. Heat of formation of MgH^+ from Keq for: $MgH^+ + Mg(s) = Mg_2H^+$.

78PO/RAD P. L. Po, T. P. Radus, and R. F. Porter, "An Energy Dependent Kinetic Study of the Reactions of Zn(g) Atoms with $H_3^+(D_3^+)$ and CH_4D^{+}", J. Phys. Chem. **82**, 520 (1978).

High pressure mass spectrometer. Bracketing.

77POL/DEV S. K. Pollack, J. L. Devlin III, K. D. Summerhays, R. W. Taft, and W. J. Hehre, "The Site of Protonation in Aniline", J. Am. Chem. Soc. **99**, 4583 (1977).

ICR. Data related to TAFT scale, corrected to 320 K.

80POL/HEH S. K. Pollack and W. J. Hehre, "Determination of the Heat of Formation of Ortho-Benzyne by Ion Cyclotron Resonance Spectroscopy", Tetrahedron Letters **21**, 2483 (1980).

ICR. Bracketing:

$(t\text{-}C_4H_9)_2S < C_6H_4 < (CH_3)_2NCOOC_2H_5$

78POL/MUN C. W. Polley and B. Munson, "The Proton Affinities of the Halogen Acids", Int. J. Mass Spectrom. Ion Phys. **26**, 49 (1978).

High pressure mass spectrometry.

Bracketing: $Br < HCl < N_2O$

$HCl < HBr < CO$

$I < HI < HBr$

81POL/RAI S. K. Pollack, B. C. Raine, and W. J. Hehre, "Determination of the Heats of Formation of the Isomeric Xylylenes by Ion Cyclotron Double Resonance Spectroscopy", J. Am. Chem. Soc. **103**, 6308 (1981).

ICR. Bracketing:

$3\text{-Clpyridine} < o\text{-}C_8H_8 < CF_3CH_2N(CH_3)_2$

$2\text{-Clpyridine} < p\text{-}C_8H_8 < C_2H_5NH_2$

77POL/WOL S. K. Pollack, J. F. Wolf, B. A. Levi, R. W. Taft, and W. J. Hehre, "Kinetic Detection of Common Intermediates in Gas Phase Ion-Molecule Reactions", J. Am. Chem. Soc. **99**, 1350 (1977).

ICR. Data related to TAFT scale; temperature assumed to be 320 K rather than 300 K.

83PRE/TZE H. F. Prest, W.-B. Tzeng, J. M. Brom, Jr., and C. Y. Ng, "Photoionization Study of $(H_2S)_2$ and $(H_2S)_3$", 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.

83RAK/BOH A. B. Rakshit and D. K. Bohme, "The Proton Affinity of C_3 and Heat of Formation of C_3H^+," Int. J. Mass Spectrom. Ion Phys., **49**, 275 (1983).

Flowing afterglow. Bracketing:

$CH_3OH < C_3 < CH_3CN$.

84RAK/BOH A. B. Raksit and D. K. Bohme, "Selected-Ion Flow Tube Methods Applied to the Bracketing of Proton Affinities. $PA(C_2N_2)$ and $PA(HC_3N)$" Int. J. Mass Spectrom. Ion Proc. **57**, 211 (1984).

Flowing afterglow. Bracketing:

$SO_2 < C_2N_2 < C_2H_4$

$CH_3NO_2 < HC_3N < CH_3CN$

80REE/FRE W. D. Reents, Jr. and B. S. Freiser, "Gas Phase Nitrosation of Benzene. Implications for Solution Electrophilic Aromatic Substitution Reactions" J. Am. Chem. Soc. **102**, 271 (1980).

ICR. Bracketing. $NH_3 < C_6H_5NO < (i\text{-}C_3H_7)_2O$

68REF/CHU K. M. A. Refaey and W. A. Chupka, "Photoionization of the Lower Aliphatic Alcohols with Mass Analysis", J. Chem. Phys. **48**, 5205 (1968).

Determination of appearance potentials of fragment ions from alcohols.

75RID D. P. Ridge, "Gas Phase Proton Affinities of Several Fluoroethylenes", J. Am. Chem. Soc. **97**, 5670 (1975).

ICR. Bracketing:

$H_2O < C_2H_3F \sim H_2S$

$C_2H_5I < CH_2CF_2 < CH_3OH$

$C_2H_5F < CHFCHF < H_2O$

$H_2O < C_2HF_3 < H_2S$

71ROC/SUT A. E. Roche, M. M. Sutton, D. K. Bohme, and H. I. Schiff, "Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. I. Relative Proton Affinities", J. Chem. Phys. **55**, 5480 (1971).

Flowing afterglow. Bracketing:

$N_2 < CF_4$, $NO < CH_4$

$Ar < H_2, O_2$ (Not included in Table)

82ROS/BUF H. M. Rosenstock, R. Buff, M. A. A. Ferreira, S. G. Lias, A. C. Parr, R. L. Stockbauer, and J. L. Holmes, "Fragmentation Mechanism and Energetics of Some Alkyl Halide Ions", J. Am. Chem. Soc. **104**, 2337 (1982).

Appearance potentials of $C_2H_5^+$ and $C_3H_7^+$ from alkyl halides.

77ROS/DRA H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, "Energetics of Gaseous Ions," J. Phys. Chem. Ref. Data **6**, Suppl. 1 (1977).

82ROY/MCM M. Roy and T. B. McMahon, "The Proton Affinity of Thioformaldehyde. Implications for the Heat of Formation of Thioformaldehyde and Thiomethyl Carbonium Ion from Ion Cyclotron Resonance Investigations of the Proton Transfer Reactions of $[CH_2SH]^{+}$", Org. Mass Spectrom. **17**, 392 (1982).

ICR. Bracketing:

$CF_3CO_2C_2H_5 < CH_2S < CH_3CHO$

79SAL/KEB P. P. S. Saluja and P. Kebarle, "Heat of Formation of the 2-Norbornyl Cation in the Gas Phase," J. Am. Chem. Soc. **101**, 1084 (1979).

High pressure mass spectrometer. Proton transfer equilibria observed in norbornene: anisole ($\Delta G_{560} = 1.5$ kcal/mol) and anisole: cyclohexanone ($\Delta G_{560} = -1.9$ kcal/mol) systems.

75SCH/BOH H. I. Schiff and D. K. Bohme, "Flowing Afterglow Studies at York University", Int. J. Mass Spectrom. Ion Phys. **16**, 167 (1975).

Review. Flowing afterglow.

84SHA/BLA R. B. Sharma, A. T. Blades, and P. Kebarle, "Protonation of Polyethers, Glymes and Crown Ethers in the Gas Phase," J. Am. Chem. Soc. **106**, 510 (1984).

High pressure mass spectrometer. Entropy changes determined.

81SHA/KEB D. K. Sen Sharma and P. Kebarle, "Stability and Reactivity of the Benzyl and Tropylium Cations in the Gas Phase," Can. J. Chem. **59**, 1592 (1981).

Determination of equilibrium constant of reaction: $C_6H_5CH_2^+ + (CH_3)_3CCl \rightleftharpoons (CH_3)_3C^+ + C_6H_5CH_2Cl$.

78SHE/GOB K. J. Shea, R. Gobeille, J. Bramblet, and E. Thompson, "Gas Phase Basicities of Silanamines", 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.

81SMI/ADA D. Smith, N. G. Adams, and W. Lindinger, "Reactions of the H_nS^+ Ions ($n=0$ to 3) with Several Molecular Gases at Thermal Energies", J. Chem. Phys. **75**, 3365 (1981).

SIFT. Bracketing: $CO < COS < S$

78SMI/MUN D. E. Smith and B. Munson, "Proton Affinities of Some Sulfur-Oxygen Compounds", J. Am. Chem. Soc. **100**, 497 (1978).

Bracketing. $CH_3F < SO_2F_2 < SO_2 < HSO_3F < C_2H_4$

$H_2O < H_2SO_4 \sim CF_3SO_3H < H_2S$

75SOL/FIE J. J. Solomon and F. H. Field, "Reversible Reactions of Gaseous Ions. IX. The Stability of C_4-C_7 Tertiary Alkyl Carbonium Ions", J. Am. Chem. Soc. **97**, 2625 (1975).

Heats of formation of alkyl ions from hydride transfer equilibria; related to the heat of formation of t $C_4H_9^+ = 165.8$ kcal/mol.

76SOL/FIE J. J. Solomon and F. H. Field, "Reversible Reactions of Gaseous Ions. X. The Intrinsic Stability of the Norbornyl Cation", J. Am. Chem. Soc. **98**, 1567 (1976).

Hydride transfer equilibrium constant determined for $t\text{-}C_4H_9^+ + \text{Norbornane} \rightarrow \text{Norbornyl}^+ + iso\text{-}C_4H_{10}$. Heat of formation of $t\text{-}C_4H_9^+$ taken as 165.8 kcal/mol.

75SOL/HAR B. H. Solka and A. G. Harrison, "Bimolecular Reactions of Trapped Ions. Part XI. Rates and Equilibria in Proton Transfer Reactions of $CH_3SH_2^{+}$", Int. J. Mass Spectrom. Ion Phys. **17**, 379 (1975).

Equilibrium:

$CH_3CHOH^+ + CH_3SH$, $\Delta G = -0.5$ kcal/mol

$CH_3SH_2^+ + C_2H_5CHO$, $\Delta G = -2$ kcal/mol
$CH_3SH_2^+ + (CH_3)_2O$, $\Delta G = -4$ kcal/mol

72SOL/POR J. J. Solomon and R. F. Porter, "Chemical Ionization Mass Spectrometry of Selected Boron Hydrides", J. Am. Chem. Soc. **94**, 1443 (1972).
Bracketing: $H_2O < B_5H_9 < H_2S$

74STA/BEA R. H. Staley and J. L. Beauchamp, "Basicities and Ion-Molecule Reactions of the Methylphosphines in the Gas Phase by Ion Cyclotron Resonance Spectroscopy", J. Am. Chem. Soc. **96**, 6252 (1974).
ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

74STA/BEA(2) R. H. Staley and J. L. Beauchamp, "Relationship of Nitrogen Lone Pair Interactions to Thermodynamic Parameters Associated with Amine Basicities", J. Am. Chem. Soc. **96**, 1604 (1974).
ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

75STA/BEA R. H. Staley and J. L. Beauchamp, "Equilibrium Studies of Gas Phase Ion-Molecule Reactions. Ion Cyclotron Resonance Results for the Reaction $CO_2H^+ + CH_4 = CH_5^+ + CO_2$", J. Chem. Phys. **62**, 1998 (1975).
ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

76STA/KLE R. H. Staley, J. E. Kleckner, and J. L. Beauchamp, "Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles", J. Am. Chem. Soc. **98**, 2081 (1976).
ICR. Data relative to TAFT scale; temperature assumed to be 320 K.

77STA/TAA R. H. Staley, M. Taagepera, W. G. Henderson, I. Koppel, J. L. Beauchamp, and R. W. Taft, "Effects of Alkyl and Fluoroalkyl Substitution on the Heterolytic and Homolytic Bond Dissociation Energies of Protonated Amines", J. Am. Chem. Soc. **99**, 326 (1977).
ICR. Data related to TAFT scale; temperature assumed to be 320 K.

77STA/WIE R. H. Staley, R. D. Wieting, and J. L. Beauchamp, "Carbenium Ion Stabilities in the Gas Phase and Solution. An Ion Cyclotron Resonance Study of Bromide Transfer Reactions Involving Alkali Ions, Alkyl Carbenium Ions, Acyl Cations, and Cyclic Halonium Ions", J. Am. Chem. Soc. **99**, 5964 (1977).
ICR. Data related to TAFT scale; temperature assumed to be 320 K.

79STE/BEA A. E. Stevens and J.L. Beauchamp, "Gas Phase Organometallic Chemistry. Mechanism and Energetics of Methane Formation Resulting from Protonation of $(CO)_5MnCH_3$", J. Am. Chem. Soc. **101**, 245 (1979).
ICR. Bracketing:
$CH_3CH{=}CH_2 < (CO)_5MnCH_3 \sim CH_3OH < CH_3CHO$

81STE/BEA A. E. Stevens and J. L. Beauchamp, "Metal-Hydrogen Bond Energies in Protonated Transition Complexes", 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 for $(C_5H_5)_2Ni$ results. Entropy corrections unknown.

80STO/CAM J. A. Stone, J. R. M. Camicioli, and M. C. Baird, "Protonation of Dimethylmercury. Complexing Reactions of CH_3Hg^+ in the Gas Phase", Inorg. Chem. **19**, 3128 (1980).
ICR. Bracketing:
$C_6H_6 < (CH_3)_2Hg < C_6H_5CH_3$

82STO/SPL J. A. Stone, D. E. Splinter, and S. Y. Kong, "A Comparison of the Relative Binding Energies of H^+ and NO^+ to Aromatic and Haloaromatic Bases by High Pressure Mass Spectrometry", Can. J. Chem. **60**, 910 (1982).
High pressure mass spectrometer. Proton transfer equilibrium constants in mixtures of methyl formate with toluene, 3-fluorotoluene, 2-fluorotoluene, and 4-fluorotoluene.

77SUM/POL K. D. Summerhays, S. K. Pollack, R. W. Taft, and W. J. Hehre, "Gas Phase Basicities of Substituted Anilines. Inferences About the Role of Solvent in Dictating Site of Protonation", J. Am. Chem. Soc. **99**, 4585 (1977).
ICR. Data related to TAFT scale; temperature assumed to be 320 K.

81TAA/SUM M. Taagepera, K. D. Summerhays, W. J. Hehre, R. D. Topsom, A. Pross, L. Radom, and R. W. Taft, " Analysis of the Acidities of 3- and 4- Substituted Pyridinium and Anilinium Ions", 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 R. W. Taft, R. McIver, W. J. Hehre, 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, private 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".

75TAF R. W. Taft, "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 R. W. Taft, "Protonic Acidities and Basicities in the Gas Phase and in Solution: Substituent and Solvent Effects", 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".

73TAF/TAA R. W. Taft, M. Taagepera, K. D. Summerhays, and J. Mitsky, "Regarding Heats of Solution of Gaseous Anilinium and Pyridinium Ions in Water and Intrinsic Basicities in Aqueous Solution", J. Am. Chem. Soc. **95**, 3811 (1973).
ICR. See comments under TAFT.

78TAF/WOL R. W. Taft J. F. Wolf, J. L. Beauchamp, G. Scorrano, and E. M. Arnett, "Solvent Effects of Water and Fluorosulfuric Acid on Proton Transfer Equilibria and the Energies of Solvation of Gaseous Onium Ions", J. Am. Chem. Soc. **100**, 1240 (1978).
ICR. See comments under TAFT.

78TAN/MAC K. Tanaka, G. I. Mackay, and D. K. Bohme, "Rate and Equilibrium Constant Measurements for Gas-Phase Proton Transfer Reactions Involving H_2O, H_2S, HCN, and H_2CO", Can. J. Chem. **56**, 193 (1978).
Flowing afterglow.

79TAN/MAC S. D. Tanner, G. I. Mackay, A. C. Hopkinson, and D. K. Bohme, "Proton Transfer Reactions of HCO^+ at 298 K", Int. J. Mass Spectrom. Ion Phys. **29**, 153 (1979).
Flowing afterglow.

79TIE/AND P. W. Tiedemann, S. L. Anderson, S. T. Ceyer, T.

Hirooka, C. Y. Ng, B. H. Mahan, and Y. T. Lee, "Proton Affinities of Hydrogen Halides Determined by the Molecular Beam Photoionization Method", J. Chem. Phys. **71**, 605 (1979).

Appearance energies of fragment ions from molecular clusters.

81TRA J. C. Traeger, "Heat of Formation for sec-Butyl Cation in the Gas Phase", Org. Mass Spec. **16**, 193 (1981).

Appearance potential of sec-$C_4H_9^+$ from halogenated butanes, and correction to 298 K.

81TRA/MCL J. C. Traeger and R. G. McLoughlin, "Absolute Heats of Formation for Gas Phase Cations", 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 J. C. Traeger, R. G. McLoughlin and A. J. C. Nicholson, "Heat of Formation of Acetyl Cation in the Gas Phase", J. Am. Chem. Soc. **104**, 5318 (1982).

Appearance potentials of CH_3CO^+ ions; correction to 298 K.

78TSA W. Tsang, "Thermal Stability of Primary Amines," Int. J. Chem. Kinet. **10**, 41 (1978).

Heats of formation of benzyl, tert-butyl radicals.

79VAJ/HAR J. H. Vajda and A. G. Harrison, "Proton Affinities of Some Olefinic Carbonyl Compounds and Heats of Formation of $C_nH_{2n-1}O^+$ Ions", Int. J. Mass Spectrom. Ion Phys. **30**, 293 (1979).

High pressure mass spectrometer. Crotonaldehyde measured vs. acetone, methyl acetate, and ethyl acetate; methacrolein measured vs. acetone, p-dioxane, and n-butyl formate; acrolein measured vs. ethyl formate.

82VIL/FUT H. Villinger, J. H. Futrell, F. Howorka, N. Duric, and W. Lindinger, "The Proton Transfer from ArH^+ to Various Neutrals", J. Chem. Phys. **76**, 3529 (1982).

75VOG/BEA J. Vogt and J. L. Beauchamp, "Reactions of CHF_2^+ with n-Donor Bases by Ion Cyclotron Resonance Spectroscopy. The Proton Affinity of Difluorocarbene", J. Am. Chem. Soc. **97**, 6682 (1975).

ICR. Bracketing: $HCN < CF_2 < CH_2O$

77WAN/DES J.-S. Wang, A. J. DeStefano, and R. F. Porter, "Acidity of $B_5H_9^+$ and Stability of the B_5H_8 Radical", Inorg. Chem. **17**, 1374 (1978).

High pressure mass spectrometer. Bracketing:

$C_6H_6 < B_5H_8 < CH_3CHO$.

74WAR P. Warneck, "Heat of Formation of the HCO Radical", Z. Naturforsch. 29a, 350 (1974).

79WIB/FIS N. Wiberg, G. Fischer and H. Bachhuber, "Diazen und andere Distickstoffhydride: Bildungswarmen, Dissoziationsenergien, Auftrittspotentiale, Protonenaffinitaten", Z. Naturforsch. **34b**, 1385 (1979).

Ionization and appearance potentials in HN=NH, $H_2N=N$, and N_2H_4.

80WIG/BEA C. A. Wight and J. L. Beauchamp, "Acidity, Basicity, and Ion-Molecule Reactions of Isocyanic Acid in the Gas Phase by Ion Cyclotron Resonance Spectroscopy", J. Phys. Chem. **84**, 2503 (1980).

ICR: Related to TAFT scale; temperature corrected to 320 K.

76WIL/LEB A. D. Williamson, P. R. LeBreton, and J. L. Beauchamp, "Photoionization Mass Spectrometry of 2-Fluoropropane and 2,2-Difluoropropane. A Novel Determination of the Proton Affinity of Vinyl Fluoride and 1,1-Difluoroethylene", 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).

76WIL/LOS C. Willis, F. P. Lossing and R. A. Back, "The Heat of Formation of N_2H_2 and the Proton Affinity of N_2", Can. J. Chem. **54**, 1 (1976).

Heat of formation of N_2H^+ as a fragment ion in N_2H_2.

75WIL/MCC M. S. Wilson and J. A. McCloskey, "Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity", J. Am. Chem. Soc. **97**, 3436 (1975).

High pressure mass spectrometer. Bracketing: All compounds bracketed relative to NH_3, CH_3NH_2, $(CH_3)_2NH$, and $(CH_3)_3N$.

77WOL/ABB J. F. Wolf, J. L. M. Abboud, and R. W. Taft, "Regarding Polarizability Effects of Hydrocarbon Substituents on Base Strengths in Solution", J. Org. Chem. **42**, 3316 (1977).

ICR. Results given in figure form.

75WOL/HAR J. F. Wolf, P. G. Harch, and R. W. Taft, "Concerning Negligible Aqueous Solvent Effects on Proton Transfer Equilibria of Aryl Carbocations", J. Am. Chem. Soc. **97**, 2904 (1975).

ICR: Related to TAFT scale. Data corrected from 300 K to 320 K.

77WOL/STA J. F. Wolf, R. H. Staley, I. Koppel, M. Taagepera, R. T. McIver, Jr., J. L. Beauchamp, and R. W. Taft, "Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements", J. Am. Chem. Soc. **99**, 5417 (1977).

ICR. Data corrected from 300 K to 320 K (R. W. Taft, personal communication).

73YAM/KEB R. Yamdagni and P. Kebarle, "Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of a,w-Diamines", J. Am. Chem. Soc. **95**, 3504 (1973).

High pressure mass spectrometer.

76YAM/KEB R. Yamdagni and P. Kebarle, "Gas Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements" J. Am. Chem. Soc. **98**, 1320 (1976).

High pressure mass spectrometer. Data assumed to have been superseded by data in LAU/KEB, when species studied have been duplicated. Other data corrected to LAU/KEB scale; free energy change values multiplied by 1.05.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species

(Prepared in collaboration with Mahnaz Motevalli-Aliabadi)

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H$(MH^+)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[Ar]	Ar RN 7440-37-1	88.6	371.	0.	0.	DEF	277.	1159.
[AsC_3H_9]	$(CH_3)_3As$ RN 593-88-4	213.4	893.	3.	13.(10)	[77PED/RYL]	155.	650.
[AsF_3]	AsF_3 RN 7784-35-2	155.	648.	-188.	-786.	[82/TN270]	23.	95.5
[AsH_3]	AsH_3 RN 7784-42-1	179.2	750.	16.	66.	[82/TN270]	202.	846.
[B_2H_6]	B_2H_6 RN 19287-45-7	~146	~611	9.	36.	[82/TN270]	228.	955.
[$B_3H_5N_3$]	B-Borazinyl radical RN xxxxx	193.6	810.					
[$B_3H_6N_3$]	Borazine RN 6569-51-3	194.1	812.	-122.	-512.	[82/TN270]	49.	206.
[$B_4C_2H_6$]	1,6-$C_2B_4H_6$ RN 20693-67-8	207.	866.	-90.	-378.	Est	68.	286.
[B_4H_8]	B_4H_8 RN 12007-71-5	188	787					
[B_4H_{10}]	B_4H_{10} RN 18283-93-7	~144	~602	16.	66.	[82/TN270]	237.	993.5
[$B_5C_2H_7$]	2,4-$C_2B_5H_7$ RN 20693-69-0	168.	703.	-85.	-356.	Est	113.	471.
[B_5H_8]	B_5H_8 RN 65930-58-7	184.	770.					
[B_5H_9]	B_5H_9 RN 19624-22-7	169.	707.	17.	73.	[82/TN270]	214.	896.
[Br]	Br RN 10097-32-2	132.0	552.	26.7	111.7	[82/TN270]	259.3	1085.
[$BrCH_3$]	CH_3Br RN 74-83-9	165.7	693.	-9.	-37.(1)	[77PED/RYL]	191.	800.
[BrCN]	BrCN RN 506-68-3	178.3	746.	43.	181.(4)	[77PED/RYL]	231.	965.
[BrC_5H_4N]	4-Bromopyridine RN 1120-87-2	217.9	912.	38.	161.	Est	186.	779.
[BrC_5H_4N]	3-Bromopyridine RN 626-55-1	215.1	900.	38.	161.	Est	189.	791.
[BrC_5H_4N]	2-Bromopyridine RN 109-04-6	214.7	898.	38.	161.	Est	189.	793.
[BrC_6H_5]	Bromobenzene RN 108-86-1	182.4	763.	25.	104.(3)	[77PED/RYL]	208.	871.
[BrC_6H_6N]	3-$BrC_6H_4NH_2$ RN 591-19-5	208.1	871.	26.	108.	Est	183.	767.
[$BrC_7H_{12}N$]	3-Bromo-1-azabicyclo[2.2.2]-octane RN xxxxx	227.1**	950.**	1.	3.	Est	139.	583.
[BrH]	HBr RN 10035-10-6	136	569	-9.	-36.	[82/TN270]	221.	925.
[$CClH_3$]	CH_3Cl RN 74-87-3	~168	~703	-19.5	-82.(1)	[79KUD/KUD]	178.	745.
[CClN]	ClCN RN 506-77-4	175.7	735.	32.	133.(1)	[77PED/RYL]	222.	928.
[CCl_2]	CCl_2 RN 1605-72-7	~200.0	~837.	45.	189.	[78AUS/LIA]	211.	882.
[CFH_3]	CH_3F RN 593-53-3	150.	628.	-56.	-234.(8)	[78KUD/KUD]	160.	668.
[CF_2]	CF_2 RN 2154-59-8	171.9	719.	-52.	-217.	[77LIA/AUS]	142.	594.
[CF_2H_2]	CH_2F_2 RN 75-10-5	147.	615.	-108.	-453.(8)	[78KUD/KUD]	110.	462.
[CF_2O]	F_2CO RN 353-50-4	160.5	671.5	-153.	-640.(1)	[77PED/RYL]	52.	218.5
[CF_3H]	CHF_3 RN 75-46-7	147.	615.	-166.	-695.(8)	[78KUD/KUD]	52.5	220.
[CF_3HO_3S]	CF_3SO_3H RN 1493-13-6	~169	~707	-282.	-1179.	Est	-85.	-356.
[CF_3NO]	CF_3NO RN 334-99-6	169	707	-126.	-529.	Est	70.	294.
[CF_4]	CF_4 RN 75-73-0	~126	~527	-223.	-933.(8)	[81BOM/BER]	17.	70.
[CHN]	HNC RN xxxxx	190.2	796.	51.	212.(8)	[82PAU/HEH]	226.	947.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton	Affinity	$\Delta_f H$(M)		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[CHN]	HCN RN 74-90-8	171.4	717.	32.	135.	[82/TN270]	226.	947.
[CHNO]	HNCO RN 75-13-8	173.3	725.	-25.	-105.(13)	[75COM]	167.	700.
[CHO]	HCO RN 17030-74-9	152.	636.	9.	37.(5)	[82MCM/GOL]	223.	931.
[CH_2N_2]	CH_2N_2 RN 334-88-3	205.	858.	55.	230.(17)	[78VOG/WIL]	216.	902.
[CH_2O]	HCOH RN xxxxx	229.	958.	31.	131.	[82PAU/HEH2]	168.	703.
[CH_2O]	H_2CO RN 50-00-0	171.7	718.	-26.	-109.(1)	[77PED/RYL]	168.	703.
[CH_2O_2]	HCOOH RN 64-118-6	178.8	748.	-90.5	-379.(1)	[78CHA/ZWO]	96.	403.
[CH_2S]	CH_2S RN 865-36-1	186.	778.	21.5	90.(8)	[82ROY/MCM]	201.	842.
[CH_3I]	CH_3I RN 74-88-4	~171	~715	3.5	15.(1)	[77PED/RYL]	198.	830.
[CH_3NO]	$HCONH_2$ RN 75-12-7	198.4	830.	-44.	-186.	[69BEN/CRU]	123.	514.
[CH_3NO_2]	CH_3ONO RN 624-91-9	192.5	805.	-16.	-67.(2)	[74BAT/CHR]	157.	658.
[CH_3NO_2]	CH_3NO_2 RN 75-52-5	179.2	750.	-18.	-75.(1)	[77PED/RYL]	168.5	705.
[CH_4]	CH_4 RN 74-82-8	132.0	552.	-18.	-75.	[74SCO]	216.	903.
[CH_4N]	CH_2NH_2 RN 54088-53-8	199	833	36.	149.(8)	[82MCM/GOL]	202.	846.
[CH_4O]	CH_3OH RN 67-56-1	181.9	761.	-48.	-202.(1)	[77PED/RYL]	135.5	567.
[CH_4S]	CH_3SH RN 74-93-1	187.4	784.	-5.	-23.(1)	[77PED/RYL]	173.	723.
[CH_5N]	CH_3NH_2 RN 74-89-5	214.1	896.	-5.	-23.(1)	[77PED/RYL]	146.	611.
[CH_5P]	CH_3PH_2 RN 593-54-4	204.1	854.	-7.	-30.	Est	154.	646.
[CH_6N_2]	CH_3NHNH_2 RN 60-34-4	214.1**	896.**	23.	95.(1)	[77PED/RYL]	174.	729.
[CO]	CO RN 630-08-0	141.9	594.	-26.5	-111.	[82/TN270]	197.	824.
[COS]	COS RN 463-58-1	151.	632.	-34.	-142.(1)	[77PED/RYL]	181.	756.
[CO_2]	CO_2 RN 124-38-9	130.9	548.	-94.	-393.	[82/TN270]	141.	589.
[CS]	CS RN 2944-05-0	175	732	56.	234.	[82/TN270]	247.	1032.
[CS_2]	CS_2 RN 75-15-0	167.1	699.	28.	117.(1)	[77PED/RYL]	226.5	948.
[C_2BrH_5]	C_2H_5Br RN 74-96-4	~171	~715	-15.	-62.(2)	[77PED/RYL]	180.	753.
[C_2ClH_2N]	$ClCH_2CN$ RN 107-14-2	179.5	751.	20.5	86.	Est	207.	865.
[$C_2ClH_3O_2$]	$CH_2ClCOOH$ RN 79-11-8	182.4	763.	-104.	-435.(9)	[77PED/RYL]	79.	332.
[C_2ClH_5]	C_2H_5Cl RN 75-00-3	169.	707.	-27.	-112.(1)	[77PED/RYL]	170.	711.
[$C_2Cl_3HO_2$]	CCl_3COOH RN 76-03-9	183.5	768.	-106.	-444.(10)	Est	76.	318.
[$C_2Cl_3H_3O$]	Cl_3CCH_2OH RN 115-20-8	177.4	742.	-70.	-293.	Est	118.	495.
[C_2Cl_3N]	CCl_3CN RN 545-06-2	175.8	735.5	19.5	82.	Est	209.	876.5
[C_2D_6O]	$(CD_3)_2O$ RN 17222-37-6	190.6	797.	-44.	-184.(1)	[77PED/RYL]	131.	549.
[C_2FH_3]	C_2H_3F RN 75-02-5	175.	732.	-33.	-139.(2)	[76WIL/LEB]	157.	659.
[$C_2FH_3O_2$]	CH_2FCOOH RN 144-49-0	183.5	768.	-140.	-586.	Est	42.	176.
[C_2FH_5]	C_2H_5F RN 353-36-6	165.	690.	-63.	-263.(2)	[75CHE/ROD]	138.	577.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_2FH_6N]$	$CH_2FCH_2NH_2$ RN 406-34-8	212.3	888.	-55.	-229.	Est	99.	413.
$[C_2F_2H_2]$	CH_2CF_2 RN 75-38-7	176	736	-82.	-345.(10	[76WIL/LEB]	107.	449.
$[C_2F_2H_2]$	(E)-CHFCHF RN 1630-78-0	166	694	-70.	-293.	[80STA/VOG]	130.	543.
$[C_2F_2H_4O]$	CF_2HCH_2OH RN 359-13-7	176.2	737.	-155.	-649.	Est	34.	144.
$[C_2F_2H_5N]$	$CF_2HCH_2NH_2$ RN 430-67-1	207.5	868.	110.	462.(6)	Est	269.	1124.
$[C_2F_3H]$	C_2F_3H RN 359-11-5	~169	~707	-117.	-491.(8)	[77PED/RYL]	79.	332.
$[C_2F_3HO]$	CF_3CHO RN 75-90-1	165.1	691.	-189.	-790.(50)	[75HAR/THY]	12.	49.
$[C_2F_3HO_2]$	CF_3COOH RN 76-05-1	169.0	707.	-246.	-1031.(1)	[77PED/RYL]	-50.	-208.
$[C_2F_3H_3O]$	CF_3CH_2OH RN 75-89-8	169.0	707.	-212.	-888.(5)	[77PED/RYL]	-15.5	-65.
$[C_2F_3H_4N]$	$CF_3CH_2NH_2$ RN 753-90-2	202.5	847.	-167.5	-701.	Est	-4.	-18.
$[C_2F_3N]$	CF_3CN RN 353-85-5	166.1	695.	-118.	-495.(3)	[71JANAF]	81.	340.
$[C_2F_4O]$	CF_3CFO RN 354-34-7	160.2	670.	-249.	-1042.	Est	-43.5	-182.
$[C_2H_2]$	C_2H_2 RN 74-86-2	153.3	641.	54.	228.(1)	[82/TN270]	266.9	1117.
$[C_2H_2O]$	$CH_2C{=}O$ RN 463-51-4	198.0	828.	-11.	-48.(8)	[71NUT/LAU]	157.	657.
$[C_2H_3]$	C_2H_3 radical RN 2669-89-8	~181	~757	70.5	295.(8)	[82MCM/GOL]	255.	1068.
$[C_2H_3N]$	CH_3CN RN 75-05-8	188.4	788.	18.	74.(1)	[83AN/MAN]	195.	816.
$[C_2H_3NS]$	CH_3SCN RN 556-64-9	195.9	820.	38.	160.	[82/TN270]	208.	870.
$[C_2H_3NS]$	CH_3NCS RN 556-61-6	195.9	820.	31.	131.	[82/TN270]	201.	841.
$[C_2H_4]$	C_2H_4 RN 74-85-1	162.6	680.	12.	52.(1)	[77PED/RYL]	215.6	902.
$[C_2H_4N_2]$	$NCCH_2NH_2$ RN xxxxx	197.4	826.	26.	108.	Est	194.	812.
$[C_2H_4O]$	c-C_2H_4O (Oxirane) RN 75-21-8	187.9	786.	-13.	-53.(1)	[77PED/RYL]	165.	691.
$[C_2H_4O]$	CH_3CHO RN 75-07-0	186.6	781.	-40.	-166.(1)	[77PED/RYL]	139.	583.
$[C_2H_4O_2]$	CH_3COOH RN 64-19-7	190.2	796.	-103.	-432.(1)	[77PED/RYL]	72.	302.
$[C_2H_4O_2]$	HCO_2CH_3 RN 107-31-3	188.9	790.	-85.	-356.(1)	[77PED/RYL]	92.	384.
$[C_2H_4S]$	c-C_2H_4S (Thiirane) RN 420-12-2	194.6	814.	19.5	82.(1)	[77PED/RYL]	191.	798.
$[C_2H_5I]$	C_2H_5I RN 75-03-6	~176	~736	-2.	-9.(1)	[77PED/RYL]	187.5	785.
$[C_2H_5N]$	Aziridine (Azirane) RN 151-56-4	215.7	902.	30.	127.(1)	[77PED/RYL]	180.	755.
$[C_2H_5N]$	$CH_2{=}CHNH_2$ RN 593-67-9	219.1	917.	7.	29.	[81ELL/DIX]	154.	643.
$[C_2H_5N]$	$CH_3CH{=}NH$ RN 20729-41-3	213.9	895.	2.	8.(17)	[79ELL/EAD]	154.	643.
$[C_2H_5NO]$	CH_3CONH_2 RN 60-35-5	206.2	863.	-57.	-238.(1)	[77PED/RYL]	103.	429.
$[C_2H_5NO]$	$HCONHCH_3$ RN 123-39-7	205.8	861.	-45.	-187.(3)	Est	115.	481.
$[C_2H_5NO_2]$	NH_2CH_2COOH (Glycine) RN 56-40-6	211.6	885.	-93.	-391.(5)	[77NGA/SAB]	61.	254.
$[C_2H_5NO_2]$	C_2H_5ONO RN 109-95-5	197.3	825.5	-25.	-103.	[74BAT/CHR]	144.	601.5

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_fH(M)$		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_2H_5NO_2$]	$C_2H_5NO_2$ RN 79-24-3	184.8	773.	-24.	-102.(1)	[77PED/RYL]	156.5	655.
[C_2H_5P]	c-C_2H_4PH (Phosphirane) RN 6569-82-0	191.4	801.	-16.	-69.(2)	Est	158.	660.
[C_2H_6]	C_2H_6 RN 74-84-0	143.6	601.	-20.	-84.	[74SCO]	202.	845.
[C_2H_6Hg]	CH_3HgCH_3 RN 593-74-8	~186	~778	22.	94.(1)	[77PED/RYL]	202.	846.
[$C_2H_6N_2$]	(E)-$CH_3N=NCH_3$ RN 4143-41-3	206.9	866.	36.	149.	[82PAM/ROG]	194.	813.
[C_2H_6O]	$(CH_3)_2O$ RN 115-10-6	192.1	804.	-44.	-184.(1)	[77PED/RYL]	130.	542.
[C_2H_6O]	C_2H_5OH RN 64-17-5	188.3	788.	-56.	-235.(1)	[77PED/RYL]	121.	507.
[C_2H_6OS]	$(CH_3)_2SO$ RN 67-68-5	211.3	834.	-36.	-151.(1)	[77PED/RYL]	118.	495.
[C_2H_6S]	$(CH_3)_2S$ RN 75-18-3	200.6	839.	-9.	-38.(1)	[77PED/RYL]	156.	653.
[C_2H_6S]	C_2H_5SH RN 75-08-1	190.8	798.	-11.	-46.(1)	[77PED/RYL]	164.	686.
[$C_2H_6S_2$]	CH_3SSCH_3 RN 624-92-0	~196	~820	-6.	-24.(1)	[77PED/RYL]	164.	686.
[C_2H_7N]	$(CH_3)_2NH$ RN 124-40-3	220.6	923.	-4.5	-19.(1)	[77PED/RYL]	140.5	588.
[C_2H_7N]	$C_2H_5NH_2$ RN 75-04-7	217.0	908.	-11.	-48.(1)	[77PED/RYL]	137.	574.
[C_2H_7NO]	$NH_2(CH_2)_2OH$ RN 141-43-5	221.3	926.	-48.	-202.	[77REI/PRA]	96.	402.
[$C_2H_7O_3P$]	$(CH_3O)_2PHO$ RN 868-85-9	207.2	867.					
[C_2H_7P]	$(CH_3)_2PH$ RN 676-59-5	216.3	905.	-16.	-66.	Est	134.	559.
[$C_2H_8N_2$]	1,2-Diaminoethane RN 107-15-3	225.9	945.	-4.	-18.(2)	[77PED/RYL]	135.	567.
[$C_2H_8N_2$]	$(CH_3)_2NNH_2$ RN 57-14-7	219.9	920.	20.	84.(2)	[77PED/RYL]	166.	694.
[C_2N_2]	NCCN RN xxxxx	162.	678.					
[C_3]	C_3 RN 12075-35-3	~185	~774	200(4)	837(17)	[83RAK/BOH]	~381.	~1593.
[C_3ClH_4N]	$Cl(CH_2)_2CN$ RN 542-76-7	187.5	784.5	10.	41.	Est	188.	786.5
[C_3FH_5O]	CH_3COCH_2F RN 430-51-3	192.0	803.	-91.5	-383.	Est	82.	344.
[C_3FH_8N]	$FCH_2CH_2CH_2NH_2$ RN 462-41-9	217.8	911.	-61.	-254.	Est	87.	365.
[$C_3F_2H_4O$]	CFH_2COCFH_2 RN 453-14-5	187	782	-126.	-529.	Est	52.	219.
[$C_3F_3H_3O$]	CH_3COCF_3 RN 421-50-1	174.2	729.	-194.	-812.	Est	-3.	-11.
[$C_3F_3H_3O_2$]	$HCOOCH_2CF_3$ RN 32042-38-9	179.4	751.	-256.	-1073.	Est	-70.	-293.5
[$C_3F_3H_3O_2$]	CF_3COOCH_3 RN 431-47-0	178.8	748.	-242.	-1013.	Est	-55.	-231.
[$C_3F_3H_6N$]	$CF_3CH_2CH_2NH_2$ RN 460-39-9	210.6	881.	-175.	-731.	Est	-20.	-82.
[$C_3F_3H_6N$]	$CF_3CH_2NHCH_3$ RN 2730-67-8	209.8	878.	-167.	-699.	Est	-11.	-47.
[$C_3F_3H_6N$]	$CF_3N(CH_3)_2$ RN 677-41-8	193.8	811.	-187.	-784.(15)	Est	-15.	-65.
[$C_3F_4H_2O$]	CF_2HCOCF_2H RN 360-52-1	170.	711.	-228.	-953.	Est	-32.	-134.
[C_3F_5N]	C_2F_5CN RN 422-04-8	167.1	699.	-219.	-917.(29)	[73THY/HAR]	-20.5	-86.
[$C_3F_6H_2O$]	$(CF_3)_2CHOH$ RN 920-66-1	165.0	690.	-381	-1595.	Est	-180.	-754.
[C_3F_6O]	$(CF_3)_2CO$ RN 684-16-2	161.5	676.	-334.	-1397.	[72GOR/T600]	-130.	-543.
[C_3GeH_8]	$(CH_3)_2Ge=CH_2$ RN 82064-99-1	204.9	857.	19.	81.	[82PIE/HEH]	180.	754.
[C_3HN]	HCCCN RN xxxxx	184.	770.					

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H$(MH^+)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_3H_2N_2$]	$CH_2(CN)_2$ RN 109-77-3	175.6	735.	63.5	266.(2)	[77PED/RYL]	254.	1061.
[C_3H_3]	c-C_3H_3 radical RN xxxxx	175.8	735.	99.	414.(17)	[82MCM/GOL]	289.	1210.
[C_3H_3N]	CH_2=CHCN RN 107-13-1	189.7	794.	44.	184.	[82CHU/NGU]	220.	920.
[C_3H_3NO]	Oxazole RN 288-42-6	208.4	872.	-4.	-16.(1)	[78MCC/HAM]	153.	642.
[C_3H_3NO]	Isooxazole RN 288-14-2	202.3	846.	19.	79.(1)	[78MCC/HAM]	182.	763.
[C_3H_3NS]	Thiazole RN 288-47-1	213.2	892.	36.5	153.(10)	Est	189.	791.
[$C_3H_3N_3$]	1,3,5-Triazine RN 290-87-9	201.1	841.	54.	226.(1)	[82BYS]	219.	915.
[C_3H_4]	Cyclopropene RN 2781-85-3	198	828	66.	277.(3)	[77PED/RYL]	234.	979.
[C_3H_4]	H_2C=C=CH_2 RN 463-49-0	186.3	779.	46.	191.(1)	[77PED/RYL]	225.	942.
[C_3H_4]	CH_3CCH RN 74-99-7	182	761	45.	187.(2)	[77PED/RYL]	228.	956.
[$C_3H_4N_2$]	Imidazole RN 288-32-4	219.8	920.	35.	145.(2)	[80SAB]	180.5	755.
[$C_3H_4N_2$]	Pyrazole RN 288-13-1	209.8	878.	44.	185.(2)	[80SAB]	200.	837.
[C_3H_4O]	CH_3CH=CO RN 6004-44-0	199.4	834.	-25.	-105.	[80DEM/WUL]	141.	591.
[C_3H_4O]	CH_2=CHCHO RN 107-02-8	193.9	811.	-18.	-77.	[79VAJ/HAR]	153.	642.
[C_3H_5]	c-C_3H_5 radical RN xxxxx	188.	787.	62.	261.	[80DEF/MCI]	240.	1004.
[C_3H_5]	CH_2=CH-CH_2 radical RN xxxxx	175.8	735.	43.	179.	[81TSA]	229.	958.5
[C_3H_5N]	1-Azabicyclo[1.1.0]butane RN 19540-05-7	212**	887**	75.	314.	Est	229.	957.
[C_3H_5N]	$HCCCH_2NH_2$ RN 2450-71-7	210.8	882.	53.	222.	Est	208.	870.
[C_3H_5N]	C_2H_5CN RN 107-12-0	192.6	806.	12.	51.	[82CHU/NGU]	185.	775.
[$C_3H_5O_3P$]	2,6,7-Trioxa-1-phospha-bicyclo[2.2.1.]heptane RN 279-53-8	194.0	812.	-146.5	-613.	Est	25.	105.
[C_3H_6]	c-C_3H_6 RN 75-19-4	179.8	752.	13.	53.(1)	[77PED/RYL]	198.5	831.
[C_3H_6]	CH_3CH=CH_2 RN 115-07-1	179.5	751.	5.	20.(1)	[77PED/RYL]	191.	799.
[$C_3H_6N_2$]	$H_2N(CH_2)_2CN$ RN 151-18-8	207.0	866.	22.	91	Est	180.	755.
[$C_3H_6N_2$]	CH_3NHCH_2CN RN 5616-32-0	206.0	862.	25.5	107.	Est	185.	775.
[C_3H_6O]	CH_2=$CHOCH_3$ RN 107-25-5	207.4	868.	-24.	-100.(7)	Est	134.	562.
[C_3H_6O]	c-C_3H_6O (Oxetane) RN 503-30-0	196.9	824.	-19.	-81.(1)	[77PED/RYL]	149.	625.
[C_3H_6O]	$(CH_3)_2CO$ RN 67-64-1	196.7	823.	-52.	-217.(1)	[76CHA/ZWO]	117.	490.
[C_3H_6O]	2-Methyloxirane RN 75-56-9	194.7	815.	-23.	-95.(1)	[77PED/RYL]	148.	620.
[C_3H_6O]	C_2H_5CHO RN 123-38-6	189.6	793.	-45.	-187.(2)	[77PED/RYL]	131.	550.
[$C_3H_6O_2$]	CH_3COOCH_3 RN 79-20-9	197.8	828.	-99.	-414.(1)	[*80SVO/UCH]	69.	288.
[$C_3H_6O_2$]	$HCO_2C_2H_5$ RN 109-94-4	193.1	808.	-92.	-387.	Est	80.	335.
[$C_3H_6O_2$]	C_2H_5COOH RN 79-09-4	191.8	802.	-107.	-448.(2)	[77PED/RYL]	67.	279.5
[$C_3H_6O_3$]	$(CH_3O)_2CO$ RN 616-38-6	200.2	838.	-131.5	-550.	Est	34.	142.
[C_3H_6S]	Thietane RN 287-27-4	201.3**	842.**	14.5	61.(1)	[77PED/RYL]	179.	749.
[C_3H_6S]	2-Methylthiirane RN 1072-43-1	200.6**	839.**	11.	46.(2)	[77PED/RYL]	176.	737.
[C_3H_7]	i-C_3H_7 RN 19252-53-0	159.8	669.	21.5	91.	[81TSA]	227.4	951.5

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_fH(M)$		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_3H_7N]$	$CH_2{=}C(CH_3)NH_2$ RN 4427-28-5	226.3	947.	8.	32.	Est	147.	615.
$[C_3H_7N]$	Azetidine RN 503-29-7	223.5	935.	24.	99.(4)	Est	166.	694.
$[C_3H_7N]$	N-Methylaziridine RN 1072-44-2	221.6	927.	30.	127.	Est	174.	730.
$[C_3H_7N]$	$(CH_3)_2C{=}NH$ RN 38697-07-3	221	925	2.	10.	[70BEN/O`N]	147.	615.
$[C_3H_7N]$	2-Methylaziridine RN 75-55-8	219.2**	917.**	22.	91.(6)	Est	168.	704.
$[C_3H_7N]$	$H_2C{=}CHCH_2NH_2$ RN 107-11-9	215.8	903.	14.	57.	Est	163.5	684.
$[C_3H_7N]$	c-$C_3H_5NH_2$ RN 765-30-0	215.0**	899.**	18.	77.(1)	[77PED/RYL]	169.	708.
$[C_3H_7NO]$	$(CH_3)_2NCHO$ RN 68-12-2	211.4	884.	-46.	-192.(2)	[77PED/RYL]	108.	453.5
$[C_3H_7NO_2]$	Sarcosine RN xxxxx	218.7	915.	-88.	-367.(1)	[78SAB/LAF]	59.	248.
$[C_3H_7NO_2]$	L-Alanine RN 56-41-7	214.8	899.	-99.	-415.(4)	[77NGA/SAB]	52.	216.
$[C_3H_7NO_2]$	i-C_3H_7ONO RN 541-42-4	201.9	845.	-32.	-133.(4)	[74BAT/CHR]	132.	552.
$[C_3H_7NO_2S]$	L-Cysteine RN 3374-22-9	214.3	897.					
$[C_3H_7NO_3]$	L-Serine RN 302-84-1	216.8	907.	-134.	-561.	Est	15.	62.
$[C_3H_7O_3P]$	2-Methoxy-1,3,2-dioxaphospholane RN 3741-36-4	212.7	890.	-164.	-688.	Est	-11.	-48.
$[C_3H_8]$	C_3H_8 RN 74-98-6	150.	628.	-25.	-105.	[74SCO]	191.	797.
$[C_3H_8O]$	$CH_3OC_2H_5$ RN 540-67-0	196.4	822.	-52.	-216.(1)	[77PED/RYL]	118.	492.
$[C_3H_8O]$	i-C_3H_7OH RN 67-63-0	191.2	800.	-65.	-273.(1)	[77PED/RYL]	109.	457.
$[C_3H_8O]$	n-C_3H_7OH RN 71-23-8	190.8	798.	-61.	-255.(1)	[77PED/RYL]	114.	476.
$[C_3H_8Pb]$	$(CH_3)_2Pb{=}CH_2$ RN 82065-01-8	223.9	937.	59.	247.	[82PIE/HEH]	200.	840.
$[C_3H_8S]$	$CH_3SC_2H_5$ RN 624-89-5	203.5	851.	-14.	-60.(1)	[77PED/RYL]	148.	619.
$[C_3H_8S]$	i-C_3H_7SH RN 75-33-2	194.1	812.	-18.	-76.(1)	[77PED/RYL]	153.	642.
$[C_3H_8S]$	n-C_3H_7SH RN 107-03-9	191.6	802.	-16.	-68.(1)	[77PED/RYL]	158.	660.
$[C_3H_8Si]$	$(CH_3)_2Si{=}CH_2$ RN 4112-23-6	226.4	947.	-1.	-5.	[82PIE/HEH]	138.	579.
$[C_3H_8Sn]$	$(CH_3)_2Sn{=}CH_2$ RN 82065-00-7	215.8	903.	31.5	132.	[82PIE/HEH]	181.	759.
$[C_3H_9N]$	$(CH_3)_3N$ RN 75-50-3	225.1	942.	-6.	-24.(1)	[77PED/RYL]	135.	564.
$[C_3H_9N]$	$(CH_3)(C_2H_5)NH$ RN 624-78-2	222.8	932.	-11.	-46.(2)	Est	132.	552.
$[C_3H_9N]$	i-$C_3H_7NH_2$ RN 75-31-0	218.6	915.	-20.	-84.(1)	[*79MAJ/SVO]	127.	531.
$[C_3H_9N]$	n-$C_3H_7NH_2$ RN 107-10-8	217.9	912.	-17.	-70.(1)	[*79MAJ/SVO]	131.	548.
$[C_3H_9NO]$	$NH_2(CH_2)_3OH$ RN 156-87-6	228.6	956.5	-52.	-218.	Est	85.	356.
$[C_3H_9NO]$	$CH_3OCH_2CH_2NH_2$ RN 109-85-3	223.3	934.	-44.	-184.(3)	Est	98.	412.
$[C_3H_9O_3P]$	$P(OCH_3)_3$ RN 121-45-9	220.6	923.	-167.	-697.(20)	Est	-21.	-92.
$[C_3H_9O_3PS]$	$SP(OCH_3)_3$ RN 29952-66-7	214.5	897.	-183.	-767.	Est	-32.	-134.
$[C_3H_9O_4P]$	$OP(OCH_3)_3$ RN 512-56-1	212.0	887.	-264.5	-1107.	Est	-111.	-464.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H$(MH$^+$)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_3H_9P]$	$(CH_3)_3P$ RN 594-09-2	227.1	950.	-24.	-101.(5)	[77PED/RYL]	114.	479.
$[C_3H_{10}N_2]$	1,3-Diaminopropane RN 109-76-2	234.1	979.	-8.	-32.	Est	124.	518.
$[C_3H_{10}OSi]$	$(CH_3)_3SiOH$ See References to Table 1: 75PIT/BUR							
$[C_4F_2H_7NO]$	$CF_2HCON(CH_3)_2$ RN 667-50-5	207.2	867.					
$[C_4F_3H_5O_2]$	$CF_3CO_2C_2H_5$ RN 383-63-1	184.6	772.	-249.	-1042.	Est	-68.	-284.
$[C_4F_3H_7O]$	$C_2H_5OCH_2CF_3$ RN 461-24-5	186.4	780.	-216.	-904.	Est	-37.	-154.
$[C_4F_3H_8N]$	$CF_3CH_2N(CH_3)_2$ RN 819-06-7	215.0	900.	-167.	-700.	Est	-17.	-69.
$[C_4F_3H_8N]$	$CF_3(CH_2)_3NH_2$ RN 819-46-5	214.3	897.	-180.	-755.	Est	-29.	-121.5
$[C_4F_4H_4O_2]$	$CF_3COOCH_2CH_2F$ RN 1683-88-1	178.6	747.	-292.5	-1224.	Est	-105.	-441.
$[C_4F_6H_4O]$	$(CF_3)_2C(CH_3)OH$ RN 1515-14-6	167.0	699.	-391.	-1636.	Est	-192.	-805.
$[C_4F_7N]$	C_3F_7CN RN 375-00-8	167.4	700.	-308.	-1290.(40)	[73THY/HAR]	-110.	-460.
$[C_4F_9HO]$	$(CF_3)_3COH$ RN 2378-02-1	163.1	682.	-549.	-2297.	Est	-346.	-1449.
$[C_4F_9H_2N]$	$(CF_3)_3CNH_2$ RN 2809-92-9	191.5**	801.**	-503.	-2104.	Est	-329.	-1375.
$[C_4H_4N_2]$	Pyridazine RN 289-80-5 (1,2-Diazine)	215.6	902.	66.	278.(1)	[77PED/RYL]	216.5	906.
$[C_4H_4N_2]$	Pyrimidine (1,3-Diazine) RN 289-95-2	210.5	881.	46.	193.(2)	[77NAB/SAB]	201.	842.
$[C_4H_4N_2]$	Pyrazine (1,4-Diazine) RN 290-37-9	209.0	874.	47.	196.(2)	[81STE/BAR]	203.5	852.
$[C_4H_4N_2O]$	2(1H)-Pyrimidinone RN 557-01-7	~208	~870	-11.	-47.	Est	146.	613.
$[C_4H_4N_2O_2]$	Uracil RN 66-22-8	~208	~870	-72.	-303.(2)	[77NAB/SAB]	85.	357.
$[C_4H_4N_2S_2]$	Dithiouracil RN 2001-93-6	~217	~907	51.	214.	Est	200.	836.
$[C_4H_4O]$	Furan RN 110-00-9	192.2	804.	-8.	-35.(1)	[77PED/RYL]	165.	691.
$[C_4H_4S]$	$c-C_4H_4S$ (Thiophene) RN 110-02-1	196.5	822.	27.	115.(1)	[81KUD/KUD3]	197.	823.
$[C_4H_5N]$	Pyrrole RN 109-97-7	207.6	868.	26.	108.	[80WIL/BAE]	184.	769.
$[C_4H_5N]$	$c-C_3H_5CN$ RN 5500-21-0	195.4	817.5	44.	183.(1)	[82FUC/HAL]	214.	895.5
$[C_4H_5NO_2]$	$NCCOOC_2H_5$ RN 623-49-4	179.5	751.	-52.	-217.	Est	134.	562.
$[C_4H_5N_3O]$	Cytosine RN 71-30-7	223.8	936.	-14.	-59.(10	[80SAB2]	128.	535.
$[C_4H_6]$	1-Methylcyclopropene RN 3100-04-7	206	862	58.	244.(1)	[77PED/RYL]	218.	912.
$[C_4H_6]$	$(E)-CH_2=CHCH=CH_2$ RN 106-99-0	193**	807.5*	26.	110.(1)	[77PED/RYL]	199.	832.5
$[C_4H_6]$	Cyclobutene RN 822-35-5	191**	799**	37.5	157.(2)	[77PED/RYL]	212.	888.
	Note: Heat of formation of cyclobutyl ion = 225 kcal/mol, 941 kJ/mol							
$[C_4H_6]$	CH_3CCCH_3 RN 503-17-3	187**	782**	35.	145.(1)	[77PED/RYL]	213.	893.
$[C_4H_6N_2]$	1-Methylimidazole RN 616-47-7	228.9	958.	43.5	182.	Est	180.	754.
$[C_4H_6N_2]$	4-Methylimidazole RN 822-36-6	224.4	939.	26.	110.	Est	167.	701.
$[C_4H_6O]$	$CH_2=CHCOCH_3$ RN 78-94-4	200.2	838.	-29.	-125.	[79VAJ/HAR]	136.	567.
$[C_4H_6O]$	$CH_3CH=CHCHO$ RN 4170-30-3	199.7	835.5	-22.	-91.(E)	[79VAJ/HAR]	144.	603.5
$[C_4H_6O]$	$CH_2=C(CH_3)CHO$ RN 78-85-3	195.2	817.	-25.	-106.	[79VAJ/HAR]	145.	607.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H$(MH$^+$)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_4H_6O_2$]	$CH_3COCOCH_3$ RN 431-03-8	194.8	815.	-78.	-327.	[77PED/RYL]	93.	388.
[C_4H_7N]	i-C_3H_7CN RN 78-82-0	194.3	813.	5.	23.	[82CHU/NGU]	177.	740.
[C_4H_7N]	n-C_3H_7CN RN 109-74-0	193.7	810.	7.	31.	[82CHU/NGU]	179.	751.
[$C_4H_7NO_4$]	L-Aspartic Acid RN 617-45-8	216.7	907.	-193.	-808.	Est	-44.	-184.5
[$C_4H_7O_2$]	1,4-Dioxyl radical RN 4598-47-4	193.8	811.					
[$C_4H_7O_3P$]	2,6,7-Trioxa-1-phosphabicyclo-[2.2.2]octane RN 280-45-5	207.1	866.5	-128.5	-538.	Est	30.	125.5
[$C_4H_7O_3P$]	1-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.1]heptane RN 61580-09-4	198.1	829.	-154.	-646.	Est	13.	55.
[C_4H_8]	$(CH_3)_2C=CH_2$ RN 115-11-7	195.9	820.	-4.	-17.(1)	[77PED/RYL]	166.	693.
[C_4H_8]	E-$CH_3CH=CHCH_3$ RN 624-64-6	179.4	751.	-3.	-12.(1)	[77PED/RYL]	183.	767.
[$C_4H_8N_2$]	$NCCH_2N(CH_3)_2$ RN 926-64-7	211.1	883.	34.	141.	Est	188.	788.
[$C_4H_8N_2O_3$]	L-Asparagine RN 3130-87-8	219.8	920.	-141.	-591.	Est	5.	19.
[C_4H_8O]	$C_2H_5OCH=CH_2$ RN 109-92-2	208.2	871.	-34.	-141.(1)	[77PED/RYL]	124.	518.
[C_4H_8O]	$CH_3COC_2H_5$ RN 78-93-3	199.8	836.	-57.	-239.(1)	[76CHA/ZWO]	109.	455.
[C_4H_8O]	c-C_4H_8O (Tetrahydrofuran) RN 109-99-9	198.8	831.	-44.	-184.(1)	[77PED/RYL]	123.	514.
[C_4H_8O]	i-C_3H_7CHO RN 78-84-2	192.6	806.	-52.	-216.(1)	[77PED/RYL]	121.	508.
[C_4H_8O]	n-C_3H_7CHO RN 123-72-8	191.5	801.	-50.	-208.(2)	[77PED/RYL]	124.	521.
[$C_4H_8O_2$]	$C_2H_5COOCH_3$ RN 554-12-1	200.2	838.	-103.	-432.	[80HOL/LOS]	62.	260.
[$C_4H_8O_2$]	1,3-Dioxane RN 505-22-6	198.8	832.	-81.	-338.(1)	[82BYS/MAN]	86.	360.
[$C_4H_8O_2$]	1,4-Dioxane RN 123-91-1	193.8	811.	-75.5	-316.(1)	[82BYS/MAN]	96.	403.
[$C_4H_8O_2$]	$CH_3COOC_2H_5$ RN 141-78-6	200.7	840.	-106.	-443.(1)	[*80SVO/UCH]	59.	247.
[$C_4H_8O_2$]	$HCOOCH(CH_3)_2$ RN 625-55-8	196.0	820.	-97.	-405.	[70BEN/O'N]	73.	305.
[$C_4H_8O_2$]	$HCO_2(n\text{-}C_3H_7)$ RN 110-74-7	194.2	812.5	-110.	-462.	[*80SVO/UCH]	61.	255.5
[$C_4H_8O_2S$]	$C_2H_5S(OCH_3)CO$ RN 38103-96-7	201.0	841.	-100.	-420.	Est	64.	269.
[$C_4H_8O_3$]	$C_2H_5OCOOCH_3$ RN 623-53-0	202.7	848.	-141.	-592.	Est	21.5	90.
[C_4H_9N]	$(CH_3)_2NCH=CH_2$ RN 5763-87-1	227.8	953.	15.	62.	Est	153.	639.
[C_4H_9N]	Pyrrolidine RN 123-75-1	225.2	942.	-1.	-3.(1)	[77PED/RYL]	140.	585.
[C_4H_9N]	$CH_3CH=NC_2H_5$ RN 1190-79-0	222.7	932.	4.	18.(1)	Est	147.	616.
[C_4H_9N]	$CH_2=C(CH_3)CH_2NH_2$ RN 2878-14-0	218.2**	913.**	5.	21.	Est	152.5	638.
[C_4H_9NO]	Morpholine RN 110-91-8	219.4	918.	12.	51.	Est	158.	663.
[C_4H_9NO]	Dimethylacetamide RN 127-19-5	216.8	907.	-55.6	-233.	[*78BEA/LEE]	93.	390.
[C_4H_9NO]	n-C_3H_7NHCHO RN 6281-94-3	210.0**	879.	-61.	-256.	Est	94.5	395.
[$C_4H_9NO_2$]	t-C_4H_9ONO RN 540-80-7	205.7	861.	-41.	-172.(4)	[74BAT/CHR]	119.	497.
[$C_4H_9NO_3$]	L-Threonine RN xxxxx	218.6	915.	-141.	-592.	Est	6.	23.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_4H_9O_3P$]	2-Methoxy-1,3,2-dioxaphosphorinane RN 31121-06-9	219.4	918.	-175.	-733.	Est	-29.	-121.
[C_4H_{10}]	iso-C_4H_{10} RN 75-28-5	163.3	683.	-32.	-135.	[74SCO]	170.	712.
[$C_4H_{10}N_2$]	Piperazine RN 110-85-0	224.2	938.	6.	25.(1)	Est	147.	617.
[$C_4H_{10}N_2$]	c-C(CH_3)(C_2H_5)NHNH RN 4901-75-1	214.9**	899.**	32.	133.(17)	Est	182.5	764.
[$C_4H_{10}O$]	t-C_4H_9OH RN 75-65-0	193.7	810.	-75.	-312.(3)	[77PED/RYL]	97.	408.
[$C_4H_{10}O$]	n-C_4H_9OH RN 71-36-3	191.1	799.5	-66.	-275.(1)	[77PED/RYL]	109.	455.5
[$C_4H_{10}O$]	$(C_2H_5)_2O$ RN 60-29-7	200.2	838.	-60.	-252.(1)	[*80MAJ/WAC]	105.5	440.
[$C_4H_{10}O_2$]	$HO(CH_2)_4OH$ RN 110-63-4	212**	887**	-102.	-427.(3)	Est	52.	216.
[$C_4H_{10}O_2$]	$CH_3OCH_2CH_2OCH_3$ RN 110-71-4	204.9	857.	-81.	-340.	[67LOU/LAI]	79.5	333.
[$C_4H_{10}S$]	$(C_2H_5)_2S$ RN 352-93-2	205.0	858.	-22.	-94.(1)	[77PED/RYL]	138.	578.
[$C_4H_{10}S$]	t-C_4H_9SH RN 75-66-1	196.9	824.	-26.	-110.(1)	[77PED/RYL]	142.5	596.
[$C_4H_{11}N$]	$(CH_3)_2(C_2H_5)N$ RN 598-56-1	227.5	952.	-11.	-47.(2)	Est	127.	531.
[$C_4H_{11}N$]	$(C_2H_5)_2NH$ RN 109-89-7	225.9	945.	-17.	-73.(1)	[*79MAJ/SVO]	125.	512.
[$C_4H_{11}N$]	t-$C_4H_9NH_2$ RN 75-64-9	220.8	924.	-29.	-121.(1)	[77PED/RYL]	116.	485.
[$C_4H_{11}N$]	sec-$C_4H_9NH_2$ RN 13952-84-6	220.5	922.	-25.	-105.(1)	[*79MAJ/SVO]	120.	502.5
[$C_4H_{11}N$]	i-$C_4H_9NH_2$ RN 78-81-9	218.8	915.	-24.	-100.(1)	[*79MAJ/SVO]	123.	515.
[$C_4H_{11}N$]	n-$C_4H_9NH_2$ RN 109-73-9	218.4	914.	-22.	-92.(1)	[*79MAJ/SVO]	125.	524.
[$C_4H_{11}NO$]	$NH_2(CH_2)_4OH$ RN 13325-10-5	233.8	978.	-57.	-240.	Est	74.5	312.
[$C_4H_{12}N_2$]	1,4-Diaminobutane RN 110-60-1	237.6	994.	-13.	-53.	Est	115.	483.
[$C_4H_{12}OSi$]	$(CH_3)_3SiOCH_3$ RN 1825-61-2	~203	~849	-112.	-468.(8)	Est	51.	213.
[$C_4H_{14}OSi_2$]	$((CH_3)_2SiH)_2O$ RN 3277-26-7	~203	~849	-156.	-655.	Est	6.	26.
[C_4NiO_4]	$(CO)_4Ni$ RN 13463-39-3	180**	753**	-143.	-598.(4)	[77PED/RYL]	43.	179.
[$C_5ClH_3N_4$]	6-Chloropurine RN 87-42-3	~208	~870	43.	179.	Est	200.	839.
[C_5ClH_4N]	4-Chloropyridine RN 626-61-9	217.8	911.	26.	108.	Est	174.	727.
[C_5ClH_4N]	3-Chloropyridine RN 626-60-8	214.8	899.	26.	108.	Est	177.	739.
[C_5ClH_4N]	2-Chloropyridine RN 109-09-1	214.4	897.	25.	103.	Est	176.	736.
[C_5FH_4N]	4-Fluoropyridine RN 694-52-0	216.6	906.	-14.	-57.	Est	135.	567.
[C_5FH_4N]	3-Fluoropyridine RN 372-47-4	214.3	897.	-13.	-56.	Est	138.	577.
[C_5FH_4N]	2-Fluoropyridine RN 372-48-5	210.6	881.	-16.	-68.	Est	139.	581.
[$C_5F_3H_7O_2$]	$CF_3CO_2(n-C_3H_7)$ RN 383-66-4	185.7	777.	-254.	-1064.	Est	-74.	-311.
[C_5FeO_5]	$(CO)_5Fe$ RN 13463-40-6	~202	~845	-173.	-725.(7)	[77PED/RYL]	-9.5	-40.
[C_5HMnO_5]	$(CO)_5MnH$ RN 16972-33-1	201**	841**	-177.	-740.(10)	[82CON/ZAF]	-12.	-51.
[$C_5H_4N_2O_2$]	4-Nitropyridine RN 1122-61-8	208.5	872.	33.	137.	Est	190.	795.
[$C_5H_4N_4$]	Purine RN 120-73-0	219.3	917.5	55.	230.	Est	201.	842.5

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_5H_4N_4O$]	Hypoxanthine RN 68-94-0	~217	~907	12.	50.	[*/85CHI]	~161.	~672.
[C_5H_5]	c-C_5H_5 radical RN xxxxx	~199	~833	58.	242.(6)	[82McM/GOL]	229.	957.
[C_5H_5N]	Pyridine RN 110-86-1	220.8	924.	33.	140.(1)	[79KUD/KUD3]	178.	746.
[C_5H_5NNiO]	(C_5H_5)NiNO RN 12071-73-7	200.1**	837.**					
[C_5H_5NO]	Pyridine-N-oxide RN 694-59-7	220.3	922.	14.5	61.	Est	160.	669.
[$C_5H_5N_5$]	Adenine RN 73-24-5	223.5	935.	49.	207.(8)	[83KIR/DOM]	191.	802.
[$C_5H_5N_5O$]	Guanine RN 73-40-5	~223	~933	0.5	2.	[*/85CHI]	~143	~599.
[C_5H_6]	c-C_5H_6 RN 542-92-7	199.6	835.	31.	131.(4)	[77PED/RYL]	197.	826.
[$C_5H_6N_2$]	2-Pyridinamine RN 504-29-0	223.8	936.	28.	118.(1)	[84BIC/PIL]	170.	711.
[$C_5H_6N_2$]	3-Pyridinamine RN 462-08-8	221.0	925.	34.	144.(2)	[84BIC/PIL]	179.	749.
[$C_5H_6N_2$]	4-Pyridinamine RN 504-24-5	230*	962*	31.	130.(1)	[84BIC/PIL]	167.	697.
[$C_5H_6N_2O_2$]	Thymine RN 65-71-4	208.8	874.	-79.	-329.(4)	[77NAB/SAB]	78.	327.
[C_5H_6O]	2-Methylfuran RN 534-22-5	205.6	860.	-19.	-80.	Est	141.	590.
[C_5H_6S]	2-Methylthiophene RN 554-14-3	205.7	861.	20.	84.(1)	[77PED/RYL]	180.	753.
[C_5H_8]	3,3-Dimethylcyclopropene RN 3907-06-0	203	849	50.	209.	[79AUE/BOW]	213.	890.
[C_5H_8]	(E)-1,3-Pentadiene RN 2004-70-8	201.8**	844.**	18.	77.(1)	[77PED/RYL]	182.	763.
[C_5H_8]	1-Methylcyclobutene RN xxxxx	201	841	28.	118.	[79AUE/BOW]	193.	807.
[C_5H_8]	$CH_2=CHC(CH_3)=CH_2$ RN 78-79-5	200.4**	838.**	18.	75.(1)	[77PED/RYL]	183.	767.
[C_5H_8]	$(CH_3)_2CHCCH$ RN 598-23-2	198**	828**	32.5	136.	[69BEN/CRU]	200.	838.
[C_5H_8]	c-$C_3H_5CH=CH_2$ RN 693-86-7	197.6	827.	36.	149.(1)	[*81CHI/HYM]	204.	852.
[C_5H_8]	$C_2H_5CCCH_3$ RN 627-21-4	196**	820**	30.5	128.(4)	[77PED/RYL]	200.	838.
[C_5H_8]	c-C_5H_8 RN 142-29-0	183.4	767.5	9.	36.(2)	[82ALL/DOD]	191.	799.
[C_5H_8O]	c-$C_3H_5COCH_3$ RN 765-43-5	205.1	858.	-28.	-119.(1)	[83FUC/SMI]	133.	555.
[C_5H_8O]	Cyclopentanone RN 120-92-3	198.8	832.	-46.	-194.(2)	[*76MEY/HOT]	121.	506.
[$C_5H_8O_2$]	$CH_3COCH=C(OH)CH_3$ RN 123-54-6	207.8	869.	-92.	-384.(1)	[79HAC/PIL]	66.	277.
[$C_5H_8O_2$]	c-$C_3H_5COOCH_3$ RN 2868-37-3	202.9	849.	-74.	-308.	[83FUC/SMI]	89.	373.
[C_5H_9N]	n-C_4H_9CN RN 110-59-8	194.0	812.	2.	10.	[82CHU/NGU]	174.	728.
[C_5H_9NO]	c-$C_4H_6N(2-OCH_3)$ RN 5264-35-7	225.9	945.	-36.	-152.	Est	103.	433.
[C_5H_9NO]	1-Methyl-2-pyrrolidinone RN 872-50-4	216.8	907.	-50.	-211.	[*72GAF]	98.	412.
[$C_5H_9NO_2$]	c-$C_4H_7NH(2-COOH)$ (L-Proline) RN 609-36-9	220.2	921.	-87.	-366.(4)	[78SAB/LAF]	58.	243.
[$C_5H_9NO_3$]	$CH_3CONHCH_2COOCH_3$ RN xxxxx	217.7	911.	-140.	-585.	Est	8.	34.
[$C_5H_9NO_4$]	L-Glutamic Acid RN 617-65-2	216.5	906.	-120.	-503.	Est	29.	121.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity kcal/mol	Proton Affinity kJ/mol	$\Delta_f H(M)$ kcal/mol	$\Delta_f H(M)$ kJ/mol	Reference	$\Delta_f H(MH^+)$ kcal/mol	$\Delta_f H(MH^+)$ kJ/mol
[$C_5H_9O_3P$]	4-Methyl-3,6,7,-trioxa-1-phospha-[2.2.2.]-octane RN 1449-91-8	210.0	879.	-136.	-571.	Est	19.	80.
[C_5H_{10}]	$(CH_3)_2C{=}CHCH_3$ RN 513-35-9	196.4	822.	-10.	-42.(1)	[77PED/RYL]	159.	666.
[$C_5H_{10}N_2O_3$]	L-Glutamine RN 585-21-7	218.4	914.	-74.5	-312.	Est	73.	304.
[$C_5H_{10}O$]	c-$C_4H_7O(2\text{-}CH_3)$ RN 96-47-9	203.6	852	-52.	-218.	Est	110.	461.
[$C_5H_{10}O$]	$(C_2H_5)_2CO$ RN 96-22-0	201.4	843.	-62.	-258.(1)	[*79SAL/PEA]	102.	429.
[$C_5H_{10}O$]	$(i\text{-}C_3H_7)COCH_3$ RN 563-80-4	201.1	841.	-63.	-262.(1)	[77PED/RYL]	102.	427.
[$C_5H_{10}O$]	c-$C_5H_{10}O$ RN 142-68-7	199.7	835.5	-53.	-223.(1)	[77PED/RYL]	113.	471.5
[$C_5H_{10}O$]	n-C_4H_9CHO RN 110-62-3	192.6	806.	-55.	-231.(3)	[77PED/RYL]	118.	493.
[$C_5H_{10}O_2$]	i-$C_3H_7COOCH_3$ RN 547-63-7	201.6	843.	-109.	-456.(1)	[83FUC/SMI]	55.	231.
[$C_5H_{10}O_2$]	$CH_3COOC_3H_7$ RN 109-60-4	200.6	839.	-108.5	-454.	[70BEN/O'N]	57.	237.
[$C_5H_{10}O_2$]	$C_3H_7COOCH_3$ RN 623-42-7	200.1	837.	-108.	-452.	[70HOL/LOS]	57.	241.
[$C_5H_{10}O_2$]	$HCO_2(n\text{-}C_4H_9)$ RN 592-84-7	194.8	815.	-103.	-430.	Est	68.	285.
[$C_5H_{11}N$]	$CH_3CH{=}CHN(CH_3)_2$ RN 6163-56-0	229.4	960.	6.	26.	Est	142.	596.
[$C_5H_{11}N$]	$(CH_3)_2C{=}NC_2H_5$ RN 15673-04-8	229.5**	960.**	-9.	-36.(9)	Est	127.5	534.
[$C_5H_{11}N$]	N-Methylpyrrolidine RN 120-94-5	228.7	957.	-0.5	-2.(2)	Est	136.5	571.
[$C_5H_{11}N$]	Piperidine RN 110-89-4	226.4	947.	-12.	-49.(2)	[77PED/RYL]	128.	535.5
[$C_5H_{11}NO_2$]	$(CH_3)_2CHCH(NH_2)COOH$ (L-Valine) RN 72-18-4	217.0	908.	-109.	-455.(1)	[77PED/RYL]	40.	167.
[$C_5H_{11}NO_2$]	$(CH_3)_2NCOOC_2H_5$ RN 687-48-9	213.7	894.	-109.	-456.	Est	43.	180.
[$C_5H_{11}NO_2S$]	L-Methionine RN 59-51-8	221.4	926.	-99.	-414.(4)	[81SAB/MIN]	45.	190.
[$C_5H_{12}O$]	$C_2H_5O(i\text{-}C_3H_7)$ RN 625-54-7	203.5	851.	-68.	-286.	Est	94.	393.
[$C_5H_{12}O$]	t-$C_4H_9OCH_3$ RN 1634-04-4	202.2	846.	-69.	-288.(4)	Est	95.	396.
[$C_5H_{12}O_2$]	$CH_3O(CH_2)_3OCH_3$ RN 17081-21-9	213.8	894.					
[$C_5H_{13}N$]	$(CH_3)(C_2H_5)_2N$ RN 616-39-7	230.0	962.	-17.	-70.	Est	119.	498.
[$C_5H_{13}N$]	$(CH_3)_2(i\text{-}C_3H_7)N$ RN 996-35-0	229.8	961.	-24.	-99.	Est	112.	470.
[$C_5H_{13}N$]	$(C_2H_5)(i\text{-}C_3H_7)NH$ RN 19961-27-4	227.4	951.	-25	-105.	Est	113.	474.
[$C_5H_{13}N$]	t-$C_5H_{11}NH_2$ RN 594-39-8	222.3	930.	-31.5	-132.	Est	112.	468.
[$C_5H_{13}N$]	neo-$C_5H_{11}NH_2$ RN 5813-64-9	219.3	917.5	-30.	-127.	Est	115.	480.5
[$C_5H_{13}N$]	n-$C_5H_{11}NH_2$ RN 110-58-7	218.9	916.	-26.	-110.	Est	120.5	504.
[$C_5H_{14}N_2$]	1,5-Diaminopentane RN 462-94-2	238.1	996.	-17.	-73.	Est	110.	461.
[$C_5H_{14}N_2$]	$(CH_3)_2N(CH_2)_3NH_2$ RN 109-55-7	236.4	989.	-7.	-30.	Est	122.	511.
[$C_5H_{15}NSi$]	$(CH_3)_3SiN(CH_3)_2$ RN 18135-05-2	~226	~946	-59(1)	-248(3)	[77PED/RYL]	81.	336.
[C_6ClH_5]	Chlorobenzene RN 108-90-7	181.7	760.	12.	51.(1)	[77PED/RYL]	196.	821.
[C_6ClH_6N]	2-Chloro-6-methylpyridine RN 18368-63-3	219**	916**	14.5	61.	Est	161.	675.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species—Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[C_6ClH_6N]	2-Chloro-4-methylpyridine RN 3678-62-4	218.6**	915.**	16.	66.	Est	163.	681.
[C_6ClH_6N]	4-Chlorobenzenamine RN 106-47-8	208.6	873.	13.	55.	Est	170.	712.
[C_6ClH_6N]	3-Chlorobenzeneamine RN 108-42-9	207.2	867.	13.	55.	Est	172.	718.
[C_6ClH_6NO]	6-Chloro-1-methyl-2(1H)-pyridinone RN 17228-63-6	217.8	911.	-21.	-88.(16)	Est	127.	531.
[C_6ClH_6NO]	2-Chloro-6-methoxypyridine RN 17228-64-7	215.9	903.	-21.	-89.	Est	128.5	538.
[C_6CrO_6]	$(CO)_6Cr$ RN 13007-92-6	180**	753**	-217.	-908.(1)	[77PED/RYL]	-31.	-131.
[C_6FH_5]	Fluorobenzene RN 462-06-6	182.6	764.	-28.	-116.(1)	[77PED/RYL]	155.	650.
[C_6FH_6N]	4-Fluorobenzenamine RN 371-40-4	208.1	871.	-26.	-109.	Est	131.5	550.
[C_6FH_6N]	3-Fluorobenzenamine RN 372-19-0	207.0	866.	-27.	-112.	Est	132.	552.
[$C_6F_2H_4$]	1,2-Difluorobenzene RN 367-11-3	181.8	761.	-70.	-294.(1)	[77PED/RYL]	114.	475.
[$C_6F_2H_4$]	1,3-Difluorobenzene RN 372-18-9	181.5	759.	-74.	-309.(1)	[77PED/RYL]	110.	462.
[$C_6F_2H_4$]	1,4-Difluorobenzene RN 540-36-3	181.2	758.	-73.	-307.(1)	[77PED/RYL]	111.	465.
[$C_6F_3H_3$]	1,2,4-$C_6H_3F_3$ RN 367-23-7	181.4	759.	-115.	-482.(1)	Est	69.	289.
[$C_6F_3H_3$]	1,3,5-$C_6H_3F_3$ RN 372-38-3	181.	757.	-122.	-512.(3)	Est	62.	261.
[$C_6F_3H_4N$]	4-Trifluoromethylpyridine RN 3796-24-5	212.8	890.	-128.	-536.	Est	25.	104.
[$C_6F_3H_4N$]	3-Trifluoromethylpyridine RN 3796-23-4	212.6	889.	-128.	-537.	Est	25.	103.5
[$C_6F_3H_4N$]	2-Trifluoromethylpyridine RN 368-48-9	211.5	885.	-127.	-532.	Est	27.	113.
[$C_6F_3H_9O_2$]	$CF_3CO_2(n-C_4H_9)$ RN 367-64-6	185.8	777.	-259.	-1085.	Est	-79.	-332.
[$C_6F_3H_{10}NO$]	$CF_3CONH(n-C_4H_9)$ RN 400-59-9	203.6	852.	-216.	-904.	Est	-54.	-226.
[$C_6F_4H_2$]	1,2,3,4-$C_6H_2F_4$ RN 551-62-2	181.1	758.	-152.	-638.(1)	Est	32.	134.
[$C_6F_4H_2$]	1,2,3,5-$C_6H_2F_4$ RN 2367-82-0	180.6	756.	-157.	-657.(1)	Est	28.	117.
[$C_6F_4H_2$]	1,2,4,5-$C_6H_2F_4$ RN 327-54-8	179.7	752.	-155.	-647.(3)	[78HAR/HEA]	31.	131.
[C_6F_5H]	C_6HF_5 RN 363-72-4	179.9	753.	-193.	-806.(7)	[77PED/RYL]	-7.	-29.
[C_6F_6]	C_6F_6 RN 392-56-3	177.7	743.	-226.	-946.(8)	[79PRI/SAP]	-38.	-159.
[$C_6H_3MnO_5$]	$(CO)_5MnCH_3$ RN 13601-24-6	183	766	-180.	-753.(4)	[82CON/ZAF]	3.	11.
[$C_6H_3O_5Re$]	$(CO)_5ReCH_3$ RN 14524-92-6	187**	782**	-183.	-765.(10)	[77TEL/RAB]	-4.	-17.
[C_6H_4]	o-Benzyne RN xxxxx	213.0	891.	119.	497.	[80POL/HEH]	271.	1136.
[$C_6H_4N_2$]	2-Pyridinecarbonitrile RN 100-70-9	208.1	871.	67.	281.(2)	[84BIC/PIL]	225.	940.
[$C_6H_4N_2$]	3-Pyridinecarbonitrile RN 100-54-9	209.3	876.	66.	278.(2)	[84BIC/PIL]	222.	932.
[$C_6H_4N_2$]	4-Pyridinecarbonitrile RN 100-48-1	210.3	880.	68.	284.(1)	[84BIC/PIL]	223.	934.
[C_6N_5NO]	Nitrosobenzene RN 586-96-9	204.8	857.					

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species—Continued

Formula	Compound (M)	Proton Affinity		Δ_fH(M)		Reference	Δ_fH(MH$^+$)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_6H_5NO]$	4-Pyridinecarboxaldehyde RN 872-85-5	215.2**	900.**	6.	24.	Est	156.	654.
$[C_6H_5NO_2]$	$C_6H_5NO_2$ RN 98-95-3	193.4	809.	16.	68.(1)	[77PED/RYL]	188.5	789.
$[C_6H_5O]$	C_6H_5O radical RN xxxxx	~204	~853	11.	48.	[82MCM/GOL]	173.	724.5
$[C_6H_6]$	Benzene RN 71-43-2	181.3	759.	20.	83.(1)	[77PED/RYL]	204.	854.5
$[C_6H_6IN]$	3-$IC_6H_4NH_2$ RN 626-01-7	208.9	874.	40.	166.	Est	196.	822.
$[C_6H_6N]$	C_6H_5NH radical RN xxxxx	219	916	57.	237.(8)	[82MCM/GOL]	198.4	830.
$[C_6H_6N_4]$	6-Methylpurine RN 2004-03-7	~223	~933	42.5	178.	Est	185.	775.
$[C_6H_6O]$	C_6H_5OH RN 108-95-2	196.3	821.	-23.	-96.(1)	[78KUD/KUD]	146.	613.
$[C_6H_6O]$	$(HCCCH_2)_2O$ RN 6921-27-3	190.8	798.	71.	299.	Est	246.	1031.
$[C_6H_7N]$	4-Methylpyridine RN 108-89-4	225.2	942.	25.	104.(1)	[77PED/RYL]	165.	692.
$[C_6H_7N]$	2-Methylpyridine RN 109-06-8	225.0	942.	24.	99.(1)	[77PED/RYL]	164.	688.
$[C_6H_7N]$	3-Methylpyridine RN 108-99-6	224.1	938.	25.	106.(1)	[77PED/RYL]	167.	698.
$[C_6H_7N]$	$(HCCCH_2)_2NH$ RN 6921-28-4	216.1	904.	113.	472.(4)	Est	262.	1098.
$[C_6H_7N]$	$C_6H_5NH_2$ RN 62-53-3	209.5	876.	21.	87.(1)	[78COL/BEN]	177.	740.5
$[C_6H_7NO]$	4-Methoxypyridine RN 620-08-6	227.6	952.	-3.	-13.	Est	135.	565.
$[C_6H_7NO]$	3-Methoxypyridine RN 7295-76-3	223.6	935.	-4.	-16.	Est	138.	578.5
$[C_6H_7NO]$	2-Methoxypyridine RN 1628-89-3	221.9	928.	-12.	-52.	Est	131.	550.
$[C_6H_7NO]$	1-Methyl-2-pyridinone RN 694-85-9	220.2	921.	-20.	-85.(10)	Est	125.	524.
$[C_6H_7NO]$	2-$(OH)C_6H_4NH_2$ RN xxxxx	214.2	896.	-20.	-85.	Est	131.	549.
$[C_6H_7NO]$	3-$(OH)C_6H_4NH_2$ RN 591-27-5	214.2	896.	-23.	-95.	Est	129.	539.
$[C_6H_7NS]$	4-(Methylthio)-pyridine RN 22581-72-2	225.5**	943.**	37.	155.	Est	177.	741.5
$[C_6H_7NS]$	2-(Methylthio)-pyridine RN 18438-38-5	222.0	929.	33.	138.	Est	177.	739.
$[C_6H_8]$	1-Methyl-3-methylenecyclobutene RN 15082-13-0	212**	887**	48.	202.	[79AUE/BOW]	202.	845.
$[C_6H_8N_2]$	1,2-$C_6H_4(NH_2)_2$ RN 95-54-5	212.8	890.	22.	92.(5)	Est	175.	732.
$[C_6H_8N_2]$	1,3-$C_6H_4(NH_2)_2$ RN 108-45-2	222.4	930.5	21.	88.	Est	164.	687.5
$[C_6H_8N_2]$	1,4-$C_6H_4(NH_2)_2$ RN 106-50-3	215.9	903.	23.	97.	Est	173.	723.
$[C_6H_8O]$	2,5-Dimethylfuran RN 625-86-5	209.1	875.	-30.	-125.	Est	127.	530.
$[C_6H_8O_2]$	1,3-Cyclohexanedione RN 504-02-9	211.9	886.	-79.	-330.	Est	75.	313.
$[C_6H_8O_2]$	1,2-Cyclohexanedione RN 765-87-7	204.8	857.	-70.	-293.(2)	Est	91.	380.
$[C_6H_9N]$	2,5-Dimethylpyrrole RN 625-84-3	218.4	914.	9.5	40.(1)	[77PED/RYL]	157.	656.
$[C_6H_9N_3O_2]$	L-Histidine RN xxxxx	231.9	970.	-31.	-129.	Est	103.	431.
$[C_6H_9O_3P]$	2,8,9,-Trioxa-1-phosphadamantane RN 281-33-4	213.8	894.	-166.	-694.	Est	-14.	-58.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_6H_{10}]$	1,3,3-Trimethylcyclopropene RN 3664-56-0	214.**	895**	41.	173.	[80WOL/HOL]	193.	808.
$[C_6H_{10}]$	$c-C_3H_5C(CH_3)=CH_2$ RN 4663-22-3	209.0	874.	22.	94.	[82KOZ/MAS]	179.	750.
$[C_6H_{10}]$	$CH_3CH=CHC(CH_3)=CH_2$ RN 1118-58-7	207.9**	870.**	11.	46.	Est(E)	169.	706.
$[C_6H_{10}]$	$CH_2=CH(CH_3)C(CH_2)_2$ RN 16906-27-7	206	862	21.	88.	[79AUE/BOW]	181.	756.
$[C_6H_{10}]$	$CH_3CH=C(CH_3)CH=CH_2$ RN 4549-74-0	205.7**	860.6**	10.	43.	[80WOL/HOL]	170.	712.
$[C_6H_{10}]$	$CH_2=C(CH_3)C(CH_3)=CH_2$ RN 513-81-5	202.1**	846.**	10.5	44.(1)	[77PED/RYL]	174.	728.5
$[C_6H_{10}]$	1,2-Dimethylcyclobutene RN 1501-58-2	201	841	17.	73.	[76JEN]	182.	762.
$[C_6H_{10}]$	$c-C_5H_8=CH_2$ RN 1528-30-9	200.8	840.	3.	12.(2)	[82ALL/DOD]	168.	702.
$[C_6H_{10}]$	1-Methylcyclopentene RN 693-89-0	196.9	824.	-1.	-4.(1)	[82ALL/DOD]	168.	702.
$[C_6H_{10}]$	$c-C_6H_{10}$ RN 110-83-8	189.3	792.	-1.	-5.(1)	[77PED/RYL]	175.	733.
$[C_6H_{10}O]$	Cyclohexanone RN 108-94-1	201.4	843.	-54.	-226.(2)	[*76MEY/HOT]	110.	461.
$[C_6H_{10}O]$	$(CH_2=CHCH_2)_2O$ RN 557-40-4	200.4	838.	-7.	-31.	Est	158.	661.
$[C_6H_{10}O_2]$	$CH_3COCH_2CH_2COCH_3$ RN 110-13-4	213.2	892.	-89.	-372.	Est	63.5	266.
$[C_6H_{11}N]$	$(CH_2=CHCH_2)_2NH$ RN 124-02-7	224.7	940.	34.	146.(6)	Est	175.	735.
$[C_6H_{11}NO]$	$c-C_5H_8N(2-OCH_3)$ RN 53687-79-9	228.1	954.	-42.	-176.(8)	Est	95.5	400.
$[C_6H_{11}NO]$	$c-C_5H_8N(2-O)1-CH_3$ RN 931-20-4	219.3	917.5	-57.	-237.(3)	[*74BEA/MUE]	90.	375.5
$[C_6H_{11}NO_3]$	$CH_3CONHCH(CH_3)COOCH_3$ (N-Acetyl alanine methyl ester) RN xxxxx	224.5	939.	-145.5	-609.	Est	-4.	-18.
$[C_6H_{12}]$	$(CH_3)_2C=C(CH_3)_2$ RN 563-79-1	199.0	833.	-16.	-69.(1)	[77PED/RYL]	150.	628.
$[C_6H_{12}]$	$CH_3CH=C(CH_3)C_2H_5$ RN 922-61-2	198.2	829.	-15.	-64.(1) (E)	[77PED/RYL]	152.	638.
$[C_6H_{12}]$	$(CH_3)_2C=CHCH_2CH_3$ RN 625-27-4	197.9	828.	-16.	-67.(1)	[77PED/RYL]	152.	635.
$[C_6H_{12}]$	$c-C_6H_{12}$ RN 110-82-7	~169	~707	-29.	-123.(1)	[77PED/RYL]	167.	700.
$[C_6H_{12}N_2]$	1,4-Diazabicyclo[2.2.2]octane RN 280-57-9	229.0	958.	21.	89.(7)	[71RAP/WES]	158.	661.
$[C_6H_{12}O]$	$t-C_4H_9COCH_3$ RN 75-97-8	202.3	846.	-69.	-290.(1)	[77PED/RYL]	94.	394.
$[C_6H_{12}O]$	2,2-Dimethyltetrahydrofuran	205.4	859.					
$[C_6H_{12}O]$	$c-C_6H_{12}O$ (Oxepane) RN 592-90-5	202	845	-3.	-12.	Est	161.	673.
$[C_6H_{12}O_2]$	$t-C_4H_9COOCH_3$ RN 598-98-1	202.8	848.5	-117.	-491.(1)	[*82FUC]	45.5	190.5
$[C_6H_{13}N]$	$(CH_3)_2NC(CH_3)=CHCH_3$ RN 52113-79-8	237	992	0.2	1.	Est	129.	539.
$[C_6H_{13}N]$	$(CH_3)_2C=CHN(CH_3)_2$ RN xxxxx	229.5	960.					
$[C_6H_{13}N]$	1-Methylpiperidine RN 626-67-5	229.7	961.	-12.	-50.(4)	Est	124.	519.
$[C_6H_{13}N]$	$n-C_3H_7CH=NC_2H_5$ RN 1611-12-7	225.3**	943.**	-5.	-21.	Est	135.	566.
$[C_6H_{13}N]$	$c-C_6H_{11}NH_2$ RN 108-91-8	221.2	925.5	-25.	-105.(1)	[79STE]	120.	500.
$[C_6H_{13}NO_2]$	$L-C_2H_5CH(CH_3)CH(NH_2)COOH$ RN 73-32-5	218.9	916.	-116.	-487.(10)	Est	30.	127.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_6H_{13}NO_2$]	$(CH_3)_2CHCH_2CH(NH_2)COOH$ (L-Leucine) RN 61-90-5	218.1	912.5	-117.	-488.(3)	[77PED/RYL]	31.	129.5
[$C_6H_{13}O_3P$]	cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane RN 7735-82-2	226.2	946.	-182.	-760.	Est	-42.	-176.
[$C_6H_{13}O_3P$]	trans-2-Methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane RN 41821-91-4	225	941	-182.	-760.	Est	-41.	-171.
[$C_6H_{14}N_2O_2$]	L-Lysine RN 56-87-1	230.3	963.5	-125.	-522.	Est	11.	44.5
[$C_6H_{14}O$]	$(i\text{-}C_3H_7)_2O$ RN 108-20-3	206.0	862.	-76.	-319.(2)	[*80MAJ/WAG]	84.	350.
[$C_6H_{14}O$]	$C_2H_5O(t\text{-}C_4H_9)$ RN 637-92-3	205.3	859.	-77.	-324.	Est	83.	347.
[$C_6H_{14}O$]	$(n\text{-}C_3H_7)_2O$ RN 111-43-3	202.3	846.	-70.	-293.(2)	[*80MAJ/WAG]	93.	391.
[$C_6H_{14}O_2$]	$CH_3O(CH_2)_4OCH_3$ RN 13179-96-9	221.8	928.	-98.	-408.	Est	46.	194.
[$C_6H_{14}OSi$]	$CH_2{=}C(CH_3)OSi(CH_3)_3$ RN 1833-53-0	221.	925.	-104.	-437.	Est	40.	168.
[$C_6H_{14}O_3$]	$CH_3(OCH_2CH_2)_2OCH_3$ RN 111-96-6	219.4	918.	-119.	-498.	Est	27.	114.
[$C_6H_{14}S$]	$(i\text{-}C_3H_7)_2S$ RN 625-80-9	209.6	877.	-34.	-142.(1)	[77PED/RYL]	122.	511.
[$C_6H_{14}S$]	$(n\text{-}C_3H_7)_2S$ RN 111-47-7	206.5	864.	-30.	-125.(1)	[77PED/RYL]	129.	541.
[$C_6H_{15}N$]	$(C_2H_5)_3N$ RN 121-44-8	232.3	972.	-22.	-93.(1)	[*79MAJ/SVO]	111.	465.
[$C_6H_{15}N$]	$(CH_3)_2(t\text{-}C_4H_9)N$ RN 918-02-5	232.0	971.	-24.	-102.	Est	109.	457.
[$C_6H_{15}N$]	$(i\text{-}C_3H_7)_2NH$ RN 108-18-9	230.2	963.	-34.	-144.(1)	[*79PET/MAJ]	101.	423.
[$C_6H_{15}N$]	$(n\text{-}C_3H_7)_2NH$ RN 142-84-7	227.5	952.	-28.	-116.(1)	[77PED/RYL]	110.	462.
[$C_6H_{15}N$]	$n\text{-}C_6H_{13}NH_2$ RN 111-26-2	218.9	916.	-31.	-130.	Est	116.	484.
[$C_6H_{15}NO$]	$NH_2(CH_2)_6OH$ RN 4048-33-3	231.0**	966.5**	-67.	-279.	Est	68.	284.5
[$C_6H_{15}O_4P$]	$OP(OC_2H_5)_3$ RN 78-40-0	~217	~910	-284.	-1187.(6)	[77PED/RYL]	-135.	-565.
[$C_6H_{15}P$]	$(C_2H_5)_3P$ RN 554-70-1	231.7**	969.**	-12.	-49.(13)	[77PED/RYL]	122.	512.
[$C_6H_{16}N_2$]	1,6-diaminohexane RN 124-09-4	237.7	994.4	-22.	-94.	Est	105.5	441.5
[$C_6H_{16}N_2$]	$(CH_3)_2N(CH_2)_2N(CH_3)_2$ RN 110-18-9	235.7	986.	-4.	-16.(2)	Est	126.	528.
[$C_6H_{17}NSi$]	$(CH_3)_3SiCH_2N(CH_3)_2$ RN 18182-40-6	231.5	968.	-49.	-207.	Est	85.	354.
[$C_6H_{18}OSi_2$]	$((CH_3)_3Si)_2O$ RN 107-46-0	~203	~849	-185.	-777.(6)	[77PED/RYL]	-23.	-96.
[C_6MoO_6]	$(CO)_6Mo$ RN 13939-06-5	185**	774**	-219.	-916.(2)	[77PED/RYL]	-38.	-160.
[C_6O_6V]	$(CO)_6V$ RN 20644-87-5	194.5**	814.**	-204.	-854.(29)	[67BID/MCI]	-33.	-138.
[C_6O_6W]	$(CO)_6W$ RN 14040-11-0	184**	770**	-211.	-883.(3)	[77PED/RYL]	-29.	-123.
[C_7ClH_5O]	$4\text{-}ClC_6H_4CHO$ RN 104-88-1	200.2	838.	-16.	-69.	Est	149.	623.
[$C_7ClH_{10}N$]	3-Chloro-1-azabicyclo[2.2.2]-oct-2-ene RN xxxxx	224.0**	937.**	25.	104.(10)	Est	166.5	697.
[$C_7ClH_{12}N$]	3-Chloro-1-azabicyclo[2.2.2]-octane RN 42332-45-6	225.8**	945.**	-10.5	-44.	Est	129.	541.
[$C_7ClH_{14}N$]	$c\text{-}C_5H_9N,2\text{-}CH_2Cl,1\text{-}CH_3$ RN 49665-74-9	227.6**	952.**	-23.	-97.	Est	115.	481.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_fH(M)$		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_7CoH_5O_2]$	$(C_5H_5)Co(CO)_2$ RN 12078-25-0	~204**	853**					
$[C_7CrH_5NO_3]$	$(C_5H_5)Cr(CO)_2NO$ RN 36312-04-6	196.9**	824.**					
$[C_7D_3H_5]$	$C_6H_5CD_3$ RN 1124-18-1	189.8	794.	12.	50.(1)	[77PED/RYL]	188.	786.
$[C_7FH_5O]$	4-FC_6H_4CHO RN 459-57-4	199.2	833.	-56.	-235.	Est	110.	462.
$[C_7FH_5O]$	3-FC_6H_4CHO RN 456-48-4	196.4	822.	-56.	-236.	Est	113.	472.
$[C_7FH_6]$	3-$FC_6H_4CH_2$ radical RN xxxxx	~200	~837					
$[C_7FH_7]$	3-$FC_6H_4CH_3$ RN 352-70-5	189.3	792.	-36.	-150.	Est	140.	587.
$[C_7FH_7]$	2-$FC_6H_4CH_3$ RN 95-52-3	186.6	781.	-36.	-149.	Est	143.	600.
$[C_7FH_7]$	4-$FC_6H_4CH_3$ RN 352-32-9	185.8	777.	-35.	-148.(1)	[77PED/RYL]	144.5	605.
$[C_7FH_{12}N]$	3-Fluoro-1-azabicyclo[3.2.1]-octane RN xxxxx	228.1**	954.**	22.	94.	Est	160.	670.
$[C_7F_2H_{11}N]$	3,3-Difluoro-1-azabicyclo-[2.2.2]octane RN xxxxx	221.8**	928.**	-101.	-423.	Est	43.	179.
$[C_7F_3H_6N]$	3-$CF_3C_6H_4NH_2$ RN 98-16-8	204.2	854.	-142.	-595.	Est	19.	81.
$[C_7H_5N]$	C_6H_5CN RN 100-47-0	195.9	820.	52.	219.	[82CHU/NGU]	222.	929.
$[C_7H_5O_2Rh]$	$(C_5H_5)Rh(CO)_2$ RN 12192-97-1	212**	887.**					
$[C_7H_6N_2]$	m-$NCC_6H_4NH_2$ RN 2237-30-1	200.7	840.	53.	222.	Est	218.	912.
$[C_7H_6O]$	4-Methylene-2,5-cyclohexadiene-1-one RN 502-87-4	~222	~929	10.	40.(4)	Est	153.	641.
$[C_7H_6O]$	2,4,6-Cycloheptatriene-1-one RN 539-80-0	219	918	10.5	44.(3)	[77PED/RYL]	157.	656.
$[C_7H_6O]$	C_6H_5CHO RN 100-52-7	200.2	838.	-9.	-37.(2)	[77PED/RYL]	157.	655.
$[C_7H_6O_2]$	C_6H_5COOH RN 65-85-0	198.2	829.	-70.	-294.(2)	[77PED/RYL]	97.	407.
$[C_7H_7]$	c-C_7H_7 radical RN 3551-27-7	199.4	834.	65.	271.(8)	[82MCM/GOL]	227.	951.
$[C_7H_7]$	$C_6H_5CH_2$ RN 2154-56-5	199.1	833.	49.	204.	[81TSA]	215.	901.
$[C_7H_7N]$	3,4-Cyclobutenopyridine RN xxxxx	225.9**	945.**	60.	252.	Est	200.	837.
$[C_7H_7N]$	2,3-Cyclobutenopyridine RN xxxxx	223.3**	934.**	60.	250.	Est	202.	846.
$[C_7H_7N]$	4-Vinylpyridine RN 100-43-6	223.2**	934.**	48.	202.	Est	191.	798.
$[C_7H_7NO]$	1-(4-Pyridinyl)-ethanone RN 1122-54-9	217.4	910.	-6.	-26.	Est	142.	594.
$[C_7H_7NO]$	1-(3-Pyridinyl)-ethanone RN 350-03-8	217.2	909.	-6.	-26.	Est	142.	595.
$[C_7H_8]$	$C_6H_5CH_3$ RN 108-88-3	189.8	794.	12.	50.(1)	[77PED/RYL]	188.	786.
$[C_7H_8O]$	$C_6H_5OCH_3$ RN 100-66-3	200.3	838.	-16.	-68.(1)	[77PED/RYL]	149.	624.
$[C_7H_9N]$	2,3-Dimethylpyridine RN 583-61-9	226.2	946.	16.	68.(1)	[77PED/RYL]	156.	652.
$[C_7H_9N]$	2,4-Dimethylpyridine RN 108-47-4	227.3	951.	15.	64.(2)	[77PED/RYL]	153.	643.
$[C_7H_9N]$	2,5-Dimethylpyridine RN 589-93-5	226.2	946.	16.	67.(1)	[77PED/RYL]	155.5	651.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		Δ_fH(M)		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[C_7H_9N]	2,6-Dimethylpyridine RN 108-48-5	228.2	955.	14.	59. (2)	[77PED/RYL]	152.	634.
[C_7H_9N]	3,4-Dimethylpyridine RN 583-58-4	226.0	946.	17.	70. (1)	[77PED/RYL]	157.	654.
[C_7H_9N]	3,5-Dimethylpyridine RN 591-22-0	225.5	943.	17.	73. (1)	[77PED/RYL]	158.	661.
[C_7H_9N]	2-Ethylpyridine RN 100-71-0	226.2	946.	19.	81.	Est	159.	665.
[C_7H_9N]	3-Ethylpyridine RN 536-78-7	223.9	937.	20.5	86.	Est	162.	679.
[C_7H_9N]	4-Ethylpyridine RN 536-75-4	224.6**	940.**	20.	83.	Est	161.	672.
[C_7H_9N]	$C_6H_5NHCH_3$ RN 100-61-8	218.1	912.5	20.	85.	[78COL/BEN]	168.	702.5
[C_7H_9N]	$C_6H_5CH_2NH_2$ RN 100-46-9	216.8	907.	20.	84. (3)	[77CAR/LAY]	169.	707.
[C_7H_9N]	4-$CH_3C_6H_4NH_2$ RN 106-49-0	213.7	894.	14.	59.	Est	166.	695.
[C_7H_9N]	3-$CH_3C_6H_4NH_2$ RN 108-44-1	213.4	893.	13.	54. (2)	Est	165.	691.
[C_7H_9NO]	Pyridine-2-methoxymethyl RN 23579-92-2	226.0**	945.5**	-5.	-22.	Est	134.	562.5
[C_7H_9NO]	3-$CH_3OC_6H_4NH_2$ RN 536-90-3	217.6	910.	-16.	-67.	Est	132.	553.
[C_7H_9NO]	2-$CH_3OC_6H_4NH_2$ (o-Anisidine) RN 90-04-0	214.7	898.	-14.	-57.	Est	137.	575.
[C_7H_9NO]	4-$CH_3OC_6H_4NH_2$ RN 104-94-9	214.3	897.	-14.	-58.	Est	137.5	575.
[C_7H_9NS]	3-$CH_3SC_6H_4NH_2$ RN 1783-81-9	214.5	897.	24.	102.	Est	175.5	735.
[C_7H_{10}]	Bicyclo[2.2.1]hept-2-ene RN 498-66-8	200.4	838.	21.5	90. (4)	[80ROG/CHO]	187.	782.
[$C_7H_{10}N_2$]	N,N-Dimethyl-2-pyridinamine RN 5683-33-0	229.2	959.	31.5	132.	[84BIC/PIL]	168.	703.
[$C_7H_{10}N_2$]	N,N-Dimethyl-3-pyridinamine RN 18437-57-5	229.9**	962.**	38.	158.	[84BIC/PIL]	174.	726.
[$C_7H_{10}N_2$]	N,N-Dimethyl-4-pyridinamine RN 1122-58-3	236.2	988.	34.	144.	[84BIC/PIL]	163.5	686.
[$C_7H_{10}O$]	$(c-C_3H_5)_2CO$ RN 1121-37-5	210.7	881.5	39.	163.	Est	194.	811.5
[$C_7H_{11}N$]	1-Azabicyclo[2.2.2]oct-2-ene RN 13929-94-7	228.5**	956.**	37.	156.	Est	174.5	730.
[$C_7H_{11}NO$]	1-Azabicyclo[2.2.2]octan-3-one RN 3731-38-2	221.9**	928.**	-28.	-116.	Est	116.	486.
[C_7H_{12}]	$(CH_3)_2C=CHC(CH_3)=CH_2$ RN xxxxx	213.1**	892.	4.	17.	[79AUE/BOW]	157.	655.
[C_7H_{12}]	1-Methylcyclohexene RN 591-49-1	198.8	832.	-10.	-43. (1)	[77PED/RYL]	157.	655.
[C_7H_{12}]	c-C_5H_6-1,2-$(CH_3)_2$ RN 765-47-9	198.1	829.	-10.	-41.	[82ALL/DOD]	158.	660.
[$C_7H_{13}N$]	1-Azabicyclo[2.2.2]octane (Quinuclidine) RN 100-76-5	232.1	971.	-1.	-4. (1)	[77PED/RYL]	132.6	555.
[$C_7H_{13}N$]	Bicyclo[2.2.1]heptan-2-amine, exo (2-Aminonorbornane) RN 7242-92-4	221.7**	927.**	-8.	-32. (1)	Est	136.	570.
[$C_7H_{13}N$]	Bicyclo[2.2.1]heptan-2-amine, endo (2-Aminonorbornane) RN 31002-73-0	221.7**	927.**	-7.	-28. (1)	Est	137.	574.
[C_7H_{14}]	$(CH_3)_2C=CHCH(CH_3)_2$ RN xxxxx	196.1	820.	-20.	-84. (1)	[77PED/RYL]	149.5	626.
[$C_7H_{14}N_2$]	3-Amino-1-azabicyclo[2.2.2.] octane RN 6238-14-8	231.8**	970.**	4.	17.	Est	138.	577.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		Δ_fH(M)		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_7H_{14}O]$	$(i\text{-}C_3H_7)_2CO$ RN 565-80-0	204.9	857.	-74.	-311.(1)	[77PED/RYL]	87.	363.
$[C_7H_{15}N]$	$(CH_3)_2NC(C_2H_5)$=$CHCH_3$ RN 78733-73-0	236.4	989.	-2.	-10.	Est	127.	531.
$[C_7H_{16}O]$	$(i\text{-}C_3H_7)O(t\text{-}C_4H_9)$ RN 17348-59-3	208.8**	874.**	-81.	-339.	Est	76.	317.
$[C_7H_{16}O_2]$	$CH_3O(CH_2)_5OCH_3$ RN 111-89-7	221.8	928.	-104.	-436.	Est	40.	167.
$[C_7H_{17}N]$	$(C_2H_5)_2(n\text{-}C_3H_7)N$ RN 4458-31-5	232.0**	971.**	-27.	-114.	Est	106.	445.
$[C_7H_{17}N]$	$(CH_3)_2(neo\text{-}C_5H_{11})N$ RN 10076-31-0	229.9	962.	-28.	-118.	Est	107.5	450.
$[C_7H_{17}N]$	$n\text{-}C_7H_{15}NH_2$ RN 111-68-2	219.0	916.	-36.	-151.	Est	111.	463.
$[C_7H_{18}N_2]$	$(CH_3)_2N(CH_2)_3N(CH_3)_2$ RN 110-95-2	238.8	999.	-7.	-29.	Est	120.	502.
$[C_7H_{18}N_2]$	1,7-Diaminoheptane RN 646-19-5	238.	996.	-27.	-115.	Est	100.	419.
$[C_7H_{19}NSi]$	$(CH_3)_3Si(CH_2)_2N(CH_3)_2$ RN 23138-94-5	231.8	970.	-54.	-228.	Est	79.	332.
$[C_8F_3H_5O]$	$p\text{-}CF_3C_6H_4CHO$ RN 455-19-6	191.0	799.	-172.	-721.	Est	2.	10.
$[C_8FeH_8O_2]$	$(C_5H_5)Fe(CO)_2CH_3$ RN 12080-06-7	190.6**	797.**					
$[C_8H_5NO]$	$4\text{-}(CN)C_6H_4CHO$ RN 105-07-7	187.0	782.	25.5	107.	Est	204.	855.
$[C_8H_6N_2]$	Cinnoline RN 253-66-7	223.2	934.	81.	338.(10)	Est	223.	934.
$[C_8H_6N_2]$	Quinoxaline RN 91-19-0	214.4	897.	63.	262.(4)	[81STE/BAR]	214.	895.
$[C_8H_8]$	C_6H_5CH=CH_2 RN 100-42-5	202.0	845.	35.	148.(1)	[77PED/RYL]	199.	833.
$[C_8H_8]$	$1,2\text{-}C_6H_4(=CH_2)_2$ RN xxxxx	214.8	899.	55.	230.(17)	[81POL/RAI]	206.	861.
$[C_8H_8]$	$1,4\text{-}C_6H_4(=CH_2)_2$ RN xxxxx	215.7	902.	56.	234.(17)	[81POL/RAI]	207.	865.
$[C_8H_8O]$	$C_6H_5COCH_3$ RN 98-86-2	205.4	859.	-21.	-87.(2)	[77PED/RYL]	140.	584.
$[C_8H_8O]$	$4\text{-}(CH_3)C_6H_4CHO$ RN 104-87-0	203.7	852.	-18.	-75.	Est	144.	603.
$[C_8H_8O_2]$	$4\text{-}CH_3OC_6H_4CHO$ RN 123-11-5	213.5	893.	-48.5	-203.(5)	[77PED/RYL]	104.	434.
$[C_8H_8O_2]$	$C_6H_5CO_2CH_3$ RN 95-58-3	203.7	852.	-69.	-288.(7)	[77PED/RYL]	93.	390.
$[C_8H_9]$	$C_6H_5CHCH_3$ radical RN xxxxx	~201	~841	44.	184.	[82MAU]	209.	875.
$[C_8H_9N]$	3,4-Cyclopentenopyridine RN xxxxx	226.8**	949.**	27.	113.	Est	166.	695.
$[C_8H_9N]$	2,3-Cyclopentenopyridine RN xxxxx	225.8**	945.**	27.	111.	Est	166.	696.
$[C_8H_{10}]$	m-Xylene RN 108-38-3	195.9	820.	4.	17.(1)	[77PED/RYL]	174.	727.
$[C_8H_{10}]$	o-Xylene RN 95-47-6	193.3	809.	4.	18.(1)	[77PED/RYL]	177.	739.
$[C_8H_{10}]$	p-Xylene RN 106-42-3	192.0	803.	4.	18.(1)	[77PED/RYL]	178.	745.
$[C_8H_{10}]$	$C_2H_5C_6H_5$ RN 100-41-4	191.6	802.	7.	29.(1)	[77PED/RYL]	181.	757.
$[C_8H_{11}N]$	2-Isopropylpyridine RN 75981-47-4	227.2	951.	13.	56.	Est	152.	635.
$[C_8H_{11}N]$	$C_6H_5N(CH_3)_2$ RN 121-69-7	223.4	935.	24.	101.(3)	[82FUR/SAK]	166.	696.
$[C_8H_{11}N]$	$C_6H_5NHC_2H_5$ RN 103-69-5	221.8	928.	13.	56.(6)	[69BEN/CRU]	157.	658.
$[C_8H_{11}N]$	$3\text{-}C_2H_5C_6H_4NH_2$ RN 587-02-0	214.0	895.	6.	27.	Est	158.	662.
$[C_8H_{11}P]$	$C_6H_5P(CH_3)_2$ RN 672-66-2	229.6	961.	19.5	82.	Est	156.	651.
$[C_8H_{12}]$	$(c\text{-}C_3H_5)_2C$=CH_2 RN 822-93-5	216.5	906.	51.	213.	[70BEN/O`N]	200.	837.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		Δ_fH(M)		Reference	Δ_fH(MH$^+$)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_8H_{12}]$	2-Methylenebicyclo[2.2.1]heptane RN 497-35-8	207**	866**	12.	50.	[79AUE/BOW]	171.	714.
$[C_8H_{12}]$	2-Methylbicyclo[2.2.1]hept-2-ene RN xxxxx	206	862	11.	46.	Est	171.	714.
$[C_8H_{13}N]$	1-Azabicyclo[2.2.2]-oct-2-ene,3-methyl RN xxxxx	231.0**	966.5**	30.	124.	Est	164.	687.5
$[C_8H_{13}N]$	1-Azabicyclo[2.2.2]-octane,3-methylene RN 22207-84-7	230.1**	963.**	20.	84.	Est	156.	651.
$[C_8H_{14}]$	$(CH_3)_2C{=}C(CH_3)C(CH_3){=}CH_2$ RN xxxxx	210.6**	881.**	-3.	-13.	[79AUE/BOW]	152.	636.
$[C_8H_{14}O]$	c-$C_6H_{11}COCH_3$ RN 823-76-7	202.4	847.	-65.	-273.	Est	98.	410.
$[C_8H_{14}O_2]$	c-$C_6H_{11}COOCH_3$ RN 4630-82-4	203.7	852.	-111.	-466.	Est	51.	212.
$[C_8H_{15}N]$	3-Methyl-1-azabicyclo[2.2.2.]-octane RN-695-88-5	231.7**	969.**	-8.	-33.	Est	126.	528.
$[C_8H_{15}N]$	1,4,4-Trimethyl-1,2,3,4-tetrahydropyridine RN 35079-50-6	234.2**	980.**					
$[C_8H_{15}NO]$	cis-3-Aminobicyclo[2.2.2]octan-2-ol RN 17997-65-8	223.9	937.	-57.	-240.	Est	84.	353.
$[C_8H_{15}NO]$	trans-3-Aminobicyclo[2.2.2]-octan-2-ol RN 40335-14-6	220.6	923.	-59.0	-248.	Est	86.	359.
$[C_8H_{16}O_4]$	1,4,7,10-Tetraoxa-cyclododecane (12-Crown-4) RN 294-93-9	221.6	927.	-151.	-631.	[82BYS/MAN]	-7.	-29.
$[C_8H_{17}N]$	1,4,4-Trimethylpiperidine RN 1003-84-5	230.8**	966.**					
$[C_8H_{18}O]$	$(n\text{-}C_4H_9)_2O$ RN 142-96-1	203.7	852.	-79.5	-333.(1)	[*80MAJ/WAG]	82.	345.
$[C_8H_{18}O]$	$(sec\text{-}C_4H_9)_2O$ RN 6863-58-7	209.0	874.	-88.	-370.(2)	[77PED/RYL]	68.	286.
$[C_8H_{18}O]$	$(t\text{-}C_4H_9)_2O$	See References to Table 1: 75PIT/BUR						
$[C_8H_{18}O_4]$	$CH_3(OCH_2CH_2)_3OCH_3$ RN 112-49-2	224.1	938.	-157.	-656.	Est	-15.	-64.
$[C_8H_{18}S]$	$(t\text{-}C_4H_9)_2S$ RN 107-47-1	212.8	890.	-45.	-189.(1)	[77PED/RYL]	108.	451.
$[C_8H_{18}S]$	$(n\text{-}C_4H_9)_2S$ RN 544-40-1	208.7	873.	-40.	-167.(1)	[77PED/RYL]	117.	490.
$[C_8H_{19}N]$	$(i\text{-}C_3H_7)_2(C_2H_5)N$ RN 7087-68-5	235.3	984.	-33.	-140.	Est	97.	405.5
$[C_8H_{19}N]$	$(t\text{-}C_4H_9)_2NH$ RN 21981-37-3	233.2	976.	-41.	-172.(3)	[81SUR/HAC]	91.	382.
$[C_8H_{19}N]$	$(sec\text{-}C_4H_9)_2NH$ RN 626-23-3	231.8	970.	-37.5	-157.	Est	96.	403.
$[C_8H_{19}N]$	$(CH_3)_3C(CH_2)_2N(CH_3)_2$ RN 15673-04-8	230.4	964.	-36.	-149.(3)	Est	100.	417.
$[C_8H_{19}N]$	$(i\text{-}C_4H_9)_2NH$ RN 110-96-3	228.6	956.	-43.	-179.(8)	[73PEP/GAF]	94.	395.
$[C_8H_{19}N]$	$(n\text{-}C_4H_9)_2NH$ RN 111-92-2	228.4	956.	-37.5	-157.(1)	[77PED/RYL]	100.	417.
$[C_8H_{19}N]$	n-$(C_8H_{17})NH_2$ RN 111-86-4	220.4**	922.**	-41.	-172.	Est	104.	436.
$[C_8H_{20}N_2]$	$(CH_3)_2N(CH_2)_4N(CH_3)_2$ RN 111-51-3	240.4	1006.	-12.	-51.(1)	Est	113.	473.
$[C_8H_{21}NSi]$	$(CH_3)_3Si(CH_2)_3N(CH_3)_2$ RN 28247-29-2	231.8	970.	-59.	-248.	Est	75.	312.
$[C_8H_{21}NSi]$	$(CH_3)_2(t\text{-}C_4H_9)SiN(CH_3)_2$ RN 66365-05-7	229.7	961.	-68.	-286.(23)	Est	68.	283.
$[C_8H_{22}OSi_2]$	$((CH_3)_3SiCH_2)_2O$	See References to Table 1: 75PIT/BUR						
$[C_9ClH_9]$	4-$ClC_6H_4C(CH_3){=}CH_2$ RN 1712-70-5	205.0	858.	19.	81.	Est	180.	753.
$[C_9CrH_8O_3]$	$(C_5H_5)Cr(CO)_3CH_3$ RN 41311-89-1	206**	862**					
$[C_9FH_9]$	4-$FC_6H_4C(CH_3){=}CH_2$ RN 350-40-3	206.7	865.	-20.5	-86.	Est	138.	579.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_fH(M)$		Reference	$\Delta_fH(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_9H_7MnO_3]$	$(CH_3C_5H_4)Mn(CO)_3$ RN 12108-13-3	200.6**	839.**	-121.	-508.	Est	44.	183.
$[C_9H_7N]$	Quinoline RN 91-22-5	226.5	948.	50.	211.(1)	[79VIS]	190.	793.
$[C_9H_7N]$	Isoquinoline RN 119-65-3	225.9	945.	50.	208.(1)	[79VIS/WIL]	190.	793.
$[C_9H_7NO]$	Quinoline-1-oxide RN 1613-37-2	224.6	940.	31.	131.	Est	172.	721.
$[C_9H_9N]$	$(HCCCH_2)_3N$ RN 6921-29-5	220.2	921.	174.	727.	Est	319.	1336.
$[C_9H_{10}]$	$C_6H_5C(CH_3)=CH_2$ RN 98-83-9	207.0	866.	27.	113.	[69BEN/CRU]	186.	777.
$[C_9H_{10}O]$	$(4-CH_3)C_6H_4COCH_3$ RN xxxxx	208.7	873.	-29.	-120.	Est	128.	535.
$[C_9H_{11}]$	$C_6H_5C(CH_3)_2$ radical RN xxxxx	202.4	847.	33.	139.	[82MCM/GOL]	202.	846.
$[C_9H_{11}]$	$C_6H_5(CHC_2H_5)$ radical RN xxxxx	~202	~845	39	164	[82MAU]	203.	849.
$[C_9H_{11}N]$	2,3-Cyclohexenopyridine RN 10500-57-9	227.7**	953.**	18.	74.	Est	156.	651.
$[C_9H_{11}N]$	3,4-Cyclohexenopyridine RN 36566-06-6	227.7**	953.**	18.	76.	Est	156.	653.
$[C_9H_{11}NO_2]$	$C_6H_5CH_2CH(NH_2)COOH$ (L-Phenylalanine) RN 150-30-1	216.5	906.	-75.	-313.(1)	[77PED/RYL]	74.	311.
$[C_9H_{11}NO_3]$	L-Tyrosine RN xxxxx	222.3	930.	-116.	-486.	Est	27.	114.
$[C_9H_{12}]$	Mesitylene RN 108-67-8	200.7	840.	-4.	-16.(1)	[77PED/RYL]	161.	674.
$[C_9H_{12}]$	$n-C_3H_7C_6H_5$ RN 103-65-1	192.4	805.	2.	8.(1)	[77PED/RYL]	175.	733.
$[C_9H_{12}]$	$i-C_3H_7C_6H_5$ RN 98-82-8	192.1	804.	1.	4.(1)	[77PED/RYL]	174.5	730.
$[C_9H_{12}N_2O_6]$	Uridine RN 58-96-8	~208	~870	-223.	-935.	Est	-66.	-275.
$[C_9H_{12}O_3]$	$1,3,5-C_6H_3(OCH_3)_3$ RN 621-23-8	220.6	923.	-90.5	-379.	Est	54.5	228.
$[C_9H_{13}N]$	2,6-Diethylpyridine RN 935-28-4	231.1	967.	4.5	19.(2)	Est	139.	582.
$[C_9H_{13}N]$	$C_6H_5CH_2N(CH_3)_2$ RN 103-83-3	228.1**	954.**	20.	84.	Est	158.	660.
$[C_9H_{13}N]$	$C_6H_5N(CH_3)(C_2H_5)$ RN 613-97-8	227.1	950.	17.	71.	Est	156.	651.
$[C_9H_{13}N]$	2-t-Butylpyridine RN 5944-41-2	227.4**	951.**	7.	28.	Est	145.	607.
$[C_9H_{13}N]$	4-t-Butylpyridine RN 3978-81-2	225.9	945.	8.	32.	Est	147.	617.
$[C_9H_{13}N]$	$3-CH_3C_6H_4N(CH_3)_2$ RN 121-72-2	224.5	939.	16.	67.	Est	157.	658.
$[C_9H_{13}N]$	$4-CH_3C_6H_4N(CH_3)_2$ RN 99-97-8	225.6	944.	17.	70.	Est	157.	656.
$[C_9H_{14}N_2O_6]$	5,6-Dihydrouridine RN 5627-05-4	~208	~870	-233.5	-977.	Est	-76.	-317.
$[C_9H_{15}N]$	$(CH_2=CHCH_2)_3N$ RN 102-70-5	230.0	962.	53.5	224.	Est	189.	792.
$[C_9H_{17}N]$	1-Cyclopentylpyrrolidine RN 18707-33-0	233.1**	975.**					
$[C_9H_{17}N]$	$c-C_5H_{10}NCH=C(CH_3)_2$ RN 673-33-6	230.7**	965.**	-7.	-31.	Est	127.5	534.
$[C_9H_{17}NO_2]$	3,3-Dimethoxy-1-azabicyclo[2.2.2]octane RN xxxxx	232**	971**	-78.	-326.	Est	56.	233.
$[C_9H_{18}O]$	$(tert-C_4H_9)_2CO$ RN 815-24-7	206.5	864.	-83.	-345.8	[77PED/RYL]	77.	320.
$[C_9H_{18}N_2]$	1,5-Diazabicyclo[3.3.3]-undecane RN 283-58-9	232.4	972.	33.	138.	[81ALD/ARR]	166.	696.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_9H_{19}N]$	2,2,6,6,-Tetramethyl-piperidine RN 768-66-1	231.7**	969.**	-38.	-160.(3)	[81SUR/HAC]	96.	401.
$[C_9H_{19}N]$	N-Isobutylpiperidine RN 10315-89-6	232.9**	974.**					
$[C_9H_{21}N]$	$(t-C_4H_9)C(CH_3)_2N(CH_3)_2$ RN 3733-36-6	235.1	984.	-34.	-142.	Est	97.	404.
$[C_9H_{21}N]$	$(n-C_3H_7)_3N$ RN 102-69-2	234.0	979.	-38.	-161.	Est	93.	390.
$[C_9H_{21}N]$	$(t-C_5H_{11})(t-C_4H_9)NH$ RN 58471-09-3	232.5	973.	-46.	-191.(4)	Est	87.5	366.
$[C_{10}ClH_{14}N]$	$4-ClC_6H_4N(C_2H_5)_2$ RN 2873-89-4	225.6	944.	2.	8.	Est	142.	594.
$[C_{10}CrH_7O_3]$	$(C_6H_5CH_2)Cr(CO)_3$ RN 32984-97-7	205**	858**					
$[C_{10}F_3H_9]$	$4-CF_3C_6H_4C(CH_3)CH_2$ RN 55186-75-9	199.6	835.	-131.	-549.	Est	35.	146.
$[C_{10}FeH_{10}]$	$(C_5H_5)_2Fe$ RN 102-54-5	~210	~879.	58.	242.(3)	[77PED/RYL]	213.5	893.
$[C_{10}H_8]$	Azulene RN 275-51-4	220.	921.	69.	289.(3)	[77PED/RYL]	215.	898.
$[C_{10}H_8]$	Naphthalene RN 91-20-3	194.7	815.	36.	150.(1)	[*82COL/JIM]	207.	865.
$[C_{10}H_9N]$	1-Naphthalenamine RN 134-32-7	216.9	907.5	38.	158.(7)	[77PED/RYL]	186.5	780.5
$[C_{10}H_{10}N_2]$	1,8-Diaminonaphthalene RN 479-27-6	223.8	936.	46.	193.	Est	188.	787.
$[C_{10}H_{10}Ni]$	$(C_5H_5)_2Ni$ RN 1271-28-9	223.	933.	85.	357.(5)	[77PED/RYL]	228.	954.
$[C_{10}H_{10}Ru]$	$(C_5H_5)_2Ru$ RN 1287-13-4	218**	912**	-62.	-260.	Est	85.5	358.
$[C_{10}H_{12}]$	1,2,3,4-tetrahydronaphthalene RN 119-64-2	194.7	815.	6.	24.(2)	[77PED/RYL]	177.	739.5
$[C_{10}H_{12}]$	$4-CH_3C_6H_4C(CH_3)CH_2$ RN 1195-32-0	211.0	883.	19.	80.	Est	174.	727.
$[C_{10}H_{12}O]$	$4-CH_3OC_6H_4C(CH_3)CH_2$ RN 1712-69-2	217.4	910.	-23.	-95.	Est	125.5	525.
$[C_{10}H_{13}N]$	N-Phenylpyrrolidine RN 4096-21-3	224.7	940.	30.	117.	Est	171.	716.
$[C_{10}H_{14}]$	$t-C_4H_9C_6H_5$ RN 98-06-6	193.0	807.	-5.	-23.(1)	[77PED/RYL]	167.	699.5
$[C_{10}H_{14}]$	$n-C_4H_9C_6H_5$ RN 104-51-8	192.1	804.	-3.	-13.(1)	[77PED/RYL]	170.	713.
$[C_{10}H_{14}N_2O_5]$	Thymidine RN 50-89-5	~208	~870	-230.	-961.	Est	-72.	-301.
$[C_{10}H_{15}N]$	$C_6H_5N(C_2H_5)_2$ RN 91-66-7	227.6	952.	9.5	40.	[69BEN/CRU]	148.	617.
$[C_{10}H_{15}N]$	$3,5-(CH_3)_2C_6H_3N(CH_3)_2$ RN 4913-13-7	227.0	950.	8.	35.	Est	147.	615.
$[C_{10}H_{16}]$	1,5,5-Trimethyl-3-methylenecyclohexene RN 16609-28-2	216.1**	904.**	-2.	-8.	[79AUE/BOW]	148.	618.
$[C_{10}H_{16}N_2]$	$1,2-(N(CH_3)_2)_2C_6H_4$ RN 704-01-8	235.2	984.	36.	151.	Est	167.	697.
$[C_{10}H_{17}NO]$	cis-3-Amino-2-twistanol RN xxxxx	224.0	937.	-47.	-197.	Est	95.	396.
$[C_{10}H_{17}NO]$	trans-3-Amino-2-twistanol RN xxxxx (isomer 1)	221.5	927.	-49.	-205.	Est	95.	398.
$[C_{10}H_{17}NO]$	trans-3-Amino-2-twistanol RN xxxxx (isomer 2)	220.0	920.	-49.	-205.	Est	97.	405.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
$[C_{10}H_{19}N]$	1-Azabicyclo[3.3.3]undecane (Manxine) RN 31023-92-4	230.1	963.	5.	20.(20)	Est	140.	587.
$[C_{10}H_{19}NO]$	4-Aminodecahydro-3-naphthalenol RN xxxxx	222.1	929.	-77.	-321.	Est	67.	280.
$[C_{10}H_{20}O_5]$	1,4,7,10,13-Pentaoxacyclopentadecane (15-Crown-5) RN 33100-27-5	223.6	936.	-186.	-780.(2)	[82BYS/MAN]	-44.	-184.
$[C_{10}H_{22}O]$	$(n\text{-}C_5H_{11})_2O$ RN 693-65-2	205.2**	859.**	-90.	-375.	Est	71.	296.5
$[C_{10}H_{22}O_5]$	$CH_3(OCH_2CH_2)_4OCH_3$ RN 143-24-8	227.2	951.					
$[C_{10}H_{23}N]$	$n\text{-}(C_{10}H_{21})NH_2$ RN 2016-57-1	220.7**	923.**	-51.	-214.	Est	94.	393.
$[C_{10}H_{24}N_2]$	$(CH_3)_2N(CH_2)_6N(CH_3)_2$ RN 111-18-2	237.9	995.	-22.	-91.	Est	106.	444.
$[C_{11}H_{10}]$	1-Methylnaphthalene RN 90-12-0	200.7	840.	27.	113.(2)	[74SAB/CHA]	192.	803.
$[C_{11}H_{10}]$	2-Methylnaphthalene RN 91-57-6	200.0	837.	26.5	111.(2)	[74SAB/CHA]	192.	804.
$[C_{11}H_{12}N_2O_2]$	L-Tryptophan RN 54-12-6	225.4	943.	-58.	-243.	Est	82.	344.
$[C_{11}H_{13}N]$	1,4-Dihydro-1,4-ethanoquinoline RN 4363-25-1	232.0	971.	41.	173.	Est	175.	732.
$[C_{11}H_{15}N]$	1-Phenylpiperidine RN 4096-2-2	225.8	945.	14.	57.	Est	154.	642.
$[C_{11}H_{17}N]$	2,6-Diisopropylpyridine RN 6832-21-9	232.9	974.	-8.	-33.	Est	125.	523.
$[C_{11}H_{17}N]$	$2\text{-}C_6H_{13}(c\text{-}C_5H_4N)$ RN 1129-69-7	228.9	958.	0.	0.	Est	137.	572.
$[C_{11}H_{17}N]$	$3\text{-}CH_3C_6H_4N(C_2H_5)_2$ RN 91-67-8	228.9	956.	1.	4.	Est	138.	578.
$[C_{11}H_{17}N]$	$4\text{-}CH_3C_6H_4N(C_2H_5)_2$ RN 613-48-9	228.6	956.	3.	12.	Est	140.	587.
$[C_{12}H_8]$	Biphenylene RN 259-79-0	203.4	851.	104.	437.(13)	[77PED/RYL]	267.	1116.
$[C_{12}H_8N_2]$	Phenazine RN 92-82-0	223.7	936.	82.	344.(3)	[80ARS]	224.	938.
$[C_{12}H_{10}]$	Acenaphthene RN 83-32-9	203.5	851.	37.	155.(1)	[81KUD/KUD]	199.	834.
$[C_{12}H_{10}]$	Biphenyl RN 92-52-4	196.1	820.	43.	182.(1)	[77PED/RYL]	213.	892.
$[C_{12}H_{14}N_2]$	N,N'-Dimethyl-1,8-naphthalenediamine RN 20734-56-9	230.0	962.	45.	189.	Est	181.	757.
$[C_{12}H_{16}N_2O_6]$	2',3'-O-Isopropylideneuridine RN 362-43-6	~208	~870	-218.	-911.	Est	-60.	-251.
$[C_{12}H_{18}]$	$(CH_3)_6C_6$ RN 87-85-4	207.3	867.	-21.	-87.(3)	[77PED/RYL]	138.	576.
$[C_{12}H_{19}N]$	$C_6H_4N(CH_3)_2,2\text{-}t\text{-}C_4H_9$ RN 22025-87-2	229.3	959.	15.	63.	Est	151.5	634.
$[C_{12}H_{19}N]$	$C_6H_5N(C_3H_7)_2$ RN 2217-07-4	228.6	956.	1.	3.	Est	138.	578.
$[C_{12}H_{21}N]$	$(CH_2{=}C(CH_3)CH_2)_3N$ RN xxxxx	230.7**	965.**	28.	116.	Est	163.	684.
$[C_{12}H_{21}NO]$	3-Amino-tricyclo[7.3.0.0^{4,8}]dodecan-2-ol RN xxxxx	220.0	920.	-63.	-263.	Est	83.	347.
$[C_{12}H_{24}N_2]$	1,6-Diazabicyclo[4.4.4]-tetradecane RN 71058-67-8	226.0	946.	-23.	-95.	[81ALD/ARR]	116.	489.5
$[C_{12}H_{24}O_6]$	1,4,7,10,13,16-Hexaoxacyclooctadecane (18-Crown-6) RN 17455-13-9	230.	962.	-227.	-950.	Est	-91.	-382.
$[C_{12}H_{27}N]$	$(n\text{-}C_4H_9)_3N$ RN 102-82-9	234.8	982.	-53.	-222.(1)	Est	78.	326.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species—Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H$(M)		Reference	$\Delta_f H$(MH^+)	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_{13}H_9N$]	Acridine RN 260-94-6	231.9	970.	70.	291.(1)	[81KUD/KUD2]	203.	851.
[$C_{13}H_{10}$]	Fluorene RN 86-73-7	200.0	837.	45.	187.(1)	[81KUD/KUD]	210.	880.
[$C_{13}H_{10}O$]	$(C_6H_5)_2CO$ RN 119-61-9	210.9	882.	12.	50.(3)	[78SAB/LAF2]	167.	698.
[$C_{13}H_{13}P$]	$(C_6H_5)_2(CH_3)P$ RN 1486-28-8	230.3	963.5	44.	185.	Est	180.	751.5
[$C_{13}H_{16}N_2$]	N,N,N'-Trimethyl-1,8-naphthalenediamine RN 20723-57-0	235.6	986.	-52.	-217.	Est	78.	327.
[$C_{13}H_{21}N$]	2,6-Di-t-butylpyridine RN 585-48-4	233.4	976.	-19.	-81.	Est	113.	472.5
[$C_{13}H_{21}N$]	2,4-Di-t-butylpyridine RN 29939-31-9	231.4**	968.**	-19.	-79.	Est	115.	483.
[$C_{13}H_{25}N$]	2,6-Di-t-butylpiperidine RN xxxxx	234.3	980.	-76.	-317.	Est	56.	233.
[$C_{13}H_{25}N$]	out-6H-1-Azabicyclo[4.4.4] tetradecane RN xxxxx	214.3	896.	-11.	-47.	[81ALD/ARR]	140.	586.
[$C_{14}H_{10}$]	Anthracene RN 120-12-7	207.0	866.	55.	230.(1)	[79KUD/KUD4]	214.	894.
[$C_{14}H_{10}$]	Phenanthrene RN 85-01-8	198.7	831.	49.	207.(1)	[79KUD/KUD4]	216.	906.
[$C_{14}H_{12}$]	$(C_6H_5)_2C{=}CH_2$ RN 530-48-3	211.9	887.	59.	246.(4)	[77PED/RYL]	212.5	889.
[$C_{14}H_{14}$]	$C_6H_5(CH_2)_2C_6H_5$ RN 103-29-7	194.6	814.	34.	143.(2)	[77PED/RYL]	205.	859.
[$C_{14}H_{18}$]	1,2,3,4,5,6,7,8-Octahydrophenanthrene RN 5325-97-3	204.7	856.	-8.	-34.(8)	[77SHA/GOL]	153.	640.
[$C_{14}H_{18}$]	1,2,3,4,5,6,7,8-Octahydroanthracene RN 1079-71-6	202.6	848.	-9.	-37.(3)	[77PED/RYL]	154.	645.
[$C_{14}H_{18}N_2$]	N,N,N',N'-Tetramethyl-1,8-naphthalenediamine RN 20734-58-1	241.8	1012.	63.	262.	Est	186.5	780.
[$C_{14}H_{27}N$]	1-Methyl-2,6-t-butylpiperidine RN xxxxx	239.2	1001.	-67.	-311.	Est	60.	250.
[$C_{15}H_{12}$]	9-Methylanthracene RN 779-02-2	213.9	895.	48.	201.	Est	200.	836.
[$C_{15}H_{12}$]	2-Methylanthracene RN 613-12-7	210.3	880.	45.	187.	Est	200.	837.
[$C_{15}H_{18}$]	1,4-Dimethyl-7-isopropylazulene RN 489-84-9	233.	975.	33.	139.	Est	165.	694.
[$C_{16}H_{10}$]	Pyrene RN 129-00-0	206.1	862.	52.	216.(1)	[79KUD/KUD2]	211.	884.
[$C_{16}H_{10}$]	Fluoranthene RN 206-44-0	199.3	834.	69.	289.(1)	[81KUD/KUD]	235.	985.
[$C_{16}H_{16}$]	$(4\text{-}CH_3C_6H_4)_2C{=}CH_2$ RN xxxxx	215.4	901.	43.	180.	Est	193.	809.
[$C_{16}H_{18}$]	$C_6H_5(CH_2)_4C_6H_5$ RN 1083-56-3	195.9	820.	24.	100.	Est	194.	810.
[$C_{18}H_{12}$]	Tetracene RN 92-24-0	217.8	911.	67.	284.(1)	[79KUD/KUD2]	216.	903.
[$C_{18}H_{12}$]	Chrysene RN 218-01-9	201.6	843.	63.	263.(1)	[79KUD/KUD2]	227.	949.5
[$C_{18}H_{12}$]	Triphenylene RN 217-59-4	198.5	830.5	64.5	270.(1)	[79KUD/KUD2]	232.	969.5
[$C_{18}H_{15}P$]	$(C_6H_5)_3P$ RN 603-35-0	~230.	~962.	78.	328.(21)	[79STE]	214.	896.
[$C_{20}H_{12}$]	Perylene RN 198-55-0	211.4	884.	74.	308.(4)	[77PED/RYL]	228.	953.5

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species—Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[$C_{22}H_{12}$]	1,12-Benzoperylene RN 191-24-2	208.5	872.	72.	302.	[77STE/GOL]	229.	960.
[$C_{22}H_{14}$]	Picene RN 213-46-7	203.4	851.	78.	326.	Est	240.	1005.
[$C_{24}H_{12}$]	Coronene RN 191-07-1	205.0	858.	77.	323.	[77STE/GOL]	238.	995.
[Cl]	Cl RN 22537-15-1	123.6	517.	29.1	122.	[82/TN270]	271.8	1137.
[ClH]	HCl RN 7647-01-0	134.8	564.	-22.	-92.	[82/TN270]	209.	874.
[F]	F RN 14762-94-8	81.0	339.	19.	79.	[82/TN270]	>303.3	1270.
[FH]	HF RN 7664-39-3	117.	489.5	-65.	-271.	[82/TN270]	184.	770.
[F_2O_2S]	F_2SO_2 RN 2699-79-8	159.0	665.	-181.	-759.(8)	[82JANAF]	25.	106.
[F_3N]	NF_3 RN 7783-54-2	144	604	-30.	-125.	[82/TN270]	192.	802.5
[F_3OP]	OPF_3 RN 13478-20-1	167.8	702.	-289.	-1211.	[82/TN270]	-91.5	-383.
[F_3P]	PF_3 RN 7783-55-3	166.5	697.	-220.	-919.	[82/TN270]	-20.	-85.5
[HI]	HI RN 10034-85-2	150.	628.	6.	26.	[82/TN270]	222.	928.
[HNO_3]	HNO_3 See References to Table 1:	75FEH/HOW						
[HO_2]	HO_2 RN 3170-83-0	~158.	~661.	3.	11.(4)	[82BAU/COX]	210.	880.
[H_2]	H_2 RN 1333-74-0	101.3	424.	0.	0.	DEF	264.	1106.
[H_2O]	H_2O RN 7732-18-5	166.5	697.	-58.	-242.	[82/TN270]	141.	591.
[H_2O_2]	H_2O_2 RN 7722-84-1	162.	678.	-32.5	-136.	[82BAU/COX]	171.	716.
[H_2O_4S]	H_2SO_4 RN 7664-93-9	~169	~707	-176.	-735.(8)	[82JANAF]	21.	88.
[H_2S]	H_2S RN 7783-06-4	170.2	712.	-5.	-21.	[82/TN270]	190.	797.
[H_2Se]	H_2Se RN 7783-07-5	171.3	717.	7.	30.	[82/TN270]	201.5	843.
[H_2N]	NH_2 RN 15194-15-7	187	782	44.	185.(5)	[82MCM/GOL]	223.	935.
[H_3N]	NH_3 RN 7664-41-7	204.0	853.5	-11.	-46.	[82/TN270]	151.	630.5
[H_3P]	PH_3 RN 7803-51-2	188.6	789.	1.	5.	[82/TN270]	178.	746.
[H_4N_2]	H_2NNH_2 RN 302-01-2	204.7	856.	23.	95.	[82/TN270]	184.	770.
[H_4Si]	SiH_4 RN 7803-62-5	~155	~648	8.	35.	[81BEL/PER]	219.	916.5
[He]	He RN 7440-59-7	42.5	178.	0.	0.	DEF	323.	1352.
[I]	I RN 14362-44-8	145.4	608.	25.5	107.	[82/TN270]	246.	1029.
[Kr]	Kr RN 7439-90-9	101.6	425.	0.	0.	DEF	264.	1105.
[Mg]	Mg See References to Table 1:	77PO/POR						
[Mg_2]	Mg_2 RN 29904-79-8	~219	916.					
[NO]	NO RN 10102-43-9	~127	~531	21.5	90.	[82BAU/COX]	260.	1089.
[N_2]	N_2 RN 7727-37-9	118.2	494.5	0.	0.	DEF	247.5	1035.5
[N_2O]	N_2O RN 10024-97-2	136.5	571.	20.	82.	[82/TN270]	249.	1041.
[Ne]	Ne RN 7440-01-9	48.1	201.	0.	0.	DEF	318.	1329.

Table 2. Proton affinities and heats of formation of molecules and corresponding protonated species--Continued

Formula	Compound (M)	Proton Affinity		$\Delta_f H(M)$		Reference	$\Delta_f H(MH^+)$	
		kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol
[O]	O RN 17778-80-2	116.3	487.	59.5	249.	[82/TN270]	309.	1293.
[OSi]	SiO See References to Table 1:	81FAH/FEH						
[O_2]	O_2 RN 7782-44-7	100.9	422.	0.	0.	DEF	265.	1108.
[O_2S]	SO_2 RN 7446-09-5	161.6	676.	-71.	-297.	[82/TN270]	133.	557.
[O_3S]	SO_3 RN 7446-11-9	~138	~577	-95.	-396.	[82/TN270]	133.	557.
[S]	S RN 7704-34-9	158.3	662.	67.	279.	[82/TN270]	274.	1147.
[Xe]	Xe RN 7440-63-3	118.6	496.	0.	0.	DEF	247.	1034.
[Zn]	Zn RN 7440-66-6	156	653	31.	131.	[82/TN270]	241.	1008.

References to Table 2

A reference of the form *00ABC/DEF means that a condensed phase heat of formation from 77PED/RYL has been used with a heat of vaporization or sublimation from the designated reference.

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

82ALL/DOD N.L. Allinger, H. Dodziuk, D.W. Rogers and S.N. Naik, Tetrahedron **38**, 1593 (1982).

83AN/MAN X.-W. An and M. Mansson, J. Chem. Thermodyn. **15**, 587 (1983).

80ARS M.R. Arshadi, J. Chem. Thermodyn. **12**, 903 (1980).

79AUE/BOW D.H. Aue and M.T. Bowers, "Stabilities of Positive Ions from Equilibrium Gas-Phase Basicity Measurements," in *Gas Phase Ion Chemistry*, M.T. Bowers Editor, Vol. 2, pp. 1-51 Academic Press, New York (1979).

78AUS/LIA P. Ausloos and S. G. Lias, J. Am. Chem. Soc. 100, 4594 (1978).

74BAT/CHR L. Batt, K. Christie, R.T. Milne, and A.J. Summers, Int. J. Chem. Kinet. **6**, 877 (1974).

82BAU/COX D.L. Baulch, R.A. Cox, P.J. Crutzen, R.F. Hampson, Jr., J.A. Kerr, J. Troe, and R.T. Watson, J. Phys. Chem. Ref. Data **11**, 327 (1982).

78BEA/LEE P. Beak, J.K. Lee, and J.M. Ziegler, J. Org. Chem. **43**, 1536 (1978).

74BEA/MUE P. Beak, D.S. Mueller, and J. Lee, J. Am. Chem. Soc. **96**, 3867 (1974).

81BEL/PER T.N. Bell, K.A. Perkins, and P.G. Perkins, J. Chem. Soc. Faraday Trans. I **77**, 1779 (1981).

69BEN/CRU S.W. Benson, F.R. Cruickshank, D.M. Golden, G.R. Haugen, H.E. O'Neal, A.S. Rodgers, R. Shaw and R. Walsh, Chem. Rev. **69**, 279 (1969).

70BEN/O'N S.W. Benson and H.E. O'Neal, "Kinetic Data on Gas Phase Unimolecular Reactions," NSRDS-NBS **21**, (1970).

84BIC/PIL J. Bickerton, G. Pilcher, G. Al-Takhin, J. Chem. Thermodyn. **16**, 373 (1984).

67BID/MCI D.R. Bidinosti, N.S. McIntyre, Can. J. Chem. **45**, 641 (1967).

81BOM/BER D.S. Bomse, D.W. Berman, and J.L. Beauchamp, J. Am. Chem. Soc. **103**, 3967 (1981).

82BYS K. Bystrom, J. Chem. Thermodyn. **14**, 865 (1982).

82BYS/MAN K. Bystrom and M. Mansson, J. Chem. Soc. Perkins 2, 505 (1982).

77CAR/LAY J.A.S. Carson, P.G. Laye, and M. Yureali, J. Chem. Thermodyn. **9**, 827 (1977).

76CHA/ZWO J. Chao and B.J. Zwolinski, J. Phys. Chem. Ref. Data **5**, 319 (1976).

78CHA/ZWO J. Chao and B.J. Zwolinski, J. Phys. Chem. Ref. Data **7**, 363 (1978).

75CHE/ROD S.S. Chen, A.S. Rodgers, J. Chao, R.C. Wilhoit, and B.J. Zwolinski, J. Phys. Chem. Ref. Data **4**, 441 (1977).

85CHI J. S. Chickos, "Heat of Sublimation" in "Molecular Structures and Energetics" (ed. J. F. Liebman and A. Greenberg, Verlag Chemie, Weinheim, in press).

81CHI/HYM J. S. Chickos, A. S. Hyman, L. H. Ladon, and J. F. Liebman, J. Org. Chem. **46**, 4294 (1981). Rule 2 from this reference was used to estimate heats of vaporization of liquid hydrocarbons.

82CHU/NGU J.Y. Chu, T.T. Nguyen, and K.D. King, J. Phys. Chem. **86**, 443 (1982).

78COL/BEN A.J. Colussi and S.W. Benson, Int. J. Chem. Kinet. **10**, 1139 (1978).

82COL/JIM M. Colomina, P. Jimenez, and C. Turrion, J. Chem. Thermodyn. **14**, 779 (1982).

75COM F. Compernolle, Org. Mass. Spectrom. **10**, 289 (1975).

82CON/ZAF J.A. Connor, M.T. Zafarani-Moattar, J. Bickerton, N.I. El-Saied, S. Suradi, R. Carson, G. Al Takkhin, and H.A. Skinner, Organometallics **1**, 1166 (1982).

80DEF/MCI D. J. DeFrees, R. T. McIver, Jr. and W. J. Hehre, J. Am. Chem. Soc. **103**, 3334 (1980).

80DEM/WUL R.L. Deming and C.A. Wulff, "The Thermodynamics of Allenes, Ketenes and Related Compounds," in *The Chemistry of Ketenes, Allenes and Related Compounds,* S. Patai, Editor, part 1, pp. 155-164, J. Wiley and Sons, New York (1980).

81ELL/DIX M. R. Ellenberger, D. A. Dixon, and W. E. Farneth, J. Am. Chem. Soc. **103**, 5377 (1981).

79ELL/EAD M.R. Ellenberger, R.A. Eades, M.W. Thomsen, W.E. Farneth and D.A. Dixon, J. Am. Chem. Soc. **101**, 7151 (1979).

82FUC R. Fuchs, personal communication of unpublished heat of vaporization data.

82FUC/HAL R. Fuchs, J.H. Hallman and M.O. Perlman, Can. J. Chem. **60**, 1832 (1982).

83FUC/SMI R. Fuchs and N. Smith, personal communication of unpublished heat of formation and heat of vaporization data.

82FUR/SAK J. Furukawa, M. Sakiyama, S. Seki, Y. Saito, K. Kusano, Bull. Chem. Soc. Jpn. **55**, 3329 (1982).

72GAF "M-PYROL: "N-Methylpyrrolidone" (GAF Corporation, New York, 1972). "M-PYROL" is a registered tradename of this compound by GAF corporation. Neither our citing this name nor reference thereto should be viewed as an endorsement by the authors or the U.S. government.

72GOR A.S. Gordon, Int. J. Chem. Kinet. **4**, 541 (1972).

79HAC/PIL J.M. Hacking and G. Pilcher, J. Chem. Thermodyn. **11**, 1015 (1979).

78HAR/HEA D. Harrop and A.J. Head, J. Chem. Thermodyn. **10**, 705 (1978).

75HAR/THY P.W. Harland, and T.C.J. Thynne, Int. J. Mass Spectrom. Ion Phys. **18**, 73 (1975).

80HOL/LOS J.L. Holmes and F.P. Lossing, J. Am. Chem. Soc. **12**, 1591 (1980).

71JANAF D.R. Stull and H. Prophet, "JANAF Thermochemical Tables, 2nd Edition" NSRDS-NBS **37**, (1971).

82JANAF M.W. Chase, Jr., J.L. Curnutt, J.R. Downy Jr., R.A. McDonald, A.N. Syverrud, and E.A. Valenzuela, "JANAF Thermochemical Tables 1982 Supplement," J. Phys. Chem. Ref. Data **11**, 695 (1982).

76JEN J.L. Jensen, "Heats of Hydrogenation: A Brief Survey," Prog. Phys. Org. Chem. **12**, 189 (1976).

83KIR/DOM* D. R. Kirklin and E. S. Domalski, J. Chem. Thermodyn. **15**, 941 (1983). Heat of sublimation from 77PED/RYL.

82KOZ/MAS M. P. Kozina, V. S. Mastryunov, and E. M. Mil'vitshaya, Russian Chemical Review (Engl. Trans.) **51**, 765 (1982).

78KUD/KUD S.A. Kudchadker, A.P. Kudchadker, R.C. Wilhoit, and B.J. Zwolinski, J. Phys. Chem. Ref. Data **7**, 417 (1978).

79KUD/KUD S.A. Kudchadker, A.P. Kudchadker, R.C. Wilhoit, and B.J. Zwolinski, Thermochim. Acta **30**, 319 (1979).

79KUD/KUD2 A.P. Kudchadker, S.A. Kudchadker, and R.C. Wilhoit, "Four-Ring Condensed Aromatic Compounds," *API Monograph 709–79*, American Petroleum Institute, Washington, D.C. (1979).

79KUD/KUD3 A.P. Kudchadker and S.A. Kudchadker, "Pyridine and Phenylpyridines," *API Monograph 710–79*, American Petroleum Institute, Washington, D.C. (1979).

79KUD/KUD4 S.A. Kudchadker, A.P. Kudchadker, and B.J. Zwolinski, J. Chem. Thermodyn. **11**, 1051 (1979).

81KUD/KUD A.P. Kudchadker, S.A. Kudchadker, R.C. Wilhoit, and S.K. Gupta, "Acenaphthylene, Acenaphthene, Fluorene, and Fluoranthene," *API Monograph, 715–81*, American Petroleum Institute, Washington, D.C. (1981).

81KUD/KUD2 A.P. Kudchadker, S.A. Kudchadker, R.C. Wilhoit, and S.K. Gupta, "Carbazole, 9-Methylcarbazole and Acridine," in *API Monograph, 71681*, American Petroleum Institute, Washington, D.C. (1981).

81KUD/KUD3 A.P. Kudchadker, S.A. Kudchadker, R.C. Wilhoit, and S.K. Gupta, "Thiophene, 2,3- and 2,5-Dihydrothiophene and Tetrahydrothiophene," *API Monograph 717–81*, American Petroleum Institute, Washington, D.C. (1981).

77LIA/AUS S.G. Lias and P. Ausloos, Int. J. Mass Spectrom. Ion Phys. **23**, 273 (1977).

67LOU/LAI L.F. Loucks, K.J. Laidler, Can. J. Chem. **45**, 2785 (1967).

79MAJ/SVO V. Majer, V. Svoboda, J. Koubeck, and J. Pick, Collect. Czech. Chem. Commun. **44**, 3521 (1979).

80MAJ/WAG V. Majer, Z. Wagner, V. Svoboda, and V. Cadek, J. Chem. Thermodyn. **12**, 387 (1980).

82MAU M. Mautner, J. Am. Chem. Soc. **104**, 5 (1982).

78MCC/HAM D.G. McCormick and W.S. Hamilton, J. Chem. Thermodyn. **10**, 275 (1978).

82MCM/GOL D.F. McMillen and D.M. Golden, *The Annual Review of Physical Chemistry*, Vol. 33, Annual Reviews, Palo Alto, CA. (1982).

76MEY/HOT E.F. Meyer and C.A. Hotz, J. Chem. Eng. Data **21**, 274 (1974).

77NAB/SAB M. Nabavian, R. Sabbah, R. Chastel, and M. Laffitte, J. Chim. Phys. **74**, 115 (1977).

77NGA/SAB S.N. Ngauv, R. Sabbah, and M. Laffitte, Thermochim. Acta **20**, 371 (1977).

71NUT/LAU R. L. Nuttall, A. H. Laufer, and M. V. Kilday, J. Chem. Thermodyn. **3**, 107 (1971).

82PAM/ROG K.M. Pamidimukkala, D. Rogers, and G.B. Skinner, J. Phys. Chem. Ref. Data **11**, 83 (1982).

82PAU/HEH C.F. Pau and W.J. Hehre, J. Phys. Chem. **86**, 321 (1982).

82PAU/HEH2 C.F. Pau and W.J. Hehre, J. Phys. Chem. **86**, 1282 (1982).

73PEP/GAF V.I. Pepekin, R.G. Gafurov, Yu.A. Lebedev, T. Eremenko, E.M. Sogomonyan, and A.Ya. Apin, Bull. Acad. Sci. U.S.S.R. Div. Chem. Sci. **22**, 304 (1973).

77PED/RYL J.B. Pedley and J. Rylance, "Sussex-N.P.L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds", University of Sussex (1977).

79PET/MAJ L. Petros, V. Majer, J. Koubeck, V. Svoboda, and J. Pick, Collect. Czech. Chem. Commun. **44**, 3533 (1979).

82PIE/HEH W.J. Pietro, and W.J. Hehre, J. Am. Chem. Soc. **104**, 4329 (1982).

80POL/HEH S.K. Pollack and W.J. Hehre, Tetrahedron Lett. **21**, 2483 (1980).

81POL/RAI S.K. Pollack, B.C. Raine, and W.J. Hehre, J. Am. Chem. Soc. **103**, 6308 (1981).

79PRI/SAP S.J.W. Price and H.J. Sapiano, Can. J. Chem. **57**, 685 (1979).

83RAK/BOH A. B. Rakshit and D. K. Bohme, Int. J. Mass Spectrom. Ion Phys., **49**, 275 (1983).

71RAP/WES N.J. Rapport, E.F. Westrum Jr., and J.T.J. Andrews, J. Am. Chem. Soc. **93**, 4363 (1971).

77REI/PRA R.C. Reid, J.M. Prausnitz and T.K. Sherwood, *The Properties of Gases and Liquids*, 3rd Edition, McGraw Hill, New York, (1977).

80ROG/CHO D.W. Rogers, L.S. Choi, R.S. Girellini, T.J. Holmes and N.L. Allinger, J. Phys. Chem. **84**, 1810 (1980).

82ROY/MCM M. Roy and T.B. McMahon, Org. Mass Spectrom. **17**, 392 (1982).

80SAB R. Sabbah, Thermochim. Acta **41**, 33 (1980).

80SAB2 R. Sabbah, Thermochim. Acta **35**, 73 (1980).

74SAB/CHA R. Sabbah, R. Chastel, and M. Laffitte, Thermochim. Acta **10**, 353 (1974).

78SAB/LAF R. Sabbah and M. Laffitte, J. Chem. Thermodyn. **10**, 101 (1978).

78SAB/LAF2 R. Sabbah and M. Laffitte, Bull. Soc. Chim. Fr. 1–50 (1978).

81SAB/MIN R. Sabbah and C. Mindakis, Thermochim. Acta **43**, 269 (1981).

79SAL/PEA P.P.S. Saluja, L.A. Peacock, and R. Fuchs, J. Am. Chem. Soc. **101**, 1958 (1979).

74SCO D.W. Scott, "Chemical Thermodynamic Properties of Hydrocarbons and Related Substances: Properties of Alkane Hydrocarbons C1 through C10 The Ideal Gas State from 0 through 1500 K," APIRP62 Report *39*, (U.S. Dept. of Interior, Bureau of Mines, 1974).

77SHA/GOL R. Shaw, D.M. Golden and S.W. Benson, J. Phys. Chem. **81**, 1716 (1977).

80STA/VOG J.P. Stadelmann and J. Vogt, Int. J. Mass Spectrom. Ion Phys. **35**, 83 (1980).

79STE W.V. Steele, J. Chem. Thermodyn. **11**, 1185 (1979).

81STE/BAR S.E. Stein and B.D. Barton, Thermochim. Acta **44**, 265 (1981).

77STE/GOL S.E. Stein, D.M. Golden, and S.W. Benson, J. Phys. Chem. **81**, 314 (1977). We chose the results from group additivity values suggested by these authors as opposed to any other theoretical values also presented in this paper.

81SUR/HAC S. Suradi, J.M. Hacking, G. Pilcher, I. Gumrukcu, and M.F. Lappert, J. Chem. Thermodyn. **13**, 857 (1981).

80SVO/UCH V. Svoboda, V. Uchytilova, V. Majer, and J. Pick, Collect. Czech. Chem. Commun. **45**, 3233 (1980).

77TEL/RAB V.I. Tel'noi and I.B. Rabinovich, Russ. Chem. Rev. (Engl. Trans.) **46**, 1337 (1977).

73THY/HAR T.C.J. Thynne and P.W. Harland, Int. J. Mass Spectrom. Ion Phys. **11**, 399 (1973).

82/TN270 D.D. Wagman, W.H. Evans, V.P. Parker, R.H. Schumm, I. Halow, S.M. Bailey, K.L. Churney, and R.L. Nuttall, "The

NBS Tables of Chemical Thermodynamic Properties," J. Chem. Ref. Data **11**, Suppl. No. 2, 1982.

81TSA W. Tsang in "Shock Tubes in Chemistry," (A. Lifshitz, Editor; Dekker, 1981), p. 59.

79VAJ/HAR J.H. Vajda and A.G. Harrison, Int. J. Mass Spectrom. Ion Phys. **30**, 293 (1979).

79VIS D.S. Viswanath, "Quinoline," *API Monograph*, American Petroleum Institute, Washington, D.C. (1979).

79VIS/WIL D.S. Viswanath and R.C. Wilhoit, "Isoquinoline," in *API Monograph 712-79*, American Petroleum Institute, Washington, D.C. (1979).

78VOG/WIL J. Vogt, A.D. Williamson, and J.L. Beauchamp, J. Am. Chem. Soc. **100**, 3478 (1978).

80WIL/BAE G.D. Willett and T. Baer, J. Am. Chem. Soc. **102**, 6774 (1980).

76WIL/LEB A.D. Williamson, P.R. LeBreton, and J.L. Beauchamp, J. Am. Chem. Soc. **98**, 2705 (1976).

80WOL/HOL P. Wolkoff, J.L. Holmes and F.P. Lossing, Can. J. Chem. **58**, 251 (1980).