Summary of the Apparent Standard Partial Molal Gibbs Free Energies of Formation of Aqueous Species, Minerals, and Gases at Pressures 1 to 5000 Bars and Temperatures 25 to 1000 °C

Eric H. Oelkers

Laboratoire de Géochimie, CNRS-Université Paul Sabatier, 38 rue des Trente Six Ponts, 31400 Toulouse, France

Harold C. Helgeson

Department of Geology and Geophysics, University of California, Berkeley, CA 94720

Everett L. Shock

Department of Earth and Space Sciences, Washington University, St. Louis, MO 63130

Dimitri A. Sverjensky

Department of Earth and Space Sciences, The Johns Hopkins University, Baltimore MD 21218

James W. Johnson

Earth Sciences Division, Lawrence Livermore National Laboratory, L-219, P.O. Box 808, Livermore, CA 94550

and

Vitalii A. Pokrovskii

Department Erdwissen-schaften, ETH Zentrum, Zurich, CH-8092, Switzerland

Received March 1, 1993; revised manuscript received October 27, 1994

Accurate values of the apparent standard partial molal Gibbs free energies of formation ($\Delta\overline{G}°$) of aqueous species, minerals, and gases at high temperatures and pressures are a requisite for characterizing a variety of industrial and natural processes including corrosion of metals, solvent extraction, crystal growth, metamorphism, and the formation of hydrothermal ore deposits. Revision of the HKF equations of state for aqueous species other than H_2O (Helgeson, Kirkham and Flowers, 1981) by Tanger and Helgeson (1988) and Shock *et al.* (1992) permits calculation of $\Delta\overline{G}°$ for these species at temperatures to 1000 °C and pressures to 5000 bars. The revised equations of state were combined with parameters generated by Shock and Helgeson (1988, 1990), Shock *et al.* (1989), Sassani and Shock (1990), Shock and McKinnon (1993), Shock and Koretsky (1993), Schulte and Shock (1993), Pokrovskii and Helgeson (1995 a, b, and c), and Sverjensky *et al.* (1995) together with densities and electrostatic properties of H_2O computed from equations summarized by Johnson and Norton (1991) to calculate values of $\Delta\overline{G}°$ for aqueous species as a function of temperature and pressure. The results of these calculations are tabulated for 348 such species, including both inorganic and organic aqueous ions, neutral species, and metal ligand complexes. Similar calculations using equations, parameters, and thermodynamic data taken from Kelley (1960), Helgeson *et al.* (1978), Wagman *et al.* (1982), Hill (1990), Shock (1993), and Pokrovskii and Helgeson (1995 a and b) were used to generate tables of $\Delta\overline{G}°$ for H_2O, 22 minerals, and 18 gases. The tabulated values of $\Delta\overline{G}°$, which were generated with the aid of SUPCRT92 (Johnson *et al.*, 1992), facilitate considerably assessment of the thermodynamic behavior of chemical processes at both high and low temperatures and pressures. ©*1995 American Institute of Physics and American Chemical Society.*

Key words: aqueous species; electrolyte solutions; gases; Gibbs free energies of formation; H_2O; and water/mineral interaction.

Contents

1. Introduction 1402
2. Standard State Conventions 1402
3. Thermodynamic Relations 1403
4. Calculations 1404
5. Computational Uncertainties 1404
6. Concluding Remarks 1405
7. Acknowledgements 1558
8. References 1558

List of Figures

1. Logarithms of equilibrium constants for reactions among aqueous species as a function of temperature at pressure corresponding to liquid/vapor equilibrium for H_2O. 1406

2. Logarithms of equilibrium constants for reactions among aqueous species as a function of temperature in °C and pressure. 1406
3. Logarithms of equilibrium constants for reactions among aqueous species and minerals as a function of temperature at various pressures 1407
4. Logarithms of equilibrium constants for reactions among gases and aqueous species as a function of temperature at the pressures corresponding to liquid/vapor equilibrium for H_2O 1407

List of Tables

1. Apparent standard partial molal Gibbs free energies of formation of aqueous species other than H_2O 1408
2. Apparent standard molal Gibbs free energies of formation of H_2O. 1542
3. Apparent standard molal Gibbs free energies of formation of minerals 1544
4. Apparent standard molal Gibbs free energies of formation of gases. 1553
5. Chemical formulas of aqueous organic species considered in this study 1554
6. Index of aqueous species considered in this study. 1555
7. Index of minerals considered in this study 1558

1. Introduction

Because aqueous species play such a major role in a wide variety of chemical and geological processes, extensive efforts have been made over the past several decades to characterize the thermodynamic behavior of these species at both high and low temperatures and pressures (Helgeson and Kirkham, 1974a, b, 1976; Helgeson *et al.*, 1981, 1988a, b; Helgeson, 1982, 1985, 1992 a and b; Haar *et al.* 1984; Jackson and Helgeson, 1985; Sverjensky, 1987; Tanger and Helgeson, 1988; Shock and Helgeson, 1988, 1989, 1990; Oelkers and Helgeson, 1988, 1990, 1991, 1993a, 1993b; Shock *et al.* 1989, 1992; Sassani and Shock, 1990, 1992; Johnson and Norton, 1991; Shock, 1992, 1993, 1995; Schulte and Shock, 1993; Shock and Koretsky, 1993; Sverjensky *et al.* 1995; Pokrovskii and Helgeson, 1995 a, b, and c). As a consequence, it is now possible to compute with the aid of SUPCRT92 (Johnson *et al.*, 1992) the standard partial molal thermodynamic properties of 348 aqueous organic and inorganic ions and neutral species including H_2O and metal ligand complexes at temperatures to 1000 °C and pressures to 5000 bars[1] SUPCRT92 can also be used to calculate the standard partial molal properties of minerals and gases at high pressures and temperatures using equations, parameters, and thermodynamic data taken from Kelley (1960), Helgeson *et al.* (1978), Wagman *et al.* (1982), Haar *et al.* (1984), Shock (1993), and Pokrovskii and Helgeson (1995 a and b).

Equilibrium constants for reactions among the aqueous species, minerals, and gases can be used to interpert phase relations and equilibrium constraints in a wide variety of chemical, industrial, and geochemical systems. Such equilibrium constants can also be generated using SUPCRT92. Alternatively, computed values of the apparent standard partial molal Gibbs free energies of formation ($\Delta\overline{G}^\circ$) of aqueous species, minerals, and gases at high temperatures and pressures can be taken from tables to generate equilibrium constants (K) for reactions from

$$K = e^{-\Delta\overline{G}^\circ_r/RT} \tag{1}$$

where R refers to the gas constant (1.9872 cal $mol^{-1}K^{-1}$), T stands for temperature in K, and $\Delta\overline{G}^\circ_r$ denotes the standard partial molal Gibbs free energy of reaction computed from

$$\Delta\overline{G}^\circ_r = \sum_i n_{i,r}\Delta\overline{G}^\circ_i \tag{2}$$

where $n_{i,r}$ represents the stoichiometric reaction coefficient of the ith species in the rth reaction, which is positive for products and negative for reactants, and $\Delta\overline{G}^\circ_i$ designates the apparent standard partial molal Gibbs free energy of formation from the elements (see below) of the subscripted reactant or product. The purpose of the present communication is to facilitate calculations of this kind by providing in tabular form values of $\Delta\overline{G}^\circ_i$ for aqueous species, minerals, and gases which can be used together with Eqs. (1) and (2) to compute equilibrium constants for a wide variety of chemical reactions at temperatures from 25 to 1000 °C and pressures from 1 to 5000 bars.

2. Standard State Conventions

The standard state convention for aqueous species adopted in the present study is one of unit activity of the species in a hypothetical one molal solution referenced to infinite dilution at any pressure or temperature. The standard state for minerals and H_2O corresponds to unit activity of the pure solid or liquid at any pressure and temperature, but that for gases calls for unit fugacity of the hypothetical perfect gas at 1 bar and any temperature.

The standard partial molal Gibbs free energies given in the present communication are apparent standard partial molal Gibbs free energies of formation ($\Delta\overline{G}^\circ$) defined by (Benson, 1968; Helgeson *et al.*, 1978, 1981)

$$\Delta\overline{G}^\circ = \Delta\overline{G}^\circ_f + (\overline{G}^\circ_{P,T} - \overline{G}^\circ_{P_r,T_r}) \tag{3}$$

where $\Delta\overline{G}^\circ_f$ stands for the standard partial molal Gibbs free energy of formation of an aqueous species, mineral, or gas from the elements in their stable form at the reference pressure (P_r) and temperature (T_r) of 1 bar and 298.15 K, and $(\overline{G}^\circ_{P,T} - \overline{G}^\circ_{P_r,T_r})$ denotes the difference in the standard partial molal Gibbs free energy of the aqueous species, mineral, or gas at the pressure (P) and temperature (T) of interest and that at P_r and T_r.

The apparent standard partial molal Gibbs free energies of formation of aqueous species tabulated below are conven-

ional properties. $\Delta\bar{G}^\circ$ of an aqueous species is related to the absolute apparent standard partial molal Gibbs free energy of formation of the species ($\Delta\bar{G}^{\circ\,abs}$) by

$$\Delta\bar{G}^\circ = \Delta\bar{G}^{\circ abs} - Z\Delta\bar{G}^{\circ,abs}_{H^+} \tag{4}$$

where $\Delta\bar{G}^{\circ,abs}_{H^+}$ refers to the absolute apparent standard partial molal Gibbs free energy of formation of the hydrogen ion and Z represents the formal charge on the aqueous species of interest. Hence, for neutral species, $\Delta\bar{G}^\circ = \Delta\bar{G}^{\circ abs}$. Note also that it follows from Eq. (4) that $\Delta\bar{G}^\circ_{H^+} = 0$, which permits calculation of $\Delta\bar{G}^\circ$ for individual ions from those of electrolytes using the additivity principle (Millero, 1972; Fortier *et al.*, 1974; Helgeson and Kirkham, 1976; Tanger and Helgeson, 1988).

3. Thermodynamic Relations

The parenthetical term in Eq. (3) for an aqueous species other than H_2O can be expressed as (Tanger and Helgeson, 1988; Shock *et al.*, 1989)

$$\bar{G}^\circ_{P,T} - \bar{G}^\circ_{P_r,T_r} = -\bar{S}^\circ_{P_r,T_r}(T-T_r) - c_1\left(T\ln\left(\frac{T}{T_r}\right) - T + T_r\right)$$

$$+a_1(P-P_r) + a_2\ln\left(\frac{\Psi+P}{\Psi+P_r}\right)$$

$$-c_2\left(\left(\left(\frac{1}{T-\Theta}\right)-\left(\frac{1}{T_r-\Theta}\right)\right)\left(\frac{\Theta-T}{\Theta}\right)-\left(\frac{T}{\Theta^2}\right)\ln\left(\frac{T_r(T-\Theta)}{T(T_r-\Theta)}\right)\right)$$

$$+\left(\frac{1}{T-\Theta}\right)\left(a_3(P-P_r)+a_4\ln\left(\frac{\Psi+P}{\Psi+P_r}\right)\right)$$

$$+\omega\left(\frac{1}{\epsilon}-1\right)-\omega_{P_r,T_r}\left(\frac{1}{\epsilon_{P_r,T_r}}-1\right)+\omega_{P_r,T_r}Y_{P_r,T_r}(T-T_r) \tag{5}$$

where $\bar{S}^\circ_{Pr,Tr}$ stands for the standard partial molal entropy of the species at the reference pressure and temperature, ϵ and ϵ_{P_r,T_r} designate the dielectric constant of H_2O at the temperature and pressure of interest and P_r, T_r, respectively, $Y_{Pr,\,Tr}$ is given by

$$Y_{P_r,T_r} = \frac{1}{\epsilon_{P_r,T_r}}\left(\left(\frac{\partial\ln\epsilon}{\partial T}\right)_{P_r,T_r}\right) = \frac{1}{\epsilon^2_{P_r,T_r}}\left(\left(\frac{\partial\epsilon}{\partial T}\right)_{P_r,T_r}\right) \tag{6}$$

and a_1, a_2, a_3, a_4, c_1, and c_2 refer to temperature/pressure independent equation of state parameters for the species. Ψ and Θ in Eq. (5) denote solvent constants equal to 2600 bars and 228 °K, respectively. ω represents the conventional Born coefficient of the species, which can be expressed as

$$\omega = \eta(Z^2(r_{e,P_r,T_r}+|Z|g)^{-1} - Z(3.082+g)^{-1}) \tag{7}$$

where g designates a solvent function of temperature and density given by Shock *et al.* (1992), $\eta = 1.66027\times10^5$ Å cal mol^{-1}, Z again stands for the formal charge on the species, r_{e,P_r,T_r} refers to the effective electrostatic radius of the species at the reference pressure and temperature, which for monatomic ions is given by (Helgeson and Kirkham, 1976)

$$r_{e,P_r,T_r} = r_x + k_z|Z| \tag{8}$$

and for charged aqueous species by (Shock and Helgeson, 1988)

$$r_{e,P_r,T_r} = \frac{Z^2(\eta Y_{P_r,T_r}-\kappa_z)}{\bar{S}^\circ_{P_r,T_r}-\alpha_Z} \tag{9}$$

where r_x denotes the crystallographic radius of the ion, k_Z designates a constant equal to 0.94 Å for cations and 0.0 Å for anions, κ_Z represents a correlation parameter equal to 100 Å cal mol^{-1} K^{-1}, $\bar{S}^\circ_{P_r,T_r}$ stands for the standard partial molal entropy of the species at the subscripted pressure and temperature, and α_Z is defined by

$$\alpha_Z \equiv 71.5\ |Z| \text{ cal mol}^{-1}\text{ K}^{-1}. \tag{10}$$

The conventional Born correlation parameters of neutral aqueous species are taken to be independent of pressure and temperature. Hence, for these species

$$\omega = (-1514.4\text{ K})\ \bar{S}^\circ_{P_r,T_r} + \beta_Z \tag{11}$$

where β_Z refers to a correlation parameter equal to 0.0 cal mol^{-1} for noble or diatomic gases and 34,000 cal mol^{-1} for polyatomic and neutral aqueous species (Shock and Helgeson, 1990).

The parenthetical term in Eq. (3) for the stable phase of H_2O at a given pressure and temperature can be computed from (Johnson and Norton, 1991)

$$(\bar{G}^\circ_{H_2O,P,T} - \bar{G}^\circ_{H_2O,P_r,T_r}) = \bar{A}^\circ_{P,T} + \rho_{P,T}\left(\frac{\partial\bar{A}^\circ}{\partial\rho}\right)_T - (\bar{G}^\circ_{H_2O,P_r,T_r} - \bar{G}^\circ_{H_2O,tr}) \tag{12}$$

where $\rho_{P,T}$ and $\bar{A}^\circ_{P,T}$ represent the density and standard partial molal Helmholtz free energy of H_2O, respectively, at the subscripted pressure and temperature, and ($\bar{G}^\circ_{H_2O,P_r,T_r} - \bar{G}^\circ_{H_2O,tr}$) stands for the difference between the standard partial molal Gibbs free energy of H_2O at P_r, T_r and its value at the triple point of H_2O (0.0061173 bars and 273.16 K); this difference is equal to −398 cal mol^{-1}. The density of H_2O in Eq. (12) can be expressed as (Haar *et al.*, 1984; Johnson and Norton, 1991)

$$\rho_{P,T} = (PCM)^{1/2}\left(\frac{\partial\bar{A}^\circ}{\partial\rho}\right)^{-1/2}_T \tag{13}$$

where C stands for a conversion factor (0.02390054 cal bar^{-1} cm^{-3}), M signifies the molecular weight of H_2O (18.0152 g mol^{-1}) and P again represents the pressure of interest. Equations (3), (12) and (13) were used together with values of $\bar{A}^\circ_{P,T}$ and $(\partial\bar{A}^\circ/\partial\rho)_T$ computed from equations reported by Hill (1990) to calculate values of $\Delta\bar{G}^\circ_{H_2O}$. The Hill (1990) formulation of the Helmholtz function is based on a fit

of experimental data obtained at temperatures from 0 to 900 °C and pressures from 0 to 10 kbar. The formulation was demonstrated to permit regular extrapolations of thermodynamic properties to a maximum temperature of 2000 °C and a maximum pressure of 250 kbar.

The parenthetical term in Eq. (3) for minerals and gases can be computed from (Helgeson *et al.* 1978)

$$\overline{G}^{\circ}_{P,T}-\overline{G}^{\circ}_{P_r,T_r} = -\overline{S}^{\circ}_{P_r,T_r}(T-T_r)+a\left(T-T_r-T\ln\left(\frac{T}{T_r}\right)\right) -\left(\frac{(c+bT_r^2T)(T-T_r)^2}{2T_r^2T}\right)+\overline{V}^{\circ}_{P_r,T_r}(P-P_r) \quad (14)$$

where a, b, and c stand for temperature/pressure-independent coefficients characteristic of the mineral and $\overline{V}^{\circ}_{P_r,T_r}$ refers to the standard molal volume of the mineral at the subscripted temperature and pressure. Equation (14) is compatible with the Maier-Kelley power function (Kelley, 1960) for the standard partial molal heat capacities of minerals and gases. The last term in Eq. (14) for minerals is predicated on the observation that their standard partial molal expansibilities and compressibilities in the crust of the Earth are small and have an opposing effect on the standard partial molal volumes of the minerals with increasing temperature and pressure. Consequently, $\overline{V}^{\circ}_{P,T}$ for minerals can be taken to be equal to $\overline{V}^{\circ}_{P_r,T_r}$ without introducing undue uncertainty in calculated values of $(\overline{G}^{\circ}_{P,T}-\overline{G}^{\circ}_{P_r,T_r})$ at pressures ≤ 10 kbar (Helgeson *et al.*, 1978).[2] As a consequence of the standard state for gases adopted in the present study, the standard partial molal volumes of gases, and therefore the last term on the right side of Eq. (14) for gases are equal to zero.

4. Calculations

Calculated values of $\Delta\overline{G}^{\circ}$ for 348 aqueous species other than H_2O are listed in Table 1 for temperatures and pressures ranging from 25 °C and 1 bar to 1000 °C and 5 kbar. The values of $\Delta\overline{G}^{\circ}$ shown in the table were calculated from Eqs. (3) and (5) using equations and parameters taken from the sources listed in Table 6. The species are arranged in alphabetical order in these tables.

Values of $\Delta\overline{G}^{\circ}$ for H_2O calculated from Eqs. (3), (12) and (13) using equations and parameters taken from Hill (1990) are listed in Table 2 for temperatures and pressures from 25 °C and 1 bar to 2000 °C and 200 kbar. The minimum temperatures for which $\Delta\overline{G}^{\circ}$ values are given in this table are limited at high pressures by the ice VII-H_2O melting curve (Lei *et al.*, 1993). Corresponding values of $\Delta\overline{G}^{\circ}$ for 22 minerals and 18 gases computed from Eqs. (3) and (14) using parameters reported by Kelley (1960), Helgeson *et al.* (1978), Wagman *et al.* (1982), Shock (1993), and Pokrovskii and Helgeson (1995a and b) are given in Tables 3 and 4 for temperatures from 25° to 1000 °C and pressures from 1 bar to 5 kbar.[3] The values of $\Delta\overline{G}^{\circ}$ given in Table 3 are consistent with experimental solubility and phase equilibrium data, but not necessarily with metastable phase relations in nature. A list of chemical formulas of the organic aqueous species denoted by name in Table 1 appears in Table 5. Indexes of the aqueous species and minerals for which values of $\Delta\overline{G}^{\circ}$ are given in Tables 1 and 2, respectively, are shown in Tables 6 and 7.

5. Computational Uncertainties

Detailed analysis of the magnitudes and sources of uncertainties in values of $\Delta\overline{G}^{\circ}$ computed from Eqs. (3) to (11) can be found in Shock and Helgeson (1988, 1990), Shock *et al.* (1989), and Sverjensky *et al.* (1995). These uncertainties vary considerably depending on the species, pressure and temperature. Uncertainties associated the $\Delta\overline{G}^{\circ}$ values of aqueous species listed in Table 1 stem from uncertainties associated with both the standard partial molal Gibbs free energies of formation from the elements at 25 °C and 1 bar and the equations of state parameters (a_1, a_2, a_3, a_4, c_1, c_2, and ω). Typical uncertainties in values of $\Delta\overline{G}^{\circ}$ at 25 °C and 1 bar for aqueous species are of the order of ±200 to ±600 cal mol^{-1} (Wagman *et al.* 1982). In accord with Shock and Helgeson (1988), in the unlikely event that all of the average uncertainties in estimated equations of state parameters lead to uncertainties in calculated values of $\Delta\overline{G}^{\circ}$ of the same sign, the combined effect of these uncertainties would be ±0 at 25 °C and 1 bar, ~±700 cal/mol at 500 °C and 2 kbar, and ~±1500 cal/mol at 1000 °C and 5 kbar. However, it appears likely that uncertainties arising from the various equations of state parameters would tend to cancel out with increasing temperature and pressure. Under these circumstances, uncertainties associated with the $\Delta\overline{G}^{\circ}$ values listed in Table 1 would probably be less than ~±1000 cal mol^{-1}. The uncertainties in the values of $\Delta\overline{G}^{\circ}$ for H_2O given in Table 2 tend to be substantially lower than those for the aqueous species shown in Table 1.

Uncertainties in the calculated values of $\Delta\overline{G}^{\circ}$ for the minerals and gases listed in Tables 3 and 4 arise from uncertainties both in $\Delta\overline{G}^{\circ}_f$ in Eq. (3) and those associated with the thermodynamic parameters used to calculate $(\overline{G}^{\circ}_{P,T}-\overline{G}^{\circ}_{P_r,T_r})$ from Eq. (14). The values of $\Delta\overline{G}^{\circ}_f$ for most of the minerals shown in Table 3 were obtained by regression of experimental mineral solubilities and/or critical evaluation of phase relations at high temperatures and pressures, which generally lead to uncertainties in $\Delta\overline{G}^{\circ}_f$ of ~±300 cal mol (Pokrovskii and Helgeson, 1995a and b). The contribution of uncertainties in the thermodynamic parameters that appear in Eq. (14) to the overall uncertainty of the $\Delta\overline{G}^{\circ}$ values given in Tables 3 and 4 can be estimated by considering the individual contributions of uncertainties associated with standard molal entropies, heat capacities, and volumes. The standard molal entropies and heat capacities of minerals at 25 °C and 1 bar adopted by Pokrovskii and Helgeson (1995 a and b) are based on calorimetric measurements. These values are generally uncertain to

[2]The one exception to this approximation for minerals in the present study is the volume of quartz, which is taken to be a function of temperature and pressure in accord with expansibility and compressibility measurements (Helgeson *et al.* 1978).

[3]Corresponding values for more than 100 additional minerals will appear in a subsequent publication.

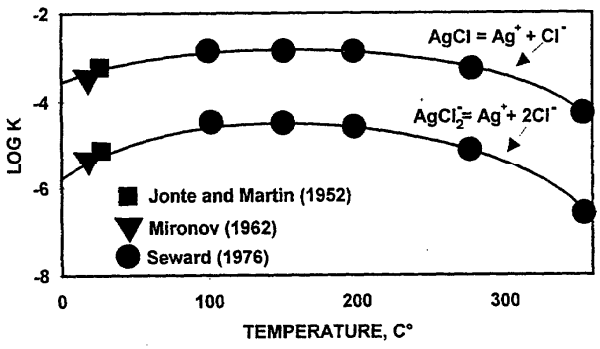
the extent of a few tenths of a cal mol^{-1} (Helgeson *et al.*, 1978). Taking account of Eqs. (3) and (14), an uncertainty in $\overline{S}^{\circ}_{P_r,T_r}$ for a given mineral of ± 0.2 cal mol^{-1} would lead to an uncertainty in $\Delta\overline{G}^{\circ}$ of ± 95 cal mol^{-1} at 500 °C and ± 195 cal mol^{-1} at 1000 °C. Similarly, uncertainty in the standard molal heat capacities of ± 0.2 cal $mol^{-1}K^{-1}$ introduce uncertainties in $\Delta\overline{G}^{\circ}$ of $\sim\pm 50$ cal mol^{-1} at 500 °C and $\sim\pm 175$ cal mol^{-1} at 1000 °C. The molal volumes of minerals at 25° and 1 bar are generally accurate within ± 0.1 cm^3 mol^{-1}, which introduces a corresponding uncertainty in $\Delta\overline{G}^{\circ}$ of 12 cal mol^{-1} at 5 kbar. Uncertainties associated with the assumption that the volumes of the minerals are independent of temperature and pressure are probably no more than 100 cal mol^{-1} over the temperature and pressure range considered in Table 3 (Helgeson *et al.*, 1978). It follows that the overall uncertainty in the values of $\Delta\overline{G}^{\circ}$ for minerals given in Table 3 is of the order of a kcal mol^{-1} or less. The uncertainties in the values of $\Delta\overline{G}^{\circ}$ for gases in Table 4 are generally smaller than the minerals in Table 3.

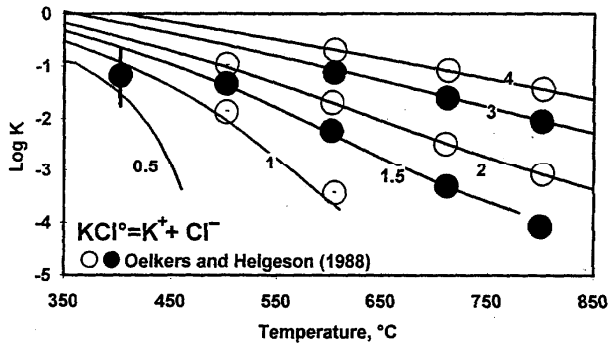
It follows from the discussion in the preceding paragraphs that the overall uncertainty in the values of $\Delta\overline{G}^{\circ}$ for aqueous species, minerals, and gases computed above is of the order of a kcal mol^{-1} or less at high temperatures and pressures. However, because uncertainties in $\Delta\overline{G}^{\circ}$ tend to cancel in reactions (Helgeson *et al.*, 1978), the relative uncertainties in $\Delta\overline{G}^{\circ}_r$ are much smaller. For example, the logarithms of equilibrium constants generated using values of $\Delta\overline{G}^{\circ}$ taken from Tables 1 to 4 are generally within 0.2 units of their experimental counterparts at all temperatures and pressures (see below).

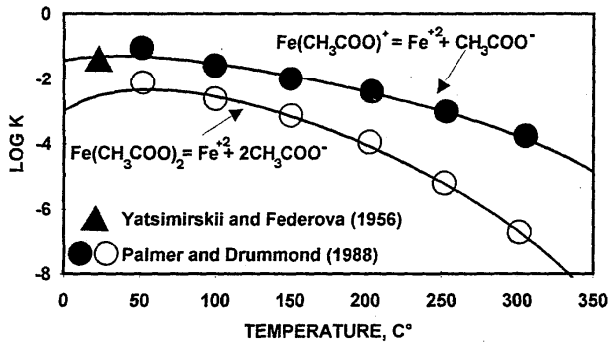
The general validity of the thermodynamic data and equations of state used to generate the values of $\Delta\overline{G}^{\circ}$ given in Tables 1–4 can be assessed in Figures 1–4, where logarithms of equilibrium constants for various reactions generated using values of $\Delta\overline{G}^{\circ}$ taken from these tables represented by the curves can be compared with their experimental counterparts denoted by the symbols. It can be seen in these figures that the computed values are in close agreement with the log K values determined experimentally. Numerous other such comparisons can be found in Helgeson *et al.* (1978), Sverjensky (1987), Shock and Helgeson (1988, 1990), Shock *et al.* (1989), Shock (1993), Shock and Koretsky (1993), Sverjensky *et al.* (1995) and Pokrovskii and Helgeson (1995 a, b, and c).

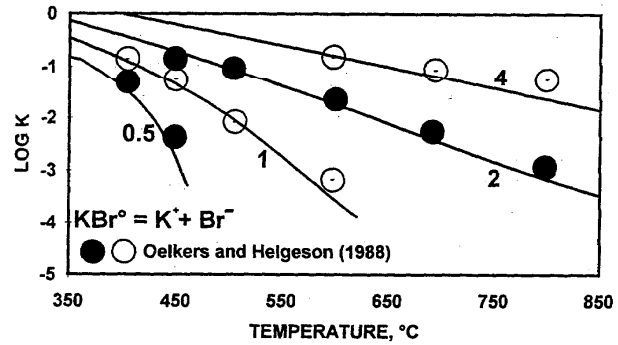
6. Concluding Remarks

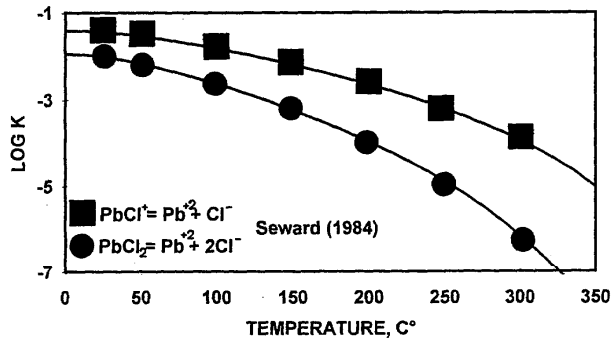
The values of $\Delta\overline{G}^{\circ}$ for aqueous species, minerals, and gases listed in Tables 1–4 can be used to calculate without a computer equilibrium constants from Eqs. (1) and (2) for a wide variety of chemical reactions. The equations summarized above, together with corresponding equations for the apparent standard partial molal enthalpies of formation and the standard partial molal entropies, volumes, and heat capacities of aqueous species, minerals, and gases have been incorporated into computer program SUPCRT92 (Johnson *et al.* 1992) which can be obtained at no cost from the Laboratory of Theoretical Geochemistry at the University of California, Berkeley.

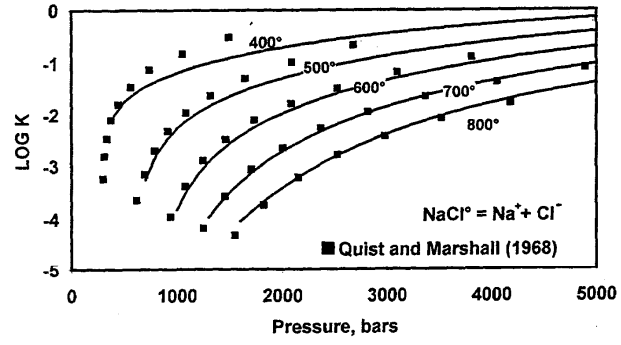


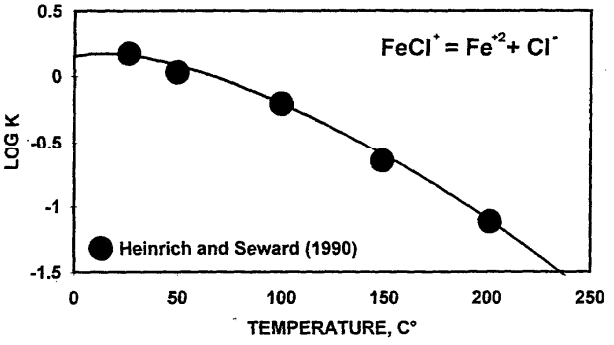












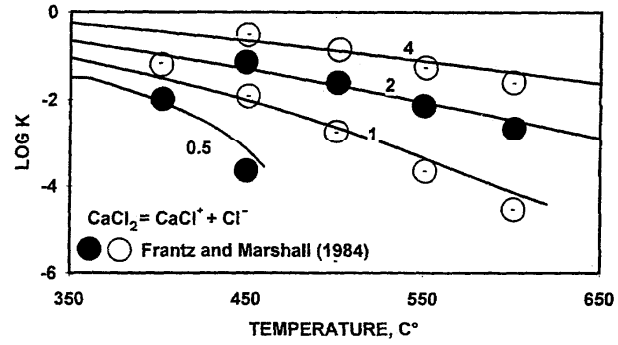


FIG. 1. Logarithms of equilibrium constants (Log k) for reactions among aqueous species as a function of temperature at pressure corresponding to liquid/vapor equilibrium for H_2O. The symbols represent experimentally derived equilibrium constants taken from the sources listed in the figure, but the curves were generated from Eqs. (1)–(3) using values of $\Delta\bar{G}°$ taken from Table 1.

FIG. 2. Logarithms of equilibrium constants (Log k) for reactions among aqueous species as a function of temperature in °C and pressure (labeled in kilobars). The symbols represent experimentally derived equilibrium constants taken from the sources listed in the figure, but the curves were generated from Eqs. (1)–(3) together with values of $\Delta\bar{G}°$ taken from Table 1.

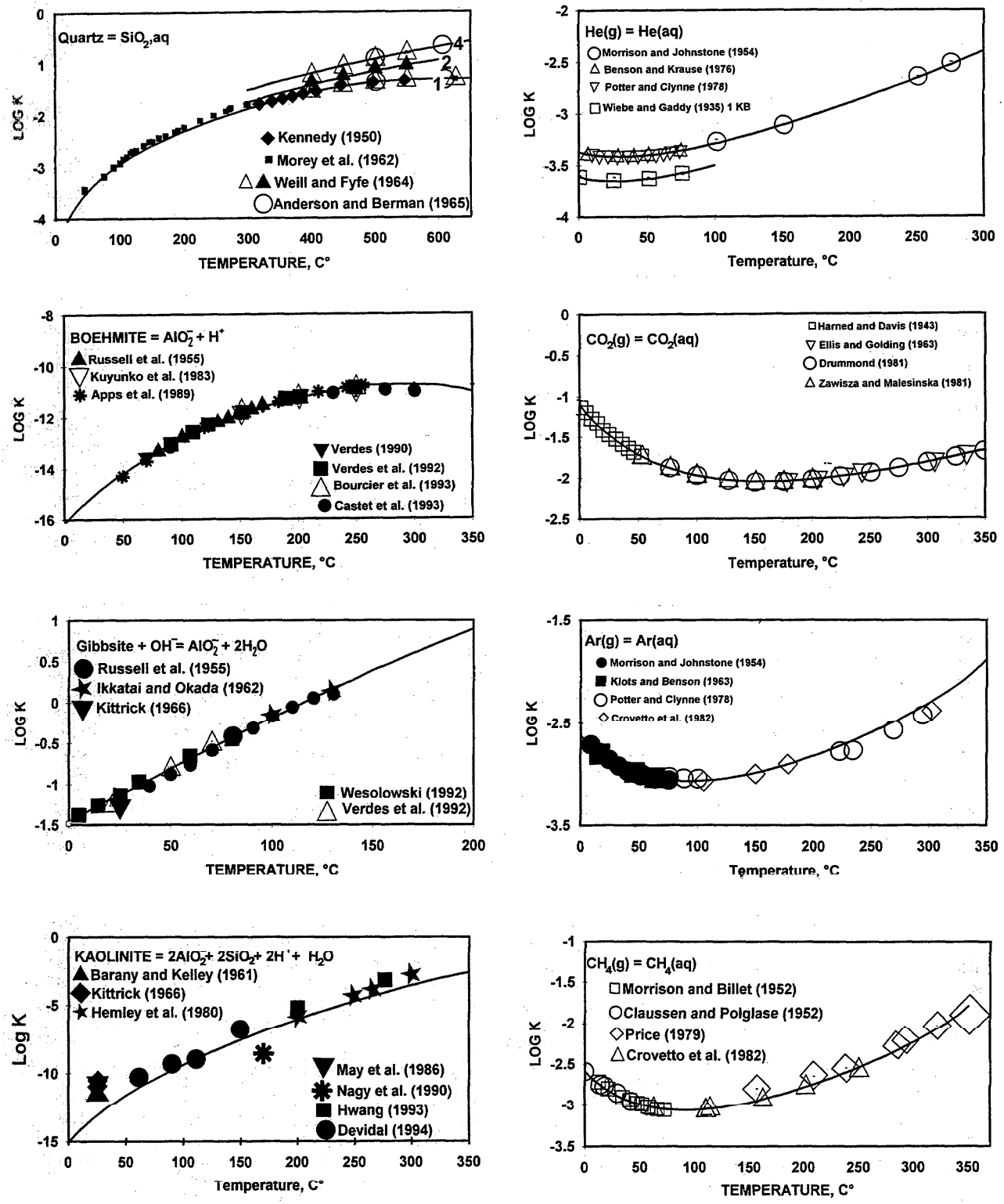


FIG. 3. Logarithms of equilibrium constants (Log k) for reactions among aqueous species and minerals as a function of temperature at various pressures (labeled in kilobars). Unlabled curves designate pressures corresponding to liquid/vapor equilibrium for H_2O. The symbols represent experimentally derived equilibrium constants taken from the sources listed in the figure, but the curves were generated from Eqs. (1)–(3) together with values of $\Delta\overline{G}°$ taken from Tables 1 and 3.

FIG. 4. Logarithms of equilibrium constants (Log k) for reactions among gases and aqueous species as a function of temperature at the pressures corresponding to liquid/vapor equilibrium for H_2O. The symbols in this figure represent experimentally derived equilibrium constants taken from the sources listed in the figure, but the curves were generated from Eqs. (1)–(3) using values of $\Delta\overline{G}°$ taken from Tables 1 and 4.

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text).

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Butanamide				
25	9.41	10.46	11.47	12.45	13.40	15.27	17.08	18.86
50	8.13	9.18	10.19	11.16	12.11	13.96	15.75	17.51
75	6.65	7.71	8.72	9.69	10.64	12.48	14.26	16.00
100	5.00	6.06	7.07	8.05	9.00	10.83	12.61	14.34
125	3.19	4.25	5.27	6.24	7.19	9.03	10.80	12.53
150	1.23	2.29	3.31	4.29	5.24	7.07	8.84	10.57
175	−0.89	0.18	1.20	2.19	3.14	4.98	6.75	8.48
200	−3.14	−2.07	−1.04	−0.05	0.91	2.75	4.53	6.25
225	−5.52	−4.46	−3.41	−2.42	−1.45	0.40	2.18	3.91
250	−8.04	−6.98	−5.91	−4.91	−3.93	−2.07	−0.29	1.44
300	−13.49	−12.41	−11.29	−10.24	−9.25	−7.36	−5.56	−3.82
350	−19.79	−18.41	−17.14	−16.04	−15.01	−13.08	−11.25	−9.49
400		−25.21	−23.49	−22.27	−21.18	−19.19	−17.33	−15.55
450		−33.90	−30.40	−28.94	−27.76	−25.67	−23.77	−21.96
500		−45.07	−37.94	−36.06	−34.73	−32.52	−30.55	−28.71
550		−55.66	−46.20	−43.63	−42.08	−39.70	−37.66	−35.78
600		−65.51	−55.06	−51.65	−49.80	−47.20	−45.08	−43.15
700		−84.30	−73.58	−68.78	−66.23	−63.09	−60.77	−58.73
800		−102.76	−92.43	−86.90	−83.76	−80.06	−77.50	−75.36
900		−121.34	−111.46	−105.62	−102.09	−97.92	−95.17	−92.95
1000		−140.24	−130.75	−124.79	−121.03	−116.55	−113.67	−111.42
				1-Butanol				
25	−38.84	−37.83	−36.85	−35.90	−34.97	−33.15	−31.38	−29.63
50	−40.12	−39.11	−38.13	−37.19	−36.27	−34.48	−32.73	−31.02
75	−41.59	−40.58	−39.61	−38.67	−37.76	−35.98	−34.25	−32.56
100	−43.25	−42.24	−41.27	−40.33	−39.41	−37.64	−35.92	−34.24
125	−45.08	−44.06	−43.09	−42.15	−41.24	−39.47	−37.75	−36.08
150	−47.06	−46.04	−45.07	−44.13	−43.21	−41.44	−39.73	−38.07
175	−49.19	−48.18	−47.20	−46.25	−45.33	−43.56	−41.85	−40.19
200	−51.47	−50.46	−49.46	−48.51	−47.60	−45.82	−44.11	−42.44
225	−53.89	−52.87	−51.87	−50.91	−49.99	−48.21	−46.49	−44.82
250	−56.44	−55.42	−54.41	−53.44	−52.51	−50.72	−49.00	−47.33
300	−61.97	−60.93	−59.85	−58.85	−57.90	−56.09	−54.35	−52.67
350	−68.36	−67.02	−65.80	−64.74	−63.75	−61.89	−60.14	−58.44
400		−73.91	−72.25	−71.07	−70.03	−68.11	−66.32	−64.61
450		−82.69	−79.26	−77.86	−76.72	−74.71	−72.88	−71.14
500		−93.93	−86.93	−85.10	−83.81	−81.68	−79.79	−78.01
550		−104.61	−95.31	−92.80	−91.29	−88.99	−87.03	−85.21
600		−114.58	−104.28	−100.95	−99.15	−96.63	−94.59	−92.73
700		−133.63	−123.08	−118.37	−115.88	−112.84	−110.59	−108.62
800		−152.41	−142.24	−136.81	−133.74	−130.13	−127.66	−125.59
900		−171.34	−161.62	−155.88	−152.43	−148.36	−145.70	−143.55
1000		−190.63	−181.29	−175.43	−171.75	−167.38	−164.59	−162.41
				1-Butene				
25	20.31	21.20	22.05	22.87	23.65	25.17	26.63	28.04
50	19.12	20.05	20.93	21.77	22.58	24.13	25.63	27.08
75	17.77	18.71	19.61	20.47	21.29	22.88	24.39	25.86
100	16.26	17.23	18.14	19.01	19.84	21.45	22.98	24.47
125	14.62	15.60	16.53	17.41	18.25	19.88	21.43	22.92
150	12.86	13.86	14.79	15.69	16.54	18.18	19.74	21.25
175	10.99	11.99	12.95	13.85	14.72	16.37	17.95	19.47
200	9.00	10.02	10.99	11.91	12.79	14.46	16.05	17.58
225	6.90	7.93	8.93	9.87	10.76	12.45	14.06	15.60
250	4.68	5.74	6.77	7.73	8.64	10.35	11.97	13.53
300	−0.17	1.01	2.15	3.17	4.12	5.89	7.55	9.13
350	−6.14	−4.30	−2.90	−1.76	−0.74	1.11	2.82	4.43
400		−10.60	−8.42	−7.07	−5.95	−3.98	−2.21	0.55
450		−19.85	−14.54	−12.79	−11.49	−9.36	−7.51	5.79

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Butene — Continued				
500		−33.12	−21.44	−18.94	−17.38	−15.02	−13.06	−11.29
550		−45.04	−29.28	−25.57	−23.62	−20.96	−18.87	−17.02
600		−55.37	−37.86	−32.67	−30.20	−27.16	−24.92	−22.98
700		−73.58	−55.61	−47.97	−44.29	−40.30	−37.68	−35.56
800		−90.20	−72.90	−63.99	−59.27	−54.28	−51.27	−48.95
900		−106.10	−89.59	−80.13	−74.72	−68.92	−65.57	−63.10
1000		−121.71	−105.89	−96.22	−90.41	−84.05	−80.47	−77.95
				1-Butyne				
25	50.03	50.97	51.86	52.71	53.53	55.11	56.64	58.12
50	48.85	49.82	50.74	51.62	52.47	54.10	55.66	57.17
75	47.52	48.51	49.45	50.35	51.21	52.87	54.45	55.99
100	46.05	47.06	48.01	48.92	49.80	51.48	53.08	54.63
125	44.46	45.49	46.45	47.37	48.26	49.95	51.57	53.14
150	42.76	43.80	44.78	45.71	46.61	48.32	49.95	51.53
175	40.95	42.00	43.00	43.94	44.85	46.58	48.22	49.81
200	39.04	40.10	41.12	42.08	43.00	44.74	46.40	48.00
225	37.02	38.10	39.14	40.12	41.05	42.82	44.49	46.10
250	34.89	36.00	37.07	38.07	39.02	40.81	42.50	44.12
300	30.24	31.46	32.65	33.71	34.70	36.55	38.28	39.93
350	24.51	26.38	27.83	29.00	30.06	31.99	33.77	35.45
400		20.33	22.55	23.94	25.10	27.15	28.99	30.72
450		11.34	16.70	18.49	19.83	22.04	23.96	25.75
500		−1.64	10.08	12.63	14.23	16.66	18.69	20.54
550		−13.25	2.55	6.30	8.29	11.03	13.19	15.11
600		−23.26	−5.70	−0.47	2.04	5.15	7.47	9.48
700		−40.77	−22.76	−15.08	−11.35	−7.29	−4.60	−2.40
800		−56.64	−39.30	−30.35	−25.58	−20.52	−17.43	−15.05
900		−71.73	−55.18	−45.68	−40.23	−34.35	−30.93	−28.39
1000		−86.49	−70.63	−60.92	−55.07	−48.63	−44.98	−42.39
				1-Heptanamine				
25	16.91	18.51	20.04	21.51	22.94	25.71	28.39	31.00
50	15.07	16.68	18.21	19.68	21.11	23.86	26.52	29.11
75	12.93	14.54	16.08	17.55	18.97	21.72	24.37	26.95
100	10.51	12.13	13.67	15.14	16.57	19.32	21.96	24.54
125	7.84	9.46	11.00	12.48	13.91	16.66	19.31	21.88
150	4.92	6.55	8.10	9.59	11.02	13.78	16.42	18.99
175	1.77	3.40	4.97	6.46	7.90	10.67	13.32	15.89
200	−1.59	0.04	1.62	3.12	4.57	7.35	10.01	12.58
225	−5.17	−3.54	−1.94	−0.42	1.04	3.83	6.50	9.08
250	−8.97	−7.33	−5.69	−4.15	−2.68	0.13	2.81	5.40
300	−17.24	−15.53	−13.79	−12.19	−10.67	−7.81	−5.10	−2.49
350	−26.95	−24.66	−22.65	−20.94	−19.36	−16.43	−13.67	−11.03
400		−35.13	−32.32	−30.40	−28.71	−25.66	−22.84	−20.16
450		−48.91	−42.90	−40.56	−38.70	−35.49	−32.59	−29.86
500		−67.08	−54.56	−51.45	−49.32	−45.87	−42.87	−40.08
550		−84.12	−67.42	−63.07	−60.54	−56.79	−53.66	−50.79
600		−99.78	−81.28	−75.42	−72.36	−68.22	−64.93	−61.98
700		−129.25	−110.28	−101.91	−97.61	−92.50	−88.83	−85.69
800		−157.89	−139.62	−129.95	−124.58	−118.46	−114.39	−111.05
900		−186.55	−169.08	−158.85	−152.79	−145.83	−141.41	−137.92
1000		−215.58	−198.82	−188.37	−181.90	−174.37	−169.72	−166.18
				1-Heptanol				
25	−32.00	−30.45	−28.97	−27.54	−26.15	−23.46	−20.86	−18.32
50	−33.98	−32.42	−30.94	−29.51	−28.12	−25.45	−22.87	−20.35
75	−36.28	−34.72	−33.23	−31.80	−30.42	−27.75	−25.17	−22.67
100	−38.88	−37.31	−35.82	−34.38	−33.00	−30.33	−27.76	−25.26

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Heptanol — Continued				
125	−41.76	−40.18	−38.68	−37.24	−35.85	−33.18	−30.61	−28.11
150	−44.89	−43.31	−41.80	−40.35	−38.96	−36.28	−33.71	−31.21
175	−48.27	−46.68	−45.16	−43.70	−42.30	−39.61	−37.04	−34.54
200	−51.89	−50.29	−48.75	−47.28	−45.87	−43.17	−40.59	−38.08
225	−55.73	−54.13	−52.56	−51.08	−49.66	−46.94	−44.34	−41.83
250	−59.81	−58.19	−56.59	−55.09	−53.65	−50.91	−48.30	−45.78
300	−68.71	−67.00	−65.27	−63.70	−62.21	−59.42	−56.77	−54.23
350	−79.19	−76.80	−74.78	−73.08	−71.52	−68.64	−65.95	−63.37
400		−88.07	−85.16	−83.22	−81.54	−78.53	−75.77	−73.15
450		−103.01	−96.52	−94.12	−92.25	−89.05	−86.20	−83.52
500		−122.82	−109.05	−105.80	−103.62	−100.18	−97.20	−94.45
550		−141.36	−122.92	−118.28	−115.66	−111.87	−108.75	−105.92
600		−158.31	−137.87	−131.54	−128.34	−124.11	−120.81	−117.89
700		−190.11	−169.15	−160.02	−155.42	−150.11	−146.39	−143.25
800		−220.92	−200.72	−190.14	−184.35	−177.90	−173.74	−170.38
900		−251.66	−232.37	−221.16	−214.59	−207.21	−202.65	−199.13
1000		−282.75	−264.25	−252.80	−245.78	−237.76	−232.95	−229.37
				1-Heptene				
25	26.45	27.88	29.24	30.52	31.76	34.13	36.38	38.56
50	24.70	26.19	27.58	28.91	30.19	32.62	34.95	37.19
75	22.68	24.20	25.62	26.98	28.28	30.76	33.12	35.40
100	20.43	21.97	23.42	24.79	26.11	28.63	31.02	33.33
125	17.97	19.53	21.00	22.39	23.73	26.27	28.69	31.02
150	15.31	16.90	18.39	19.80	21.15	23.72	26.16	28.51
175	12.48	14.08	15.60	17.03	18.39	20.99	23.45	25.82
200	9.48	11.10	12.64	14.09	15.48	18.10	20.58	22.96
225	6.30	7.94	9.52	11.00	12.40	15.05	17.56	19.96
250	2.95	4.62	6.25	7.76	9.18	11.87	14.40	16.82
300	−4.40	−2.56	−0.77	0.84	2.33	5.10	7.68	10.15
350	−13.38	−10.60	−8.42	−6.66	−5.07	−2.18	0.48	3.00
400		−20.12	−16.81	−14.73	−12.98	−9.93	−7.17	−4.59
450		−33.98	−26.09	−23.42	−21.42	−18.12	−15.25	−12.59
500		−53.74	−36.54	−32.77	−30.39	−26.76	−23.72	−20.97
550		−71.55	−48.37	−42.84	−39.88	−35.81	−32.59	−29.73
600		−87.05	−61.31	−53.61	−49.90	−45.27	−41.82	−38.83
700		−114.52	−88.11	−76.82	−71.33	−65.31	−61.32	−58.05
800		−139.72	−114.29	−101.15	−94.13	−86.65	−82.08	−78.53
900		−163.92	−139.65	−125.70	−117.69	−109.01	−103.94	−100.18
1000		−187.75	−164.49	−150.23	−141.63	−132.14	−126.73	−122.90
				1-Heptyne				
25	56.73	58.21	59.60	60.93	62.20	64.63	66.95	69.20
50	54.98	56.52	57.95	59.32	60.63	63.14	65.53	67.84
75	52.98	54.55	56.01	57.41	58.75	61.30	63.73	66.08
100	50.76	52.35	53.84	55.26	56.61	59.20	61.66	64.04
125	48.34	49.95	51.46	52.90	54.27	56.89	59.38	61.77
150	45.74	47.37	48.91	50.36	51.75	54.39	56.90	59.32
175	42.97	44.62	46.18	47.65	49.06	51.72	54.26	56.69
200	40.04	41.71	43.29	44.78	46.21	48.90	51.46	53.91
225	36.94	38.63	40.25	41.77	43.21	45.94	48.51	50.98
250	33.67	35.39	37.06	38.61	40.08	42.84	45.44	47.93
300	26.52	28.40	30.24	31.88	33.41	36.26	38.91	41.45
350	17.76	20.57	22.79	24.60	26.23	29.20	31.93	34.51
400		11.28	14.65	16.76	18.55	21.69	24.52	27.16
450		−2.34	5.62	8.33	10.37	13.75	16.70	19.43
500		−21.86	−4.56	−0.75	1.68	5.39	8.50	11.32
550		−39.40	−16.11	−10.52	−7.52	−3.36	−0.06	2.87
600		−54.61	−28.74	−20.98	−17.22	−12.51	−8.98	5.93
700		−81.43	−54.89	−43.53	−37.99	−31.88	−27.81	−24.47

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	Pressure, kbar 0.5	1.0	1.5	2.0	3.0	4.0	5.0
1-Heptyne — Continued								
800		−105.91	−80.36	−67.13	−60.06	−52.49	−47.84	−44.22
900		−129.34	−104.95	−90.92	−82.84	−74.07	−68.91	−65.08
1000		−152.34	−128.96	−114.62	−105.95	−96.36	−90.88	−86.97
1-Hexanamine								
25	14.86	16.27	17.63	18.94	20.21	22.67	25.06	27.40
50	13.21	14.63	15.98	17.29	18.56	21.01	23.38	25.69
75	11.29	12.71	14.07	15.38	16.64	19.09	21.45	23.74
100	9.12	10.55	11.91	13.22	14.49	16.93	19.28	21.57
125	6.73	8.16	9.53	10.84	12.11	14.55	16.90	19.19
150	4.12	5.55	6.93	8.24	9.52	11.96	14.32	16.61
175	1.30	2.74	4.13	5.45	6.73	9.18	11.54	13.83
200	−1.71	−0.26	1.13	2.47	3.75	6.21	8.58	10.87
225	−4.90	−3.46	−2.05	−0.70	0.59	3.07	5.44	7.73
250	−8.29	−6.84	−5.40	−4.04	−2.73	−0.24	2.13	4.44
300	−15.66	−14.17	−12.63	−11.22	−9.88	−7.35	−4.94	−2.62
350	−24.28	−22.31	−20.54	−19.03	−17.64	−15.04	−12.60	−10.25
400		−31.60	−29.16	−27.47	−25.99	−23.29	−20.79	−18.42
450		−43.73	−38.57	−36.53	−34.90	−32.06	−29.50	−27.08
500		−59.61	−48.92	−46.23	−44.36	−41.33	−38.68	−36.21
550		−74.56	−60.31	−56.57	−54.37	−51.08	−48.31	−45.78
600		−88.34	−72.57	−67.54	−64.90	−61.28	−58.38	−55.77
700		−114.40	−98.23	−91.07	−87.37	−82.92	−79.71	−76.94
800		−139.82	−124.24	−115.98	−111.37	−106.06	−102.50	−99.57
900		−165.31	−150.42	−141.68	−136.48	−130.46	−126.60	−123.54
1000		−191.17	−176.88	−167.96	−162.40	−155.90	−151.85	−148.75
1-Hexanol								
25	−35.49	−34.11	−32.79	−31.51	−30.27	−27.86	−25.53	−23.25
50	−37.26	−35.87	−34.55	−33.27	−32.03	−29.64	−27.33	−25.07
75	−39.29	−37.90	−36.57	−35.30	−34.06	−31.67	−29.37	−27.13
100	−41.58	−40.18	−38.85	−37.57	−36.33	−33.95	−31.65	−29.41
125	−44.09	−42.69	−41.35	−40.07	−38.83	−36.44	−34.14	−31.91
150	−46.82	−45.41	−44.07	−42.78	−41.54	−39.14	−36.84	−34.61
175	−49.76	−48.34	−46.99	−45.69	−44.44	−42.04	−39.74	−37.50
200	−52.89	−51.47	−50.10	−48.80	−47.54	−45.13	−42.81	−40.57
225	−56.22	−54.79	−53.40	−52.08	−50.81	−48.39	−46.07	−43.82
250	−59.74	−58.30	−56.88	−55.54	−54.26	−51.82	−49.49	−47.23
300	−67.40	−65.89	−64.36	−62.97	−61.65	−59.16	−56.79	−54.52
350	−76.40	−74.32	−72.54	−71.04	−69.66	−67.09	−64.69	−62.38
400		−83.99	−81.45	−79.74	−78.26	−75.59	−73.12	−70.78
450		−96.78	−91.19	−89.09	−87.44	−84.61	−82.07	−79.68
500		−113.72	−101.92	−99.09	−97.18	−94.14	−91.49	−89.05
550		−129.56	−113.78	−109.77	−107.48	−104.14	−101.38	−98.86
600		−144.05	−126.56	−121.11	−118.32	−114.61	−111.69	−109.09
700		−171.20	−153.26	−145.42	−141.45	−136.81	−133.54	−130.76
800		−197.48	−180.20	−171.12	−166.13	−160.53	−156.87	−153.91
900		−223.68	−207.18	−197.56	−191.90	−185.50	−181.52	−178.41
1000		−250.17	−234.34	−224.51	−218.47	−211.53	−207.32	−204.16
1-Hexene								
25	24.37	25.62	26.81	27.94	29.03	31.11	33.10	35.02
50	22.81	24.11	25.33	26.50	27.62	29.76	31.81	33.78
75	21.01	22.34	23.59	24.77	25.92	28.10	30.18	32.19
100	19.00	20.35	21.62	22.83	23.99	26.20	28.31	30.34
125	16.82	18.19	19.47	20.70	21.87	24.11	26.23	28.29
150	14.46	15.85	17.16	18.39	19.58	21.84	23.99	26.06
175	11.95	13.35	14.68	15.94	17.14	19.42	21.58	23.67
200	9.29	10.71	12.06	13.33	14.55	16.85	19.04	21.14

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Hexene — Continued				
225	6.47	7.91	9.29	10.59	11.82	14.15	16.36	18.47
250	3.49	4.96	6.39	7.71	8.97	11.33	13.56	15.69
300	−3.02	−1.40	0.17	1.58	2.89	5.33	7.60	9.78
350	−11.00	−8.53	−6.61	−5.06	−3.66	−1.12	1.23	3.44
400		−16.98	−14.04	−12.21	−10.67	−7.98	−5.55	−3.28
450		−29.31	−22.27	−19.91	−18.15	−15.24	−12.70	−10.36
500		−46.90	−31.54	−28.20	−26.09	−22.88	−20.20	−17.78
550		−62.75	−42.04	−37.12	−34.50	−30.89	−28.05	−25.52
600		−76.53	−53.53	−46.66	−43.37	−39.27	−36.22	−33.58
700		−100.91	−77.31	−67.24	−62.35	−57.00	−53.47	−50.59
800		−123.25	−100.53	−88.80	−82.54	−75.89	−71.84	−68.71
900		−144.68	−123.00	−110.55	−103.40	−95.68	−91.18	−87.85
1000		−165.77	−144.99	−132.26	−124.59	−116.14	−111.35	−107.95
				1-Hexyne				
25	54.42	55.72	56.94	58.11	59.23	61.38	63.44	65.43
50	52.87	54.21	55.48	56.68	57.84	60.05	62.17	64.21
75	51.09	52.46	53.76	54.98	56.16	58.42	60.57	62.64
100	49.12	50.52	51.83	53.08	54.28	56.56	58.74	60.83
125	46.98	48.40	49.73	50.99	52.21	54.51	56.71	58.83
150	44.69	46.12	47.47	48.75	49.97	52.31	54.52	56.66
175	42.24	43.69	45.06	46.36	47.60	49.95	52.19	54.34
200	39.65	41.12	42.51	43.83	45.08	47.46	49.72	51.89
225	36.92	38.40	39.83	41.17	42.44	44.85	47.12	49.31
250	34.03	35.55	37.02	38.38	39.68	42.11	44.41	46.61
300	27.72	29.38	31.00	32.45	33.80	36.31	38.66	40.90
350	19.98	22.48	24.44	26.04	27.47	30.09	32.51	34.79
400		14.28	17.26	19.13	20.71	23.48	25.98	28.32
450		2.22	9.30	11.70	13.51	16.49	19.10	21.51
500		−15.09	0.32	3.70	5.85	9.14	11.88	14.38
550		−30.63	−9.88	4.91	2.25	1.43	4.35	6.94
600		−44.08	−21.04	−14.13	−10.80	−6.62	−3.50	−0.80
700		−67.77	−44.13	−34.02	−29.09	−23.66	−20.06	−17.11
800		−89.36	−66.59	−54.82	−48.52	−41.80	−37.68	−34.47
900		−109.99	−88.26	−75.77	−68.58	−60.78	−56.21	−52.81
1000		−130.23	−109.40	−96.63	−88.91	−80.39	−75.52	−72.06
				1-Octanamine				
25	18.96	20.74	22.43	24.07	25.66	28.72	31.68	34.57
50	16.93	18.72	20.42	22.05	23.64	26.69	29.63	32.49
75	14.57	16.36	18.06	19.70	21.28	24.33	27.26	30.11
100	11.89	13.69	15.39	17.03	18.62	21.66	24.59	27.44
125	8.91	10.72	12.44	14.08	15.67	18.72	21.65	24.49
150	5.67	7.48	9.21	10.86	12.45	15.51	18.44	21.29
175	2.17	3.99	5.73	7.39	8.99	12.05	14.99	17.84
200	−1.58	0.24	2.00	3.67	5.28	8.36	11.31	14.16
225	−5.57	−3.74	−1.96	−0.27	1.35	4.45	7.41	10.27
250	−9.80	−7.96	−6.14	−4.43	−2.79	0.32	3.30	6.16
300	−19.03	−17.12	−15.17	−13.39	−11.70	−8.53	−5.52	−2.62
350	−29.90	−27.32	−25.07	−23.15	−21.39	−18.13	−15.07	−12.14
400		−39.04	−35.87	−33.71	−31.83	−28.43	−25.30	−22.33
450		−54.56	−47.70	−45.07	−42.99	−39.40	−36.18	−33.14
500		−75.12	−60.76	−57.25	−54.85	−51.00	−47.65	−44.55
550		−94.37	−75.20	−70.26	−67.41	−63.20	−59.70	−56.51
600		−112.00	−90.77	−84.09	−80.63	−75.98	−72.30	−69.01
700		−145.12	−123.35	−113.78	−108.89	−103.12	−99.01	−95.50
800		−177.25	−156.28	−145.21	−139.09	−132.15	−127.58	−123.85
900		−209.35	−189.31	−177.60	−170.68	−162.78	−157.80	−153.90
1000		−241.85	−222.63	−210.66	−203.27	−194.72	−189.48	−185.52

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Octanol				
25	−30.25	−28.52	−26.86	−25.27	−23.72	−20.74	−17.85	−15.03
50	−32.26	−30.51	−28.86	−27.27	−25.72	−22.75	−19.88	−17.09
75	−34.62	−32.87	−31.21	−29.62	−28.08	−25.11	−22.25	−19.47
100	−37.32	−35.56	−33.90	−32.30	−30.76	−27.79	−24.93	−22.16
125	−40.32	−38.56	−36.89	−35.29	−33.74	−30.77	−27.91	−25.14
150	−43.61	−41.85	−40.16	−38.56	−37.00	−34.03	−31.17	−28.39
175	−47.18	−45.41	−43.71	−42.09	−40.53	−37.54	−34.68	−31.90
200	−51.00	−49.23	−47.51	−45.88	−44.31	−41.31	−38.44	−35.66
225	−55.08	−53.30	−51.56	−49.91	−48.33	−45.31	−42.43	−39.64
250	−59.40	−57.62	−55.85	−54.18	−52.58	−49.54	−46.64	−43.85
300	−68.87	−67.00	−65.10	−63.37	−61.73	−58.63	−55.70	−52.87
350	−79.98	−77.47	−75.27	−73.41	−71.69	−68.51	−65.53	−62.67
400		−89.47	−86.38	−84.28	−82.44	−79.13	−76.08	−73.18
450		−105.22	−98.54	−95.97	−93.94	−90.45	−87.30	−84.34
500		−125.93	−111.94	−108.51	−106.18	−102.43	−99.16	−96.14
550		−145.41	−126.73	−121.92	−119.14	−115.04	−111.63	−108.52
600		−163.36	−142.67	−136.15	−132.78	−128.25	−124.66	−121.46
700		−197.28	−176.06	−166.73	−161.97	−156.35	−152.34	−148.92
800		−230.37	−209.93	−199.15	−193.19	−186.42	−181.97	−178.33
900		−263.57	−244.04	−232.63	−225.88	−218.18	−213.33	−209.53
1000		−297.27	−278.53	−266.88	−259.67	−251.34	−246.23	−242.37
				1-Octene				
25	28.72	30.34	31.85	33.30	34.69	37.33	39.86	42.29
50	26.78	28.46	30.02	31.52	32.95	35.68	38.27	40.78
75	24.54	26.25	27.85	29.37	30.83	33.61	36.26	38.81
100	22.04	23.77	25.40	26.94	28.43	31.24	33.92	36.50
125	19.30	21.06	22.71	24.28	25.77	28.62	31.33	33.94
150	16.35	18.13	19.81	21.39	22.91	25.79	28.52	31.15
175	13.21	15.01	16.71	18.31	19.84	22.75	25.51	28.15
200	9.86	11.68	13.41	15.04	16.60	19.53	22.31	24.98
225	6.33	8.17	9.94	11.60	13.17	16.15	18.95	21.64
250	2.59	4.47	6.30	7.99	9.59	12.60	15.43	18.14
300	−5.58	−3.52	−1.52	0.28	1.95	5.05	7.95	10.71
350	−15.57	−12.47	−10.04	−8.07	−6.29	−3.05	−0.07	2.74
400		−23.07	−19.38	−17.06	−15.11	−11.68	−8.60	−5.72
450		−38.47	−29.71	−26.74	−24.51	−20.82	−17.60	−14.63
500		−60.40	−41.35	−37.16	−34.50	−30.44	−27.05	−23.98
550		−80.17	−54.51	−48.37	−45.08	−40.54	−36.93	−33.74
600		−97.39	−68.90	−60.37	−56.24	−51.08	−47.23	−43.89
700		−127.95	−98.71	−86.22	−80.12	−73.42	−68.97	−65.33
800		−156.00	−127.86	−113.31	−105.53	−97.21	−92.12	−88.17
900		−182.98	−156.12	−140.67	−131.78	−122.15	−116.50	−112.31
1000		−209.54	−183.80	−168.01	−158.48	−147.94	−141.93	−137.66
				1-Octyne				
25	58.86	60.52	62.08	63.56	64.98	67.70	70.29	72.79
50	56.93	58.65	60.26	61.79	63.26	66.06	68.72	71.29
75	54.71	56.47	58.11	59.67	61.17	64.02	66.74	69.35
100	52.25	54.03	55.70	57.28	58.80	61.69	64.44	67.09
125	49.56	51.36	53.06	54.66	56.20	59.12	61.90	64.57
150	46.67	48.50	50.21	51.84	53.39	56.34	59.15	61.84
175	43.59	45.43	47.18	48.82	50.39	53.38	56.20	58.92
200	40.32	42.18	43.96	45.63	47.22	50.23	53.08	55.82
225	36.87	38.76	40.57	42.27	43.88	46.93	49.80	52.56
250	33.22	35.15	37.02	38.75	40.39	43.47	46.37	49.15
300	25.26	27.35	29.40	31.24	32.95	36.13	39.09	41.92
350	15.50	18.62	21.10	23.12	24.94	28.25	31.30	34.18
400		8.28	12.01	14.37	16.37	19.86	23.02	25.97
450		−6.86	1.95	4.96	7.23	11.00	14.29	17.33

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Octyne — Continued				
500		−28.49	−9.40	−5.17	−2.47	1.66	5.12	8.27
550		−47.96	−22.26	−16.07	−12.74	−8.12	−4.45	−1.19
600		−64.86	−36.33	−27.75	−23.58	−18.34	−14.42	−11.02
700		−94.72	−65.44	−52.90	−46.77	−39.99	−35.47	−31.76
800		−122.02	−93.84	−79.24	−71.42	−63.03	−57.87	−53.85
900		−148.19	−121.29	−105.80	−96.87	−87.16	−81.44	−77.19
1000		−173.91	−148.12	−132.29	−122.71	−112.10	−106.02	−101.67
				1-Pentanamine				
25	12.80	14.03	15.21	16.36	17.47	19.64	21.74	23.79
50	11.34	12.57	13.76	14.90	16.01	18.15	20.23	22.27
75	9.64	10.88	12.07	13.21	14.32	16.46	18.53	20.55
100	7.74	8.98	10.17	11.31	12.42	14.56	16.62	18.63
125	5.64	6.88	8.08	9.22	10.33	12.47	14.53	16.54
150	3.35	4.60	5.80	6.94	8.06	10.20	12.26	14.27
175	0.89	2.14	3.34	4.50	5.61	7.76	9.82	11.83
200	−1.74	−0.49	0.73	1.89	3.01	5.16	7.23	9.24
225	−4.53	−3.28	−2.05	−0.88	0.25	2.41	4.49	6.50
250	−7.48	−6.23	−4.98	−3.79	−2.66	−0.48	1.60	3.62
300	−13.90	−12.61	−11.28	−10.06	−8.89	−6.68	−4.58	−2.55
350	−21.36	−19.69	−18.17	−16.86	−15.65	−13.39	−11.26	−9.21
400		−27.73	−25.66	−24.21	−22.92	−20.58	−18.40	−16.32
450		−38.14	−33.82	−32.08	−30.67	−28.22	−25.98	−23.87
500		−51.64	−42.78	−40.50	−38.90	−36.28	−33.98	−31.82
550		−64.39	−52.60	−49.46	−47.59	−44.76	−42.36	−40.15
600		−76.20	−63.16	−58.96	−56.72	−53.62	−51.11	−48.85
700		−98.62	−85.26	−79.31	−76.20	−72.42	−69.65	−67.25
800		−120.59	−107.71	−100.85	−96.99	−92.50	−89.45	−86.92
900		−142.65	−130.34	−123.08	−118.74	−113.66	−110.37	−107.73
1000		−165.06	−153.25	−145.84	−141.21	−135.74	−132.29	−129.61
				1-Pentanol				
25	−38.47	−37.27	−36.12	−35.01	−33.92	−31.80	−29.74	−27.73
50	−39.93	−38.73	−37.58	−36.47	−35.39	−33.30	−31.27	−29.28
75	−41.63	−40.43	−39.28	−38.17	−37.09	−35.01	−32.99	−31.02
100	−43.54	−42.34	−41.19	−40.08	−39.00	−36.92	−34.91	−32.95
125	−45.65	−44.45	−43.29	−42.18	−41.11	−39.03	−37.02	−35.07
150	−47.95	−46.75	−45.59	−44.47	−43.39	−41.31	−39.31	−37.36
175	−50.43	−49.22	−48.06	−46.94	−45.86	−43.77	−41.76	−39.81
200	−53.08	−51.87	−50.69	−49.57	−48.48	−46.39	−44.38	−42.43
225	−55.90	−54.69	−53.49	−52.36	−51.26	−49.16	−47.15	−45.19
250	−58.87	−57.66	−56.45	−55.30	−54.19	−52.08	−50.06	−48.10
300	−65.35	−64.10	−62.81	−61.62	−60.48	−58.34	−56.30	−54.32
350	−72.87	−71.23	−69.76	−68.49	−67.31	−65.11	−63.04	−61.05
400		−79.35	−77.32	−75.90	−74.65	−72.37	−70.26	−68.24
450		−89.82	−85.56	−83.85	−82.48	−80.09	−77.92	−75.87
500		−103.39	−94.59	−92.35	−90.79	−88.24	−86.00	−83.90
550		−116.22	−104.51	−101.41	−99.57	−96.81	−94.47	−92.33
600		−128.11	−115.16	−111.00	−108.80	−105.77	−103.32	−101.12
700		−150.74	−137.45	−131.55	−128.48	−124.78	−122.07	−119.73
800		−172.92	−160.12	−153.31	−149.50	−145.09	−142.10	−139.63
900		−195.22	−182.99	−175.79	−171.49	−166.50	−163.27	−160.69
1000		−217.90	−206.16	−198.81	−194.23	−188.83	−185.45	−182.84
				1-Pentene				
25	22.47	23.54	24.56	25.53	26.47	28.27	29.99	31.66
50	21.10	22.21	23.26	24.26	25.23	27.08	28.85	30.56
75	19.52	20.66	21.73	22.75	23.73	25.62	27.42	29.16
100	17.76	18.92	20.01	21.05	22.05	23.95	25.77	27.53

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Pentene — Continued				
125	15.85	17.02	18.13	19.18	20.19	22.12	23.96	25.74
150	13.79	14.98	16.10	17.17	18.19	20.14	21.99	23.78
175	11.60	12.80	13.94	15.02	16.06	18.02	19.90	21.70
200	9.27	10.49	11.65	12.75	13.80	15.79	17.67	19.49
225	6.81	8.05	9.24	10.36	11.42	13.43	15.34	17.17
250	4.22	5.48	6.71	7.85	8.93	10.97	12.89	14.74
300	−1.47	−0.07	1.29	2.50	3.64	5.74	7.71	9.58
350	−8.44	−6.29	−4.63	−3.28	−2.07	0.13	2.15	4.07
400		−13.66	−11.10	−9.51	−8.18	−5.85	−3.75	−1.78
450		−24.45	−18.27	−16.22	−14.69	−12.17	−9.97	−7.94
500		−39.88	−26.36	−23.44	−21.60	−18.82	−16.50	−14.40
550		−53.77	−35.53	−31.21	−28.93	−25.80	−23.33	−21.14
600		−65.82	−45.56	−39.54	−36.66	−33.08	−30.44	−28.15
700		−87.12	−66.33	−57.48	−53.19	−48.52	−45.45	−42.94
800		−106.59	−86.58	−76.26	−70.77	−64.96	−61.43	−58.70
900		−125.26	−106.17	−95.21	−88.93	−82.17	−78.24	−75.35
1000		−143.61	−125.31	−114.11	−107.37	−99.96	−95.78	−92.82
				1-Pentyne				
25	52.16	53.28	54.33	55.34	56.32	58.18	59.97	61.71
50	50.79	51.95	53.04	54.09	55.09	57.01	58.85	60.62
75	49.24	50.42	51.54	52.60	53.62	55.58	57.44	59.25
100	47.52	48.73	49.86	50.94	51.97	53.95	55.84	57.67
125	45.66	46.88	48.03	49.12	50.17	52.17	54.08	55.92
150	43.66	44.89	46.06	47.16	48.23	50.25	52.17	54.03
175	41.53	42.78	43.96	45.09	46.16	48.20	50.14	52.01
200	39.28	40.54	41.75	42.89	43.97	46.04	47.99	49.88
225	36.90	38.19	39.42	40.58	41.68	43.77	45.74	47.64
250	34.40	35.71	36.98	38.16	39.28	41.39	43.39	45.30
300	28.92	30.35	31.76	33.01	34.18	36.36	38.40	40.35
350	22.18	24.36	26.07	27.45	28.70	30.98	33.07	35.06
400		17.24	19.84	21.47	22.84	25.25	27.42	29.46
450		6.72	12.94	15.03	16.60	19.20	21.47	23.56
500		−8.43	5.13	8.10	9.98	12.83	15.22	17.40
550		−22.01	−3.73	0.63	2.96	6.16	8.71	10.96
600		−33.74	−13.43	−7.37	−4.45	−0.80	1.92	4.28
700		−54.34	−33.51	−24.61	−20.28	−15.54	−12.39	−9.82
800		−73.06	−53.01	−42.65	−37.12	−31.22	−27.62	−24.82
900		−90.93	−71.79	−60.79	−54.47	−47.63	−43.63	−40.67
1000		−108.42	−90.08	−78.84	−72.06	−64.57	−60.31	−57.29
				1-Propanamine				
25	7.01	7.88	8.72	9.54	10.34	11.90	13.43	14.93
50	5.91	6.78	7.62	8.43	9.23	10.78	12.28	13.76
75	4.66	5.53	6.37	7.18	7.98	9.52	11.01	12.48
100	3.28	4.15	4.99	5.80	6.59	8.13	9.62	11.08
125	1.76	2.64	3.48	4.29	5.08	6.62	8.10	9.56
150	0.12	1.00	1.85	2.66	3.45	4.99	6.47	7.92
175	−1.62	−0.75	0.10	0.92	1.71	3.25	4.73	6.18
200	−3.48	−2.61	−1.75	−0.93	−0.13	1.40	2.89	4.34
225	−5.45	−4.58	−3.71	−2.88	−2.08	−0.54	0.95	2.40
250	−7.51	−6.65	−5.77	−4.93	−4.13	−2.58	−1.08	0.37
300	−11.97	−11.10	−10.17	−9.31	−8.49	−6.92	−5.42	−3.96
350	−17.07	−15.99	−14.96	−14.05	−13.20	−11.60	−10.08	−8.61
400		−21.49	−20.13	−19.14	−18.25	−16.60	−15.05	−13.57
450		−28.42	−25.73	−24.57	−23.60	−21.89	−20.31	−18.81
500		−37.20	−31.83	−30.35	−29.27	−27.46	−25.84	−24.31
550		−45.57	−38.46	−36.47	−35.23	−33.30	−31.62	−30.06
600		−53.40	−45.56	−42.94	−41.48	−39.39	−37.65	−36.06
700		−68.42	−60.39	−56.74	−54.77	−52.27	−50.38	−48.71

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Propanamine — Continued				
800		−83.26	−75.51	−71.32	−68.91	−65.99	−63.94	−62.18
900		−98.22	−90.81	−86.39	−83.69	−80.43	−78.23	−76.42
1000		−113.47	−106.35	−101.84	−98.97	−95.47	−93.18	−91.34
				1-Propanol				
25	−41.91	−41.08	−40.28	−39.50	−38.73	−37.22	−35.75	−34.31
50	−43.03	−42.20	−41.40	−40.62	−39.86	−38.38	−36.93	−35.51
75	−44.31	−43.48	−42.68	−41.91	−41.15	−39.67	−38.24	−36.83
100	−45.74	−44.91	−44.11	−43.33	−42.58	−41.11	−39.68	−38.28
125	−47.31	−46.47	−45.67	−44.90	−44.14	−42.67	−41.25	−39.86
150	−49.01	−48.17	−47.37	−46.59	−45.83	−44.36	−42.94	−41.55
175	−50.83	−49.99	−49.18	−48.40	−47.64	−46.17	−44.75	−43.36
200	−52.76	−51.93	−51.11	−50.33	−49.57	−48.09	−46.67	−45.28
225	−54.81	−53.98	−53.16	−52.36	−51.60	−50.12	−48.70	−47.31
250	−56.97	−56.14	−55.31	−54.51	−53.74	−52.25	−50.82	−49.43
300	−61.65	−60.80	−59.92	−59.09	−58.30	−56.80	−55.36	−53.96
350	−67.00	−65.93	−64.93	−64.06	−63.24	−61.71	−60.25	−58.84
400		−71.70	−70.36	−69.40	−68.54	−66.95	−65.47	−64.05
450		−78.94	−76.24	−75.10	−74.16	−72.51	−71.00	−69.55
500		−88.12	−82.64	−81.17	−80.12	−78.37	−76.81	−75.34
550		−96.87	−89.61	−87.61	−86.40	−84.52	−82.90	−81.40
600		−105.08	−97.05	−94.42	−92.97	−90.93	−89.25	−87.71
700		−120.87	−112.65	−108.94	−106.97	−104.51	−102.67	−101.05
800		−136.49	−128.56	−124.30	−121.88	−118.99	−116.97	−115.27
900		−152.28	−144.70	−140.20	−137.47	−134.23	−132.07	−130.31
1000		−168.38	−161.10	−156.51	−153.61	−150.12	−147.86	−146.08
				1-Propene				
25	17.91	18.62	19.30	19.96	20.60	21.83	23.02	24.18
50	16.91	17.65	18.36	19.03	19.69	20.95	22.17	23.36
75	15.77	16.53	17.25	17.94	18.61	19.89	21.13	22.33
100	14.52	15.29	16.02	16.72	17.40	18.70	19.95	21.16
125	13.16	13.94	14.68	15.39	16.08	17.39	18.65	19.87
150	11.69	12.49	13.24	13.96	14.65	15.98	17.25	18.48
175	10.14	10.94	11.71	12.44	13.14	14.48	15.76	17.00
200	8.49	9.30	10.09	10.83	11.54	12.90	14.19	15.44
225	6.74	7.58	8.38	9.14	9.86	11.23	12.54	13.79
250	4.91	5.76	6.59	7.37	8.10	9.49	10.81	12.08
300	0.88	1.84	2.77	3.59	4.37	5.80	7.15	8.44
350	−4.08	−2.55	−1.41	−0.48	0.34	1.85	3.24	4.56
400		−7.78	−5.97	−4.87	−3.96	−2.35	−0.91	0.45
450		−15.50	−11.04	−9.60	−8.54	−6.79	−5.28	−3.88
500		−26.60	−16.77	−14.69	−13.40	−11.47	−9.86	−8.41
550		−36.56	−23.27	−20.17	−18.55	−16.37	−14.65	−13.14
600		−45.17	−30.40	−26.04	−23.99	−21.48	−19.64	−18.05
700		−60.29	−45.13	−38.71	−35.63	−32.31	−30.16	−28.41
800		−74.05	−59.46	−51.96	−48.00	−43.84	−41.35	−39.44
900		−87.18	−73.26	−65.30	−60.76	−55.91	−53.13	−51.10
1000		−100.05	−86.71	−78.57	−73.69	−68.37	−65.40	−63.32
				1-Propyne				
25	47.88	48.64	49.36	50.05	50.73	52.03	53.28	54.50
50	46.89	47.68	48.42	49.14	49.83	51.16	52.45	53.70
75	45.78	46.58	47.34	48.07	48.78	50.13	51.44	52.70
100	44.56	45.38	46.15	46.89	47.61	48.98	50.30	51.58
125	43.24	44.07	44.86	45.61	46.33	47.72	49.05	50.34
150	41.84	42.68	43.48	44.24	44.97	46.37	47.71	49.01
175	40.35	41.20	42.01	42.78	43.52	44.94	46.29	47.59
200	38.77	39.64	40.46	41.25	42.00	43.43	44.79	46.10

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				1-Propyne — Continued				
225	37.11	37.99	38.84	39.64	40.40	41.84	43.22	44.54
250	35.37	36.26	37.14	37.96	38.73	40.20	41.58	42.92
300	31.54	32.54	33.51	34.38	35.19	36.71	38.13	39.49
350	26.82	28.38	29.57	30.53	31.40	32.98	34.44	35.83
400		23.40	25.25	26.39	27.35	29.03	30.54	31.97
450		15.95	20.45	21.93	23.04	24.85	26.44	27.91
500		5.13	15.01	17.13	18.46	20.47	22.14	23.67
550		−4.52	8.81	11.96	13.61	15.88	17.66	19.25
600		−12.80	2.01	6.41	8.50	11.08	13.00	14.66
700		−27.23	−12.03	−5.57	−2.44	0.95	3.17	4.99
800		−40.24	−25.61	−18.07	−14.06	−9.83	−7.27	−5.29
900		−52.57	−38.60	−30.60	−26.02	−21.09	−18.24	−16.14
1000		−64.58	−51.20	−43.02	−38.10	−32.70	−29.66	−27.51
				2-Butanone				
25	−36.73	−35.77	−34.84	−33.93	−33.05	−31.32	−29.65	−28.00
50	−38.07	−37.10	−36.17	−35.27	−34.39	−32.69	−31.03	−29.40
75	−39.56	−38.59	−37.66	−36.76	−35.89	−34.19	−32.54	−30.93
100	−41.20	−40.22	−39.29	−38.39	−37.51	−35.82	−34.18	−32.57
125	−42.97	−41.99	−41.05	−40.15	−39.27	−37.58	−35.94	−34.34
150	−44.86	−43.88	−42.94	−42.03	−41.15	−39.46	−37.82	−36.22
175	−46.87	−45.89	−44.94	−44.03	−43.15	−41.45	−39.81	−38.21
200	−49.00	−48.02	−47.06	−46.14	−45.25	−43.55	−41.90	−40.30
225	−51.25	−50.26	−49.28	−48.36	−47.46	−45.75	−44.10	−42.50
250	−53.60	−52.61	−51.62	−50.68	−49.78	−48.05	−46.39	−44.79
300	−58.69	−57.65	−56.59	−55.61	−54.68	−52.93	−51.25	−49.63
350	−64.60	−63.20	−61.97	−60.93	−59.96	−58.15	−56.45	−54.81
400		−69.53	−67.80	−66.62	−65.58	−63.71	−61.97	−60.31
450		−77.87	−74.13	−72.70	−71.55	−69.57	−67.78	−66.09
500		−88.91	−81.09	−79.17	−77.86	−75.74	−73.88	−72.15
550		−99.19	−88.75	−86.06	−84.50	−82.18	−80.24	−78.47
600		−108.55	−96.99	−93.35	−91.46	−88.90	−86.86	−85.03
700		−125.99	−114.14	−108.93	−106.26	−103.09	−100.82	−98.87
800		−142.76	−131.34	−125.32	−121.98	−118.17	−115.65	−113.58
900		−159.39	−148.48	−142.10	−138.32	−134.00	−131.25	−129.09
1000		−176.12	−165.65	−159.14	−155.10	−150.42	−147.54	−145.34
				2-Heptanone				
25	−30.43	−28.93	−27.48	−26.10	−24.74	−22.13	−19.60	−17.13
50	−32.33	−30.82	−29.38	−27.99	−26.64	−24.04	−21.53	−19.08
75	−34.50	−32.98	−31.53	−30.14	−28.80	−26.20	−23.70	−21.27
100	−36.91	−35.39	−33.94	−32.55	−31.20	−28.60	−26.11	−23.68
125	−39.56	−38.03	−36.57	−35.17	−33.82	−31.23	−28.73	−26.30
150	−42.42	−40.88	−39.42	−38.01	−36.66	−34.05	−31.55	−29.13
175	−45.49	−43.94	−42.46	−41.05	−39.69	−37.08	−34.57	−32.14
200	−48.75	−47.20	−45.71	−44.28	−42.91	−40.29	−37.78	−35.34
225	−52.21	−50.66	−49.14	−47.70	−46.32	−43.68	−41.15	−38.71
250	−55.87	−54.30	−52.75	−51.29	−49.89	−47.23	−44.70	−42.25
300	−63.83	−62.17	−60.50	−58.97	−57.53	−54.82	−52.25	−49.78
350	−73.22	−70.92	−68.96	−67.31	−65.80	−63.00	−60.39	−57.88
400		−80.98	−78.17	−76.30	−74.67	−71.75	−69.07	−66.52
450		−94.50	−88.25	−85.94	−84.12	−81.03	−78.26	−75.65
500		−112.63	−99.40	−96.26	−94.15	−90.81	−87.93	−85.26
550		−129.46	−111.75	−107.28	−104.76	−101.08	−98.06	−95.31
600		−144.73	−125.09	−119.00	−115.91	−111.82	−108.63	−105.79
700		−173.05	−152.91	−144.14	−139.71	−134.58	−130.99	−127.94
800		−200.22	−180.83	−170.65	−165.08	−158.86	−154.84	−151.59
900		−227.15	−208.62	−197.85	−191.53	−184.41	−180.01	−176.60
1000		−254.25	−236.48	−225.47	−218.71	−210.99	−206.34	−202.88

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				2-Hexanone				
25	−32.48	−31.16	−29.89	−28.66	−27.47	−25.15	−22.91	−20.72
50	−34.19	−32.86	−31.59	−30.37	−29.18	−26.88	−24.65	−22.49
75	−36.13	−34.80	−33.52	−32.30	−31.11	−28.82	−26.60	−24.45
100	−38.28	−36.94	−35.67	−34.44	−33.25	−30.96	−28.75	−26.60
125	−40.63	−39.29	−38.01	−36.78	−35.59	−33.29	−31.08	−28.93
150	−43.17	−41.82	−40.53	−39.29	−38.10	−35.80	−33.59	−31.44
175	−45.88	−44.53	−43.23	−41.99	−40.79	−38.48	−36.26	−34.11
200	−48.77	−47.41	−46.09	−44.84	−43.63	−41.32	−39.10	−36.94
225	−51.82	−50.46	−49.12	−47.85	−46.64	−44.31	−42.08	−39.92
250	−55.04	−53.67	−52.30	−51.02	−49.79	−47.44	−45.20	−43.03
300	−62.03	−60.59	−59.12	−57.78	−56.51	−54.12	−51.85	−49.67
350	−70.26	−68.26	−66.55	−65.11	−63.78	−61.31	−59.00	−56.79
400		−77.07	−74.63	−72.99	−71.56	−68.99	−66.62	−64.37
450		−88.85	−83.45	−81.43	−79.85	−77.13	−74.68	−72.39
500		−104.59	−93.19	−90.47	−88.63	−85.70	−83.16	−80.81
550		−119.22	−103.97	−100.11	−97.90	−94.69	−92.03	−89.61
600		−132.51	−115.60	−110.34	−107.65	−104.08	−101.28	−98.78
700		−157.18	−139.85	−132.27	−128.44	−123.97	−120.82	−118.15
800		−180.87	−164.17	−155.40	−150.58	−145.18	−141.66	−138.81
900		−204.34	−188.40	−179.11	−173.64	−167.47	−163.63	−160.64
1000		−227.98	−212.68	−203.19	−197.35	−190.65	−186.60	−183.56
				2-Octanone				
25	−28.38	−26.69	−25.08	−23.53	−22.02	−19.11	−16.29	−13.55
50	−30.47	−28.77	−27.16	−25.61	−24.10	−21.20	−18.41	−15.68
75	−32.86	−31.16	−29.54	−27.99	−26.49	−23.59	−20.80	−18.09
100	−35.54	−33.83	−32.21	−30.65	−29.14	−26.25	−23.46	−20.76
125	−38.48	−36.76	−35.13	−33.57	−32.06	−29.16	−26.37	−23.67
150	−41.67	−39.94	−38.30	−36.73	−35.22	−32.31	−29.52	−26.81
175	−45.09	−43.36	−41.70	−40.12	−38.60	−35.68	−32.88	−30.17
200	−48.74	−47.00	−45.32	−43.73	−42.20	−39.26	−36.46	−33.74
225	−52.61	−50.86	−49.16	−47.54	−46.00	−43.05	−40.23	−37.51
250	−56.70	−54.94	−53.20	−51.56	−50.00	−47.02	−44.19	−41.46
300	−65.62	−63.76	−61.88	−60.17	−58.55	−55.52	−52.65	−49.89
350	−76.18	−73.57	−71.37	−69.52	−67.82	−64.69	−61.77	−58.97
400		−84.89	−81.71	−79.60	−77.78	−74.51	−71.51	−68.66
450		−100.15	−93.05	−90.44	−88.40	−84.93	−81.83	−78.92
500		−120.66	−105.60	−102.05	−99.68	−95.93	−92.70	−89.71
550		−139.70	−119.53	−114.46	−111.61	−107.48	−104.09	−101.01
600		−156.95	−134.58	−127.66	−124.16	−119.56	−115.97	−112.80
700		−188.93	−165.98	−156.00	−150.98	−145.19	−141.15	−137.73
800		−219.58	−197.48	−185.91	−179.59	−172.55	−168.02	−164.37
900		−249.95	−228.85	−216.59	−209.41	−201.35	−196.39	−192.56
1000		−280.52	−260.28	−247.76	−240.08	−231.32	−226.08	−222.19
				2-Pentanone				
25	−34.39	−33.25	−32.15	−31.09	−30.05	−28.03	−26.07	−24.15
50	−35.90	−34.75	−33.66	−32.59	−31.56	−29.56	−27.62	−25.73
75	−37.60	−36.45	−35.35	−34.29	−33.26	−31.27	−29.34	−27.46
100	−39.48	−38.33	−37.23	−36.16	−35.13	−33.14	−31.22	−29.34
125	−41.53	−40.37	−39.26	−38.20	−37.16	−35.17	−33.25	−31.38
150	−43.73	−42.57	−41.45	−40.38	−39.35	−37.35	−35.43	−33.56
175	−46.08	−44.91	−43.79	−42.72	−41.68	−39.67	−37.75	−35.88
200	−48.57	−47.40	−46.27	−45.18	−44.14	−42.13	−40.20	−38.32
225	−51.21	−50.03	−48.88	−47.78	−46.73	−44.71	−42.77	−40.90
250	−53.98	−52.80	−51.62	−50.51	−49.45	−47.42	−45.47	−43.59
300	−59.98	−58.75	−57.49	−56.33	−55.24	−53.17	−51.20	−49.30
350	−67.01	−65.33	−63.87	−62.62	−61.48	−59.35	−57.35	−55.43
400		−72.85	−70.78	−69.38	−68.15	−65.94	−63.89	−61.94
450		−82.84	−78.33	−76.61	−75.25	−72.91	−70.80	−68.81

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				2-Pentanone — Continued				
500		−96.10	−86.63	−84.33	−82.76	−80.25	−78.06	−76.02
550		−108.45	−95.80	−92.55	−90.69	−87.94	−85.65	−83.56
600		−119.69	−105.67	−101.28	−99.01	−95.96	−93.55	−91.40
700		−140.63	−126.25	−119.94	−116.73	−112.94	−110.25	−107.95
800		−160.76	−146.91	−139.61	−135.58	−131.02	−128.02	−125.57
900		−180.73	−167.50	−159.77	−155.21	−150.02	−146.75	−144.19
1000		−200.84	−188.15	−180.26	−175.39	−169.76	−166.32	−163.72
				A-Aminobutyric Acid				
25	−87.12	−86.23	−85.36	−84.52	−83.69	−82.09	−80.52	−78.97
50	−88.34	−87.44	−86.58	−85.74	−84.92	−83.33	−81.78	−80.26
75	−89.67	−88.77	−87.90	−87.07	−86.25	−84.67	−83.13	−81.62
100	−91.09	−90.19	−89.32	−88.48	−87.67	−86.09	−84.56	−83.06
125	−92.61	−91.70	−90.83	−89.99	−89.18	−87.60	−86.07	−84.57
150	−94.21	−93.30	−92.43	−91.59	−90.77	−89.19	−87.66	−86.17
175	−95.90	−94.99	−94.11	−93.26	−92.44	−90.85	−89.32	−87.83
200	−97.66	−96.75	−95.86	−95.01	−94.19	−92.60	−91.06	−89.57
225	−99.51	−98.60	−97.70	−96.84	−96.01	−94.41	−92.87	−91.38
250	−101.44	−100.52	−99.60	−98.73	−97.90	−96.29	−94.75	−93.25
300	−105.57	−104.62	−103.64	−102.74	−101.88	−100.25	−98.69	−97.18
350	−110.36	−109.10	−107.98	−107.01	−106.12	−104.45	−102.86	−101.34
400		−114.20	−112.64	−111.56	−110.61	−108.88	−107.26	−105.72
450		−121.01	−117.70	−116.40	−115.35	−113.53	−111.87	−110.30
500		−130.11	−123.26	−121.53	−120.34	−118.39	−116.67	−115.07
550		−138.52	−129.38	−126.98	−125.57	−123.45	−121.67	−120.02
600		−146.08	−135.96	−132.74	−131.04	−128.71	−126.84	−125.15
700		−159.98	−149.60	−145.01	−142.63	−139.78	−137.70	−135.91
800		−173.14	−163.15	−157.85	−154.89	−151.48	−149.18	−147.28
900		−186.06	−176.51	−170.90	−167.56	−163.69	−161.21	−159.23
1000		−198.96	−189.79	−184.06	−180.50	−176.32	−173.71	−171.70
				Acetate				
25	−88.27	−87.80	−87.32	−86.86	−86.39	−85.47	−84.55	−83.64
50	−88.79	−88.32	−87.85	−87.38	−86.93	−86.01	−85.11	−84.22
75	−89.33	−88.86	−88.40	−87.94	−87.49	−86.59	−85.70	−84.82
100	−89.89	−89.43	−88.97	−88.52	−88.07	−87.19	−86.31	−85.44
125	−90.45	−90.00	−89.56	−89.12	−88.68	−87.82	−86.95	−86.10
150	−91.01	−90.59	−90.17	−89.74	−89.32	−88.47	−87.62	−86.77
175	−91.57	−91.19	−90.78	−90.38	−89.96	−89.14	−88.31	−87.48
200	−92.11	−91.78	−91.41	−91.02	−90.63	−89.83	−89.02	−88.20
225	−92.62	−92.36	−92.03	−91.67	−91.30	−90.53	−89.75	−88.95
250	−93.08	−92.93	−92.65	−92.33	−91.98	−91.25	−90.49	−89.72
300	−93.71	−93.94	−93.85	−93.63	−93.36	−92.73	−92.04	−91.31
350	−93.26	−94.63	−94.96	−94.90	−94.73	−94.24	−93.63	−92.97
400		−94.87	−95.89	−96.09	−96.08	−95.76	−95.27	−94.69
450		−92.38	−96.48	−97.15	−97.36	−97.29	−96.94	−96.45
500			−96.53	−98.02	−98.55	−98.80	−98.61	−98.24
550			−95.86	−98.63	−99.62	−100.27	−100.29	−100.04
600			−94.64	−99.00	−100.56	−101.70	−101.96	−101.85
700				−99.31	−102.10	−104.41	−105.23	−105.44
800					−103.51	−106.96	−108.38	−108.93
900					−105.15	−109.49	−111.46	−112.29
1000						−112.19	−114.58	−115.51
				Acetic Acid				
25	−94.76	−94.15	−93.56	−92.99	−92.43	−91.34	−90.28	−89.23
50	−95.87	−95.25	−94.65	−94.06	−93.50	−92.39	−91.32	−90.27
75	−97.06	−96.43	−95.82	−95.23	−94.66	−93.55	−92.47	−91.41
100	−98.33	−97.69	−97.07	−96.48	−95.90	−94.78	−93.70	−92.64

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Acetic Acid — Continued				
125	−99.67	−99.02	−98.40	−97.80	−97.22	−96.10	−95.01	−93.95
150	−101.08	−100.43	−99.80	−99.20	−98.61	−97.48	−96.39	−95.33
175	−102.55	−101.90	−101.26	−100.66	−100.07	−98.94	−97.84	−96.78
200	−104.09	−103.43	−102.79	−102.18	−101.59	−100.45	−99.35	−98.28
225	−105.68	−105.03	−104.38	−103.76	−103.17	−102.02	−100.92	−99.84
250	−107.34	−106.69	−106.03	−105.40	−104.80	−103.64	−102.54	−101.46
300	−110.86	−110.19	−109.49	−108.84	−108.23	−107.05	−105.93	−104.85
350	−114.84	−113.98	−113.19	−112.50	−111.86	−110.65	−109.52	−108.42
400		−118.20	−117.13	−116.36	−115.68	−114.44	−113.28	−112.17
450		−123.53	−121.35	−120.44	−119.70	−118.40	−117.21	−116.08
500		−130.36	−125.91	−124.74	−123.90	−122.52	−121.29	−120.14
550		−136.77	−130.87	−129.26	−128.29	−126.80	−125.53	−124.35
600		−142.67	−136.14	−134.01	−132.86	−131.23	−129.90	−128.69
700		−153.75	−147.07	−144.06	−142.47	−140.51	−139.05	−137.78
800		−164.46	−158.02	−154.56	−152.60	150.29	−148.69	−147.34
900		−175.10	−168.93	−165.28	−163.08	−160.47	−158.75	−157.35
1000		−185.79	−179.87	−176.14	−173.80	−170.99	−169.19	−167.77
				Acetone				
25	−38.50	−37.72	−36.95	−36.21	−35.48	−34.06	−32.66	−31.29
50	−39.67	−38.88	−38.12	−37.38	−36.66	−35.25	−33.87	−32.52
75	−40.95	−40.16	−39.40	−38.66	−37.94	−36.54	−35.18	−33.84
100	−42.34	−41.55	−40.78	−40.05	−39.33	−37.93	−36.57	−35.24
125	−43.82	−43.03	−42.26	−41.52	−40.80	−39.41	−38.05	−36.73
150	−45.40	−44.60	−43.84	−43.09	−42.37	−40.98	−39.62	−38.30
175	−47.07	−46.27	−45.50	−44.75	−44.03	−42.63	−41.27	−39.95
200	−48.82	−48.02	−47.24	−46.49	−45.76	−44.36	−43.00	−41.68
225	−50.66	−49.86	−49.07	−48.31	−47.58	−46.17	−44.81	−43.48
250	−52.58	−51.78	−50.97	−50.20	−49.47	−48.05	−46.68	−45.35
300	−56.71	−55.87	−55.01	−54.22	−53.46	−52.01	−50.64	−49.30
350	−61.48	−60.36	−59.37	−58.51	−57.72	−56.24	−54.84	−53.49
400		−65.44	−64.05	−63.10	−62.25	−60.72	−59.29	−57.92
450		−72.10	−69.13	−67.97	−67.04	−65.42	−63.95	−62.56
500		−80.87	−74.68	−73.15	−72.08	−70.35	−68.83	−67.41
550		−89.04	−80.79	−78.64	−77.38	−75.50	−73.91	−72.45
600		−96.47	−87.33	−84.44	−82.92	−80.85	−79.18	−77.68
700		−110.30	−100.93	−96.79	−94.66	−92.11	−90.26	−88.67
800		−123.56	−114.53	−109.75	−107.10	−104.04	−102.00	−100.31
900		−136.68	−128.05	−123.00	−119.99	−116.53	−114.31	−112.55
1000		−149.85	−141.58	−136.42	−133.21	−129.47	−127.13	−125.35
				Acetyl Chloride				
25	−54.10	−53.39	−52.70	−52.02	−51.35	−50.05	−48.77	−47.51
50	−55.35	−54.64	−53.95	−53.28	−52.62	−51.33	−50.07	−48.83
75	−56.69	−55.98	−55.28	−54.61	−53.95	−52.67	−51.42	−50.20
100	−58.11	−57.39	−56.70	−56.02	−55.37	−54.09	−52.84	−51.63
125	−59.60	−58.88	−58.18	−57.51	−56.85	−55.57	−54.33	−53.12
150	−61.17	−60.44	−59.74	−59.06	−58.40	−57.13	−55.89	−54.67
175	−62.81	−62.08	−61.37	−60.69	−60.02	−58.74	−57.50	−56.29
200	−64.51	−63.78	−63.06	−62.37	−61.70	−60.42	−59.17	−57.96
225	−66.29	−65.55	−64.82	−64.12	−63.45	−62.15	−60.90	−59.69
250	−68.14	−67.38	−66.64	−65.93	−65.25	−63.94	−62.69	−61.47
300	−72.09	−71.28	−70.47	−69.72	−69.02	−67.68	−66.41	−65.18
350	−76.71	−75.53	−74.56	−73.75	−73.01	−71.63	−70.33	−69.08
400		−80.38	−78.95	−78.02	−77.21	−75.77	−74.43	−73.16
450		−87.02	−83.71	−82.54	−81.63	−80.09	−78.71	−77.41
500		−96.06	−88.96	−87.33	−86.27	−84.60	−83.15	−81.82
550		−104.32	−94.77	−92.43	−91.13	−89.28	−87.76	−86.38
600		−111.63	−101.04	−97.81	−96.21	−94.13	−92.52	−91.09
700		−124.83	−113.96	−109.27	−106.94	−104.29	−102.47	−100.93

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
Acetyl Chloride — Continued								
800		−137.11	−126.65	−121.20	−118.25	−115.01	−112.95	−111.29
900		−149.01	−139.02	−133.24	−129.88	−126.15	−123.89	−122.15
000		−160.76	−151.18	−145.28	−141.68	−137.62	−135.22	−133.45
Alanine								
25	−88.80	−88.09	−87.40	−86.72	−86.06	−84.75	−83.47	−82.21
50	−89.84	−89.12	−88.43	−87.76	−87.10	−85.82	−84.56	−83.32
75	−90.94	−90.23	−89.54	−88.87	−88.21	−86.93	−85.69	−84.46
100	−92.11	−91.39	−90.70	−90.03	−89.38	−88.11	−86.86	−85.65
125	−93.34	−92.62	−91.93	−91.26	−90.61	−89.34	−88.10	−86.89
150	−94.63	−93.91	−93.22	−92.55	−91.89	−90.62	−89.38	−88.18
175	−95.98	−95.26	−94.56	−93.89	−93.23	−91.96	−90.72	−89.51
200	−97.39	−96.67	−95.96	−95.28	−94.62	−93.35	−92.11	−90.90
225	−98.84	−98.12	−97.41	−96.73	−96.06	−94.78	−93.54	−92.33
250	−100.36	−99.64	−98.91	−98.22	−97.55	−96.26	−95.02	−93.81
300	−103.58	−102.84	−102.07	−101.35	−100.67	−99.36	−98.11	−96.89
350	−107.26	−106.31	−105.44	−104.68	−103.97	−102.63	−101.36	−100.14
400		−110.22	−109.03	−108.19	−107.44	−106.06	−104.77	−103.52
450		−115.36	−112.91	−111.90	−111.08	−109.64	−108.31	−107.05
500		−122.16	−117.13	−115.82	−114.90	−113.36	−112.00	−110.71
550		−128.45	−121.77	−119.97	−118.89	−117.23	−115.82	−114.50
600		−134.12	−126.73	−124.33	−123.04	−121.24	−119.76	−118.41
700		−144.55	−136.98	−133.59	−131.81	−129.62	−128.00	−126.58
800		−154.44	−147.14	−143.24	−141.04	−138.45	−136.67	−135.17
900		−164.13	−157.16	−153.04	−150.56	−147.64	−145.71	−144.16
1000		−173.79	−167.09	−162.89	−160.25	−157.10	−155.09	−153.52
Asparagine								
25	−128.65	−127.75	−126.87	−126.03	−125.20	−123.58	−122.00	−120.44
50	−130.06	−129.16	−128.28	−127.44	−126.61	−125.01	−123.45	−121.92
75	−131.54	−130.63	−129.75	−128.91	−128.08	−126.49	−124.94	−123.42
100	−133.07	−132.15	−131.28	−130.43	−129.61	−128.01	−126.47	−124.96
125	−134.66	−133.74	−132.86	−132.01	−131.19	−129.59	−128.05	−126.54
150	−136.31	−135.39	−134.50	−133.65	−132.82	−131.22	−129.68	−128.17
175	−138.01	−137.08	−136.19	−135.33	−134.50	−132.90	−131.35	−129.84
200	−139.77	−138.84	−137.93	−137.06	−136.23	−134.62	−133.07	−131.56
225	−141.59	−140.65	−139.73	−138.85	−138.00	−136.38	−134.82	−133.31
250	−143.47	−142.52	−141.57	−140.68	−139.82	−138.19	−136.62	−135.11
300	−147.48	−146.45	−145.42	−144.48	−143.60	−141.93	−140.34	−138.81
350	−152.23	−150.73	−149.51	−148.49	−147.56	−145.83	−144.21	−142.65
400		−155.69	−153.88	−152.70	−151.69	−149.88	−148.22	−146.63
450		−162.81	−158.64	−157.16	−156.02	−154.09	−152.36	−150.74
500		−172.90	−163.93	−161.88	−160.54	−158.44	−156.64	−154.98
550		−181.91	−169.86	−166.91	−165.28	−162.95	−161.05	−159.33
600		−189.68	−176.30	−172.23	−170.21	−167.60	−165.59	−163.80
700		−203.21	−189.49	−183.57	−180.63	−177.30	−175.02	−173.09
800		−215.35	−202.15	−195.27	−191.55	−187.47	−184.88	−182.82
900		−226.80	−214.19	−206.90	−202.66	−197.97	−195.13	−192.95
1000		−237.88	−225.79	−218.34	−213.80	−208.69	−205.68	−203.46
Aspartic Acid								
25	−172.40	−171.56	−170.75	−169.95	−169.18	−167.66	−166.18	−164.72
50	−173.80	−172.96	−172.15	−171.36	−170.58	−169.08	−167.62	−166.19
75	−175.27	−174.42	−173.61	−172.82	−172.05	−170.55	−169.10	−167.68
100	−176.79	−175.94	−175.12	−174.33	−173.57	−172.07	−170.63	−169.21
125	−178.38	−177.52	−176.70	−175.91	−175.14	−173.64	−172.20	−170.79
150	−180.02	−179.16	−178.33	−177.53	−176.76	−175.27	−173.82	−172.41
175	−181.72	−180.85	−180.02	−179.21	−178.44	−176.94	−175.49	−174.08
200	−183.47	−182.60	−181.75	−180.94	−180.16	−178.65	−177.20	−175.79

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Aspartic Acid — Continued				
225	−185.29	−184.41	−183.54	−182.72	−181.93	−180.41	−178.95	−177.54
250	−187.16	−186.27	−185.38	−184.55	−183.75	−182.22	−180.75	−179.33
300	−191.17	−190.19	−189.23	−188.35	−187.52	−185.95	−184.46	−183.02
350	−195.91	−194.47	−193.31	−192.35	−191.47	−189.84	−188.32	−186.87
400		−199.41	−197.67	−196.56	−195.60	−193.90	−192.33	−190.84
450		−206.50	−202.42	−201.01	−199.93	−198.10	−196.48	−194.95
500		−216.51	−207.70	−205.73	−204.45	−202.46	−200.75	−199.19
550		−225.48	−213.62	−210.74	−209.18	−206.96	−205.17	−203.54
600		−233.20	−220.04	−216.06	−214.11	−211.61	−209.70	−208.02
700		−246.69	−233.19	−227.39	−224.53	−221.32	−219.14	−217.32
800		−258.82	−245.82	−239.07	−235.44	−231.50	−229.02	−227.06
900		−270.27	−257.86	−250.70	−246.56	−242.01	−239.28	−237.21
1000		−281.36	−269.46	−262.15	−257.71	−252.75	−249.85	−247.74
				Ag^+				
25	18.43	18.43	18.45	18.49	18.54	18.66	18.81	18.98
50	17.98	17.99	18.01	18.04	18.09	18.21	18.34	18.50
75	17.52	17.52	17.54	17.58	17.62	17.73	17.86	18.01
100	17.03	17.04	17.06	17.09	17.14	17.24	17.37	17.50
125	16.54	16.54	16.56	16.59	16.63	16.73	16.85	16.99
150	16.03	16.03	16.05	16.08	16.11	16.21	16.32	16.45
175	15.51	15.50	15.52	15.54	15.58	15.67	15.78	15.91
200	14.98	14.97	14.97	15.00	15.03	15.12	15.22	15.34
225	14.44	14.42	14.42	14.44	14.47	14.55	14.65	14.77
250	13.89	13.86	13.86	13.87	13.89	13.97	14.06	14.18
300	12.81	12.73	12.70	12.70	12.71	12.77	12.85	12.96
350	11.77	11.60	11.51	11.49	11.49	11.53	11.60	11.69
400		10.36	10.30	10.26	10.24	10.25	10.31	10.38
450		9.13	9.06	8.99	8.96	8.94	8.98	9.04
500			7.80	7.71	7.65	7.60	7.61	7.66
550			6.53	6.40	6.32	6.23	6.22	6.25
600			5.24	5.08	4.97	4.84	4.80	4.81
700				2.33	2.22	2.01	1.91	1.87
800					−0.62	−0.87	−1.06	−1.14
900					−3.54	−3.82	−4.08	−4.21
1000						−6.86	−7.17	−7.32
				Ag^{+2}				
25	64.30	64.09	63.92	63.77	63.65	63.45	63.30	63.19
50	64.83	64.61	64.43	64.27	64.14	63.92	63.74	63.60
75	65.36	65.14	64.94	64.78	64.64	64.40	64.20	64.04
100	65.90	65.66	65.46	65.28	65.13	64.87	64.66	64.49
125	66.45	66.19	65.98	65.79	65.63	65.35	65.12	64.93
150	67.02	66.73	66.50	66.30	66.12	65.82	65.58	65.37
175	67.60	67.29	67.03	66.81	66.61	66.29	66.03	65.80
200	68.20	67.85	67.56	67.32	67.11	66.76	66.48	66.23
225	68.83	68.44	68.11	67.84	67.61	67.23	66.92	66.66
250	69.51	69.05	68.67	68.37	68.12	67.69	67.36	67.07
300	71.02	70.34	69.83	69.46	69.15	68.63	68.23	67.89
350	72.59	71.82	71.02	70.58	70.20	69.58	69.09	68.70
400		72.25	72.17	71.71	71.27	70.54	69.96	69.49
450		70.87	73.22	72.84	72.36	71.51	70.83	70.28
500			74.01	73.94	73.46	72.50	71.71	71.07
550			74.37	74.98	74.57	73.51	72.61	71.87
600			74.24	75.91	75.69	74.57	73.54	72.70
700				77.21	77.94	76.87	75.56	74.48
800					80.21	79.47	77.84	76.50
900					82.66	82.34	80.37	78.78
1000						85.34	83.04	81.32

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Ag(CH_3COO)^\circ$				
25	−70.84	−70.27	−69.73	−69.20	−68.68	−67.67	−66.69	−65.72
50	−71.88	−71.30	−70.73	−70.19	−69.66	−68.63	−67.62	−66.65
75	−73.04	−72.45	−71.87	−71.32	−70.78	−69.74	−68.73	−67.74
100	−74.31	−73.70	−73.12	−72.56	−72.02	−70.97	−69.95	−68.96
125	−75.66	−75.05	−74.47	−73.90	−73.36	−72.30	−71.28	−70.28
150	−77.10	−76.49	−75.90	−75.33	−74.78	−73.72	−72.69	−71.69
175	−78.61	−78.00	−77.41	−76.84	−76.29	−75.22	−74.19	−73.19
200	−80.19	−79.59	−78.99	−78.42	−77.86	−76.79	−75.76	−74.76
225	−81.83	−81.24	−80.64	−80.07	−79.51	−78.44	−77.40	−76.39
250	−83.54	−82.96	−82.36	−81.78	−81.22	−80.15	−79.11	−78.10
300	−87.11	−86.57	−85.96	−85.38	−84.82	−83.74	−82.70	−81.69
350	−90.89	−90.42	−89.80	−89.21	−88.64	−87.56	−86.51	−85.50
400		−94.50	−93.84	−93.24	−92.67	−91.58	−90.53	−89.51
450		−98.88	−98.08	−97.46	−96.88	−95.78	−94.73	−93.70
500		−103.61	−102.51	−101.86	−101.27	−100.16	−99.10	−98.07
550		−108.42	−107.14	−106.43	−105.82	−104.69	−103.63	−102.60
600		−113.30	−111.94	−111.17	−110.53	−109.39	−108.31	−107.28
700		−123.34	−121.96	−121.07	−120.38	−119.19	−118.10	−117.05
800		−133.78	−132.42	−131.48	−130.74	−129.50	−128.39	−127.34
900		−144.61	−143.29	−142.32	−141.55	−140.27	−139.14	−138.09
1000		−155.81	−154.53	−153.54	−152.75	−151.45	−150.32	−149.26
				$Ag(CH_3COO)_2^-$				
25	−158.99	−157.80	−156.67	−155.59	−154.54	−152.53	−150.60	−148.73
50	−160.40	−159.17	−158.00	−156.89	−155.82	−153.76	−151.78	−149.87
75	−162.06	−160.82	−159.64	−158.51	−157.43	−155.34	−153.34	−151.40
100	−163.95	−162.70	−161.52	−160.38	−159.29	−157.19	−155.18	−153.22
125	−166.03	−164.78	−163.60	−162.46	−161.36	−159.26	−157.24	−155.28
150	−168.27	−167.03	−165.85	−164.72	−163.63	−161.52	−159.50	−157.54
175	−170.65	−169.44	−168.27	−167.15	−166.06	−163.96	−161.94	−159.98
200	−173.16	−171.99	−170.84	−169.72	−168.64	−166.55	−164.54	−162.58
225	−175.76	−174.67	−173.54	−172.44	−171.37	−169.29	−167.29	−165.34
250	−178.45	−177.45	−176.36	−175.28	−174.22	−172.17	−170.18	−168.24
300	−183.91	−183.28	−182.31	−181.30	−180.29	−178.30	−176.35	−174.43
350	−188.88	−189.28	−188.61	−187.71	−186.77	−184.87	−182.97	−181.10
400		−195.16	−195.13	−194.45	−193.62	−191.84	−190.02	−188.19
450		−199.00	−201.73	−201.42	−200.77	−199.16	−197.43	−195.66
500			−208.18	−208.56	−208.16	−206.80	−205.19	−203.49
550			−214.30	−215.80	−215.77	−214.71	−213.25	−211.64
600			−220.24	−223.10	−223.56	−222.88	−221.58	−220.07
700				−238.10	−239.65	−239.91	−239.01	−237.73
800					−256.60	−257.80	−257.34	−256.29
900					−274.61	−276.57	−276.51	−275.64
1000						−296.30	−296.52	−295.72
				$Ag(CO_3)^-$				
25	−111.43	−111.42	−111.38	−111.33	−111.26	−111.09	−110.90	−110.69
50	−111.50	−111.48	−111.45	−111.40	−111.34	−111.19	−111.01	−110.82
75	−111.55	−111.55	−111.52	−111.48	−111.42	−111.29	−111.12	−110.94
100	−111.59	−111.60	−111.58	−111.55	−111.51	−111.39	−111.24	−111.07
125	−111.62	−111.64	−111.64	−111.62	−111.59	−111.49	−111.36	−111.20
150	−111.62	−111.67	−111.70	−111.69	−111.67	−111.59	−111.48	−111.34
175	−111.59	−111.69	−111.73	−111.75	−111.75	−111.69	−111.60	−111.48
200	−111.53	−111.67	−111.76	−111.80	−111.82	−111.80	−111.73	−111.62
225	−111.41	−111.63	−111.76	−111.84	−111.88	−111.90	−111.86	−111.77
250	−111.22	−111.54	−111.74	−111.86	−111.93	−112.00	−111.99	−111.93
300	−110.48	−111.20	−111.60	−111.84	−112.00	−112.18	−112.25	−112.25
350	−108.63	−110.42	−111.31	−111.71	−111.99	−112.33	−112.50	−112.58
400		−109.38	−110.78	−111.46	−111.89	−112.43	−112.74	−112.91
450		−105.98	−109.90	−111.02	−111.68	−112.48	−112.95	−113.23

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Ag(CO_3)^-$ — Continued				
500			−108.49	−110.34	−111.33	−112.47	−113.12	−113.53
550			−106.42	−109.39	−110.81	−112.37	−113.24	−113.80
600			−103.87	−108.17	−110.11	−112.17	−113.31	−114.02
700				−105.33	−108.27	−111.47	−113.21	−114.30
800					−106.15	−110.40	−112.81	−114.28
900					−104.09	−109.12	−112.15	−113.94
1000						−107.86	−111.37	−113.30
				$Ag(CO_3)_2^{-3}$				
25	−236.89	−236.87	−236.82	−236.74	−236.65	−236.42	−236.14	−235.84
50	−236.39	−236.38	−236.34	−236.28	−236.20	−236.00	−235.76	−235.49
75	−235.84	−235.86	−235.85	−235.81	−235.75	−235.59	−235.38	−235.13
100	−235.24	−235.31	−235.33	−235.32	−235.29	−235.17	−235.00	−234.79
125	−234.58	−234.71	−234.78	−234.81	−234.82	−234.75	−234.62	−234.45
150	−233.83	−234.05	−234.19	−234.28	−234.32	−234.32	−234.25	−234.12
175	−232.97	−233.32	−233.55	−233.70	−233.80	−233.88	−233.87	−233.79
200	−231.98	−232.49	−232.84	−233.07	−233.24	−233.42	−233.48	−233.46
225	−230.82	−231.55	−232.05	−232.39	−232.64	−232.95	−233.10	−233.14
250	−229.40	−230.47	−231.17	−231.65	−232.00	−232.45	−232.70	−232.82
300	−225.41	−227.72	−229.09	−229.93	−230.54	−231.37	−231.87	−232.18
350	−218.18	−223.61	−226.49	−227.85	−228.82	−230.14	−230.97	−231.53
400		−219.13	−223.19	−225.32	−226.78	−228.73	−229.98	−230.82
450		−208.61	−218.87	−222.23	−224.37	−227.12	−228.86	−230.05
500			−213.08	−218.43	−221.50	−225.27	−227.60	−229.19
550			−205.55	−213.82	−218.10	−223.12	−226.14	−228.19
600			−196.84	−208.46	−214.15	−220.63	−224.46	−227.01
700				−196.73	−204.89	−214.60	−220.29	−224.01
800					−194.67	−207.26	−214.99	−219.94
900					−184.43	−199.09	−208.74	−214.72
1000						−190.83	−201.99	−208.42
				$AgCl^\circ$				
25	−17.45	−17.15	−16.85	−16.56	−16.26	−15.67	−15.08	−14.50
50	−18.31	−18.00	−17.69	−17.39	−17.08	−16.49	−15.90	−15.31
75	−19.19	−18.87	−18.55	−18.24	−17.94	−17.34	−16.74	−16.16
100	−20.08	−19.75	−19.44	−19.12	−18.82	−18.21	−17.62	−17.03
125	−20.98	−20.66	−20.34	−20.02	−19.71	−19.11	−18.51	−17.92
150	−21.91	−21.58	−21.25	−20.94	−20.63	−20.02	−19.42	−18.83
175	−22.84	−22.51	−22.19	−21.87	−21.56	−20.95	−20.35	−19.76
200	−23.79	−23.46	−23.14	−22.82	−22.50	−21.89	−21.29	−20.70
225	−24.75	−24.43	−24.10	−23.78	−23.46	−22.85	−22.25	−21.66
250	−25.72	−25.40	−25.07	−24.75	−24.44	−23.82	−23.22	−22.63
300	−27.69	−27.40	−27.06	−26.74	−26.42	−25.80	−25.20	−24.60
350	−29.73	−29.45	−29.10	−28.77	−28.45	−27.82	−27.22	−26.62
400		−31.57	−31.19	−30.84	−30.52	−29.89	−29.28	−28.68
450		−33.86	−33.33	−32.97	−32.63	−32.00	−31.38	−30.78
500		−36.35	−35.53	−35.13	−34.79	−34.14	−33.52	−32.92
550		−38.80	−37.79	−37.34	−36.98	−36.32	−35.69	−35.09
600		−41.20	−40.11	−39.60	−39.21	−38.53	−37.90	−37.29
700		−45.95	−44.84	−44.21	−43.77	−43.05	−42.40	−41.78
800		−50.70	−49.62	−48.93	−48.44	−47.67	−47.01	−46.38
900		−55.48	−54.44	−53.72	−53.20	−52.39	−51.71	−51.08
1000		−60.31	−59.30	−58.57	−58.03	−57.20	−56.51	−55.87
				$AgCl_2^-$				
25	−51.56	−50.92	−50.31	−49.71	−49.13	−47.99	−46.88	−45.80
50	−52.74	−52.09	−51.46	−50.84	−50.25	−49.09	−47.96	−46.86
75	−53.94	−53.28	−52.64	−52.02	−51.42	−50.26	−49.12	−48.01
100	−55.15	−54.49	−53.85	−53.23	−52.63	−51.46	−50.33	−49.22

BLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$AgCl_2^-$ — Continued				
125	−56.37	−55.72	−55.08	−54.47	−53.87	−52.70	−51.57	−50.46
150	−57.60	−56.95	−56.33	−55.72	−55.12	−53.96	−52.84	−51.73
175	−58.81	−58.20	−57.58	−56.99	−56.40	−55.25	−54.13	−53.03
200	−60.02	−59.44	−58.85	−58.26	−57.68	−56.55	−55.44	−54.35
225	−61.20	−60.68	−60.11	−59.55	−58.98	−57.87	−56.77	−55.69
250	−62.34	−61.91	−61.38	−60.83	−60.29	−59.20	−58.12	−57.05
300	−64.39	−64.28	−63.88	−63.41	−62.91	−61.89	−60.85	−59.81
350	−65.53	−66.39	−66.31	−65.96	−65.54	−64.61	−63.63	−62.64
400		−67.99	−68.58	−68.44	−68.14	−67.34	−66.45	−65.50
450		−67.11	−70.55	−70.81	−70.69	−70.08	−69.28	−68.40
500			−72.04	−73.02	−73.17	−72.80	−72.13	−71.33
550			−72.88	−75.01	−75.54	−75.50	−74.98	−74.27
600			−73.22	−76.77	−77.81	−78.17	−77.83	−77.22
700				−79.90	−82.06	−83.39	−83.48	−83.10
800					−86.21	−88.52	−89.06	−88.93
900					−90.56	−93.66	−94.62	−94.68
1000						−98.96	−100.21	−100.35
				$AgCl_3^{-2}$				
25	−82.71	−81.69	−80.71	−79.77	−78.85	−77.08	−75.37	−73.70
50	−83.81	−82.76	−81.76	−80.80	−79.87	−78.06	−76.32	−74.62
75	−84.93	−83.88	−82.88	−81.91	−80.97	−79.16	−77.40	−75.69
100	−86.07	−85.03	−84.03	−83.07	−82.13	−80.32	−78.57	−76.86
125	−87.21	−86.19	−85.21	−84.26	−83.34	−81.54	−79.80	−78.10
150	−88.33	−87.36	−86.41	−85.48	−84.57	−82.80	−81.07	−79.38
175	−89.43	−88.53	−87.61	−86.71	−85.83	−84.09	−82.39	−80.72
200	−90.48	−89.67	−88.82	−87.96	−87.10	−85.41	−83.74	−82.09
225	−91.45	−90.78	−90.00	−89.20	−88.38	−86.74	−85.11	−83.49
250	−92.30	−91.84	−91.17	−90.43	−89.66	−88.10	−86.51	−84.93
300	−93.38	−93.71	−93.39	−92.85	−92.22	−90.83	−89.38	−87.88
350	−92.26	−94.85	−95.37	−95.14	−94.71	−93.59	−92.29	−90.91
400		−95.03	−96.94	−97.23	−97.10	−96.32	−95.24	−94.01
450		−89.64	−97.79	−99.01	−99.32	−99.02	−98.20	−97.15
500			−97.50	−100.35	−101.31	−101.63	−101.15	−100.31
550			−95.72	−101.16	−103.02	−104.15	−104.06	−103.46
600			−92.79	−101.42	−104.43	−106.53	−106.90	−106.58
700				−100.99	−106.48	−110.89	−112.36	−112.67
800					−108.13	−114.82	−117.47	−118.43
900					−110.12	−118.59	−122.33	−123.82
1000						−122.61	−127.14	−128.85
				$AgCl_4^{-3}$				
25	−112.28	−110.82	−109.43	−108.09	−106.80	−104.31	−101.91	−99.57
50	−113.07	−111.57	−110.15	−108.79	−107.47	−104.93	−102.48	−100.10
75	−114.01	−112.52	−111.10	−109.73	−108.41	−105.86	−103.39	−101.00
100	−115.08	−113.61	−112.20	−110.85	−109.53	−106.99	−104.54	−102.14
125	−116.23	−114.81	−113.44	−112.11	−110.81	−108.30	−105.86	−103.48
150	−117.44	−116.10	−114.77	−113.48	−112.21	−109.74	−107.33	−104.97
175	−118.67	−117.44	−116.19	−114.95	−113.72	−111.31	−108.94	−106.62
200	−119.89	−118.82	−117.66	−116.49	−115.31	−112.98	−110.67	−108.38
225	−121.04	−120.20	−119.17	−118.09	−116.98	−114.75	−112.51	−110.27
250	−122.05	−121.55	−120.70	−119.73	−118.71	−116.60	−114.44	−112.26
300	−123.21	−123.99	−123.74	−123.09	−122.30	−120.50	−118.55	−116.53
350	−121.23	−125.47	−126.60	−126.45	−125.98	−124.62	−122.96	−121.14
400		−126.07	−129.02	−129.67	−129.68	−128.89	−127.59	−126.02
450		−119.08	−130.56	−132.59	−133.29	−133.26	−132.39	−131.13
500			−130.62	−135.01	−136.69	−137.65	−137.33	−136.42
550			−128.73	−136.78	−139.80	−142.02	−142.34	−141.83
600			−125.41	−137.91	−142.59	−146.31	−147.38	−147.34
700				−139.29	−147.38	−154.58	−157.41	−158.41

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$AgCl_4^{-3}$ — Continued				
800					−151.98	−162.50	−167.26	−169.35
900					−157.43	−170.51	−177.04	−180.04
1000						−179.20	−187.07	−190.45
				$AgNO_3^\circ$				
25	−7.81	−7.39	−6.98	−6.58	−6.19	−5.41	−4.65	−3.90
50	−9.08	−8.65	−8.23	−7.82	−7.41	−6.62	−5.85	−5.09
75	−10.40	−9.95	−9.52	−9.11	−8.70	−7.90	−7.12	−6.36
100	−11.75	−11.30	−10.86	−10.44	−10.03	−9.23	−8.44	−7.68
125	−13.13	−12.68	−12.24	−11.81	−11.40	−10.59	−9.81	−9.04
150	−14.54	−14.09	−13.65	−13.22	−12.80	−11.99	−11.21	−10.43
175	−15.99	−15.53	−15.09	−14.66	−14.24	−13.43	−12.64	−11.87
200	−17.45	−17.00	−16.56	−16.13	−15.71	−14.89	−14.10	−13.33
225	−18.95	−18.50	−18.05	−17.62	−17.20	−16.38	−15.59	−14.81
250	−20.46	−20.03	−19.58	−19.14	−18.72	−17.90	−17.11	−16.33
300	−23.55	−23.15	−22.69	−22.25	−21.83	−21.01	−20.21	−19.43
350	−26.74	−26.37	−25.90	−25.46	−25.03	−24.20	−23.40	−22.62
400		−29.71	−29.20	−28.74	−28.31	−27.47	−26.67	−25.89
450		−33.23	−32.58	−32.11	−31.67	−30.82	−30.01	−29.23
500		−37.00	−36.06	−35.55	−35.10	−34.24	−33.43	−32.64
550		−40.76	−39.63	−39.07	−38.60	−37.73	−36.91	−36.11
600		−44.50	−43.29	−42.66	−42.16	−41.28	−40.45	−39.65
700		−52.00	−50.77	−50.03	−49.47	−48.54	−47.70	−46.89
800		−59.60	−58.40	−57.60	−56.99	−56.02	−55.15	−54.34
900		−67.32	−66.15	−65.32	−64.69	−63.68	−62.80	−61.97
1000		−75.16	−74.02	−73.19	−72.53	−71.50	−70.61	−69.78
				Al^{+3}				
25	−116.54	−117.04	−117.48	−117.86	−118.21	−118.82	−119.34	−119.81
50	−114.49	−115.02	−115.48	−115.90	−116.27	−116.94	−117.52	−118.04
75	−112.39	−112.94	−113.43	−113.87	−114.27	−114.98	−115.61	−116.17
100	−110.23	−110.82	−111.34	−111.80	−112.22	−112.97	−113.64	−114.24
125	−108.02	−108.65	−109.20	−109.69	−110.14	−110.93	−111.63	−112.26
150	−105.75	−106.43	−107.02	−107.54	−108.02	−108.86	−109.60	−110.26
175	−103.41	−104.15	−104.79	−105.35	−105.86	−106.76	−107.53	−108.24
200	−100.99	−101.80	−102.51	−103.12	−103.67	−104.63	−105.45	−106.19
225	−98.48	−99.39	−100.17	−100.85	−101.44	−102.47	−103.35	−104.13
250	−95.86	−96.90	−97.78	−98.52	−99.17	−100.28	−101.22	−102.05
300	−90.28	−91.73	−92.87	−93.75	−94.52	−95.82	−96.91	−97.85
350	−85.14	−86.20	−87.89	−88.84	−89.73	−91.25	−92.51	−93.58
400		−83.79	−83.03	−83.90	−84.85	−86.57	−88.02	−89.25
450		−88.55	−78.63	−78.98	−79.91	−81.81	−83.45	−84.85
500			−75.28	−74.21	−74.94	−76.95	−78.79	−80.36
550			−73.66	−69.71	−69.95	−71.98	−74.02	−75.78
600			−74.01	−65.68	−64.98	−66.87	−69.12	−71.08
700				−59.51	−55.14	−56.12	−58.79	−61.23
800					−45.22	−44.48	−47.65	−50.62
900					−34.55	−31.93	−35.71	−39.19
1000						−18.77	−23.25	−27.02
				$Al(CH_3COO)^{+2}$				
25	−208.56	−208.57	−208.54	−208.51	−208.45	−208.31	−208.15	−207.96
50	−207.81	−207.82	−207.80	−207.77	−207.72	−207.60	−207.45	−207.27
75	−207.18	−207.19	−207.18	−207.16	−207.12	−207.01	−206.87	−206.72
100	−206.65	−206.67	−206.67	−206.65	−206.62	−206.53	−206.41	−206.27
125	−206.19	−206.23	−206.25	−206.24	−206.22	−206.15	−206.04	−205.92
150	−205.80	−205.87	−205.90	−205.91	−205.91	−205.86	−205.77	−205.65
175	−205.46	−205.56	−205.62	−205.66	−205.67	−205.64	−205.57	−205.47
200	−205.16	−205.31	−205.40	−205.46	−205.49	−205.50	−205.45	−205.37

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Al(CH_3COO)^{+2}$ — Continued				
225	−204.88	−205.09	−205.23	−205.32	−205.37	−205.42	−205.40	−205.34
250	−204.62	−204.91	−205.10	−205.23	−205.31	−205.40	−205.41	−205.38
300	−204.07	−204.63	−204.98	−205.18	−205.33	−205.53	−205.62	−205.64
350	−203.79	−204.38	−205.05	−205.31	−205.53	−205.85	−206.03	−206.13
400		−205.75	−205.37	−205.63	−205.91	−206.35	−206.64	−206.82
450		−210.12	−206.06	−206.15	−206.45	−207.01	−207.41	−207.69
500			−207.33	−206.90	−207.16	−207.81	−208.34	−208.71
550			−209.44	−207.91	−208.01	−208.74	−209.39	−209.87
600			−212.48	−209.25	−209.01	−209.76	−210.54	−211.14
700				−213.17	−211.47	−211.98	−213.05	−213.92
800					−214.41	−214.32	−215.72	−216.90
900					−217.53	−216.73	−218.51	−219.97
1000						−219.36	−221.52	−223.14
				$Al(CH_3COO)_2^+$				
25	−299.36	−298.80	−298.25	−297.72	−297.21	−296.20	−295.21	−294.24
50	−299.73	−299.15	−298.59	−298.05	−297.52	−296.49	−295.49	−294.51
75	−300.38	−299.79	−299.22	−298.67	−298.14	−297.10	−296.09	−295.10
100	−301.25	−300.66	−300.09	−299.54	−299.00	−297.96	−296.94	−295.95
125	−302.33	−301.73	−301.16	−300.61	−300.07	−299.03	−298.01	−297.02
150	−303.58	−302.99	−302.42	−301.87	−301.33	−300.29	−299.27	−298.28
175	−304.98	−304.41	−303.84	−303.30	−302.76	−301.72	−300.71	−299.72
200	−306.53	−305.98	−305.42	−304.88	−304.35	−303.31	−302.30	−301.32
225	−308.22	−307.69	−307.14	−306.61	−306.08	−305.05	−304.05	−303.07
250	−310.01	−309.53	−308.99	−308.47	−307.95	−306.93	−305.94	−304.96
300	−313.90	−313.56	−313.07	−312.56	−312.06	−311.07	−310.10	−309.13
350	−318.12	−317.98	−317.60	−317.12	−316.64	−315.68	−314.73	−313.78
400		−323.06	−322.54	−322.09	−321.63	−320.72	−319.79	−318.87
450		−328.74	−327.88	−327.44	−327.01	−326.14	−325.25	−324.35
500			−333.61	−333.15	−332.75	−331.92	−331.07	−330.20
550			−339.72	−339.20	−338.81	−338.04	−337.23	−336.39
600			−346.20	−345.57	−345.18	−344.46	−343.69	−342.89
700				−359.29	−358.77	−358.12	−357.47	−356.74
800					−373.41	−372.77	−372.24	−371.61
900					−389.00	−388.33	−387.92	−387.37
1000						−404.76	−404.46	−403.95
				$AlHO_2^\circ$				
25	−207.50	−207.34	−207.17	−206.99	−206.80	−206.43	−206.04	−205.64
50	−207.38	−207.21	−207.03	−206.85	−206.67	−206.29	−205.90	−205.51
75	−207.33	−207.16	−206.98	−206.80	−206.61	−206.24	−205.86	−205.47
100	−207.35	−207.18	−207.00	−206.82	−206.64	−206.26	−205.88	−205.50
125	−207.43	−207.26	−207.09	−206.91	−206.72	−206.35	−205.98	−205.60
150	−207.57	−207.40	−207.23	−207.05	−206.87	−206.50	−206.13	−205.75
175	−207.75	−207.59	−207.42	−207.25	−207.07	−206.71	−206.34	−205.97
200	−207.98	−207.83	−207.67	−207.50	−207.32	−206.97	−206.60	−206.24
225	−208.24	−208.11	−207.95	−207.79	−207.62	−207.27	−206.92	−206.55
250	−208.52	−208.42	−208.28	−208.13	−207.97	−207.63	−207.27	−206.91
300	−209.13	−209.14	−209.05	−208.92	−208.77	−208.46	−208.12	−207.77
350	−209.48	−209.89	−209.91	−209.84	−209.72	−209.44	−209.13	−208.79
400		−210.46	−210.84	−210.86	−210.79	−210.56	−210.27	−209.96
450		−209.93	−211.74	−211.94	−211.95	−211.80	−211.55	−211.26
500		−207.81	−212.52	−213.06	−213.19	−213.14	−212.94	−212.68
550		−206.52	−213.09	−214.19	−214.49	−214.58	−214.44	−214.21
600		−206.16	−213.53	−215.30	−215.84	−216.10	−216.03	−215.84
700		−207.12	−214.71	−217.59	−218.69	−219.38	−219.48	−219.37
800		−209.51	−216.79	−220.25	−221.82	−222.97	−223.24	−223.23
900		−212.85	−219.77	−223.48	−225.37	−226.88	−227.31	−227.37
1000		−216.90	−223.50	−227.31	−229.38	−231.15	−231.69	−231.76

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Al(OH)^{+2}$				
25	−166.47	−166.68	−166.84	−166.97	−167.08	−167.24	−167.34	−167.40
50	−165.31	−165.53	−165.71	−165.85	−165.97	−166.15	−166.29	−166.38
75	−164.19	−164.42	−164.61	−164.77	−164.90	−165.11	−165.26	−165.38
100	−163.10	−163.35	−163.55	−163.72	−163.86	−164.09	−164.27	−164.40
125	−162.03	−162.30	−162.52	−162.70	−162.86	−163.11	−163.31	−163.47
150	−160.97	−161.27	−161.51	−161.72	−161.89	−162.17	−162.39	−162.56
175	−159.91	−160.25	−160.53	−160.75	−160.95	−161.26	−161.50	−161.70
200	−158.85	−159.24	−159.55	−159.81	−160.03	−160.38	−160.65	−160.86
225	−157.78	−158.23	−158.59	−158.88	−159.13	−159.52	−159.82	−160.06
250	−156.68	−157.21	−157.63	−157.96	−158.24	−158.68	−159.02	−159.29
300	−154.35	−155.15	−155.74	−156.15	−156.51	−157.07	−157.50	−157.84
350	−152.32	−152.99	−153.93	−154.41	−154.83	−155.53	−156.07	−156.49
400		−152.74	−152.30	−152.74	−153.22	−154.05	−154.70	−155.22
450		−156.49	−151.02	−151.20	−151.69	−152.63	−153.41	−154.03
500			−150.42	−149.83	−150.22	−151.26	−152.16	−152.89
550			−150.84	−148.70	−148.84	−149.92	−150.95	−151.80
600			−152.41	−147.91	−147.55	−148.58	−149.75	−150.74
700				−147.61	−145.25	−145.85	−147.31	−148.58
800					−143.19	−142.89	−144.68	−146.29
900					−140.99	−139.67	−141.87	−143.80
1000						−136.38	−139.01	−141.11
				$Al(OH)_2^+$				
25	−215.47	−215.38	−215.28	−215.16	−215.03	−214.75	−214.43	−214.10
50	−215.08	−214.99	−214.89	−214.77	−214.65	−214.37	−214.07	−213.75
75	−214.76	−214.68	−214.58	−214.46	−214.34	−214.07	−213.77	−213.47
100	−214.51	−214.43	−214.34	−214.23	−214.11	−213.84	−213.56	−213.26
125	−214.32	−214.25	−214.16	−214.05	−213.94	−213.69	−213.41	−213.12
150	−214.17	−214.12	−214.04	−213.94	−213.83	−213.59	−213.33	−213.04
175	−214.07	−214.04	−213.97	−213.89	−213.79	−213.56	−213.30	−213.03
200	−214.01	−214.00	−213.95	−213.88	−213.79	−213.58	−213.33	−213.07
225	−213.98	−214.00	−213.97	−213.92	−213.84	−213.65	−213.42	−213.16
250	−213.97	−214.03	−214.03	−214.00	−213.94	−213.77	−213.55	−213.31
300	−213.99	−214.20	−214.27	−214.27	−214.25	−214.13	−213.96	−213.75
350	−214.21	−214.43	−214.67	−214.71	−214.71	−214.66	−214.54	−214.37
400		−215.58	−215.26	−215.29	−215.32	−215.33	−215.27	−215.14
450		−218.45	−216.10	−216.03	−216.07	−216.14	−216.13	−216.05
500			−217.30	−216.94	−216.96	−217.07	−217.12	−217.10
550			−219.01	−218.04	−217.96	−218.11	−218.23	−218.25
600			−221.27	−219.36	−219.09	−219.24	−219.42	−219.51
700				−222.77	−221.70	−221.71	−222.04	−222.26
800					−224.72	−224.38	−224.87	−225.26
900					−227.95	−227.22	−227.90	−228.43
1000						−230.28	−231.16	−231.77
				AlO_2^-				
25	−198.70	−198.58	−198.46	−198.32	−198.18	−197.89	−197.59	−197.28
50	−198.52	−198.38	−198.25	−198.10	−197.95	−197.65	−197.33	−197.01
75	−198.32	−198.19	−198.05	−197.90	−197.75	−197.44	−197.12	−196.80
100	−198.12	−197.99	−197.86	−197.72	−197.57	−197.27	−196.95	−196.63
125	−197.90	−197.79	−197.67	−197.54	−197.40	−197.10	−196.80	−196.48
150	−197.66	−197.58	−197.47	−197.36	−197.23	−196.95	−196.66	−196.35
175	−197.39	−197.35	−197.27	−197.18	−197.06	−196.81	−196.54	−196.24
200	−197.07	−197.09	−197.06	−196.99	−196.90	−196.68	−196.42	−196.15
225	−196.71	−196.81	−196.82	−196.79	−196.73	−196.55	−196.32	−196.06
250	−196.27	−196.48	−196.56	−196.57	−196.55	−196.41	−196.22	−195.99
300	−195.01	−195.65	−195.96	−196.09	−196.15	−196.14	−196.04	−195.87
350	−192.70	−194.40	−195.21	−195.52	−195.70	−195.85	−195.86	−195.77
400		−193.13	−194.27	−194.82	−195.16	−195.53	−195.67	−195.68
450		−190.10	−193.02	−193.96	−194.53	−195.16	−195.47	−195.60

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				AlO_2^- — Continued				
500			−191.34	−192.90	−193.76	−194.73	−195.24	−195.51
550			−189.15	−191.60	−192.84	−194.23	−194.97	−195.39
600			−186.66	−190.08	−191.77	−193.63	−194.64	−195.23
700				−186.82	−189.22	−192.12	−193.75	−194.74
800					−186.42	−190.22	−192.54	−193.94
900					−183.66	−188.09	−191.05	−192.81
1000						−185.96	−189.44	−191.35
				Ar°				
25	3.90	4.27	4.64	5.00	5.36	6.06	6.75	7.44
50	3.49	3.88	4.26	4.63	5.00	5.71	6.41	7.11
75	2.99	3.39	3.78	4.16	4.53	5.25	5.96	6.66
100	2.41	2.82	3.21	3.60	3.97	4.70	5.42	6.12
125	1.76	2.17	2.57	2.96	3.34	4.08	4.80	5.50
150	1.04	1.46	1.87	2.26	2.65	3.39	4.11	4.82
175	0.25	0.68	1.10	1.50	1.89	2.64	3.36	4.07
200	−0.59	−0.16	0.27	0.67	1.07	1.83	2.56	3.27
225	−1.50	−1.05	−0.62	−0.21	0.19	0.96	1.70	2.42
250	−2.47	−2.01	−1.56	−1.14	−0.73	0.04	0.79	1.51
300	−4.63	−4.12	−3.61	−3.16	−2.73	−1.93	−1.17	−0.43
350	−7.35	−6.51	−5.89	−5.38	−4.93	−4.09	−3.30	−2.55
400		−9.41	−8.42	−7.81	−7.31	−6.41	−5.60	−4.83
450		−13.70	−11.25	−10.46	−9.87	−8.90	−8.05	−7.25
500		−19.90	−14.47	−13.33	−12.62	−11.54	−10.64	−9.82
550		−25.49	−18.15	−16.45	−15.55	−14.34	−13.37	−12.52
600		−30.36	−22.20	−19.80	−18.67	−17.27	−16.24	−15.34
700		−39.01	−30.64	−27.09	−25.39	−23.55	−22.34	−21.36
800		−46.98	−38.92	−34.78	−32.59	−30.29	−28.90	−27.82
900		−54.68	−46.99	−42.60	−40.09	−37.40	−35.85	−34.71
1000		−62.30	−54.94	−50.44	−47.74	−44.80	−43.14	−41.98
				Au^+				
25	39.00	39.14	39.29	39.44	39.61	39.94	40.29	40.65
50	38.39	38.53	38.68	38.84	39.01	39.34	39.69	40.04
75	37.77	37.91	38.07	38.23	38.39	38.73	39.07	39.42
100	37.14	37.29	37.44	37.60	37.77	38.10	38.44	38.78
125	36.50	36.65	36.81	36.97	37.13	37.46	37.80	38.14
150	35.86	36.01	36.17	36.32	36.48	36.81	37.15	37.49
175	35.22	35.36	35.51	35.67	35.83	36.16	36.49	36.82
200	34.57	34.71	34.86	35.01	35.17	35.49	35.82	36.15
225	33.92	34.05	34.19	34.34	34.50	34.81	35.14	35.47
250	33.27	33.38	33.52	33.67	33.82	34.13	34.45	34.78
300	31.99	32.05	32.17	32.30	32.45	32.74	33.06	33.38
350	30.77	30.73	30.80	30.92	31.05	31.33	31.63	31.94
400		29.34	29.42	29.52	29.64	29.90	30.19	30.49
450		27.98	28.03	28.11	28.21	28.45	28.72	29.01
500			26.64	26.69	26.77	26.98	27.23	27.51
550			25.25	25.26	25.32	25.50	25.73	25.99
600			23.86	23.83	23.87	24.01	24.21	24.46
700				20.91	20.93	21.00	21.15	21.36
800					17.95	17.97	18.06	18.23
900					14.93	14.92	14.95	15.07
1000						11.81	11.79	11.90
				Au^{+3}				
25	103.60	103.14	102.73	102.37	102.04	101.46	100.96	100.51
50	105.08	104.60	104.17	103.79	103.44	102.82	102.27	101.78
75	106.62	106.11	105.67	105.27	104.90	104.25	103.67	103.14
100	108.21	107.68	107.21	106.79	106.40	105.72	105.11	104.55

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — *Continued*

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Au^{+3} — *Continued*				
125	109.85	109.28	108.79	108.35	107.94	107.22	106.58	106.00
150	111.55	110.94	110.41	109.94	109.51	108.75	108.08	107.48
175	113.31	112.65	112.08	111.57	111.12	110.31	109.61	108.97
200	115.15	114.42	113.79	113.25	112.76	111.90	111.16	110.49
225	117.06	116.25	115.56	114.96	114.43	113.51	112.72	112.02
250	119.08	118.15	117.37	116.72	116.14	115.15	114.31	113.57
300	123.44	122.15	121.13	120.35	119.67	118.51	117.55	116.71
350	127.69	126.51	124.99	124.12	123.33	121.98	120.87	119.91
400		128.59	128.81	127.96	127.08	125.55	124.27	123.18
450		125.89	132.36	131.81	130.92	129.20	127.75	126.52
500			135.26	135.63	134.82	132.95	131.32	129.93
550			137.03	139.30	138.77	136.82	134.98	133.43
600			137.53	142.69	142.76	140.81	138.77	137.03
700				148.22	150.78	149.28	146.81	144.65
800					158.97	158.54	155.57	152.93
900					167.75	168.54	164.99	161.91
1000						179.02	174.86	171.54
				$Au(CH_3COO)^0$				
25	−49.87	−49.15	−48.47	−47.80	−47.16	−45.91	−44.70	−43.52
50	−51.13	−50.38	−49.67	−48.99	−48.33	−47.05	−45.82	−44.62
75	−52.47	−51.72	−50.99	−50.30	−49.63	−48.34	−47.09	−45.87
100	−53.90	−53.13	−52.41	−51.71	−51.03	−49.72	−48.46	−47.24
125	−55.40	−54.63	−53.89	−53.19	−52.51	−51.19	−49.93	−48.70
150	−56.97	−56.19	−55.45	−54.74	−54.06	−52.73	−51.46	−50.23
175	−58.59	−57.82	−57.07	−56.36	−55.67	−54.34	−53.07	−51.83
200	−60.26	−59.50	−58.75	−58.04	−57.34	−56.01	−54.74	−53.49
225	−61.99	−61.24	−60.49	−59.77	−59.07	−57.74	−56.46	−55.22
250	−63.76	−63.03	−62.27	−61.55	−60.86	−59.52	−58.23	−56.99
300	−67.42	−66.75	−65.99	−65.27	−64.57	−63.22	−61.93	−60.68
350	−71.25	−70.66	−69.89	−69.16	−68.45	−67.10	−65.81	−64.55
400		−74.77	−73.96	−73.21	−72.50	−71.14	−69.85	−68.59
450		−79.14	−78.19	−77.42	−76.70	−75.34	−74.03	−72.77
500		−83.83	−82.58	−81.78	−81.05	−79.67	−78.36	−77.10
550		−88.57	−87.13	−86.28	−85.53	−84.13	−82.82	−81.55
600		−93.34	−91.83	−90.90	−90.13	−88.72	−87.39	−86.12
700		−103.09	−101.55	−100.52	−99.68	−98.23	−96.89	−95.60
800		−113.13	−111.63	−110.53	−109.65	−108.15	−106.79	−105.49
900		−123.48	−122.01	−120.89	−119.98	−118.44	−117.06	−115.76
1000		−134.13	−132.69	−131.56	−130.62	−129.06	−127.67	−126.36
				$Au(CH_3COO)_2^-$				
25	−138.24	−136.88	−135.59	−134.36	−133.18	−130.91	−128.73	−126.62
50	−139.90	−138.50	−137.17	−135.91	−134.69	−132.36	−130.12	−127.96
75	−141.77	−140.35	−139.01	−137.72	−136.49	−134.12	−131.86	−129.67
100	−143.82	−142.39	−141.04	−139.75	−138.50	−136.12	−133.84	−131.63
125	−146.03	−144.59	−143.24	−141.94	−140.69	−138.30	−136.01	−133.79
150	−148.36	−146.94	−145.59	−144.29	−143.04	−140.64	−138.35	−136.12
175	−150.81	−149.42	−148.07	−146.77	−145.52	−143.13	−140.83	−138.61
200	−153.36	−152.00	−150.67	−149.38	−148.14	−145.75	−143.45	−141.23
225	−155.99	−154.69	−153.37	−152.10	−150.87	−148.49	−146.20	−143.98
250	−158.68	−157.48	−156.18	−154.93	−153.70	−151.34	−149.06	−146.84
300	−164.12	−163.25	−162.06	−160.85	−159.67	−157.35	−155.10	−152.90
350	−169.14	−169.17	−168.22	−167.10	−165.97	−163.72	−161.51	−159.35
400		−175.00	−174.56	−173.62	−172.57	−170.42	−168.27	−166.14
450		−179.17	−180.97	−180.33	−179.43	−177.42	−175.34	−173.26
500			−187.26	−187.18	−186.48	−184.66	−182.68	−180.66
550			−193.30	−194.11	−193.71	−192.14	−190.27	−188.32
600			−199.18	−201.10	−201.09	−199.83	−198.10	−196.22
700				−215.41	−216.28	−215.77	−214.36	−212.66

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
					$Au(CH_3COO)_2^-$ — Continued			
800					−232.17	−232.41	−231.36	−229.85
900					−248.93	−249.79	−249.05	−247.68
000						−267.94	−267.43	−266.11
					Benzene			
25	32.00	32.97	33.92	34.83	35.73	37.47	39.17	40.84
50	31.02	32.00	32.94	33.85	34.74	36.47	38.15	39.79
75	29.88	30.86	31.80	32.71	33.60	35.32	36.98	38.62
100	28.59	29.58	30.52	31.42	32.31	34.02	35.68	37.30
125	27.16	28.15	29.09	30.00	30.88	32.59	34.25	35.86
150	25.60	26.58	27.53	28.44	29.32	31.03	32.68	34.30
175	23.92	24.90	25.84	26.75	27.64	29.35	31.00	32.61
200	22.12	23.09	24.04	24.95	25.84	27.55	29.20	30.82
225	20.21	21.17	22.13	23.04	23.93	25.65	27.30	28.91
250	18.19	19.14	20.10	21.03	21.92	23.64	25.29	26.91
300	13.83	14.75	15.75	16.69	17.59	19.33	20.99	22.60
350	8.92	9.92	11.00	11.97	12.90	14.65	16.32	17.95
400		4.55	5.86	6.89	7.85	9.63	11.32	12.96
450		−1.95	0.30	1.46	2.46	4.30	6.01	7.66
50(		−9.87	−5.70	−4.32	−3.24	−1.34	0.41	2.07
55(		−17.58	−12.19	−10.44	−9.24	−7.25	−5.47	−3.79
60(		−25.00	−19.09	−16.90	−15.54	−13.44	−11.61	−9.90
70(		−39.64	−33.59	−30.66	−28.94	−26.55	−24.62	−22.85
800		−54.44	−48.59	−45.28	−43.25	−40.56	−38.51	−36.69
900		−69.61	−63.99	−60.52	−58.28	−55.35	−53.20	−51.33
1000		−85.22	−79.81	−76.27	−73.92	−70.82	−68.60	−66.72
					Butanoate			
25	−84.61	−83.80	−83.02	−82.27	−81.54	−80.13	−78.76	−77.42
50	−85.45	−84.61	−83.82	−83.05	−82.30	−80.86	−79.46	−78.10
75	−86.36	−85.52	−84.71	−83.93	−83.18	−81.72	−80.32	−78.94
100	−87.33	−86.49	−85.68	−84.90	−84.15	−82.69	−81.28	−79.90
125	−88.35	−87.52	−86.71	−85.94	−85.19	−83.73	−82.32	−80.94
150	−89.41	−88.59	−87.80	−87.03	−86.29	−84.84	−83.43	−82.06
175	−90.49	−89.71	−88.93	−88.18	−87.44	−86.00	−84.60	−83.24
200	−91.59	−90.85	−90.10	−89.36	−88.64	−87.22	−85.83	−84.48
225	−92.68	−92.01	−91.30	−90.58	−89.87	−88.48	−87.11	−85.77
250	−93.75	−93.19	−92.52	−91.83	−91.15	−89.78	−88.43	−87.10
300	−95.68	−95.51	−95.00	−94.40	−93.78	−92.50	−91.20	−89.91
350	−96.64	−97.61	−97.49	−97.03	−96.50	−95.33	−94.11	−92.87
400		−99.28	−99.87	−99.67	−99.27	−98.27	−97.14	−95.97
450		−98.27	−102.00	−102.25	−102.06	−101.28	−100.28	−99.18
500			−103.66	−104.71	−104.84	−104.34	−103.49	−102.49
550			−104.65	−106.99	−107.56	−107.44	−106.77	−105.89
600			−105.16	−109.08	−110.21	−110.56	−110.11	−109.35
700				−112.99	−115.37	−116.83	−116.89	−116.41
800					−120.60	−123.17	−123.78	−123.60
900					−126.24	−129.70	−130.80	−130.87
1000						−136.57	−138.03	−138.19
					Butanoic Acid			
25	−91.19	−90.20	−89.25	−88.32	−87.42	−85.66	−83.94	−82.26
50	−92.68	−91.68	−90.73	−89.81	−88.91	−87.16	−85.47	−83.81
75	−94.31	−93.32	−92.36	−91.44	−90.54	−88.80	−87.12	−85.47
100	−96.09	−95.09	−94.14	−93.21	−92.32	−90.58	−88.90	−87.26
125	−98.01	−97.00	−96.04	−95.12	−94.22	−92.48	−90.80	−89.17
150	−100.05	−99.04	−98.07	−97.14	−96.24	−94.50	−92.82	−91.19
175	−102.22	−101.20	−100.22	−99.29	−98.38	−96.64	−94.95	−93.32
200	−104.50	−103.48	−102.49	−101.54	−100.63	−98.88	−97.19	−95.55

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Butanoic Acid — Continued				
225	−106.89	−105.87	−104.86	−103.91	−102.99	−101.22	−99.53	−97.89
250	−109.41	−108.37	−107.34	−106.37	−105.44	−103.67	−101.97	−100.32
300	−114.84	−113.74	−112.63	−111.61	−110.65	−108.83	−107.11	−105.44
350	−121.23	−119.65	−118.33	−117.23	−116.22	−114.35	−112.59	−110.90
400		−126.43	−124.51	−123.25	−122.16	−120.20	−118.39	−116.68
450		−135.59	−131.24	−129.67	−128.45	−126.36	−124.50	−122.74
500		−147.95	−138.67	−136.52	−135.09	−132.83	−130.88	−129.08
550		−159.34	−146.90	−143.81	−142.08	−139.59	−137.54	−135.69
600		−169.58	−155.78	−151.54	−149.41	−146.63	−144.46	−142.54
700		−188.36	−174.21	−168.07	−165.00	−161.48	−159.03	−156.97
800		−206.16	−192.53	−185.41	−181.53	−177.25	−174.50	−172.28
900		−223.64	−210.63	−203.08	−198.67	−193.76	−190.74	−188.42
1000		−241.11	−228.63	−220.92	−216.21	−210.86	−207.67	−205.30
				BF_4^-				
25	−355.40	−354.90	−354.41	−353.94	−353.47	−352.54	−351.64	−350.75
50	−356.47	−355.96	−355.46	−354.97	−354.49	−353.56	−352.64	−351.74
75	−357.54	−357.02	−356.51	−356.02	−355.54	−354.60	−353.68	−352.78
100	−358.60	−358.08	−357.58	−357.09	−356.61	−355.67	−354.75	−353.85
125	−359.65	−359.14	−358.64	−358.16	−357.68	−356.75	−355.83	−354.94
150	−360.69	−360.20	−359.71	−359.23	−358.76	−357.84	−356.93	−356.04
175	−361.71	−361.25	−360.78	−360.31	−359.85	−358.93	−358.04	−357.15
200	−362.71	−362.29	−361.83	−361.38	−360.93	−360.04	−359.15	−358.28
225	−363.68	−363.31	−362.88	−362.45	−362.02	−361.14	−360.27	−359.41
250	−364.59	−364.30	−363.92	−363.51	−363.10	−362.25	−361.40	−360.55
300	−366.14	−366.17	−365.94	−365.61	−365.24	−364.47	−363.67	−362.85
350	−366.71	−367.74	−367.83	−367.63	−367.35	−366.68	−365.94	−365.17
400		−368.75	−369.53	−369.56	−369.40	−368.87	−368.22	−367.50
450		−367.13	−370.89	−371.33	−371.37	−371.03	−370.48	−369.84
500			−371.71	−372.90	−373.22	−373.15	−372.73	−372.17
550			−371.83	−374.22	−374.94	−375.21	−374.96	−374.49
600			−371.41	−375.28	−376.52	−377.21	−377.15	−376.79
700				−376.91	−379.32	−381.03	−381.41	−381.31
800					−381.92	−384.65	−385.52	−385.68
900					−384.66	−388.21	−389.52	−389.88
1000						−391.87	−393.49	−393.93
				$B(OH)_3^\circ$				
25	−231.54	−231.08	−230.63	−230.19	−229.76	−228.91	−228.07	−227.25
50	−232.48	−232.00	−231.54	−231.09	−230.65	−229.79	−228.95	−228.12
75	−233.44	−232.95	−232.49	−232.03	−231.59	−230.72	−229.87	−229.04
100	−234.43	−233.93	−233.46	−233.00	−232.55	−231.68	−230.83	−229.99
125	−235.43	−234.94	−234.46	−233.99	−233.54	−232.66	−231.81	−230.97
150	−236.46	−235.96	−235.48	−235.01	−234.55	−233.67	−232.82	−231.98
175	−237.51	−237.01	−236.52	−236.05	−235.59	−234.70	−233.84	−233.00
200	−238.59	−238.08	−237.58	−237.11	−236.65	−235.75	−234.89	−234.05
225	−239.68	−239.17	−238.67	−238.19	−237.72	−236.82	−235.96	−235.11
250	−240.80	−240.29	−239.77	−239.29	−238.81	−237.91	−237.04	−236.19
300	−243.12	−242.60	−242.05	−241.54	−241.06	−240.13	−239.25	−238.39
350	−245.74	−245.04	−244.42	−243.87	−243.37	−242.42	−241.52	−240.66
400		−247.76	−246.90	−246.29	−245.75	−244.77	−243.86	−242.98
450		−251.35	−249.53	−248.80	−248.22	−247.18	−246.24	−245.35
500		−256.14	−252.38	−251.42	−250.75	−249.65	−248.68	−247.77
550		−260.49	−255.49	−254.16	−253.38	−252.18	−251.17	−250.23
600		−264.33	−258.80	−257.02	−256.08	−254.77	−253.71	−252.75
700		−271.21	−265.54	−263.02	−261.70	−260.10	−258.93	−257.91
800		−277.52	−272.06	−269.15	−267.52	−265.62	−264.32	−263.25
900		−283.55	−278.33	−275.25	−273.41	−271.26	−269.86	−268.74
1000		−289.43	−284.41	−281.27	−279.31	−276.99	−275.52	−274.39

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				BO_2^-				
25	−162.24	−162.62	−162.97	−163.30	−163.60	−164.16	−164.68	−165.18
50	−161.98	−162.34	−162.67	−162.98	−163.27	−163.80	−164.29	−164.75
75	−161.66	−162.01	−162.34	−162.64	−162.92	−163.44	−163.92	−164.37
100	−161.28	−161.64	−161.97	−162.27	−162.55	−163.07	−163.55	−164.00
125	−160.85	−161.23	−161.56	−161.87	−162.16	−162.69	−163.17	−163.62
150	−160.36	−160.76	−161.12	−161.44	−161.74	−162.28	−162.78	−163.23
175	−159.81	−160.25	−160.64	−160.98	−161.29	−161.86	−162.36	−162.83
200	−159.20	−159.69	−160.11	−160.48	−160.81	−161.40	−161.93	−162.41
225	−158.51	−159.06	−159.53	−159.94	−160.30	−160.93	−161.48	−161.98
250	−157.71	−158.37	−158.91	−159.36	−159.75	−160.43	−161.01	−161.54
300	−155.69	−156.73	−157.50	−158.06	−158.54	−159.34	−160.01	−160.60
350	−152.56	−154.57	−155.85	−156.58	−157.18	−158.15	−158.93	−159.59
400		−152.32	−153.91	−154.90	−155.66	−156.84	−157.75	−158.52
450		−148.22	−151.60	−152.98	−153.96	−155.41	−156.49	−157.36
500			−148.79	−150.78	−152.06	−153.84	−155.12	−156.13
550			−145.40	−148.27	−149.94	−152.13	−153.64	−154.81
600			−141.64	−145.49	−147.59	−150.26	−152.04	−153.38
700				−139.52	−142.33	−146.04	−148.44	−150.17
800					−136.61	−141.21	−144.30	−146.45
900					−130.73	−135.96	−139.69	−142.20
1000						−130.54	−134.79	−137.44
				Ba^{+2}				
25	−134.03	−134.16	−134.25	−134.31	−134.35	−134.37	−134.34	−134.28
50	−134.08	−134.19	−134.27	−134.33	−134.36	−134.37	−134.33	−134.26
75	−134.10	−134.22	−134.30	−134.35	−134.37	−134.38	−134.34	−134.27
100	−134.11	−134.23	−134.31	−134.36	−134.39	−134.40	−134.36	−134.29
125	−134.10	−134.23	−134.31	−134.37	−134.40	−134.42	−134.39	−134.32
150	−134.07	−134.21	−134.30	−134.37	−134.41	−134.43	−134.41	−134.35
175	−134.01	−134.17	−134.28	−134.36	−134.40	−134.44	−134.43	−134.37
200	−133.92	−134.11	−134.24	−134.33	−134.39	−134.45	−134.44	−134.40
225	−133.80	−134.02	−134.18	−134.29	−134.36	−134.44	−134.45	−134.42
250	−133.63	−133.91	−134.10	−134.23	−134.33	−134.43	−134.46	−134.44
300	−133.13	−133.59	−133.89	−134.07	−134.21	−134.38	−134.46	−134.47
350	−132.43	−133.08	−133.61	−133.85	−134.04	−134.29	−134.43	−134.49
400		−133.13	−133.29	−133.58	−133.82	−134.17	−134.37	−134.48
450		−133.90	−132.97	−133.27	−133.56	−134.00	−134.28	−134.45
500			−132.71	−132.91	−133.25	−133.79	−134.16	−134.40
550			−132.58	−132.53	−132.88	−133.53	−134.00	−134.31
600			−132.63	−132.17	−132.46	−133.22	−133.79	−134.18
700				−131.63	−131.51	−132.38	−133.19	−133.77
800					−130.43	−131.24	−132.32	−133.11
900					−129.18	−129.85	−131.21	−132.18
1000						−128.32	−129.94	−131.01
				$BaCO_3^\circ$				
25	−263.83	−263.94	−264.02	−264.08	−264.13	−264.19	−264.21	−264.21
50	−264.20	−264.31	−264.40	−264.46	−264.51	−264.58	−264.62	−264.64
75	−264.53	−264.64	−264.72	−264.79	−264.84	−264.92	−264.97	−265.00
100	−264.82	−264.93	−265.01	−265.08	−265.14	−265.22	−265.28	−265.31
125	−265.08	−265.19	−265.28	−265.35	−265.40	−265.49	−265.55	−265.59
150	−265.32	−265.43	−265.51	−265.58	−265.64	−265.73	−265.79	−265.84
175	−265.54	−265.64	−265.73	−265.80	−265.86	−265.95	−266.02	−266.06
200	−265.74	−265.84	−265.93	−266.00	−266.06	−266.15	−266.21	−266.26
225	−265.92	−266.02	−266.10	−266.17	−266.23	−266.33	−266.39	−266.44
250	−266.09	−266.18	−266.27	−266.34	−266.39	−266.49	−266.56	−266.61
300	−266.39	−266.46	−266.54	−266.61	−266.67	−266.76	−266.83	−266.88
350	−266.68	−266.70	−266.77	−266.83	−266.89	−266.98	−267.04	−267.10
400		−266.92	−266.95	−267.00	−267.05	−267.14	−267.20	−267.26
450		−267.21	−267.10	−267.13	−267.18	−267.25	−267.32	−267.37

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

				Pressure, kbar				
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$BaCO_3^o$ — Continued				
500		−267.63	−267.23	−267.23	−267.26	−267.33	−267.39	−267.44
550		−267.93	−267.35	−267.29	−267.31	−267.36	−267.42	−267.46
600		−268.12	−267.45	−267.33	−267.32	−267.36	−267.41	−267.45
700		−268.24	−267.56	−267.32	−267.26	−267.26	−267.29	−267.32
800		−268.13	−267.48	−267.19	−267.07	−267.03	−267.04	−267.07
900		−267.85	−267.22	−266.91	−266.77	−266.68	−266.68	−266.70
1000		−267.41	−266.82	−266.50	−266.33	−266.22	−266.22	−266.24
				$BaCl^+$				
25	−164.73	−164.59	−164.44	−164.28	−164.12	−163.78	−163.42	−163.06
50	−165.30	−165.15	−165.00	−164.84	−164.67	−164.33	−163.98	−163.63
75	−165.88	−165.73	−165.58	−165.41	−165.25	−164.91	−164.56	−164.21
100	−166.48	−166.33	−166.17	−166.01	−165.85	−165.51	−165.17	−164.82
125	−167.09	−166.94	−166.78	−166.62	−166.46	−166.13	−165.79	−165.44
150	−167.71	−167.57	−167.41	−167.25	−167.09	−166.76	−166.42	−166.08
175	−168.34	−168.20	−168.05	−167.89	−167.73	−167.41	−167.07	−166.73
200	−168.98	−168.85	−168.70	−168.55	−168.39	−168.07	−167.73	−167.40
225	−169.63	−169.50	−169.36	−169.21	−169.06	−168.74	−168.41	−168.08
250	−170.27	−170.17	−170.03	−169.89	−169.74	−169.42	−169.10	−168.77
300	−171.55	−171.50	−171.39	−171.26	−171.12	−170.83	−170.51	−170.19
350	−172.78	−172.84	−172.79	−172.67	−172.54	−172.27	−171.97	−171.66
400		−174.28	−174.20	−174.11	−174.00	−173.74	−173.46	−173.16
450		−175.70	−175.64	−175.57	−175.47	−175.25	−174.98	−174.70
500			−177.08	−177.04	−176.97	−176.78	−176.54	−176.27
550			−178.54	−178.54	−178.49	−178.33	−178.12	−177.87
600			−180.02	−180.05	−180.02	−179.91	−179.72	−179.49
700				−183.15	−183.14	−183.10	−182.97	−182.79
800					−186.32	−186.33	−186.28	−186.14
900					−189.58	−189.62	−189.64	−189.54
1000						−192.99	−193.06	−192.99
				BaF^+				
25	−201.12	−201.14	−201.13	−201.11	−201.08	−200.98	−200.86	−200.71
50	−201.27	−201.28	−201.28	−201.26	−201.23	−201.15	−201.04	−200.91
75	−201.44	−201.45	−201.45	−201.44	−201.41	−201.33	−201.23	−201.11
100	−201.62	−201.64	−201.64	−201.63	−201.61	−201.54	−201.44	−201.33
125	−201.82	−201.85	−201.85	−201.85	−201.83	−201.76	−201.68	−201.57
150	−202.04	−202.07	−202.08	−202.08	−202.06	−202.01	−201.93	−201.83
175	−202.26	−202.30	−202.32	−202.33	−202.32	−202.27	−202.20	−202.11
200	−202.49	−202.55	−202.58	−202.59	−202.58	−202.55	−202.48	−202.40
225	−202.72	−202.80	−202.84	−202.86	−202.86	−202.84	−202.79	−202.71
250	−202.95	−203.05	−203.11	−203.14	−203.16	−203.15	−203.10	−203.04
300	−203.38	−203.57	−203.68	−203.74	−203.77	−203.80	−203.78	−203.73
350	−203.76	−204.06	−204.28	−204.37	−204.43	−204.49	−204.50	−204.48
400		−204.86	−204.92	−205.03	−205.12	−205.22	−205.27	−205.27
450		−206.01	−205.60	−205.72	−205.83	−205.99	−206.07	−206.11
500			−206.35	−206.44	−206.58	−206.79	−206.91	−206.98
550			−207.21	−207.19	−207.34	−207.61	−207.78	−207.88
600			−208.18	−207.99	−208.12	−208.44	−208.67	−208.81
700				−209.80	−209.75	−210.13	−210.48	−210.71
800					−211.46	−211.83	−212.31	−212.63
900					−213.23	−213.55	−214.15	−214.57
1000						−215.32	−216.05	−216.52
				Be^{+2}				
25	−83.50	−83.78	−84.02	−84.23	−84.40	−84.70	−84.94	−85.14
50	−82.11	−82.40	−82.65	−82.87	−83.06	−83.39	−83.67	−83.90
75	−80.71	−81.02	−81.29	−81.52	−81.72	−82.08	−82.38	−82.64
100	−79.32	−79.65	−79.93	−80.17	−80.39	−80.77	−81.09	−81.37

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Be^{+2} — Continued				
125	−77.91	−78.27	−78.57	−78.83	−79.06	−79.47	−79.81	−80.11
150	−76.49	−76.88	−77.20	−77.49	−77.74	−78.18	−78.54	−78.86
175	−75.05	−75.48	−75.84	−76.15	−76.42	−76.89	−77.28	−77.63
200	−73.58	−74.05	−74.46	−74.80	−75.10	−75.61	−76.03	−76.40
225	−72.07	−72.61	−73.06	−73.44	−73.77	−74.33	−74.79	−75.18
250	−70.51	−71.14	−71.65	−72.08	−72.44	−73.05	−73.55	−73.98
300	−67.21	−68.11	−68.80	−69.31	−69.76	−70.50	−71.09	−71.59
350	−64.26	−64.92	−65.97	−66.54	−67.06	−67.94	−68.65	−69.24
400		−63.85	−63.29	−63.80	−64.37	−65.38	−66.21	−66.90
450		−67.52	−60.97	−61.14	−61.69	−62.82	−63.78	−64.58
500			−59.38	−58.62	−59.05	−60.25	−61.34	−62.26
550			−58.98	−56.34	−56.44	−57.66	−58.89	−59.93
600			−59.92	−54.41	−53.90	−55.03	−56.39	−57.57
700				−51.92	−49.00	−49.54	−51.19	−52.68
800					−44.21	−43.63	−45.61	−47.45
900					−39.08	−37.27	−39.65	−41.84
1000						−30.64	−33.49	−35.86
				BeO_2^{-2}				
25	−153.00	−153.28	−153.51	−153.70	−153.86	−154.12	−154.32	−154.47
50	−151.96	−152.25	−152.50	−152.71	−152.89	−153.19	−153.43	−153.62
75	−150.75	−151.07	−151.34	−151.57	−151.78	−152.11	−152.39	−152.61
100	−149.40	−149.76	−150.06	−150.32	−150.54	−150.92	−151.23	−151.48
125	−147.91	−148.32	−148.66	−148.95	−149.20	−149.62	−149.97	−150.26
150	−146.28	−146.76	−147.15	−147.48	−147.76	−148.24	−148.63	−148.95
175	−144.50	−145.06	−145.52	−145.90	−146.23	−146.77	−147.20	−147.57
200	−142.55	−143.23	−143.78	−144.22	−144.60	−145.22	−145.71	−146.12
225	−140.41	−141.25	−141.91	−142.44	−142.88	−143.59	−144.15	−144.61
250	−138.04	−139.11	−139.92	−140.54	−141.06	−141.88	−142.51	−143.03
300	−132.35	−134.26	−135.54	−136.42	−137.13	−138.22	−139.05	−139.71
350	−124.51	−128.28	−130.63	−131.85	−132.80	−134.25	−135.33	−136.17
400		−122.51	−125.11	−126.81	−128.09	−129.98	−131.35	−132.40
450		−114.21	−118.88	−121.25	−122.96	−125.38	−127.10	−128.41
500			−111.78	−115.12	−117.37	−120.46	−122.60	−124.19
550			−103.78	−108.39	−111.31	−115.19	−117.80	−119.73
600			−95.33	−101.14	−104.76	−109.55	−112.71	−115.00
700				−86.04	−90.47	−97.12	−101.54	−104.65
800					−75.11	−83.22	−89.03	−93.03
900					−59.18	−68.22	−75.36	−80.11
1000						−52.66	−60.89	−65.98
				Br^-				
25	−24.87	−24.58	−24.29	−23.99	−23.70	−23.11	−22.51	−21.92
50	−25.34	−25.04	−24.74	−24.45	−24.15	−23.56	−22.98	−22.39
75	−25.75	−25.46	−25.16	−24.87	−24.58	−24.00	−23.42	−22.84
100	−26.12	−25.84	−25.55	−25.27	−24.98	−24.41	−23.84	−23.27
125	−26.45	−26.18	−25.91	−25.63	−25.35	−24.79	−24.23	−23.68
150	−26.73	−26.48	−26.23	−25.96	−25.69	−25.15	−24.61	−24.06
175	−26.95	−26.74	−26.51	−26.26	−26.01	−25.49	−24.96	−24.43
200	−27.12	−26.96	−26.75	−26.53	−26.29	−25.80	−25.29	−24.78
225	−27.21	−27.12	−26.96	−26.76	−26.55	−26.09	−25.61	−25.11
250	−27.21	−27.22	−27.12	−26.96	−26.78	−26.36	−25.90	−25.42
300	−26.80	−27.20	−27.29	−27.24	−27.13	−26.81	−26.42	−25.99
350	−25.19	−26.70	−27.23	−27.34	−27.34	−27.16	−26.87	−26.50
400		−25.69	−26.87	−27.25	−27.40	−27.41	−27.23	−26.95
450		−21.88	−26.06	−26.90	−27.28	−27.54	−27.50	−27.31
500			−24.60	−26.25	−26.96	−27.54	−27.68	−27.61
550			−22.34	−25.25	−26.41	−27.41	−27.76	−27.82
600			−19.46	−23.92	−25.64	−27.14	−27.73	−27.94
700				−20.59	−23.51	−26.17	−27.33	−27.88

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Br^- — Continued				
800					−20.92	−24.71	−26.50	−27.39
900					−18.26	−22.93	−25.29	−26.47
1000						−21.05	−23.84	−25.14
				Br_3^-				
25	−25.59	−24.99	−24.41	−23.85	−23.30	−22.23	−21.18	−20.16
50	−26.88	−26.27	−25.68	−25.10	−24.54	−23.45	−22.38	−21.34
75	−28.19	−27.57	−26.97	−26.39	−25.82	−24.72	−23.65	−22.60
100	−29.51	−28.88	−28.28	−27.70	−27.14	−26.03	−24.96	−23.91
125	−30.83	−30.21	−29.62	−29.04	−28.47	−27.37	−26.30	−25.26
150	−32.15	−31.55	−30.96	−30.39	−29.83	−28.73	−27.67	−26.63
175	−33.47	−32.89	−32.32	−31.75	−31.20	−30.12	−29.06	−28.02
200	−34.78	−34.24	−33.68	−33.13	−32.58	−31.51	−30.46	−29.43
225	−36.06	−35.57	−35.04	−34.51	−33.97	−32.92	−31.89	−30.86
250	−37.31	−36.90	−36.40	−35.89	−35.37	−34.34	−33.32	−32.31
300	−39.58	−39.47	−39.09	−38.65	−38.18	−37.21	−36.23	−35.25
350	−41.00	−41.79	−41.71	−41.38	−40.98	−40.11	−39.18	−38.24
400		−43.64	−44.18	−44.05	−43.77	−43.01	−42.16	−41.27
450		−43.13	−46.37	−46.62	−46.50	−45.92	−45.16	−44.32
500			−48.10	−49.02	−49.16	−48.81	−48.16	−47.40
550			−49.22	−51.22	−51.72	−51.67	−51.17	−50.50
600			−49.87	−53.21	−54.18	−54.51	−54.17	−53.59
700				−56.80	−58.83	−60.07	−60.13	−59.77
800					−63.38	−65.54	−66.03	−65.89
900					−68.12	−71.02	−71.89	−71.94
1000						−76.64	−77.79	−77.91
				BrO^-				
25	−8.00	−7.88	−7.74	−7.59	−7.43	−7.10	−6.75	−6.38
50	−8.20	−8.08	−7.94	−7.80	−7.64	−7.32	−6.97	−6.62
75	−8.33	−8.21	−8.08	−7.94	−7.79	−7.47	−7.14	−6.80
100	−8.40	−8.29	−8.17	−8.03	−7.89	−7.59	−7.27	−6.93
125	−8.40	−8.31	−8.20	−8.08	−7.94	−7.66	−7.35	−7.03
150	−8.34	−8.28	−8.19	−8.08	−7.96	−7.69	−7.40	−7.09
175	−8.22	−8.19	−8.12	−8.03	−7.93	−7.68	−7.41	−7.12
200	−8.03	−8.04	−8.01	−7.95	−7.86	−7.65	−7.40	−7.12
225	−7.75	−7.84	−7.85	−7.81	−7.75	−7.57	−7.35	−7.09
250	−7.37	−7.56	−7.63	−7.64	−7.60	−7.47	−7.27	−7.04
300	−6.17	−6.75	−7.02	−7.14	−7.18	−7.16	−7.04	−6.86
350	−3.74	−5.41	−6.15	−6.43	−6.59	−6.71	−6.69	−6.58
400		−3.61	−4.95	−5.50	−5.82	−6.13	−6.23	−6.21
450		0.87	−3.29	−4.29	−4.84	−5.41	−5.66	−5.74
500			−0.97	−2.76	−3.64	−4.54	−4.97	−5.17
550			2.13	−0.87	−2.19	−3.51	−4.16	−4.50
600			5.85	1.38	−0.50	−2.32	−3.22	−3.72
700				6.53	3.54	0.55	−0.94	−1.79
800					8.10	4.01	1.87	0.66
900					12.80	7.86	5.13	3.61
1000						11.87	8.69	7.04
				BrO_3^-				
25	4.45	4.86	5.27	5.67	6.07	[illegible]	7.63	8.40
50	3.50	3.93	4.34	4.75	5.16	[illegible]	6.73	7.51
75	2.58	3.01	3.43	3.84	4.25	[illegible]	5.82	6.60
100	1.69	2.11	2.53	2.94	3.34	[illegible]	4.91	5.69
125	0.82	1.24	1.65	2.05	2.45	[illegible]	4.01	4.77
150	−0.02	0.38	0.78	1.17	1.56	[illegible]	3.10	3.86
175	−0.83	−0.46	−0.08	0.31	0.69	[illegible]	2.20	2.95
200	−1.60	−1.27	−0.91	−0.54	−0.17	[illegible]	1.31	2.05

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				BrO_3^- — Continued				
225	−2.32	−2.05	−1.72	−1.37	−1.02	−0.30	0.42	1.15
250	−2.97	−2.79	−2.50	−2.19	−1.85	−1.17	−0.46	0.25
300	−3.96	−4.11	−3.98	−3.74	−3.47	−2.86	−2.20	−1.53
350	−3.90	−5.06	−5.29	−5.19	−5.00	−4.50	−3.91	−3.29
400		−5.43	−6.35	−6.49	−6.43	−6.08	−5.59	−5.02
450		−3.04	−7.03	−7.61	−7.75	−7.60	−7.22	−6.73
500			−7.12	−8.47	−8.91	−9.04	−8.80	−8.40
550			−6.46	−9.05	−9.91	−10.40	−10.33	−10.03
600			−5.20	−9.33	−10.73	−11.66	−11.79	−11.61
700				−9.31	−11.92	−13.91	−14.51	−14.60
800					−12.81	−15.86	−16.98	−17.34
900					−13.75	−17.65	−19.23	−19.81
1000						−19.47	−21.38	−22.04
				BrO_4^-				
25	28.20	28.75	29.29	29.81	30.33	31.33	32.32	33.29
50	27.00	27.58	28.13	28.66	29.19	30.21	31.21	32.19
75	25.81	26.38	26.94	27.48	28.01	29.04	30.04	31.02
100	24.60	25.18	25.74	26.28	26.81	27.84	28.84	29.82
125	23.40	23.97	24.52	25.06	25.59	26.61	27.61	28.59
150	22.21	22.76	23.30	23.83	24.35	25.37	26.37	27.34
175	21.02	21.55	22.08	22.60	23.11	24.12	25.10	26.07
200	19.85	20.34	20.85	21.36	21.86	22.85	23.83	24.79
225	18.71	19.15	19.63	20.12	20.61	21.58	22.54	23.49
250	17.61	17.97	18.41	18.88	19.35	20.30	21.24	22.18
300	15.67	15.71	16.02	16.42	16.84	17.72	18.62	19.53
350	14.63	13.73	13.73	14.00	14.34	15.13	15.97	16.84
400		12.26	11.60	11.66	11.89	12.54	13.31	14.12
450		13.28	9.79	9.45	9.50	9.97	10.64	11.39
500			8.47	7.42	7.20	7.43	7.97	8.64
550			7.80	5.62	5.02	4.92	5.31	5.89
600			7.65	4.05	2.95	2.46	2.67	3.15
700				1.35	−0.87	−2.32	−2.53	−2.29
800					−4.54	−6.97	−7.63	−7.62
900					−8.38	−11.59	−12.66	−12.85
1000						−16.33	−17.69	−17.96
				CN^-				
25	41.20	41.49	41.77	42.06	42.35	42.94	43.53	44.12
50	40.67	40.96	41.25	41.55	41.84	42.43	43.02	43.61
75	40.18	40.48	40.77	41.06	41.35	41.93	42.52	43.10
100	39.74	40.03	40.31	40.60	40.89	41.46	42.04	42.62
125	39.34	39.61	39.89	40.17	40.45	41.01	41.58	42.15
150	38.98	39.23	39.49	39.76	40.03	40.58	41.13	41.69
175	38.67	38.89	39.13	39.38	39.64	40.17	40.71	41.25
200	38.42	38.59	38.80	39.03	39.27	39.77	40.30	40.83
225	38.23	38.33	38.50	38.70	38.92	39.40	39.90	40.42
250	38.12	38.13	38.24	38.41	38.61	39.05	39.52	40.02
300	38.29	37.93	37.86	37.93	38.06	38.40	38.81	39.26
350	39.64	38.18	37.69	37.61	37.63	37.84	38.17	38.55
400		38.99	37.82	37.47	37.34	37.37	37.59	37.90
450		42.66	38.37	37.56	37.21	37.01	37.09	37.31
500			39.58	37.94	37.27	36.75	36.66	36.78
550			41.59	38.66	37.53	36.61	36.33	36.32
600			44.23	39.71	38.02	36.60	36.08	35.94
700				42.47	39.53	36.96	35.89	35.43
800					41.46	37.75	36.09	35.29
900					43.42	38.81	36.60	35.54
1000						39.93	37.31	36.14

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				CO°				
25	−28.68	−28.29	−27.90	−27.52	−27.14	−26.41	−25.69	−24.97
50	−29.36	−28.94	−28.54	−28.15	−27.77	−27.02	−26.28	−25.56
75	−30.14	−29.71	−29.31	−28.91	−28.52	−27.76	−27.02	−26.29
100	−31.01	−30.58	−30.16	−29.76	−29.36	−28.60	−27.85	−27.12
125	−31.97	−31.53	−31.11	−30.70	−30.30	−29.52	−28.77	−28.03
150	−33.01	−32.56	−32.13	−31.71	−31.31	−30.53	−29.77	−29.03
175	−34.12	−33.66	−33.22	−32.80	−32.39	−31.60	−30.84	−30.09
200	−35.30	−34.84	−34.38	−33.95	−33.54	−32.74	−31.97	−31.22
225	−36.55	−36.08	−35.61	−35.17	−34.75	−33.94	−33.16	−32.41
250	−37.88	−37.39	−36.90	−36.45	−36.02	−35.20	−34.41	−33.65
300	−40.80	−40.22	−39.68	−39.19	−38.74	−37.88	−37.08	−36.30
350	−44.37	−43.41	−42.71	−42.16	−41.67	−40.77	−39.94	−39.15
400		−47.17	−46.04	−45.37	−44.82	−43.86	−42.99	−42.17
450		−52.63	−49.72	−48.83	−48.18	−47.12	−46.21	−45.36
500		−60.37	−53.87	−52.55	−51.75	−50.57	−49.60	−48.71
550		−67.37	−58.56	−56.56	−55.54	−54.19	−53.14	−52.22
600		−73.49	−63.69	−60.85	−59.54	−57.97	−56.84	−55.87
700		−84.39	−74.33	−70.10	−68.10	−66.00	−64.66	−63.58
800		−94.44	−84.76	−79.82	−77.23	−74.56	−73.00	−71.81
900		−104.13	−94.90	−89.65	−86.68	−83.55	−81.79	−80.52
1000		−113.71	−104.87	−99.50	−96.30	−92.85	−90.97	−89.67
				CO_2°				
25	−92.25	−91.86	−91.49	−91.11	−90.74	−90.02	−89.30	−88.59
50	−93.01	−92.61	−92.22	−91.83	−91.46	−90.72	−89.99	−89.28
75	−93.86	−93.45	−93.06	−92.67	−92.29	−91.54	−90.81	−90.09
100	−94.80	−94.39	−93.98	−93.59	−93.21	−92.46	−91.73	−91.01
125	−95.82	−95.40	−94.99	−94.60	−94.21	−93.46	−92.72	−92.00
150	−96.90	−96.48	−96.07	−95.67	−95.28	−94.53	−93.79	−93.07
175	−98.04	−97.62	−97.21	−96.81	−96.42	−95.66	−94.92	−94.20
200	−99.24	−98.82	−98.41	−98.01	−97.62	−96.86	−96.12	−95.39
225	−100.49	−100.08	−99.67	−99.26	−98.87	−98.11	−97.37	−96.64
250	−101.79	−101.39	−100.97	−100.57	−100.18	−99.41	−98.67	−97.94
300	−104.53	−104.16	−103.74	−103.33	−102.94	−102.17	−101.43	−100.70
350	−107.44	−107.12	−106.69	−106.28	−105.88	−105.11	−104.36	−103.63
400		−110.27	−109.81	−109.39	−108.99	−108.22	−107.47	−106.74
450		−113.65	−113.09	−112.66	−112.26	−111.47	−110.72	−109.99
500		−117.28	−116.53	−116.08	−115.66	−114.88	−114.12	−113.38
550		−121.00	−120.13	−119.64	−119.21	−118.41	−117.65	−116.91
600		−124.78	−123.86	−123.32	−122.88	−122.07	−121.30	−120.56
700		−132.60	−131.66	−131.05	−130.57	−129.73	−128.96	−128.21
800		−140.77	−139.85	−139.20	−138.69	−137.82	−137.03	−136.28
900		−149.27	−148.38	−147.71	−147.18	−146.28	−145.48	−144.72
1000		−158.09	−157.22	−156.54	−156.00	−155.08	−154.28	−153.52
				CO_3^{-2}				
25	−126.19	−126.24	−126.26	−126.24	−126.21	−126.10	−125.93	−125.74
50	−125.83	−125.89	−125.91	−125.91	−125.89	−125.80	−125.66	−125.50
75	−125.35	−125.43	−125.48	−125.49	−125.48	−125.42	−125.31	−125.17
100	−124.78	−124.89	−124.96	−124.99	−125.00	−124.97	−124.89	−124.77
125	−124.10	−124.26	−124.36	−124.42	−124.46	−124.46	−124.41	−124.32
150	−123.32	−123.54	−123.68	−123.78	−123.84	−123.90	−123.88	−123.82
175	−122.43	−122.72	−122.92	−123.07	−123.17	−123.28	−123.30	−123.27
200	−121.40	−121.80	−122.08	−122.28	−122.43	−122.60	−122.68	−122.69
225	−120.21	−120.76	−121.15	−121.42	−121.62	−121.88	−122.01	−122.07
250	−118.82	−119.59	−120.11	−120.47	−120.74	−121.10	−121.30	−121.41
300	−115.17	−116.76	−117.73	−118.33	−118.77	−119.38	−119.75	−119.99
350	−109.24	−112.90	−114.87	−115.82	−116.50	−117.43	−118.03	−118.42

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				CO_3^{-2} — Continued				
400		−108.66	−111.43	−112.89	−113.90	−115.26	−116.12	−116.71
450		−100.26	−107.20	−109.49	−110.95	−112.84	−114.03	−114.85
500			−101.88	−105.50	−107.58	−110.15	−111.74	−112.83
550			−95.31	−100.89	−103.78	−107.18	−109.23	−110.62
600			−87.86	−95.68	−99.52	−103.90	−106.49	−108.22
700				−84.35	−89.85	−96.39	−100.22	−102.72
800					−79.26	−87.72	−92.91	−96.23
900					−68.38	−78.23	−84.70	−88.71
1000						−68.45	−75.92	−80.23
				Ca^{+2}				
25	−132.12	−132.32	−132.48	−132.62	−132.74	−132.94	−133.09	−133.22
50	−131.78	−131.97	−132.14	−132.28	−132.41	−132.61	−132.78	−132.91
75	−131.42	−131.62	−131.79	−131.94	−132.07	−132.28	−132.46	−132.60
100	−131.05	−131.26	−131.44	−131.59	−131.73	−131.95	−132.14	−132.30
125	−130.66	−130.89	−131.08	−131.24	−131.38	−131.63	−131.82	−131.99
150	−130.26	−130.50	−130.71	−130.88	−131.04	−131.29	−131.51	−131.68
175	−129.83	−130.10	−130.33	−130.52	−130.68	−130.96	−131.19	−131.38
200	−129.37	−129.67	−129.93	−130.14	−130.32	−130.62	−130.87	−131.07
225	−128.88	−129.22	−129.51	−129.75	−129.95	−130.28	−130.55	−130.77
250	−128.34	−128.75	−129.08	−129.34	−129.57	−129.93	−130.23	−130.47
300	−127.07	−127.70	−128.15	−128.49	−128.77	−129.22	−129.57	−129.86
350	−125.70	−126.45	−127.19	−127.58	−127.92	−128.47	−128.90	−129.25
400		−126.10	−126.21	−126.64	−127.04	−127.70	−128.21	−128.63
450		−127.23	−125.30	−125.68	−126.12	−126.89	−127.50	−127.99
500			−124.58	−124.71	−125.17	−126.05	−126.76	−127.33
550			−124.20	−123.76	−124.18	−125.16	−125.99	−126.65
600			−124.20	−122.90	−123.16	−124.22	−125.16	−125.93
700				−121.59	−121.06	−122.12	−123.33	−124.32
800					−118.87	−119.68	−121.20	−122.44
900					−116.47	−116.94	−118.79	−120.26
1000						−114.05	−116.22	−117.81
				$Ca(CH_3COO)^+$				
25	−221.66	−221.31	−220.97	−220.63	−220.30	−219.63	−218.97	−218.31
50	−222.05	−221.69	−221.34	−221.00	−220.65	−219.98	−219.31	−218.65
75	−222.58	−222.22	−221.86	−221.51	−221.16	−220.48	−219.81	−219.15
100	−223.22	−222.86	−222.50	−222.15	−221.80	−221.12	−220.45	−219.79
125	−223.97	−223.60	−223.24	−222.89	−222.55	−221.87	−221.20	−220.54
150	−224.80	−224.44	−224.08	−223.73	−223.39	−222.71	−222.05	−221.39
175	−225.71	−225.36	−225.01	−224.66	−224.32	−223.65	−222.98	−222.33
200	−226.69	−226.35	−226.01	−225.67	−225.33	−224.66	−224.01	−223.35
225	−227.73	−227.42	−227.08	−226.75	−226.42	−225.76	−225.10	−224.46
250	−228.83	−228.54	−228.22	−227.90	−227.57	−226.92	−226.27	−225.63
300	−231.14	−230.97	−230.69	−230.38	−230.07	−229.45	−228.82	−228.19
350	−233.57	−233.57	−233.38	−233.10	−232.81	−232.21	−231.61	−230.99
400		−236.56	−236.28	−236.02	−235.76	−235.20	−234.62	−234.02
450		−239.86	−239.38	−239.14	−238.90	−238.38	−237.83	−237.26
500			−242.67	−242.44	−242.22	−241.75	−241.23	−240.68
550			−246.15	−245.89	−245.70	−245.28	−244.80	−244.28
600			−249.82	−249.52	−249.33	−248.96	−248.52	−248.04
700				−257.28	−257.02	−256.73	−256.39	−255.98
800					−265.23	−264.98	−264.75	−264.41
900					−273.93	−273.67	−273.55	−273.28
1000						−282.80	−282.78	−282.55

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Ca(CH_3COO)_2^\circ$				
25	−311.57	−310.62	−309.72	−308.85	−308.02	−306.40	−304.85	−303.34
50	−312.56	−311.57	−310.64	−309.75	−308.89	−307.24	−305.65	−304.10
75	−313.85	−312.85	−311.90	−310.99	−310.12	−308.44	−306.83	−305.26
100	−315.39	−314.38	−313.42	−312.50	−311.62	−309.92	−308.30	−306.72
125	−317.15	−316.13	−315.17	−314.24	−313.36	−311.65	−310.01	−308.43
150	−319.11	−318.09	−317.12	−316.20	−315.30	−313.58	−311.94	−310.35
175	−321.26	−320.24	−319.27	−318.34	−317.44	−315.71	−314.06	−312.47
200	−323.57	−322.57	−321.59	−320.65	−319.75	−318.02	−316.37	−314.76
225	−326.04	−325.05	−324.07	−323.13	−322.22	−320.49	−318.83	−317.23
250	−328.66	−327.69	−326.70	−325.76	−324.85	−323.12	−321.45	−319.84
300	−334.28	−333.40	−332.40	−331.45	−330.54	−328.80	−327.13	−325.51
350	−340.39	−339.64	−338.63	−337.67	−336.76	−335.00	−333.33	−331.71
400		−346.39	−345.34	−344.38	−343.45	−341.69	−340.01	−338.39
450		−353.70	−352.51	−351.52	−350.59	−348.82	−347.13	−345.50
500		−361.60	−360.11	−359.09	−358.14	−356.36	−354.67	−353.03
550		−369.80	−368.13	−367.05	−366.08	−364.28	−362.58	−360.95
600		−378.27	−376.52	−375.37	−374.38	−372.57	−370.86	−369.21
700		−396.07	−394.30	−393.04	−391.99	−390.13	−388.40	−386.75
800		−414.97	−413.23	−411.91	−410.81	−408.90	−407.16	−405.49
900		−434.90	−433.19	−431.84	−430.72	−428.77	−427.00	−425.33
1000		−455.78	−454.10	−452.75	−451.60	−449.62	−447.85	−446.18
				$CaCO_3^\circ$				
25	−262.85	−263.00	−263.13	−263.23	−263.31	−263.44	−263.53	−263.59
50	−262.89	−263.04	−263.17	−263.28	−263.37	−263.51	−263.62	−263.70
75	−262.89	−263.04	−263.17	−263.28	−263.38	−263.53	−263.65	−263.74
100	−262.86	−263.02	−263.15	−263.26	−263.35	−263.51	−263.64	−263.74
125	−262.81	−262.97	−263.10	−263.21	−263.31	−263.47	−263.60	−263.71
150	−262.74	−262.90	−263.03	−263.14	−263.24	−263.40	−263.54	−263.65
175	−262.66	−262.81	−262.94	−263.05	−263.15	−263.32	−263.45	−263.57
200	−262.56	−262.70	−262.84	−262.95	−263.05	−263.22	−263.35	−263.47
225	−262.44	−262.59	−262.72	−262.83	−262.93	−263.10	−263.24	−263.36
250	−262.32	−262.46	−262.59	−262.70	−262.80	−262.97	−263.11	−263.23
300	−262.05	−262.16	−262.29	−262.40	−262.50	−262.67	−262.81	−262.93
350	−261.79	−261.84	−261.95	−262.06	−262.15	−262.32	−262.46	−262.58
400		−261.50	−261.58	−261.68	−261.77	−261.93	−262.07	−262.20
450		−261.26	−261.19	−261.27	−261.35	−261.51	−261.65	−261.77
500		−261.14	−260.79	−260.83	−260.91	−261.05	−261.19	−261.31
550		−260.93	−260.39	−260.38	−260.43	−260.57	−260.70	−260.81
600		−260.60	−259.98	−259.90	−259.93	−260.05	−260.17	−260.29
700		−259.73	−259.08	−258.89	−258.87	−258.95	−259.05	−259.16
800		−258.64	−258.03	−257.79	−257.72	−257.75	−257.84	−257.93
900		−257.41	−256.83	−256.56	−256.46	−256.46	−256.53	−256.62
1000		−256.05	−255.51	−255.23	−255.11	−255.08	−255.14	−255.23
				$CaCl^+$				
25	−162.55	−162.48	−162.39	−162.30	−162.19	−161.95	−161.70	−161.43
50	−162.53	−162.46	−162.37	−162.28	−162.17	−161.94	−161.69	−161.44
75	−162.55	−162.48	−162.39	−162.30	−162.20	−161.97	−161.73	−161.48
100	−162.61	−162.54	−162.45	−162.36	−162.26	−162.04	−161.81	−161.57
125	−162.68	−162.62	−162.54	−162.45	−162.36	−162.15	−161.92	−161.69
150	−162.79	−162.73	−162.66	−162.58	−162.49	−162.29	−162.07	−161.84
175	−162.91	−162.86	−162.80	−162.73	−162.64	−162.45	−162.24	−162.02
200	−163.04	−163.01	−162.96	−162.90	−162.82	−162.64	−162.44	−162.22
225	−163.18	−163.18	−163.15	−163.09	−163.02	−162.86	−162.67	−162.46
250	−163.32	−163.36	−163.34	−163.30	−163.24	−163.09	−162.92	−162.72
300	−163.58	−163.73	−163.78	−163.77	−163.74	−163.63	−163.48	−163.31
350	−163.85	−164.10	−164.28	−164.30	−164.30	−164.24	−164.12	−163.98
400		−164.94	−164.85	−164.89	−164.92	−164.91	−164.84	−164.72
450		−166.45	−165.52	−165.55	−165.60	−165.64	−165.61	−165.53

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$CaCl^+$ — Continued				
500			−166.33	−166.26	−166.32	−166.42	−166.44	−166.40
550			−167.33	−167.04	−167.09	−167.24	−167.32	−167.32
600			−168.55	−167.91	−167.90	−168.10	−168.23	−168.28
700				−169.98	−169.65	−169.87	−170.14	−170.29
800					−171.56	−171.69	−172.10	−172.38
900					−173.55	−173.55	−174.12	−174.51
1000						−175.51	−176.23	−176.67
				$CaCl_2^\circ$				
25	−194.00	−193.62	−193.26	−192.89	−192.53	−191.82	−191.12	−190.43
50	−194.19	−193.79	−193.41	−193.04	−192.67	−191.95	−191.24	−190.54
75	−194.43	−194.03	−193.64	−193.26	−192.89	−192.16	−191.45	−190.75
100	−194.73	−194.32	−193.93	−193.55	−193.17	−192.44	−191.73	−191.02
125	−195.08	−194.67	−194.27	−193.89	−193.51	−192.77	−192.05	−191.35
150	−195.47	−195.06	−194.66	−194.27	−193.89	−193.15	−192.43	−191.73
175	−195.90	−195.49	−195.09	−194.70	−194.32	−193.58	−192.86	−192.15
200	−196.37	−195.96	−195.56	−195.17	−194.79	−194.04	−193.32	−192.61
225	−196.87	−196.47	−196.07	−195.67	−195.29	−194.55	−193.82	−193.11
250	−197.41	−197.02	−196.61	−196.22	−195.83	−195.08	−194.36	−193.65
300	−198.58	−198.21	−197.80	−197.40	−197.01	−196.26	−195.53	−194.82
350	−199.87	−199.53	−199.11	−198.70	−198.31	−197.56	−196.82	−196.11
400		−201.00	−200.54	−200.12	−199.73	−198.96	−198.23	−197.51
450		−202.69	−202.08	−201.65	−201.25	−200.48	−199.74	−199.02
500		−204.65	−203.75	−203.28	−202.86	−202.08	−201.34	−200.62
550		−206.62	−205.54	−205.01	−204.58	−203.78	−203.03	−202.31
600		−208.59	−207.43	−206.84	−206.38	−205.57	−204.81	−204.08
700		−212.63	−211.44	−210.74	−210.22	−209.37	−208.59	−207.85
800		−216.84	−215.68	−214.92	−214.36	−213.46	−212.66	−211.91
900		−221.24	−220.12	−219.33	−218.74	−217.80	−216.99	−216.23
1000		−225.83	−224.74	−223.94	−223.33	−222.36	−221.54	−220.79
				$CaHCO_3^+$				
25	−273.83	−273.71	−273.58	−273.43	−273.28	−272.97	−272.64	−272.30
50	−274.28	−274.16	−274.02	−273.88	−273.73	−273.42	−273.09	−272.76
75	−274.83	−274.70	−274.57	−274.42	−274.27	−273.97	−273.65	−273.32
100	−275.46	−275.33	−275.20	−275.05	−274.91	−274.60	−274.29	−273.97
125	−276.17	−276.04	−275.90	−275.76	−275.61	−275.31	−275.00	−274.69
150	−276.93	−276.81	−276.67	−276.53	−276.39	−276.09	−275.79	−275.48
175	−277.75	−277.63	−277.50	−277.37	−277.23	−276.94	−276.64	−276.33
200	−278.62	−278.51	−278.39	−278.26	−278.12	−277.84	−277.54	−277.24
225	−279.53	−279.44	−279.33	−279.20	−279.07	−278.79	−278.50	−278.20
250	−280.48	−280.41	−280.31	−280.19	−280.07	−279.80	−279.52	−279.22
300	−282.47	−282.48	−282.41	−282.31	−282.20	−281.95	−281.68	−281.40
350	−284.52	−284.65	−284.67	−284.59	−284.50	−284.28	−284.03	−283.76
400		−287.11	−287.07	−287.02	−286.94	−286.75	−286.53	−286.28
450		−289.75	−289.60	−289.57	−289.53	−289.37	−289.18	−288.95
500			−292.26	−292.25	−292.23	−292.12	−291.95	−291.75
550			−295.05	−295.05	−295.05	−294.99	−294.85	−294.67
600			−297.97	−297.95	−297.97	−297.96	−297.86	−297.71
700				−304.13	−304.11	−304.18	−304.17	−304.08
800					−310.62	−310.74	−310.83	−310.81
900					−317.48	−317.61	−317.80	−317.83
1000						−324.80	−325.07	−325.13
				CaF^+				
25	−200.39	−200.46	−200.51	−200.54	−200.55	−200.54	−200.50	−200.43
50	−200.19	−200.27	−200.32	−200.35	−200.37	−200.37	−200.35	−200.30
75	−200.05	−200.13	−200.18	−200.22	−200.24	−200.26	−200.24	−200.21
100	−199.95	−200.03	−200.09	−200.14	−200.16	−200.19	−200.19	−200.16

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				CaF^+ — Continued				
125	−199.89	−199.98	−200.05	−200.09	−200.13	−200.16	−200.17	−200.15
150	−199.85	−199.96	−200.03	−200.09	−200.13	−200.18	−200.19	−200.18
175	−199.84	−199.96	−200.05	−200.12	−200.17	−200.23	−200.25	−200.25
200	−199.86	−200.00	−200.10	−200.18	−200.23	−200.31	−200.35	−200.36
225	−199.88	−200.05	−200.17	−200.26	−200.33	−200.42	−200.47	−200.50
250	−199.92	−200.12	−200.26	−200.37	−200.45	−200.57	−200.63	−200.66
300	−199.98	−200.29	−200.51	−200.66	−200.77	−200.93	−201.03	−201.09
350	−200.13	−200.48	−200.85	−201.02	−201.17	−201.39	−201.53	−201.63
400		−201.33	−201.29	−201.48	−201.66	−201.93	−202.12	−202.26
450		−203.29	−201.89	−202.02	−202.22	−202.55	−202.80	−202.97
500			−202.71	−202.66	−202.85	−203.24	−203.54	−203.76
550			−203.85	−203.41	−203.55	−203.99	−204.35	−204.62
600			−205.33	−204.29	−204.32	−204.78	−205.21	−205.53
700				−206.55	−206.05	−206.46	−207.03	−207.48
800					−208.00	−208.22	−208.94	−209.53
900					−210.06	−210.03	−210.93	−211.65
1000						−211.96	−213.04	−213.83
				$CaSO_4^\circ$				
25	−312.93	−312.83	−312.72	−312.60	−312.48	−312.20	−311.92	−311.62
50	−313.03	−312.93	−312.81	−312.69	−312.57	−312.30	−312.02	−311.73
75	−313.10	−312.99	−312.88	−312.75	−312.63	−312.36	−312.08	−311.80
100	−313.14	−313.03	−312.91	−312.79	−312.66	−312.40	−312.12	−311.84
125	−313.16	−313.05	−312.93	−312.81	−312.68	−312.42	−312.14	−311.87
150	−313.17	−313.06	−312.94	−312.81	−312.68	−312.42	−312.15	−311.87
175	−313.15	−313.04	−312.92	−312.80	−312.67	−312.41	−312.13	−311.86
200	−313.13	−313.02	−312.89	−312.77	−312.64	−312.38	−312.11	−311.83
225	−313.09	−312.98	−312.85	−312.73	−312.60	−312.34	−312.07	−311.79
250	−313.03	−312.92	−312.80	−312.68	−312.55	−312.29	−312.02	−311.74
300	−312.89	−312.79	−312.67	−312.54	−312.41	−312.15	−311.88	−311.61
350	−312.69	−312.61	−312.49	−312.36	−312.23	−311.97	−311.70	−311.43
400		−312.40	−312.28	−312.15	−312.02	−311.76	−311.49	−311.22
450		−312.16	−312.03	−311.91	−311.78	−311.51	−311.25	−310.98
500		−311.90	−311.76	−311.63	−311.50	−311.24	−310.97	−310.70
550		−311.60	−311.46	−311.33	−311.20	−310.94	−310.67	−310.40
600		−311.28	−311.13	−311.00	−310.87	−310.60	−310.34	−310.07
700		−310.56	−310.41	−310.27	−310.14	−309.87	−309.60	−309.34
800		−309.74	−309.59	−309.45	−309.32	−309.05	−308.78	−308.51
900		−308.84	−308.69	−308.55	−308.42	−308.15	−307.88	−307.61
1000		−307.86	−307.72	−307.58	−307.44	−307.17	−306.91	−306.64
				Cd^{+2}				
25	−18.56	−18.72	−18.85	−18.94	−19.00	−19.08	−19.10	−19.08
50	−18.12	−18.31	−18.45	−18.57	−18.66	−18.79	−18.86	−18.90
75	−17.68	−17.89	−18.05	−18.18	−18.29	−18.45	−18.56	−18.64
100	−17.24	−17.46	−17.64	−17.79	−17.91	−18.10	−18.24	−18.34
125	−16.79	−17.03	−17.23	−17.39	−17.53	−17.74	−17.91	−18.03
150	−16.33	−16.60	−16.81	−16.99	−17.14	−17.39	−17.57	−17.72
175	−15.86	−16.15	−16.39	−16.59	−16.76	−17.03	−17.24	−17.40
200	−15.36	−15.69	−15.96	−16.19	−16.37	−16.67	−16.90	−17.09
225	−14.84	−15.22	−15.52	−15.77	−15.98	−16.32	−16.57	−16.78
250	−14.28	−14.72	−15.07	−15.35	−15.59	−15.96	−16.25	−16.48
300	−13.00	−13.65	−14.14	−14.49	−14.78	−15.25	−15.60	−15.88
350	−11.65	−12.42	−13.19	−13.60	−13.96	−14.53	−14.96	−15.31
400		−12.13	−12.25	−12.70	−13.12	−13.80	−14.33	−14.74
450		−13.40	−11.41	−11.81	−12.27	−13.06	−13.69	−14.18
500			−10.80	−10.93	−11.40	−12.31	−13.04	−13.62
550			−10.55	−10.10	−10.52	−11.54	−12.38	−13.05
600			−10.72	−9.37	−9.63	−10.72	−11.69	−12.46
700				−8.41	−7.85	−8.93	−10.17	−11.18

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Cd^{+2} — Continued				
800					−6.04	−6.86	−8.41	−9.68
900					−4.09	−4.55	−6.44	−7.93
1000						−2.13	−4.34	−5.96
				Ce^{+3}				
25	−161.60	−162.05	−162.44	−162.79	−163.10	−163.65	−164.13	−164.56
50	−160.34	−160.80	−161.21	−161.58	−161.91	−162.51	−163.03	−163.50
75	−159.02	−159.50	−159.93	−160.31	−160.67	−161.29	−161.85	−162.35
100	−157.64	−158.15	−158.60	−159.00	−159.37	−160.03	−160.61	−161.14
125	−156.22	−156.75	−157.23	−157.65	−158.04	−158.73	−159.33	−159.89
150	−154.73	−155.31	−155.81	−156.26	−156.67	−157.39	−158.03	−158.61
175	−153.18	−153.81	−154.35	−154.83	−155.26	−156.03	−156.70	−157.30
200	−151.57	−152.25	−152.84	−153.36	−153.82	−154.64	−155.34	−155.97
225	−149.87	−150.63	−151.29	−151.85	−152.35	−153.22	−153.96	−154.63
250	−148.08	−148.94	−149.68	−150.29	−150.84	−151.77	−152.56	−153.26
300	−144.16	−145.37	−146.33	−147.06	−147.70	−148.79	−149.70	−150.48
350	−140.21	−141.44	−142.87	−143.69	−144.43	−145.70	−146.74	−147.63
400		−139.36	−139.39	−140.23	−141.06	−142.50	−143.70	−144.71
450		−140.95	−136.08	−136.72	−137.59	−139.21	−140.57	−141.72
500			−133.25	−133.20	−134.04	−135.82	−137.35	−138.65
550			−131.25	−129.77	−130.41	−132.32	−134.03	−135.49
600			−130.21	−126.52	−126.72	−128.68	−130.59	−132.22
700				−120.95	−119.22	−120.93	−123.27	−125.29
800					−111.50	−112.44	−115.28	−117.73
900					−103.25	−103.27	−106.66	−109.52
1000						−93.67	−97.62	−100.70
				Cl^-				
25	−31.38	−31.17	−30.95	−30.74	−30.52	−30.06	−29.61	−29.15
50	−31.69	−31.48	−31.26	−31.05	−30.83	−30.39	−29.94	−29.49
75	−31.95	−31.74	−31.54	−31.32	−31.11	−30.68	−30.24	−29.81
100	−32.17	−31.97	−31.77	−31.57	−31.36	−30.94	−30.52	−30.09
125	−32.33	−32.16	−31.97	−31.78	−31.58	−31.18	−30.77	−30.35
150	−32.45	−32.30	−32.13	−31.95	−31.77	−31.38	−30.99	−30.59
175	−32.51	−32.40	−32.25	−32.09	−31.92	−31.57	−31.19	−30.80
200	−32.51	−32.45	−32.34	−32.20	−32.05	−31.72	−31.37	−31.00
225	−32.44	−32.44	−32.38	−32.27	−32.15	−31.85	−31.52	−31.17
250	−32.27	−32.38	−32.37	−32.31	−32.21	−31.96	−31.66	−31.33
300	−31.51	−32.01	−32.21	−32.25	−32.23	−32.08	−31.86	−31.58
350	−29.54	−31.15	−31.80	−32.01	−32.10	−32.10	−31.97	−31.77
400		−29.82	−31.09	−31.56	−31.81	−32.01	−32.00	−31.88
450		−25.80	−29.93	−30.87	−31.34	−31.79	−31.93	−31.91
500			−28.13	−29.86	−30.67	−31.45	−31.77	−31.87
550			−25.55	−28.51	−29.76	−30.96	−31.49	−31.73
600			−22.37	−26.81	−28.62	−30.32	−31.11	−31.50
700				−22.79	−25.75	−28.61	−29.98	−30.72
800					−22.39	−26.37	−28.38	−29.49
900					−18.95	−23.78	−26.39	−27.79
1000						−21.08	−24.13	−25.66
				ClO^-				
25	−8.80	−8.68	−8.54	−8.39	−8.23	−7.90	−7.55	−7.18
50	−9.00	−8.88	−8.74	−8.60	−8.44	−8.12	−7.77	−7.42
75	−9.13	−9.01	−8.88	−8.74	−8.59	−8.27	−7.94	−7.60
100	−9.20	−9.09	−8.97	−8.83	−8.69	−8.39	−8.07	−7.73
125	−9.20	−9.11	−9.00	−8.88	−8.74	−8.46	−8.15	−7.83
150	−9.14	−9.08	−8.99	−8.88	−8.76	−8.49	−8.20	−7.89
175	−9.02	−8.99	−8.92	−8.83	−8.73	−8.48	−8.21	−7.92
200	−8.83	−8.84	−8.81	−8.75	−8.66	−8.45	−8.20	−7.92

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				ClO^- — Continued				
225	−8.55	−8.64	−8.65	−8.61	−8.55	−8.37	−8.15	−7.89
250	−8.17	−8.36	−8.43	−8.44	−8.40	−8.27	−8.07	−7.84
300	−6.97	−7.55	−7.82	−7.94	−7.98	−7.96	−7.84	−7.66
350	−4.54	−6.21	−6.95	−7.23	−7.39	−7.51	−7.49	−7.38
400		−4.41	−5.75	−6.30	−6.62	−6.93	−7.03	−7.01
450		0.07	−4.09	−5.09	−5.64	−6.21	−6.46	−6.54
500			−1.77	−3.56	−4.44	−5.34	−5.77	−5.97
550			1.33	−1.67	−2.99	−4.31	−4.96	−5.30
600			5.05	0.58	−1.30	−3.12	−4.02	−4.52
700				5.73	2.74	−0.25	−1.74	−2.59
800					7.30	3.21	1.07	−0.14
900					12.00	7.06	4.33	2.81
1000						11.07	7.89	6.24
				ClO_2^-				
25	4.10	4.39	4.67	4.96	5.25	5.84	6.43	7.02
50	3.52	3.82	4.11	4.40	4.70	5.28	5.87	6.46
75	2.99	3.28	3.58	3.87	4.16	4.74	5.33	5.91
100	2.50	2.78	3.07	3.36	3.64	4.22	4.80	5.38
125	2.04	2.31	2.59	2.87	3.15	3.72	4.28	4.85
150	1.63	1.88	2.14	2.41	2.68	3.23	3.79	4.34
175	1.26	1.48	1.72	1.97	2.23	2.76	3.30	3.85
200	0.94	1.11	1.33	1.56	1.80	2.31	2.83	3.37
225	0.69	0.79	0.97	1.17	1.40	1.87	2.38	2.89
250	0.51	0.53	0.65	0.82	1.02	1.46	1.94	2.43
300	0.54	0.19	0.13	0.20	0.33	0.68	1.10	1.55
350	1.74	0.29	−0.18	−0.26	−0.23	−0.01	0.32	0.71
400		0.96	−0.20	−0.55	−0.67	−0.62	−0.40	−0.08
450		4.50	0.20	−0.61	−0.95	−1.14	−1.05	−0.82
500			1.25	−0.38	−1.04	−1.55	−1.62	−1.50
550			3.10	0.18	−0.94	−1.84	−2.11	−2.11
600			5.58	1.06	−0.62	−2.01	−2.51	−2.65
700				3.48	0.55	−2.00	−3.04	−3.49
800					2.11	−1.56	−3.20	−3.97
900					3.69	−0.88	−3.05	−4.09
1000						−0.16	−2.73	−3.87
				ClO_3^-				
25	−1.90	−1.47	−1.05	−0.63	−0.22	0.59	1.40	2.19
50	−2.86	−2.42	−1.98	−1.56	−1.14	−0.32	0.49	1.29
75	−3.80	−3.36	−2.92	−2.49	−2.08	−1.25	−0.44	0.36
100	−4.73	−4.29	−3.86	−3.43	−3.01	−2.19	−1.39	−0.59
125	−5.65	−5.21	−4.79	−4.37	−3.95	−3.14	−2.34	−1.55
150	−6.54	−6.12	−5.71	−5.30	−4.89	−4.09	−3.30	−2.51
175	−7.41	−7.02	−6.62	−6.22	−5.83	−5.04	−4.26	−3.48
200	−8.25	−7.90	−7.52	−7.14	−6.76	−5.99	−5.22	−4.45
225	−9.04	−8.75	−8.41	−8.05	−7.68	−6.93	−6.18	−5.43
250	−9.78	−9.58	−9.28	−8.94	−8.60	−7.88	−7.14	−6.41
300	−10.95	−11.08	−10.93	−10.68	−10.39	−9.75	−9.07	−8.37
350	−11.09	−12.24	−12.45	−12.33	−12.13	−11.59	−10.98	−10.33
400		−12.83	−13.74	−13.86	−13.78	−13.40	−12.88	−12.29
450		−10.69	−14.66	−15.21	−15.34	−15.16	−14.75	−14.23
500			−15.01	−16.34	−16.76	−16.86	−16.59	−16.16
550			−14.62	−17.20	−18.04	−18.49	−18.39	−18.07
600			−13.66	−17.77	−19.15	−20.05	−20.15	−19.94
700				−18.37	−20.96	−22.92	−23.49	−23.55
800					−22.52	−25.54	−26.63	−26.96
900					−24.18	−28.06	−29.60	−30.15
1000						−30.63	−32.51	−33.14

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				ClO_4^-				
25	−2.04	−1.53	−1.05	−0.60	−0.15	0.70	1.51	2.31
50	−3.13	−2.58	−2.06	−1.57	−1.09	−0.17	0.71	1.56
75	−4.22	−3.65	−3.11	−2.60	−2.10	−1.15	−0.24	0.65
100	−5.31	−4.74	−4.19	−3.67	−3.16	−2.19	−1.26	−0.36
125	−6.42	−5.84	−5.30	−4.77	−4.26	−3.28	−2.34	−1.43
150	−7.52	−6.96	−6.42	−5.90	−5.39	−4.41	−3.46	−2.54
175	−8.63	−8.09	−7.55	−7.04	−6.53	−5.56	−4.61	−3.69
200	−9.72	−9.21	−8.70	−8.19	−7.70	−6.73	−5.80	−4.88
225	−10.79	−10.34	−9.85	−9.36	−8.88	−7.93	−7.00	−6.09
250	−11.81	−11.45	−11.00	−10.53	−10.07	−9.14	−8.23	−7.33
300	−13.63	−13.59	−13.28	−12.89	−12.47	−11.61	−10.73	−9.86
350	−14.51	−15.47	−15.49	−15.22	−14.88	−14.12	−13.30	−12.47
400		−16.84	−17.54	−17.50	−17.28	−16.65	−15.91	−15.13
450		−15.63	−19.29	−19.66	−19.63	−19.19	−18.56	−17.85
500			−20.55	−21.66	−21.91	−21.73	−21.23	−20.59
550			−21.14	−23.44	−24.09	−24.25	−23.91	−23.36
600			−21.22	−25.00	−26.17	−26.74	−26.58	−26.15
700				−27.71	−30.05	−31.63	−31.91	−31.73
800					−33.83	−36.43	−37.20	−37.27
900					−37.86	−41.27	−42.47	−42.74
1000						−46.30	−47.80	−48.15
				Co^{+2}				
25	−13.00	−13.27	−13.48	−13.66	−13.82	−14.05	−14.23	−14.37
50	−12.32	−12.61	−12.85	−13.05	−13.23	−13.53	−13.76	−13.95
75	−11.63	−11.94	−12.20	−12.42	−12.62	−12.95	−13.22	−13.44
100	−10.93	−11.25	−11.53	−11.77	−11.99	−12.35	−12.65	−12.90
125	−10.21	−10.56	−10.86	−11.12	−11.35	−11.74	−12.06	−12.34
150	−9.48	−9.86	−10.18	−10.46	−10.70	−11.12	−11.47	−11.77
175	−8.73	−9.14	−9.49	−9.79	−10.05	−10.50	−10.88	−11.20
200	−7.95	−8.40	−8.79	−9.11	−9.40	−9.88	−10.28	−10.63
225	−7.13	−7.64	−8.06	−8.42	−8.73	−9.26	−9.69	−10.06
250	−6.27	−6.85	−7.33	−7.72	−8.06	−8.63	−9.09	−9.49
300	−4.37	−5.18	−5.80	−6.28	−6.68	−7.36	−7.90	−8.36
350	−2.50	−3.32	−4.26	−4.80	−5.27	−6.07	−6.71	−7.24
400		−2.74	−2.76	−3.31	−3.84	−4.76	−5.50	−6.11
450		−4.62	−1.41	−1.83	−2.39	−3.43	−4.28	−4.98
500			−0.42	−0.39	−0.93	−2.08	−3.04	−3.85
550			−0.02	0.96	0.54	−0.69	−1.78	−2.69
600			−0.29	2.15	2.01	0.75	−0.48	−1.50
700				3.80	4.94	3.84	2.32	1.04
800					7.89	7.28	5.44	3.86
900					11.07	11.07	8.86	7.01
1000						15.03	12.45	10.45
				Co^{+3}				
25	32.00	31.50	31.07	30.68	30.33	29.71	29.17	28.68
50	33.86	33.34	32.88	32.47	32.10	31.43	30.84	30.31
75	35.76	35.22	34.74	34.32	33.92	33.22	32.59	32.03
100	37.71	37.15	36.64	36.19	35.78	35.04	34.38	33.79
125	39.72	39.11	38.58	38.11	37.67	36.89	36.21	35.58
150	41.78	41.13	40.56	40.05	39.59	38.77	38.05	37.39
175	43.90	43.19	42.57	42.03	41.54	40.67	39.91	39.23
200	46.10	45.32	44.64	44.05	43.52	42.59	41.79	41.07
225	48.38	47.50	46.75	46.11	45.53	44.54	43.69	42.93
250	50.75	49.76	48.91	48.21	47.58	46.51	45.60	44.80
300	55.85	54.46	53.36	52.52	51.79	50.53	49.48	48.57
350	60.62	59.51	57.88	56.96	56.11	54.65	53.44	52.40
400		61.76	62.30	61.44	60.51	58.85	57.46	56.28
450		57.79	66.33	65.89	64.97	63.14	61.56	60.22

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Co^{+3} — Continued				
500			69.45	70.24	69.47	67.51	65.74	64.23
550			71.08	74.35	73.99	71.98	70.02	68.32
600			71.01	78.06	78.51	76.58	74.41	72.52
700				83.84	87.48	86.28	83.67	81.33
800					96.54	96.80	93.69	90.84
900					106.26	108.14	104.43	101.09
1000						120.00	115.64	112.02
				CrO_4^{-2}				
25	−173.94	−173.70	−173.45	−173.20	−172.94	−172.40	−171.84	−171.28
50	−174.18	−173.95	−173.70	−173.45	−173.19	−172.66	−172.11	−171.56
75	−174.33	−174.11	−173.87	−173.63	−173.38	−172.87	−172.34	−171.80
100	−174.40	−174.20	−173.98	−173.75	−173.51	−173.02	−172.52	−171.99
125	−174.37	−174.21	−174.02	−173.81	−173.60	−173.14	−172.65	−172.15
150	−174.26	−174.15	−174.00	−173.82	−173.63	−173.20	−172.75	−172.27
175	−174.04	−174.00	−173.90	−173.77	−173.60	−173.23	−172.81	−172.36
200	−173.70	−173.77	−173.74	−173.65	−173.53	−173.21	−172.84	−172.42
225	−173.22	−173.43	−173.49	−173.47	−173.39	−173.15	−172.83	−172.45
250	−172.55	−172.97	−173.16	−173.21	−173.20	−173.04	−172.78	−172.45
300	−170.39	−171.60	−172.20	−172.48	−172.63	−172.70	−172.58	−172.37
350	−165.86	−169.26	−170.80	−171.41	−171.79	−172.15	−172.24	−172.17
400		−166.12	−168.80	−169.95	−170.65	−171.41	−171.74	−171.84
450		−157.84	−165.96	−168.01	−169.16	−170.44	−171.08	−171.39
500			−161.89	−165.49	−167.29	−169.24	−170.25	−170.80
550			−156.33	−162.29	−164.98	−167.77	−169.22	−170.06
600			−149.65	−158.46	−162.23	−166.02	−167.98	−169.13
700				−149.64	−155.58	−161.68	−164.83	−166.70
800					−148.05	−156.32	−160.78	−163.40
900					−140.37	−150.30	−155.97	−159.20
1000						−144.09	−150.68	−154.18
				$Cr_2O_7^{-2}$				
25	−311.00	−310.16	−309.35	−308.57	−307.81	−306.34	−304.90	−303.50
50	−312.55	−311.69	−310.86	−310.07	−309.29	−307.79	−306.33	−304.91
75	−314.06	−313.20	−312.37	−311.57	−310.80	−309.29	−307.82	−306.39
100	−315.55	−314.69	−313.87	−313.08	−312.31	−310.80	−309.34	−307.91
125	−317.00	−316.17	−315.36	−314.58	−313.81	−312.32	−310.87	−309.45
150	−318.40	−317.61	−316.83	−316.07	−315.32	−313.85	−312.41	−311.00
175	−319.75	−319.02	−318.28	−317.54	−316.81	−315.37	−313.96	−312.57
200	−321.03	−320.38	−319.69	−318.99	−318.29	−316.89	−315.50	−314.13
225	−322.21	−321.69	−321.06	−320.41	−319.74	−318.40	−317.05	−315.70
250	−323.26	−322.92	−322.39	−321.80	−321.18	−319.89	−318.59	−317.27
300	−324.72	−325.09	−324.88	−324.46	−323.97	−322.85	−321.65	−320.42
350	−324.01	−326.50	−327.06	−326.93	−326.61	−325.73	−324.68	−323.55
400		−326.77	−328.75	−329.12	−329.08	−328.52	−327.66	−326.66
450		−321.41	−329.67	−330.94	−331.32	−331.19	−330.58	−329.74
500			−329.39	−332.27	−333.27	−333.72	−333.41	−332.76
550			−327.58	−333.01	−334.89	−336.10	−336.15	−335.72
600			−324.56	−333.17	−336.16	−338.30	−338.77	−338.60
700				−332.33	−337.82	−342.17	−343.65	−344.04
800					−338.89	−345.45	−348.03	−349.01
900					−340.13	−348.46	−352.03	−353.48
1000						−351.55	−355.83	−357.48
				Cs^+				
25	−69.71	−69.45	−69.17	−68.89	−68.60	−68.01	−67.41	−66.79
50	−70.50	−70.23	−69.95	−69.66	−69.37	−68.77	−68.17	−67.55
75	−71.29	−71.01	−70.72	−70.43	−70.14	−69.54	−68.94	−68.32
100	−72.08	−71.79	−71.51	−71.22	−70.92	−70.32	−69.72	−69.11

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Cs^+ — Continued				
125	−72.87	−72.59	−72.30	−72.01	−71.71	−71.11	−70.51	−69.90
150	−73.66	−73.38	−73.09	−72.80	−72.51	−71.91	−71.30	−70.69
175	−74.46	−74.18	−73.90	−73.60	−73.31	−72.71	−72.11	−71.50
200	−75.26	−74.99	−74.70	−74.41	−74.12	−73.52	−72.92	−72.31
225	−76.06	−75.80	−75.51	−75.22	−74.93	−74.34	−73.74	−73.13
250	−76.86	−76.61	−76.33	−76.04	−75.75	−75.16	−74.56	−73.96
300	−78.45	−78.25	−77.98	−77.70	−77.41	−76.82	−76.23	−75.63
350	−79.99	−79.88	−79.64	−79.36	−79.08	−78.51	−77.92	−77.32
400		−81.55	−81.31	−81.05	−80.77	−80.21	−79.63	−79.04
450		−83.18	−82.99	−82.74	−82.48	−81.93	−81.35	−80.77
500			−84.67	−84.45	−84.20	−83.66	−83.10	−82.52
550			−86.35	−86.16	−85.92	−85.40	−84.86	−84.29
600			−88.03	−87.88	−87.66	−87.16	−86.63	−86.07
700				−91.35	−91.15	−90.70	−90.20	−89.66
800					−94.69	−94.27	−93.80	−93.29
900					−98.27	−97.88	−97.44	−96.94
1000						−101.52	−101.11	−100.63
				$CsBr^\circ$				
25	−94.21	−93.52	−92.87	−92.23	−91.62	−90.42	−89.26	−88.12
50	−95.66	−94.95	−94.27	−93.62	−92.98	−91.76	−90.57	−89.42
75	−97.07	−96.34	−95.65	−94.99	−94.35	−93.11	−91.91	−90.74
100	−98.45	−97.71	−97.02	−96.35	−95.70	−94.45	−93.24	−92.06
125	−99.80	−99.07	−98.36	−97.69	−97.04	−95.78	−94.56	−93.38
150	−101.14	−100.40	−99.69	−99.02	−98.36	−97.09	−95.88	−94.69
175	−102.45	−101.72	−101.01	−100.33	−99.67	−98.40	−97.18	−95.99
200	−103.75	−103.02	−102.31	−101.63	−100.97	−99.69	−98.47	−97.28
225	−105.03	−104.31	−103.60	−102.91	−102.25	−100.97	−99.75	−98.55
250	−106.28	−105.59	−104.87	−104.19	−103.52	−102.24	−101.02	−99.82
300	−108.74	−108.11	−107.39	−106.70	−106.03	−104.75	−103.52	−102.32
350	−111.09	−110.59	−109.86	−109.17	−108.50	−107.22	−105.98	−104.78
400		−113.02	−112.30	−111.61	−110.94	−109.65	−108.41	−107.21
450		−115.43	−114.70	−114.00	−113.33	−112.04	−110.80	−109.60
500		−117.81	−117.06	−116.37	−115.70	−114.40	−113.16	−111.96
550		−120.15	−119.40	−118.70	−118.03	−116.74	−115.50	−114.29
600		−122.46	−121.71	−121.01	−120.33	−119.04	−117.80	−116.59
700		−127.00	−126.25	−125.54	−124.86	−123.57	−122.32	−121.12
800		−131.44	−130.68	−129.97	−129.30	−128.00	−126.75	−125.54
900		−135.78	−135.03	−134.32	−133.64	−132.34	−131.09	−129.88
1000		−140.05	−139.30	−138.58	−137.90	−136.60	−135.35	−134.14
				$CsCl^\circ$				
25	−100.90	−100.32	−99.76	−99.21	−98.68	−97.64	−96.64	−95.65
50	−102.19	−101.59	−101.01	−100.45	−99.91	−98.85	−97.82	−96.82
75	−103.45	−102.84	−102.25	−101.68	−101.13	−100.05	−99.02	−98.00
100	−104.69	−104.06	−103.47	−102.89	−102.33	−101.25	−100.21	−99.19
125	−105.90	−105.27	−104.67	−104.09	−103.53	−102.44	−101.39	−100.37
150	−107.09	−106.46	−105.86	−105.28	−104.71	−103.62	−102.57	−101.54
175	−108.27	−107.64	−107.03	−106.45	−105.88	−104.79	−103.73	−102.70
200	−109.42	−108.80	−108.20	−107.61	−107.04	−105.94	−104.89	−103.86
225	−110.57	−109.96	−109.35	−108.76	−108.19	−107.09	−106.03	−105.00
250	−111.69	−111.10	−110.49	−109.90	−109.33	−108.23	−107.16	−106.13
300	−113.88	−113.35	−112.74	−112.14	−111.57	−110.47	−109.40	−108.37
350	−116.00	−115.56	−114.95	−114.35	−113.78	−112.67	−111.61	−110.57
400		−117.74	−117.13	−116.53	−115.96	−114.85	−113.78	−112.74
450		−119.90	−119.27	−118.68	−118.10	−116.99	−115.92	−114.88
500		−122.03	−121.39	−120.79	−120.22	−119.11	−118.04	−117.00
550		−124.13	−123.48	−122.88	−122.31	−121.19	−120.12	−119.08
600		−126.20	−125.55	−124.95	−124.37	−123.26	−122.19	−121.14
700		−130.27	−129.62	−129.01	−128.43	−127.31	−126.24	−125.20

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$CsCl^\circ$ — Continued				
800		−134.25	−133.60	−132.99	−132.41	−131.29	−130.21	−129.17
900		−138.15	−137.50	−136.89	−136.30	−135.18	−134.11	−133.06
1000		−141.98	−141.33	−140.72	−140.13	−139.01	−137.93	−136.89
				CsI°				
25	−82.48	−81.65	−80.85	−80.09	−79.35	−77.91	−76.53	−75.19
50	−83.99	−83.13	−82.31	−81.52	−80.76	−79.29	−77.88	−76.51
75	−85.47	−84.59	−83.76	−82.96	−82.18	−80.70	−79.26	−77.87
100	−86.92	−86.03	−85.19	−84.38	−83.60	−82.10	−80.65	−79.25
125	−88.35	−87.46	−86.61	−85.79	−85.01	−83.49	−82.04	−80.63
150	−89.76	−88.86	−88.01	−87.19	−86.40	−84.88	−83.43	−82.01
175	−91.15	−90.26	−89.40	−88.58	−87.79	−86.26	−84.80	−83.38
200	−92.53	−91.64	−90.78	−89.96	−89.16	−87.63	−86.17	−84.74
225	−93.88	−93.01	−92.15	−91.32	−90.52	−88.99	−87.52	−86.10
250	−95.22	−94.37	−93.51	−92.68	−91.88	−90.34	−88.87	−87.44
300	−97.82	−97.06	−96.19	−95.36	−94.56	−93.02	−91.54	−90.11
350	−100.33	−99.71	−98.84	−98.01	−97.20	−95.66	−94.18	−92.75
400		−102.33	−101.46	−100.62	−99.81	−98.27	−96.79	−95.35
450		−104.92	−104.04	−103.20	−102.40	−100.85	−99.36	−97.93
500		−107.49	−106.60	−105.76	−104.95	−103.40	−101.91	−100.48
550		−110.03	−109.13	−108.29	−107.48	−105.92	−104.44	−103.00
600		−112.54	−111.64	−110.79	−109.98	−108.43	−106.94	−105.50
700		−117.49	−116.58	−115.73	−114.92	−113.36	−111.87	−110.43
800		−122.35	−121.44	−120.59	−119.77	−118.21	−116.72	−115.27
900		−127.13	−126.22	−125.37	−124.55	−122.99	−121.49	−120.05
1000		−131.84	−130.93	−130.08	−129.26	−127.69	−126.20	−124.75
				Cu^+				
25	11.95	11.87	11.82	11.78	11.76	11.76	11.79	11.84
50	11.69	11.61	11.56	11.52	11.49	11.48	11.49	11.52
75	11.41	11.33	11.27	11.23	11.20	11.17	11.18	11.20
100	11.10	11.02	10.96	10.91	10.88	10.85	10.84	10.86
125	10.78	10.69	10.62	10.58	10.54	10.50	10.49	10.49
150	10.43	10.34	10.27	10.22	10.18	10.13	10.11	10.11
175	10.07	9.97	9.89	9.84	9.79	9.74	9.71	9.71
200	9.70	9.59	9.50	9.44	9.39	9.33	9.30	9.29
225	9.31	9.19	9.10	9.03	8.97	8.90	8.86	8.85
250	8.92	8.78	8.68	8.60	8.54	8.46	8.41	8.39
300	8.15	7.95	7.81	7.71	7.63	7.52	7.46	7.42
350	7.41	7.12	6.89	6.77	6.67	6.53	6.44	6.39
400		6.09	5.93	5.78	5.66	5.49	5.38	5.30
450		4.94	4.93	4.76	4.62	4.41	4.26	4.16
500			3.89	3.71	3.54	3.28	3.11	2.98
550			2.80	2.63	2.43	2.12	1.91	1.76
600			1.65	1.51	1.30	0.94	0.69	0.51
700				−0.89	−1.05	−1.49	−1.84	−2.09
800					−3.50	−3.99	−4.44	−4.76
900					−6.06	−6.55	−7.10	−7.49
1000						−9.21	−9.85	−10.27
				Cu^{+2}				
25	15.68	15.40	15.17	14.98	14.80	14.51	14.28	14.08
50	16.26	15.97	15.73	15.52	15.34	15.02	14.75	14.53
75	16.84	16.54	16.29	16.07	15.87	15.53	15.24	15.00
100	17.42	17.11	16.84	16.61	16.40	16.04	15.73	15.47
125	18.00	17.67	17.39	17.14	16.92	16.54	16.22	15.93
150	18.59	18.24	17.94	17.68	17.44	17.04	16.69	16.39
175	19.20	18.82	18.49	18.21	17.95	17.52	17.15	16.83
200	19.83	19.41	19.05	18.74	18.46	18.00	17.61	17.27

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Cu^{+2} — Continued				
225	20.49	20.01	19.61	19.27	18.97	18.47	18.05	17.69
250	21.19	20.64	20.19	19.81	19.49	18.94	18.49	18.11
300	22.74	21.96	21.36	20.91	20.52	19.87	19.35	18.90
350	24.25	23.45	22.54	22.02	21.57	20.80	20.19	19.67
400		23.64	23.65	23.13	22.61	21.73	21.01	20.41
450		21.35	24.59	24.20	23.65	22.65	21.82	21.14
500			25.15	25.21	24.69	23.58	22.63	21.85
550			25.10	26.11	25.71	24.52	23.46	22.57
600			24.38	26.84	26.73	25.50	24.31	23.31
700				27.53	28.70	27.63	26.15	24.89
800					30.63	30.06	28.25	26.70
900					32.75	32.79	30.61	28.79
1000						35.65	33.10	31.13
				$Cu(CH_3COO)^{\circ}$				
25	−76.77	−76.30	−75.83	−75.38	−74.94	−74.08	−73.23	−72.40
50	−77.57	−77.08	−76.60	−76.14	−75.69	−74.81	−73.95	−73.10
75	−78.51	−78.01	−77.52	−77.05	−76.59	−75.70	−74.84	−73.99
100	−79.57	−79.06	−78.57	−78.10	−77.63	−76.73	−75.86	−75.01
125	−80.73	−80.22	−79.73	−79.25	−78.78	−77.88	−77.00	−76.15
150	−81.99	−81.48	−80.98	−80.50	−80.03	−79.13	−78.25	−77.39
175	−83.34	−82.83	−82.33	−81.85	−81.38	−80.47	−79.58	−78.72
200	−84.77	−84.26	−83.76	−83.27	−82.80	−81.89	−81.01	−80.14
225	−86.28	−85.77	−85.27	−84.78	−84.31	−83.39	−82.51	−81.64
250	−87.85	−87.36	−86.85	−86.36	−85.89	−84.97	−84.08	−83.22
300	−91.19	−90.74	−90.23	−89.73	−89.25	−88.33	−87.44	−86.57
350	−94.74	−94.39	−93.86	−93.36	−92.88	−91.95	−91.05	−90.18
400		−98.29	−97.73	−97.22	−96.73	−95.80	−94.90	−94.03
450		−102.54	−101.83	−101.30	−100.80	−99.86	−98.96	−98.08
500		−107.15	−106.15	−105.59	−105.08	−104.13	−103.22	−102.34
550		−111.88	−110.69	−110.07	−109.54	−108.58	−107.66	−106.78
600		−116.69	−115.42	−114.74	−114.19	−113.20	−112.28	−111.39
700		−126.66	−125.37	−124.57	−123.97	−122.94	−122.00	−121.10
800		−137.11	−135.85	−135.00	−134.34	−133.26	−132.31	−131.40
900		−148.03	−146.80	−145.92	−145.23	−144.12	−143.15	−142.23
1000		−159.38	−158.19	−157.30	−156.59	−155.45	−154.47	−153.55
				$Cu(CH_3COO)_2^-$				
25	−165.00	−163.91	−162.88	−161.88	−160.92	−159.07	−157.29	−155.56
50	−166.11	−164.98	−163.92	−162.90	−161.92	−160.02	−158.20	−156.43
75	−167.52	−166.38	−165.30	−164.27	−163.28	−161.36	−159.52	−157.73
100	−169.18	−168.04	−166.96	−165.92	−164.92	−162.99	−161.14	−159.34
125	−171.06	−169.92	−168.85	−167.81	−166.81	−164.88	−163.02	−161.22
150	−173.12	−172.01	−170.94	−169.91	−168.91	−166.98	−165.13	−163.33
175	−175.35	−174.27	−173.21	−172.19	−171.20	−169.28	−167.44	−165.64
200	−177.72	−176.69	−175.65	−174.65	−173.67	−171.76	−169.93	−168.14
225	−180.21	−179.25	−178.24	−177.26	−176.29	−174.41	−172.59	−170.81
250	−182.79	−181.94	−180.97	−180.01	−179.07	−177.22	−175.41	−173.64
300	−188.05	−187.60	−186.79	−185.91	−185.02	−183.25	−181.49	−179.75
350	−192.75	−193.45	−193.00	−192.26	−191.46	−189.79	−188.09	−186.41
400		−199.21	−199.47	−198.97	−198.30	−196.78	−195.17	−193.55
450		−202.67	−206.02	−205.95	−205.48	−204.17	−202.68	−201.13
500			−212.40	−213.12	−212.95	−211.92	−210.57	−209.11
550			−218.43	−220.41	−220.66	−219.99	−218.82	−217.45
600			−224.24	−227.77	−228.57	−228.34	−227.37	−226.13
700				−242.96	−244.98	−245.83	−245.34	−244.37
800					−262.36	−264.29	−264.32	−263.63
900					−280.96	−283.75	−284.25	−283.78
1000						−304.29	−305.13	−304.75

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Cu(CH_3COO)^+$				
25	−75.64	−75.38	−75.11	−74.85	−74.58	−74.04	−73.50	−72.95
50	−75.69	−75.42	−75.15	−74.88	−74.61	−74.06	−73.52	−72.98
75	−75.88	−75.61	−75.34	−75.06	−74.79	−74.25	−73.71	−73.17
100	−76.20	−75.92	−75.65	−75.38	−75.11	−74.57	−74.03	−73.49
125	−76.61	−76.34	−76.07	−75.80	−75.54	−75.00	−74.47	−73.93
150	−77.12	−76.86	−76.59	−76.33	−76.06	−75.54	−75.01	−74.48
175	−77.70	−77.46	−77.20	−76.94	−76.68	−76.16	−75.64	−75.12
200	−78.36	−78.13	−77.89	−77.64	−77.39	−76.88	−76.36	−75.84
225	−79.08	−78.88	−78.65	−78.41	−78.17	−77.67	−77.16	−76.65
250	−79.84	−79.69	−79.48	−79.25	−79.02	−78.53	−78.04	−77.54
300	−81.49	−81.47	−81.32	−81.12	−80.91	−80.47	−80.00	−79.52
350	−83.31	−83.42	−83.40	−83.23	−83.05	−82.65	−82.22	−81.77
400		−85.99	−85.71	−85.57	−85.41	−85.06	−84.67	−84.25
450		−89.36	−88.26	−88.10	−87.97	−87.68	−87.33	−86.94
500			−91.09	−90.84	−90.72	−90.48	−90.18	−89.83
550			−94.23	−93.77	−93.64	−93.45	−93.21	−92.90
600			−97.70	−96.90	−96.72	−96.58	−96.39	−96.13
700				−103.83	−103.34	−103.22	−103.16	−103.01
800					−110.52	−110.32	−110.41	−110.37
900					−118.15	−117.83	−118.07	−118.14
1000						−125.77	−126.16	−126.28
				$Cu(CH_3COO)_2^\circ$				
25	−165.82	−164.96	−164.15	−163.36	−162.60	−161.14	−159.72	−158.34
50	−166.36	−165.48	−164.63	−163.83	−163.05	−161.54	−160.09	−158.69
75	−167.22	−166.31	−165.46	−164.64	−163.84	−162.32	−160.85	−159.43
100	−168.34	−167.42	−166.56	−165.73	−164.93	−163.39	−161.91	−160.47
125	−169.69	−168.77	−167.90	−167.06	−166.25	−164.70	−163.22	−161.77
150	−171.25	−170.33	−169.45	−168.61	−167.80	−166.24	−164.75	−163.30
175	−173.00	−172.08	−171.20	−170.35	−169.54	−167.97	−166.48	−165.02
200	−174.93	−174.02	−173.13	−172.28	−171.46	−169.89	−168.39	−166.93
225	−177.01	−176.12	−175.23	−174.38	−173.56	−171.98	−170.47	−169.01
250	−179.25	−178.38	−177.49	−176.63	−175.81	−174.23	−172.72	−171.26
300	−184.15	−183.35	−182.45	−181.59	−180.76	−179.18	−177.66	−176.19
350	−189.56	−188.88	−187.96	−187.10	−186.26	−184.67	−183.15	−181.68
400		−194.94	−193.98	−193.10	−192.26	−190.67	−189.14	−187.66
450		−201.57	−200.47	−199.57	−198.73	−197.12	−195.58	−194.10
500		−208.80	−207.41	−206.48	−205.62	−204.00	−202.46	−200.97
550		−216.36	−214.78	−213.79	−212.91	−211.28	−209.73	−208.24
600		−224.20	−222.54	−221.49	−220.58	−218.93	−217.37	−215.88
700		−240.78	−239.10	−237.93	−236.97	−235.27	−233.69	−232.19
800		−258.51	−256.85	−255.63	−254.62	−252.87	−251.28	−249.76
900		−277.30	−275.69	−274.43	−273.39	−271.60	−270.00	−268.47
1000		−297.09	−295.51	−294.24	−293.18	−291.37	−289.75	−288.23
				$Cu(CH_3COO)_3^-$				
25	−255.81	−254.30	−252.87	−251.50	−250.18	−247.66	−245.24	−242.89
50	−256.59	−255.03	−253.56	−252.16	−250.80	−248.21	−245.73	−243.33
75	−257.88	−256.30	−254.81	−253.39	−252.02	−249.40	−246.88	−244.45
100	−259.58	−258.00	−256.51	−255.08	−253.70	−251.06	−248.53	−246.08
125	−261.65	−260.08	−258.58	−257.16	−255.78	−253.13	−250.60	−248.14
150	−264.04	−262.49	−261.00	−259.58	−258.20	−255.56	−253.03	−250.57
175	−266.71	−265.20	−263.73	−262.31	−260.95	−258.32	−255.79	−253.33
200	−269.62	−268.17	−266.73	−265.33	−263.98	−261.37	−258.85	−256.40
225	−272.75	−271.39	−269.99	−268.62	−267.28	−264.69	−262.19	−259.75
250	−276.05	−274.83	−273.48	−272.14	−270.83	−268.27	−265.79	−263.37
300	−282.97	−282.25	−281.08	−279.84	−278.60	−276.13	−273.71	−271.33
350	−289.54	−290.15	−289.41	−288.32	−287.18	−284.85	−282.51	−280.18
400		−298.36	−298.29	−297.47	−296.47	−294.32	−292.09	−289.84
450		−304.53	−307.52	−307.16	−306.39	−304.47	−302.38	−300.22

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Cu(CH_3COO)_3^-$ — Continued				
500			−316.83	−317.29	−316.84	−315.24	−313.32	−311.27
550			−326.02	−327.76	−327.77	−326.57	−324.85	−322.92
600			−335.22	−338.53	−339.11	−338.41	−336.92	−335.14
700				−361.20	−362.99	−363.45	−362.52	−361.06
800					−388.60	−390.19	−389.87	−388.75
900					−416.12	−418.60	−418.83	−417.99
1000						−448.72	−449.37	−448.63
				Dichloroacetate				
25	−97.53	−96.81	−96.12	−95.45	−94.78	−93.49	−92.22	−90.97
50	−98.80	−98.08	−97.38	−96.70	−96.03	−94.73	−93.47	−92.22
75	−100.10	−99.37	−98.67	−97.99	−97.33	−96.03	−94.77	−93.53
100	−101.42	−100.70	−100.00	−99.32	−98.66	−97.37	−96.11	−94.88
125	−102.76	−102.05	−101.36	−100.69	−100.03	−98.75	−97.50	−96.27
150	−104.12	−103.42	−102.74	−102.07	−101.42	−100.15	−98.91	−97.69
175	−105.48	−104.81	−104.14	−103.49	−102.84	−101.58	−100.35	−99.14
200	−106.84	−106.21	−105.56	−104.92	−104.29	−103.04	−101.83	−100.62
225	−108.19	−107.61	−106.99	−106.37	−105.75	−104.53	−103.32	−102.13
250	−109.50	−109.01	−108.43	−107.83	−107.23	−106.03	−104.84	−103.67
300	−111.94	−111.76	−111.30	−110.77	−110.22	−109.09	−107.95	−106.80
350	−113.53	−114.29	−114.14	−113.73	−113.25	−112.21	−111.12	−110.02
400		−116.37	−116.85	−116.65	−116.28	−115.37	−114.36	−113.31
450		−116.08	−119.31	−119.49	−119.29	−118.56	−117.65	−116.66
500			−121.33	−122.20	−122.26	−121.76	−120.97	−120.06
550			−122.76	−124.72	−125.16	−124.97	−124.32	−123.50
600			−123.72	−127.06	−127.97	−128.16	−127.69	−126.96
700				−131.40	−133.39	−134.52	−134.44	−133.94
800					−138.79	−140.85	−141.22	−140.95
900					−144.46	−147.28	−148.04	−147.95
1000						−153.92	−154.96	−154.95
				Dichloroacetic Acid				
25	−98.86	−98.01	−97.19	−96.41	−95.64	−94.15	−92.71	−91.30
50	−100.45	−99.58	−98.75	−97.95	−97.17	−95.67	−94.22	−92.80
75	−102.13	−101.24	−100.40	−99.60	−98.81	−97.30	−95.84	−94.42
100	−103.89	−103.00	−102.15	−101.34	−100.55	−99.03	−97.57	−96.14
125	−105.75	−104.85	−103.99	−103.17	−102.38	−100.85	−99.38	−97.95
150	−107.68	−106.78	−105.91	−105.08	−104.28	−102.74	−101.27	−99.83
175	−109.70	−108.78	−107.91	−107.07	−106.26	−104.71	−103.23	−101.79
200	−111.79	−110.87	−109.98	−109.13	−108.31	−106.75	−105.26	−103.81
225	−113.96	−113.03	−112.12	−111.26	−110.43	−108.86	−107.36	−105.91
250	−116.22	−115.27	−114.33	−113.46	−112.62	−111.03	−109.52	−108.06
300	−121.04	−120.00	−118.98	−118.06	−117.19	−115.56	−114.01	−112.53
350	−126.69	−125.16	−123.94	−122.92	−122.00	−120.31	−118.73	−117.22
400		−131.08	−129.25	−128.07	−127.06	−125.28	−123.65	−122.12
450		−139.31	−135.01	−133.51	−132.38	−130.46	−128.77	−127.19
500		−150.68	−141.37	−139.29	−137.94	−135.85	−134.08	−132.45
550		−160.97	−148.46	−145.42	−143.77	−141.44	−139.57	−137.88
600		−170.00	−156.11	−151.91	−149.85	−147.23	−145.23	−143.48
700		−186.10	−171.84	−165.72	−162.70	−159.33	−157.05	−155.15
800		−200.89	−187.17	−180.05	−176.21	−172.06	−169.46	−167.42
900		−215.09	−201.99	−194.43	−190.06	−185.27	−182.40	−180.24
1000		−229.02	−216.46	−208.74	−204.05	−198.82	−195.78	−193.57
				Dichloroacetyl Chloride				
25	−56.14	−55.19	−54.27	−53.37	−52.50	−50.80	−49.14	−47.51
50	−57.87	−56.91	−55.99	−55.10	−54.23	−52.55	−50.91	−49.30
75	−59.70	−58.74	−57.81	−56.92	−56.05	−54.37	−52.74	−51.15
100	−61.62	−60.65	−59.73	−58.83	−57.96	−56.28	−54.66	−53.07

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
Dichloroacetyl Chloride — Continued								
125	−63.63	−62.66	−61.72	−60.82	−59.95	−58.27	−56.64	−55.06
150	−65.73	−64.74	−63.80	−62.90	−62.02	−60.33	−58.71	−57.12
175	−67.91	−66.92	−65.96	−65.05	−64.17	−62.47	−60.84	−59.25
200	−70.17	−69.17	−68.20	−67.27	−66.39	−64.68	−63.04	−61.45
225	−72.53	−71.50	−70.51	−69.57	−68.67	−66.95	−65.30	−63.70
250	−74.97	−73.93	−72.90	−71.94	−71.03	−69.29	−67.63	−66.02
300	−80.22	−79.05	−77.92	−76.90	−75.94	−74.15	−72.46	−70.83
350	−86.53	−84.68	−83.27	−82.14	−81.12	−79.25	−77.51	−75.85
400		−91.24	−89.04	−87.69	−86.56	−84.58	−82.78	−81.08
450		−100.78	−95.35	−93.59	−92.28	−90.13	−88.25	−86.50
500		−114.39	−102.40	−99.87	−98.29	−95.91	−93.92	−92.11
550		−126.55	−110.35	−106.57	−104.59	−101.90	−99.78	−97.90
600		−137.01	−119.00	−113.70	−111.19	−108.11	−105.83	−103.86
700		−155.23	−136.76	−128.93	−125.16	−121.11	−118.45	−116.29
800		−171.62	−153.84	−144.70	−139.86	−134.78	−131.72	−129.36
900		−187.08	−170.12	−160.41	−154.87	−148.95	−145.54	−143.03
1000		−202.08	−185.83	−175.91	−169.96	−163.46	−159.82	−157.26
Dy^{+3}								
25	−158.70	−159.16	−159.56	−159.91	−160.24	−160.80	−161.30	−161.74
50	−157.29	−157.77	−158.19	−158.56	−158.91	−159.52	−160.05	−160.54
75	−155.83	−156.33	−156.77	−157.16	−157.52	−158.17	−158.74	−159.25
100	−154.33	−154.85	−155.31	−155.72	−156.10	−156.78	−157.38	−157.92
125	−152.78	−153.33	−153.82	−154.25	−154.65	−155.36	−155.99	−156.56
150	−151.17	−151.77	−152.29	−152.75	−153.17	−153.92	−154.58	−155.17
175	−149.51	−150.16	−150.72	−151.22	−151.67	−152.45	−153.15	−153.77
200	−147.79	−148.50	−149.11	−149.65	−150.13	−150.97	−151.70	−152.35
225	−145.98	−146.77	−147.46	−148.04	−148.56	−149.46	−150.23	−150.92
250	−144.09	−144.99	−145.75	−146.39	−146.96	−147.93	−148.75	−149.48
300	−139.97	−141.23	−142.23	−142.99	−143.66	−144.79	−145.74	−146.55
350	−135.92	−137.13	−138.62	−139.47	−140.24	−141.56	−142.65	−143.58
400		−135.17	−135.03	−135.88	−136.74	−138.24	−139.49	−140.55
450		−137.62	−131.70	−132.27	−133.16	−134.85	−136.27	−137.47
500			−128.97	−128.71	−129.53	−131.36	−132.96	−134.32
550			−127.27	−125.27	−125.84	−127.78	−129.57	−131.09
600			−126.74	−122.09	−122.11	−124.07	−126.06	−127.76
700				−116.89	−114.62	−116.19	−118.62	−120.73
800					−106.98	−107.59	−110.52	−113.09
900					−98.79	−98.28	−101.78	−104.79
1000						−88.54	−92.63	−95.88
Ethanamine								
25	6.30	6.99	7.66	8.32	8.96	10.23	11.48	12.71
50	5.40	6.09	6.76	7.41	8.05	9.31	10.53	11.74
75	4.39	5.08	5.75	6.40	7.04	8.28	9.50	10.69
100	3.28	3.97	4.64	5.29	5.93	7.17	8.37	9.56
125	2.07	2.77	3.44	4.09	4.72	5.96	7.16	8.34
150	0.78	1.47	2.14	2.79	3.42	4.66	5.86	7.03
175	−0.61	0.08	0.76	1.41	2.04	3.28	4.48	5.65
200	−2.07	−1.38	−0.71	−0.05	0.58	1.82	3.02	4.19
225	−3.61	−2.93	−2.25	−1.59	−0.95	0.29	1.49	2.66
250	−5.23	−4.55	−3.86	−3.20	−2.56	−1.32	−0.12	1.05
300	−8.69	−8.03	−7.31	−6.63	−5.98	−4.73	−3.53	−2.35
350	−12.59	−11.82	−11.04	−10.33	−9.67	−8.40	−7.18	−6.00
400		−16.03	−15.05	−14.29	−13.60	−12.30	−11.07	−9.88
450		−21.15	−19.36	−18.50	−17.76	−16.42	−15.17	−13.97
500		−27.43	−24.01	−22.95	−22.15	−20.75	−19.48	−18.26
550		−33.49	−29.02	−27.66	−26.76	−25.29	−23.98	−22.74
600		−39.27	−34.35	−32.61	−31.57	−30.00	−28.66	−27.40
700		−50.53	−45.49	−43.12	−41.77	−39.96	−38.52	−37.22

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Ethanamine — Continued				
800		−61.79	−56.93	−54.23	−52.61	−50.55	−49.01	−47.66
900		−73.23	−68.58	−65.74	−63.95	−61.67	−60.05	−58.66
1000		−84.95	−80.46	−77.57	−75.68	−73.26	−71.58	−70.18
				Ethane				
25	−3.89	−3.29	−2.72	−2.16	−1.62	−0.57	0.46	1.46
50	−4.64	−4.02	−3.43	−2.86	−2.30	−1.22	−0.18	0.84
75	−5.54	−4.91	−4.30	−3.72	−3.15	−2.06	−1.00	0.03
100	−6.57	−5.92	−5.31	−4.71	−4.14	−3.03	−1.97	−0.93
125	−7.70	−7.05	−6.42	−5.82	−5.25	−4.13	−3.05	−2.01
150	−8.94	−8.28	−7.65	−7.04	−6.45	−5.33	−4.25	−3.19
175	−10.28	−9.61	−8.96	−8.35	−7.76	−6.62	−5.53	−4.47
200	−11.71	−11.03	−10.37	−9.75	−9.15	−8.00	−6.91	−5.84
225	−13.23	−12.54	−11.87	−11.23	−10.63	−9.47	−8.36	−7.29
250	−14.84	−14.14	−13.45	−12.80	−12.18	−11.01	−9.89	−8.82
300	−18.39	−17.61	−16.85	−16.16	−15.52	−14.31	−13.17	−12.08
350	−22.68	−21.51	−20.59	−19.83	−19.14	−17.89	−16.72	−15.60
400		−26.08	−24.68	−23.80	−23.04	−21.71	−20.50	−19.36
450		−32.55	−29.21	−28.07	−27.21	−25.78	−24.52	−23.35
500		−41.54	−34.28	−32.68	−31.65	−30.08	−28.76	−27.54
550		−49.76	−39.97	−37.62	−36.36	−34.61	−33.20	−31.94
600		−57.05	−46.17	−42.91	−41.33	−39.34	−37.84	−36.53
700		−70.24	−59.09	−54.31	−51.98	−49.40	−47.67	−46.24
800		−82.62	−71.88	−66.32	−63.34	−60.15	−58.17	−56.63
900		−94.70	−84.45	−78.55	−75.15	−71.45	−69.27	−67.63
1000		−106.75	−96.92	−90.89	−87.24	−83.20	−80.87	−79.20
				Ethanol				
25	−43.33	−42.68	−42.05	−41.42	−40.81	−39.60	−38.41	−37.23
50	−44.29	−43.64	−43.01	−42.40	−41.79	−40.60	−39.44	−38.29
75	−45.37	−44.72	−44.10	−43.48	−42.88	−41.70	−40.55	−39.42
100	−46.57	−45.92	−45.29	−44.68	−44.08	−42.91	−41.76	−40.64
125	−47.86	−47.21	−46.59	−45.97	−45.38	−44.21	−43.07	−41.95
50	−49.26	−48.61	−47.98	−47.37	−46.77	−45.60	−44.47	−43.35
75	−50.75	−50.10	−49.47	−48.85	−48.25	−47.09	−45.95	−44.84
200	−52.33	−51.68	−51.04	−50.42	−49.82	−48.66	−47.52	−46.41
225	−53.99	−53.35	−52.70	−52.08	−51.48	−50.31	−49.17	−48.06
250	−55.74	−55.10	−54.44	−53.82	−53.21	−52.04	−50.90	−49.79
300	−59.49	−58.85	−58.16	−57.52	−56.90	−55.71	−54.57	−53.45
350	−63.74	−62.95	−62.18	−61.51	−60.87	−59.66	−58.50	−57.38
400		−67.52	−66.52	−65.78	−65.11	−63.86	−62.69	−61.56
450		−73.16	−71.19	−70.32	−69.60	−68.31	−67.11	−65.97
500		−80.19	−76.24	−75.14	−74.34	−72.98	−71.75	−70.59
550		−86.93	−81.72	−80.24	−79.32	−77.87	−76.60	−75.42
600		−93.30	−87.54	−85.61	−84.53	−82.96	−81.65	−80.44
700		−105.63	−99.73	−97.04	−95.58	−93.72	−92.30	−91.03
800		−117.88	−112.19	−109.11	−107.33	−105.16	−103.61	−102.29
900		−130.29	−124.85	−121.60	−119.60	−117.18	−115.53	−114.16
1000		−142.96	−137.73	−134.41	−132.30	−129.71	−127.99	−126.60
				Ethylbenzene				
25	32.44	33.76	35.03	36.26	37.46	39.78	42.03	44.23
50	31.07	32.40	33.67	34.90	36.09	38.39	40.62	42.79
75	29.48	30.81	32.08	33.31	34.50	36.79	39.01	41.17
100	27.68	29.01	30.29	31.51	32.70	34.99	37.21	39.36
125	25.68	27.02	28.30	29.53	30.72	33.01	35.22	37.37
150	23.51	24.85	26.13	27.36	28.55	30.85	33.06	35.21
175	21.17	22.51	23.80	25.03	26.22	28.52	30.73	32.88
200	18.66	20.00	21.30	22.54	23.74	26.04	28.25	30.40

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Ethylbenzene — Continued				
225	16.00	17.33	18.64	19.89	21.10	23.41	25.63	27.78
250	13.18	14.50	15.84	17.10	18.31	20.64	22.86	25.02
300	7.06	8.39	9.80	11.10	12.33	14.69	16.93	19.10
350	0.00	1.63	3.19	4.56	5.84	8.24	10.51	12.69
400		−6.05	−3.99	−2.49	−1.15	1.32	3.63	5.84
450		−15.84	−11.81	−10.06	−8.60	−6.03	−3.68	−1.44
500		−28.40	−20.36	−18.13	−16.52	−13.81	−11.38	−9.11
550		−40.33	−29.72	−26.74	−24.87	−21.97	−19.47	−17.15
600		−51.47	−39.76	−35.84	−33.66	−30.52	−27.92	−25.55
700		−72.80	−60.80	−55.34	−52.39	−48.65	−45.83	−43.33
800		−93.84	−82.27	−76.00	−72.39	−68.03	−64.96	−62.35
900		−115.07	−104.00	−97.39	−93.35	−88.48	−85.19	−82.49
1000		−136.72	−126.08	−119.33	−115.04	−109.82	−106.39	−103.66
				Ethylene				
25	19.45	19.98	20.49	20.98	21.46	22.39	23.29	24.17
50	18.67	19.23	19.76	20.27	20.77	21.73	22.66	23.57
75	17.79	18.36	18.91	19.44	19.95	20.93	21.88	22.80
100	16.82	17.40	17.96	18.50	19.02	20.02	20.98	21.91
125	15.76	16.36	16.93	17.47	18.00	19.01	19.98	20.92
150	14.63	15.24	15.82	16.37	16.90	17.92	18.90	19.86
175	13.43	14.04	14.63	15.19	15.73	16.77	17.76	18.72
200	12.15	12.78	13.38	13.95	14.50	15.54	16.54	17.51
225	10.81	11.44	12.06	12.64	13.20	14.26	15.27	16.24
250	9.39	10.04	10.68	11.27	11.84	12.91	13.93	14.92
300	6.29	7.02	7.73	8.36	8.95	10.06	11.11	12.11
350	2.52	3.64	4.51	5.21	5.85	7.01	8.08	9.10
400		−0.34	1.00	1.83	2.53	3.76	4.87	5.92
450		−6.13	−2.88	−1.81	−1.00	0.33	1.49	2.57
500		−14.37	−7.25	−5.72	−4.75	−3.28	−2.05	−0.93
550		−21.80	−12.19	−9.92	−8.72	−7.06	−5.75	−4.59
600		−28.26	−17.59	−14.41	−12.90	−11.01	−9.61	−8.39
700		−39.70	−28.75	−24.09	−21.83	−19.36	−17.74	−16.40
800		−50.19	−39.65	−34.21	−31.32	−28.25	−26.38	−24.93
900		−60.26	−50.20	−44.43	−41.12	−37.55	−35.48	−33.94
1000		−70.17	−60.53	−54.63	−51.07	−47.17	−44.95	−43.38
				Ethyne				
25	51.89	52.47	53.02	53.56	54.08	55.10	56.09	57.05
50	51.09	51.69	52.26	52.81	53.35	54.39	55.40	56.39
75	50.20	50.81	51.40	51.96	52.51	53.56	54.58	55.58
100	49.23	49.85	50.45	51.02	51.57	52.64	53.67	54.68
125	48.19	48.82	49.42	50.00	50.57	51.65	52.69	53.70
150	47.08	47.72	48.34	48.92	49.49	50.58	51.63	52.65
175	45.91	46.56	47.18	47.78	48.35	49.45	50.51	51.54
200	44.67	45.33	45.97	46.58	47.16	48.27	49.34	50.37
225	43.37	44.05	44.70	45.32	45.91	47.03	48.11	49.15
250	42.00	42.69	43.37	44.00	44.61	45.75	46.83	47.88
300	39.01	39.79	40.54	41.22	41.85	43.03	44.14	45.21
350	35.29	36.53	37.47	38.22	38.90	40.13	41.28	42.37
400		32.63	34.10	35.00	35.75	37.06	38.25	39.37
450		26.72	30.36	31.53	32.40	33.83	35.08	36.23
500		18.07	26.10	27.80	28.85	30.44	31.75	32.95
550		10.38	21.24	23.77	25.09	26.88	28.29	29.54
600		3.82	15.89	19.44	21.12	23.18	24.69	26.00
700		−7.53	4.86	10.11	12.63	15.34	17.11	18.55
800		−17.67	−5.75	0.37	3.61	7.02	9.06	10.63
900		−27.23	−15.86	−9.35	−5.64	−1.67	0.61	2.28
1000		−36.51	−25.61	−18.96	−14.97	−10.62	−8.18	−6.47

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Er^{+3}				
25	−159.90	−160.38	−160.81	−161.19	−161.53	−162.14	−162.67	−163.15
50	−158.41	−158.91	−159.36	−159.76	−160.12	−160.78	−161.35	−161.88
75	−156.87	−157.39	−157.86	−158.28	−158.66	−159.35	−159.96	−160.51
100	−155.28	−155.83	−156.31	−156.75	−157.15	−157.87	−158.51	−159.10
125	−153.63	−154.22	−154.73	−155.19	−155.61	−156.37	−157.04	−157.65
150	−151.94	−152.56	−153.11	−153.60	−154.04	−154.84	−155.54	−156.17
175	−150.18	−150.86	−151.45	−151.97	−152.44	−153.28	−154.01	−154.68
200	−148.35	−149.09	−149.74	−150.30	−150.81	−151.69	−152.47	−153.16
225	−146.45	−147.27	−147.98	−148.59	−149.14	−150.09	−150.90	−151.63
250	−144.45	−145.38	−146.18	−146.85	−147.44	−148.45	−149.32	−150.09
300	−140.12	−141.41	−142.44	−143.23	−143.93	−145.11	−146.10	−146.97
350	−135.87	−137.09	−138.61	−139.49	−140.30	−141.67	−142.80	−143.78
400		−134.96	−134.81	−135.68	−136.57	−138.13	−139.43	−140.54
450		−137.39	−131.26	−131.85	−132.77	−134.50	−135.98	−137.23
500			−128.35	−128.06	−128.90	−130.79	−132.44	−133.85
550			−126.49	−124.41	−124.98	−126.97	−128.81	−130.39
600			−125.86	−121.02	−121.02	−123.02	−125.06	−126.82
700				−115.43	−113.06	−114.64	−117.13	−119.30
800					−104.93	−105.51	−108.49	−111.13
900					−96.24	−95.65	−99.21	−102.29
1000						−85.34	−89.50	−92.82
				Eu^{+2}				
25	−129.10	−129.12	−129.11	−129.08	−129.04	−128.93	−128.79	−128.63
50	−129.05	−129.06	−129.06	−129.04	−129.00	−128.91	−128.78	−128.64
75	−129.01	−129.03	−129.03	−129.01	−128.98	−128.90	−128.79	−128.66
100	−128.98	−129.01	−129.01	−129.00	−128.98	−128.91	−128.81	−128.69
125	−128.95	−128.99	−129.01	−129.01	−129.00	−128.94	−128.85	−128.75
150	−128.93	−128.99	−129.02	−129.03	−129.03	−128.99	−128.91	−128.82
175	−128.90	−128.98	−129.04	−129.06	−129.07	−129.05	−128.99	−128.90
200	−128.86	−128.98	−129.05	−129.10	−129.12	−129.12	−129.08	−129.01
225	−128.81	−128.97	−129.07	−129.14	−129.18	−129.20	−129.18	−129.13
250	−128.72	−128.94	−129.09	−129.18	−129.24	−129.30	−129.30	−129.26
300	−128.42	−128.85	−129.11	−129.27	−129.38	−129.51	−129.57	−129.57
350	−128.01	−128.63	−129.14	−129.35	−129.52	−129.75	−129.87	−129.93
400		−129.15	−129.20	−129.45	−129.68	−130.00	−130.20	−130.32
450		−130.75	−129.33	−129.57	−129.84	−130.27	−130.56	−130.74
500			−129.61	−129.70	−130.01	−130.55	−130.93	−131.19
550			−130.16	−129.88	−130.17	−130.82	−131.31	−131.65
600			−131.00	−130.13	−130.34	−131.08	−131.68	−132.11
700				−131.04	−130.68	−131.50	−132.35	−132.99
800					−131.06	−131.74	−132.89	−133.75
900					−131.38	−131.84	−133.29	−134.36
1000						−131.92	−133.65	−134.82
				Eu^{+3}				
25	−137.30	−137.76	−138.17	−138.53	−138.86	−139.44	−139.95	−140.40
50	−135.94	−136.42	−136.85	−137.23	−137.58	−138.20	−138.75	−139.25
75	−134.52	−135.03	−135.47	−135.87	−136.24	−136.90	−137.48	−138.00
100	−133.06	−133.59	−134.05	−134.47	−134.85	−135.54	−136.15	−136.70
125	−131.54	−132.10	−132.59	−133.03	−133.43	−134.15	−134.79	−135.37
150	−129.96	−130.56	−131.09	−131.55	−131.98	−132.73	−133.40	−134.01
175	−128.32	−128.97	−129.54	−130.04	−130.49	−131.29	−131.99	−132.62
200	−126.62	−127.33	−127.95	−128.49	−128.97	−129.82	−130.55	−131.22
225	−124.83	−125.62	−126.30	−126.89	−127.41	−128.32	−129.10	−129.79
250	−122.95	−123.85	−124.61	−125.25	−125.82	−126.79	−127.62	−128.36
300	−118.86	−120.11	−121.10	−121.86	−122.53	−123.66	−124.61	−125.43
350	−114.78	−116.01	−117.48	−118.34	−119.11	−120.42	−121.51	−122.44
400		−113.93	−113.87	−114.73	−115.58	−117.08	−118.33	−119.39
450		−115.94	−110.47	−111.08	−111.98	−113.65	−115.07	−116.27

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Eu^{+3} — Continued				
500			−107.62	−107.46	−108.29	−110.13	−111.72	−113.07
550			−105.71	−103.94	−104.55	−106.49	−108.27	−109.78
600			−104.87	−100.64	−100.75	−102.72	−104.71	−106.39
700				−95.10	−93.07	−94.71	−97.13	−99.22
800					−85.19	−85.96	−88.87	−91.41
900					−76.76	−76.50	−79.97	−82.94
1000						−66.60	−70.65	−73.84
				Formaldehyde				
25	−26.13	−25.81	−25.49	−25.18	−24.87	−24.26	−23.65	−23.05
50	−26.86	−26.53	−26.20	−25.88	−25.56	−24.93	−24.32	−23.71
75	−27.63	−27.28	−26.95	−26.62	−26.29	−25.66	−25.04	−24.43
100	−28.43	−28.08	−27.73	−27.40	−27.07	−26.43	−25.81	−25.19
125	−29.27	−28.91	−28.56	−28.22	−27.89	−27.24	−26.61	−25.99
150	−30.15	−29.78	−29.43	−29.08	−28.75	−28.09	−27.46	−26.83
175	−31.07	−30.69	−30.33	−29.98	−29.63	−28.97	−28.33	−27.70
200	−32.03	−31.64	−31.26	−30.90	−30.56	−29.88	−29.24	−28.60
225	−33.03	−32.63	−32.24	−31.87	−31.51	−30.83	−30.17	−29.54
250	−34.08	−33.65	−33.24	−32.86	−32.50	−31.80	−31.14	−30.49
300	−36.37	−35.85	−35.37	−34.95	−34.56	−33.83	−33.15	−32.49
350	−39.26	−38.30	−37.67	−37.18	−36.75	−35.97	−35.26	−34.58
400		−41.28	−40.17	−39.56	−39.06	−38.22	−37.47	−36.76
450		−45.98	−42.97	−42.11	−41.51	−40.57	−39.77	−39.04
500		−53.04	−46.18	−44.87	−44.11	−43.03	−42.17	−41.39
550		−59.23	−49.90	−47.85	−46.85	−45.59	−44.65	−43.83
600		−64.40	−54.00	−51.06	−49.75	−48.26	−47.22	−46.35
700		−73.09	−62.41	−57.99	−55.94	−53.87	−52.62	−51.63
800		−80.62	−70.36	−65.16	−62.48	−59.81	−58.31	−57.22
900		−87.55	−77.76	−72.23	−69.14	−65.97	−64.27	−63.08
1000		−94.14	−84.77	−79.11	−75.78	−72.27	−70.43	−69.21
				Formate				
25	−83.86	−83.55	−83.25	−82.94	−82.63	−82.00	−81.38	−80.75
50	−84.39	−84.07	−83.76	−83.44	−83.13	−82.51	−81.88	−81.26
75	−84.90	−84.58	−84.27	−83.95	−83.64	−83.02	−82.40	−81.78
100	−85.39	−85.08	−84.77	−84.46	−84.16	−83.54	−82.93	−82.32
125	−85.87	−85.57	−85.28	−84.98	−84.68	−84.07	−83.47	−82.87
150	−86.33	−86.06	−85.78	−85.49	−85.20	−84.61	−84.02	−83.43
175	−86.77	−86.54	−86.27	−86.00	−85.72	−85.16	−84.58	−84.00
200	−87.19	−86.99	−86.76	−86.51	−86.25	−85.71	−85.15	−84.58
225	−87.55	−87.43	−87.24	−87.01	−86.77	−86.26	−85.72	−85.17
250	−87.86	−87.83	−87.69	−87.51	−87.29	−86.82	−86.30	−85.77
300	−88.15	−88.50	−88.54	−88.45	−88.31	−87.93	−87.48	−87.00
350	−87.33	−88.79	−89.25	−89.32	−89.28	−89.03	−88.67	−88.25
400		−88.59	−89.74	−90.07	−90.18	−90.11	−89.86	−89.52
450		−85.61	−89.87	−90.66	−90.99	−91.16	−91.05	−90.79
500			−89.40	−91.02	−91.68	−92.16	−92.21	−92.07
550			−88.19	−91.10	−92.21	−93.10	−93.35	−93.33
600			−86.41	−90.90	−92.58	−93.97	−94.45	−94.57
700				−90.01	−92.93	−95.47	−96.51	−96.94
800					−93.04	−96.72	−98.36	−99.13
900					−93.29	−97.87	−100.05	−101.09
1000						−99.11	−101.70	−102.86
				Formic Acid				
25	−88.98	−88.57	−88.16	−87.75	−87.34	−86.53	−85.72	−84.91
50	−89.98	−89.56	−89.15	−88.75	−88.34	−87.55	−86.76	−85.98
75	−91.01	−90.59	−90.19	−89.78	−89.38	−88.60	−87.82	−87.05
100	−92.09	−91.67	−91.26	−90.86	−90.46	−89.67	−88.90	−88.14

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Formic Acid — Continued				
125	−93.21	−92.79	−92.38	−91.97	−91.57	−90.79	−90.02	−89.26
150	−94.37	−93.95	−93.53	−93.12	−92.72	−91.94	−91.17	−90.41
175	−95.58	−95.15	−94.72	−94.31	−93.91	−93.12	−92.35	−91.60
200	−96.82	−96.38	−95.95	−95.54	−95.13	−94.34	−93.57	−92.81
225	−98.11	−97.66	−97.22	−96.80	−96.39	−95.59	−94.82	−94.06
250	−99.45	−98.99	−98.53	−98.09	−97.68	−96.87	−96.09	−95.33
300	−102.31	−101.77	−101.26	−100.79	−100.35	−99.52	−98.73	−97.96
350	−105.70	−104.80	−104.16	−103.63	−103.16	−102.29	−101.48	−100.69
400		−108.32	−107.26	−106.63	−106.10	−105.18	−104.33	−103.52
450		−113.33	−110.64	−109.80	−109.18	−108.17	−107.28	−106.45
500		−120.42	−114.39	−113.16	−112.41	−111.28	−110.34	−109.47
550		−126.76	−118.60	−116.73	−115.78	−114.49	−113.48	−112.58
600		−132.24	−123.16	−120.52	−119.29	−117.81	−116.72	−115.78
700		−141.83	−132.51	−128.59	−126.72	−124.75	−123.47	−122.43
800		−150.48	−141.51	−136.92	−134.52	−132.02	−130.53	−129.40
900		−158.65	−150.10	−145.23	−142.46	−139.54	−137.87	−136.66
1000		−166.59	−158.40	−153.41	−150.44	−147.22	−145.44	−144.20
				F^-				
25	−67.34	−67.35	−67.35	−67.34	−67.31	−67.25	−67.16	−67.06
50	−67.24	−67.25	−67.26	−67.25	−67.23	−67.19	−67.12	−67.04
75	−67.09	−67.12	−67.13	−67.13	−67.12	−67.09	−67.04	−66.98
100	−66.90	−66.94	−66.97	−66.98	−66.99	−66.97	−66.94	−66.90
125	−66.68	−66.74	−66.78	−66.81	−66.83	−66.84	−66.82	−66.79
150	−66.40	−66.50	−66.56	−66.61	−66.64	−66.68	−66.68	−66.67
175	−66.08	−66.22	−66.31	−66.38	−66.43	−66.50	−66.53	−66.54
200	−65.69	−65.89	−66.03	−66.13	−66.20	−66.30	−66.36	−66.39
225	−65.24	−65.51	−65.70	−65.84	−65.94	−66.09	−66.18	−66.23
250	−64.68	−65.07	−65.33	−65.51	−65.65	−65.85	−65.98	−66.06
300	−63.15	−63.96	−64.45	−64.76	−64.99	−65.32	−65.53	−65.68
350	−60.54	−62.35	−63.36	−63.84	−64.19	−64.69	−65.03	−65.26
400		−60.71	−62.01	−62.74	−63.26	−63.97	−64.45	−64.79
450		−57.37	−60.31	−61.43	−62.17	−63.15	−63.79	−64.25
500			−58.15	−59.86	−60.89	−62.21	−63.06	−63.66
550			−55.47	−58.01	−59.42	−61.15	−62.23	−62.99
600			−52.46	−55.91	−57.74	−59.95	−61.30	−62.23
700				−51.39	−53.87	−57.10	−59.08	−60.41
800					−49.61	−53.70	−56.37	−58.13
900					−45.22	−49.92	−53.24	−55.36
1000						−46.01	−49.86	−52.13
				Fe^{+2}				
25	−21.87	−22.11	−22.32	−22.49	−22.64	−22.89	−23.08	−23.24
50	−21.23	−21.48	−21.70	−21.88	−22.05	−22.32	−22.54	−22.73
75	−20.58	−20.85	−21.07	−21.27	−21.44	−21.74	−21.98	−22.19
100	−19.92	−20.20	−20.44	−20.65	−20.83	−21.15	−21.41	−21.64
125	−19.25	−19.55	−19.80	−20.02	−20.22	−20.56	−20.84	−21.08
150	−18.56	−18.89	−19.16	−19.40	−19.61	−19.97	−20.27	−20.53
175	−17.85	−18.21	−18.51	−18.76	−18.99	−19.38	−19.70	−19.97
200	−17.11	−17.51	−17.84	−18.12	−18.37	−18.78	−19.13	−19.43
225	−16.34	−16.79	−17.16	−17.47	−17.74	−18.19	−18.57	−18.88
250	−15.52	−16.04	−16.46	−16.81	−17.10	−17.60	−18.00	−18.34
300	−13.70	−14.45	−15.02	−15.44	−15.80	−16.40	−16.88	−17.28
350	−11.89	−12.68	−13.56	−14.04	−14.47	−15.18	−15.75	−16.22
400		−12.15	−12.13	−12.63	−13.12	−13.95	−14.62	−15.16
450		−14.00	−10.86	−11.23	−11.75	−12.70	−13.47	−14.11
500			−9.93	−9.86	−10.36	−11.42	−12.31	−13.04
550			−9.56	−8.59	−8.97	−10.11	−11.12	−11.96
600			−9.84	−7.46	−7.57	−8.75	−9.89	−10.84
700				−5.91	−4.79	−5.82	−7.25	−8.46

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Fe^{+2} — Continued				
800					−1.98	−2.54	−4.30	−5.79
900					1.05	1.07	−1.05	−2.81
1000						4.86	2.37	0.47
				Fe^{+3}				
25	−4.12	−4.60	−5.03	−5.40	−5.74	−6.34	−6.87	−7.34
50	−2.43	−2.93	−3.38	−3.78	−4.14	−4.79	−5.35	−5.87
75	−0.69	−1.21	−1.68	−2.10	−2.48	−3.16	−3.77	−4.31
100	1.10	0.55	0.06	−0.38	−0.78	−1.50	−2.13	−2.71
125	2.95	2.36	1.84	1.38	0.95	0.20	−0.47	−1.08
150	4.85	4.22	3.66	3.16	2.72	1.92	1.22	0.58
175	6.82	6.13	5.52	4.99	4.51	3.67	2.93	2.26
200	8.86	8.10	7.43	6.85	6.34	5.44	4.65	3.95
225	10.99	10.13	9.39	8.76	8.20	7.23	6.40	5.66
250	13.22	12.23	11.41	10.71	10.10	9.05	8.16	7.38
300	18.01	16.64	15.55	14.73	14.01	12.77	11.75	10.86
350	22.51	21.39	19.78	18.87	18.03	16.60	15.41	14.40
400		23.38	23.92	23.06	22.15	20.52	19.15	17.99
450		19.22	27.67	27.24	26.33	24.52	22.97	21.65
500			30.53	31.31	30.55	28.61	26.87	25.38
550			31.92	35.15	34.80	32.81	30.87	29.20
600			31.64	38.61	39.05	37.14	34.99	33.12
700				43.90	47.49	46.29	43.71	41.40
800					56.04	56.28	53.20	50.38
900					65.26	67.10	63.41	60.10
1000						78.44	74.10	70.52
				$Fe(CH_3COO)^+$				
25	−111.90	−111.61	−111.31	−111.02	−110.73	−110.14	−109.55	−108.96
50	−111.94	−111.64	−111.34	−111.04	−110.74	−110.15	−109.56	−108.97
75	−112.11	−111.81	−111.50	−111.20	−110.90	−110.31	−109.72	−109.14
100	−112.40	−112.09	−111.79	−111.49	−111.19	−110.60	−110.01	−109.43
125	−112.78	−112.48	−112.18	−111.88	−111.58	−111.00	−110.41	−109.84
150	−113.24	−112.95	−112.66	−112.36	−112.07	−111.49	−110.91	−110.34
175	−113.78	−113.50	−113.22	−112.93	−112.64	−112.07	−111.50	−110.93
200	−114.38	−114.13	−113.85	−113.57	−113.29	−112.73	−112.17	−111.60
225	−115.04	−114.81	−114.55	−114.29	−114.02	−113.47	−112.91	−112.36
250	−115.75	−115.56	−115.32	−115.07	−114.80	−114.27	−113.73	−113.18
300	−117.26	−117.21	−117.03	−116.80	−116.57	−116.07	−115.56	−115.03
350	−118.91	−119.00	−118.95	−118.76	−118.55	−118.10	−117.62	−117.12
400		−121.41	−121.10	−120.93	−120.75	−120.35	−119.91	−119.44
450		−124.63	−123.47	−123.28	−123.13	−122.78	−122.39	−121.95
500			−126.11	−125.83	−125.68	−125.39	−125.05	−124.65
550			−129.06	−128.56	−128.40	−128.16	−127.87	−127.52
600			−132.34	−131.48	−131.27	−131.07	−130.84	−130.53
700				−137.97	−137.43	−137.26	−137.15	−136.95
800					−144.12	−143.86	−143.90	−143.82
900					−151.23	−150.83	−151.03	−151.06
1000						−158.21	−158.56	−158.64
				$Fe(CH_3COO)_2^\circ$				
25	−201.80	−200.91	−200.06	−199.25	−198.46	−196.94	−195.47	−194.05
50	−202.26	−201.34	−200.47	−199.63	−198.82	−197.26	−195.76	−194.30
75	−203.02	−202.08	−201.19	−200.34	−199.52	−197.94	−196.42	−194.94
100	−204.03	−203.08	−202.18	−201.32	−200.49	−198.89	−197.36	−195.87
125	−205.26	−204.30	−203.40	−202.53	−201.69	−200.08	−198.54	−197.04
150	−206.68	−205.72	−204.81	−203.94	−203.10	−201.48	−199.93	−198.43
175	−208.28	−207.33	−206.41	−205.53	−204.69	−203.07	−201.51	−200.00
200	−210.05	−209.10	−208.18	−207.30	−206.45	−204.83	−203.27	−201.75

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Fe(CH_3COO)_2^\circ$ — Continued				
225	−211.97	−211.04	−210.11	−209.23	−208.38	−206.75	−205.18	−203.67
250	−214.03	−213.12	−212.20	−211.31	−210.46	−208.82	−207.25	−205.74
300	−218.54	−217.72	−216.78	−215.89	−215.03	−213.39	−211.81	−210.29
350	−223.54	−222.84	−221.89	−220.99	−220.12	−218.47	−216.89	−215.37
400		−228.46	−227.47	−226.56	−225.69	−224.03	−222.44	−220.91
450		−234.63	−233.50	−232.57	−231.69	−230.02	−228.43	−226.89
500		−241.38	−239.95	−238.98	−238.09	−236.41	−234.82	−233.28
550		−248.42	−246.81	−245.79	−244.88	−243.18	−241.58	−240.03
600		−255.74	−254.05	−252.96	−252.02	−250.31	−248.69	−247.14
700		−271.20	−269.49	−268.28	−267.29	−265.53	−263.90	−262.34
800		−287.74	−286.06	−284.79	−283.75	−281.95	−280.30	−278.73
900		−305.29	−303.64	−302.35	−301.28	−299.43	−297.77	−296.19
1000		−323.78	−322.16	−320.86	−319.77	−317.89	−316.22	−314.64
				$FeCl^+$				
25	−53.03	−53.01	−52.98	−52.92	−52.86	−52.71	−52.53	−52.33
50	−52.80	−52.78	−52.74	−52.69	−52.63	−52.49	−52.32	−52.14
75	−52.60	−52.59	−52.55	−52.51	−52.45	−52.32	−52.16	−51.99
100	−52.44	−52.43	−52.40	−52.36	−52.31	−52.18	−52.03	−51.87
125	−52.30	−52.30	−52.28	−52.24	−52.19	−52.08	−51.94	−51.78
150	−52.19	−52.19	−52.18	−52.15	−52.11	−52.00	−51.87	−51.72
175	−52.08	−52.11	−52.11	−52.09	−52.05	−51.96	−51.84	−51.70
200	−51.99	−52.04	−52.05	−52.04	−52.02	−51.94	−51.83	−51.70
225	−51.91	−51.98	−52.01	−52.02	−52.01	−51.94	−51.85	−51.73
250	−51.83	−51.93	−51.99	−52.01	−52.01	−51.97	−51.89	−51.78
300	−51.62	−51.86	−51.99	−52.04	−52.08	−52.08	−52.03	−51.95
350	−51.48	−51.77	−52.05	−52.14	−52.20	−52.26	−52.26	−52.21
400		−52.33	−52.19	−52.29	−52.39	−52.51	−52.55	−52.54
450		−54.02	−52.47	−52.52	−52.63	−52.81	−52.90	−52.94
500			−52.96	−52.82	−52.92	−53.16	−53.31	−53.39
550			−53.76	−53.21	−53.27	−53.55	−53.76	−53.89
600			−54.90	−53.73	−53.66	−53.97	−54.24	−54.43
700				−55.22	−54.60	−54.85	−55.27	−55.58
800					−55.70	−55.75	−56.33	−56.78
900					−56.86	−56.65	−57.41	−57.99
1000						−57.62	−58.56	−59.21
				$FeCl_2^\circ$				
25	−81.28	−80.96	−80.65	−80.34	−80.03	−79.41	−78.80	−78.19
50	−81.21	−80.88	−80.55	−80.23	−79.92	−79.29	−78.67	−78.06
75	−81.19	−80.85	−80.52	−80.20	−79.88	−79.25	−78.63	−78.02
100	−81.22	−80.88	−80.55	−80.22	−79.90	−79.26	−78.64	−78.03
125	−81.30	−80.96	−80.62	−80.29	−79.97	−79.33	−78.71	−78.09
150	−81.42	−81.08	−80.74	−80.41	−80.08	−79.44	−78.82	−78.20
175	−81.58	−81.24	−80.89	−80.56	−80.23	−79.59	−78.97	−78.35
200	−81.78	−81.43	−81.09	−80.75	−80.43	−79.78	−79.16	−78.54
225	−82.01	−81.67	−81.32	−80.98	−80.65	−80.01	−79.38	−78.76
250	−82.26	−81.93	−81.58	−81.24	−80.91	−80.27	−79.64	−79.02
300	−82.87	−82.56	−82.20	−81.86	−81.53	−80.88	−80.25	−79.63
350	−83.60	−83.31	−82.94	−82.60	−82.26	−81.61	−80.97	−80.35
400		−84.20	−83.80	−83.44	−83.10	−82.44	−81.80	−81.18
450		−85.31	−84.76	−84.38	−84.03	−83.37	−82.72	−82.10
500		−86.67	−85.84	−85.42	−85.06	−84.38	−83.74	−83.11
550		−88.05	−87.03	−86.56	−86.18	−85.49	−84.84	−84.20
600		−89.43	−88.32	−87.79	−87.38	−86.67	−86.01	−85.38
700		−92.25	−91.13	−90.48	−90.02	−89.27	−88.59	−87.95
800		−95.24	−94.14	−93.43	−92.93	−92.13	−91.43	−90.78
900		−98.39	−97.33	−96.60	−96.07	−95.23	−94.52	−93.86
1000		−101.73	−100.70	−99.96	−99.40	−98.54	−97.82	−97.16

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Glutamic Acid				
25	−173.00	−171.96	−170.95	−169.98	−169.03	−167.18	−165.38	−163.62
50	−174.81	−173.76	−172.75	−171.78	−170.84	−169.00	−167.22	−165.48
75	−176.70	−175.64	−174.64	−173.66	−172.72	−170.89	−169.12	−167.39
100	−178.67	−177.61	−176.60	−175.62	−174.68	−172.85	−171.08	−169.36
125	−180.72	−179.65	−178.64	−177.66	−176.71	−174.87	−173.11	−171.39
150	−182.85	−181.77	−180.75	−179.76	−178.80	−176.97	−175.20	−173.48
175	−185.05	−183.97	−182.93	−181.93	−180.97	−179.12	−177.35	−175.62
200	−187.33	−186.23	−185.18	−184.17	−183.20	−181.34	−179.56	−177.83
225	−189.69	−188.58	−187.49	−186.47	−185.49	−183.62	−181.82	−180.09
250	−192.14	−191.00	−189.88	−188.84	−187.84	−185.95	−184.14	−182.40
300	−197.39	−196.12	−194.88	−193.77	−192.73	−190.78	−188.94	−187.17
350	−203.73	−201.72	−200.20	−198.96	−197.85	−195.82	−193.93	−192.13
400		−208.30	−205.92	−204.45	−203.23	−201.07	−199.11	−197.27
450		−218.03	−212.18	−210.27	−208.86	−206.52	−204.48	−202.58
500		−232.10	−219.21	−216.47	−214.76	−212.18	−210.02	−208.05
550		−244.58	−227.17	−223.09	−220.95	−218.04	−215.74	−213.69
600		−255.20	−235.85	−230.14	−227.43	−224.09	−221.62	−219.49
700		−273.47	−253.62	−245.19	−241.14	−236.76	−233.88	−231.54
800		−289.66	−270.56	−260.73	−255.52	−250.04	−246.73	−244.18
900		−304.78	−286.55	−276.11	−270.15	−263.77	−260.08	−257.37
1000		−319.31	−301.85	−291.18	−284.77	−277.77	−273.84	−271.07
				Glutamine				
25	−126.60	−125.50	−124.44	−123.41	−122.41	−120.47	−118.58	−116.72
50	−128.20	−127.09	−126.03	−125.01	−124.01	−122.08	−120.21	−118.38
75	−129.88	−128.77	−127.71	−126.68	−125.69	−123.76	−121.90	−120.08
100	−131.65	−130.53	−129.46	−128.44	−127.44	−125.52	−123.66	−121.85
125	−133.49	−132.37	−131.30	−130.27	−129.28	−127.35	−125.49	−123.69
150	−135.42	−134.29	−133.21	−132.18	−131.18	−129.25	−127.39	−125.58
175	−137.42	−136.29	−135.20	−134.16	−133.15	−131.22	−129.35	−127.54
200	−139.50	−138.36	−137.26	−136.21	−135.19	−133.25	−131.38	−129.57
225	−141.65	−140.51	−139.38	−138.32	−137.30	−135.34	−133.46	−131.64
250	−143.89	−142.73	−141.58	−140.50	−139.46	−137.49	−135.60	−133.78
300	−148.69	−147.44	−146.19	−145.05	−143.98	−141.96	−140.05	−138.21
350	−154.40	−152.59	−151.11	−149.87	−148.74	−146.65	−144.70	−142.83
400		−158.58	−156.39	−154.97	−153.74	−151.55	−149.55	−147.64
450		−167.20	−162.16	−160.37	−159.00	−156.66	−154.58	−152.63
500		−179.42	−168.60	−166.13	−164.51	−161.97	−159.80	−157.79
550		−190.36	−175.83	−172.26	−170.29	−167.48	−165.19	−163.12
600		−199.80	−183.68	−178.77	−176.33	−173.18	−170.75	−168.60
700		−216.35	−199.81	−192.67	−189.13	−185.11	−182.35	−180.03
800		−231.28	−215.36	−207.07	−202.58	−197.66	−194.54	−192.05
900		−245.43	−230.23	−221.43	−216.32	−210.66	−207.24	−204.62
1000		−259.18	−244.61	−235.62	−230.15	−223.99	−220.35	−217.69
				Glycine				
25	−88.62	−88.11	−87.60	−87.10	−86.61	−85.63	−84.67	−83.71
50	−89.58	−89.06	−88.56	−88.07	−87.58	−86.62	−85.67	−84.74
75	−90.56	−90.04	−89.54	−89.05	−88.57	−87.61	−86.68	−85.76
100	−91.56	−91.05	−90.55	−90.05	−89.57	−88.63	−87.70	−86.78
125	−92.60	−92.08	−91.58	−91.08	−90.60	−89.66	−88.73	−87.82
150	−93.65	−93.14	−92.63	−92.14	−91.65	−90.71	−89.79	−88.88
175	−94.74	−94.22	−93.71	−93.21	−92.73	−91.78	−90.86	−89.96
200	−95.85	−95.33	−94.81	−94.31	−93.83	−92.88	−91.96	−91.05
225	−96.98	−96.46	−95.94	−95.43	−94.94	−93.99	−93.07	−92.17
250	−98.15	−97.62	−97.09	−96.58	−96.08	−95.13	−94.20	−93.30
300	−100.59	−100.04	−99.46	−98.93	−98.43	−97.46	−96.52	−95.61
350	−103.38	−102.62	−101.95	−101.38	−100.85	−99.86	−98.91	−97.99
400		−105.51	−104.58	−103.93	−103.37	−102.33	−101.36	−100.43
450		−109.43	−107.38	−106.60	−105.97	−104.88	−103.88	−102.93

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				Glycine — Continued				
500		−114.74	−110.44	−109.39	−108.67	−107.50	−106.46	−105.49
550		−119.55	−113.80	−112.32	−111.46	−110.19	−109.11	−108.11
600		−123.77	−117.40	−115.40	−114.36	−112.95	−111.81	−110.79
700		−131.27	−124.74	−121.87	−120.40	−118.65	−117.39	−116.30
800		−138.13	−131.84	−128.52	−126.68	−124.58	−123.18	−122.03
900		−144.66	−138.65	−135.14	−133.05	−130.67	−129.15	−127.94
1000		−151.02	−145.26	−141.67	−139.45	−136.86	−135.26	−134.04
				Ga^{+3}				
25	−38.00	−38.51	−38.95	−39.35	−39.71	−40.35	−40.91	−41.41
50	−36.00	−36.52	−36.99	−37.41	−37.79	−38.48	−39.09	−39.64
75	−33.94	−34.50	−34.98	−35.42	−35.83	−36.55	−37.19	−37.78
100	−31.85	−32.43	−32.94	−33.40	−33.82	−34.58	−35.26	−35.87
125	−29.70	−30.32	−30.86	−31.35	−31.79	−32.59	−33.30	−33.94
150	−27.50	−28.16	−28.74	−29.26	−29.73	−30.57	−31.31	−31.99
175	−25.23	−25.96	−26.59	−27.14	−27.65	−28.53	−29.31	−30.02
200	−22.90	−23.69	−24.39	−24.99	−25.53	−26.47	−27.29	−28.03
225	−20.49	−21.37	−22.13	−22.79	−23.38	−24.39	−25.26	−26.04
250	−17.97	−18.98	−19.84	−20.56	−21.19	−22.28	−23.21	−24.03
300	−12.61	−14.01	−15.12	−15.97	−16.72	−18.00	−19.07	−19.99
350	−7.57	−8.69	−10.34	−11.27	−12.13	−13.62	−14.85	−15.90
400		−6.21	−5.66	−6.53	−7.47	−9.15	−10.56	−11.76
450		−10.02	−1.39	−1.82	−2.75	−4.61	−6.21	−7.57
500			1.97	2.77	2.00	0.02	−1.78	−3.31
550			3.81	7.13	6.77	4.74	2.75	1.04
600			3.93	11.07	11.53	9.59	7.39	5.48
700				17.29	20.98	19.77	17.14	14.78
800					30.50	30.78	27.64	24.77
900					40.68	42.59	38.86	35.49
1000						54.94	50.54	46.90
				Gd^{+3}				
25	−158.60	−159.05	−159.45	−159.81	−160.13	−160.69	−161.18	−161.61
50	−157.34	−157.81	−158.23	−158.60	−158.94	−159.54	−160.08	−160.56
75	−156.02	−156.51	−156.95	−157.34	−157.69	−158.33	−158.90	−159.41
100	−154.65	−155.17	−155.62	−156.03	−156.41	−157.08	−157.67	−158.21
125	−153.23	−153.78	−154.26	−154.69	−155.08	−155.79	−156.41	−156.97
150	−151.75	−152.34	−152.85	−153.31	−153.73	−154.47	−155.12	−155.71
175	−150.21	−150.85	−151.41	−151.90	−152.34	−153.12	−153.80	−154.42
200	−148.60	−149.31	−149.91	−150.44	−150.92	−151.75	−152.47	−153.12
225	−146.92	−147.70	−148.37	−148.95	−149.46	−150.35	−151.12	−151.80
250	−145.14	−146.03	−146.78	−147.42	−147.97	−148.93	−149.74	−150.46
300	−141.25	−142.49	−143.48	−144.23	−144.88	−146.00	−146.93	−147.74
350	−137.38	−138.59	−140.06	−140.91	−141.67	−142.97	−144.04	−144.96
400		−136.74	−136.66	−137.51	−138.35	−139.84	−141.07	−142.12
450		−139.03	−133.47	−134.07	−134.96	−136.62	−138.02	−139.20
500			−130.85	−130.66	−131.49	−133.31	−134.88	−136.22
550			−129.18	−127.36	−127.95	−129.88	−131.65	−133.15
600			−128.60	−124.28	−124.37	−126.33	−128.30	−129.97
700				−119.21	−117.13	−118.75	−121.15	−123.23
800					−109.70	−110.43	−113.33	−115.86
900					−101.72	−101.40	−104.86	−107.82
1000						−91.93	−95.97	−99.16
				Heptanoate				
25	−78.39	−77.03	−75.74	−74.51	−73.32	−71.04	−68.85	−66.73
50	−79.80	−78.39	−77.07	−75.80	−74.58	−72.24	−70.00	−67.83
75	−81.39	−79.96	−78.62	−77.33	−76.09	−73.72	−71.45	−69.25
100	−83.12	−81.69	−80.34	−79.04	−77.80	−75.41	−73.12	−70.91

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Heptanoate — Continued				
125	−84.99	−83.56	−82.20	−80.91	−79.66	−77.26	−74.96	−72.74
150	−86.96	−85.55	−84.19	−82.90	−81.65	−79.25	−76.95	−74.72
175	−89.03	−87.64	−86.30	−85.01	−83.76	−81.37	−79.07	−76.84
200	−91.18	−89.83	−88.50	−87.22	−85.98	−83.60	−81.30	−79.08
225	−93.38	−92.10	−90.80	−89.53	−88.30	−85.93	−83.64	−81.42
250	−95.62	−94.44	−93.17	−91.93	−90.71	−88.36	−86.08	−83.87
300	−100.08	−99.28	−98.13	−96.94	−95.77	−93.48	−91.24	−89.05
350	−103.92	−104.15	−103.29	−102.22	−101.12	−98.90	−96.72	−94.56
400		−108.81	−108.56	−107.69	−106.70	−104.60	−102.49	−100.38
450		−111.36	−113.80	−113.30	−112.47	−110.54	−108.51	−106.46
500			−118.79	−118.96	−118.38	−116.69	−114.77	−112.79
550			−123.39	−124.63	−124.41	−123.01	−121.24	−119.34
600			−127.71	−130.28	−130.52	−129.50	−127.89	−126.08
700				−141.73	−143.03	−142.90	−141.68	−140.09
800					−156.07	−156.86	−156.06	−154.70
900					−169.90	−171.42	−171.00	−169.81
1000						−186.66	−186.51	−185.39
				Heptanoic Acid				
25	−85.15	−83.61	−82.14	−80.72	−79.35	−76.68	−74.10	−71.58
50	−87.20	−85.66	−84.19	−82.77	−81.40	−78.74	−76.18	−73.69
75	−89.53	−87.98	−86.50	−85.08	−83.71	−81.06	−78.51	−76.03
100	−92.11	−90.55	−89.07	−87.65	−86.27	−83.62	−81.07	−78.60
125	−94.92	−93.36	−91.87	−90.44	−89.06	−86.41	−83.86	−81.38
150	−97.96	−96.38	−94.88	−93.45	−92.06	−89.40	−86.85	−84.37
175	−101.20	−99.62	−98.11	−96.66	−95.27	−92.60	−90.04	−87.56
200	−104.65	−103.06	−101.53	−100.07	−98.67	−95.98	−93.41	−90.93
225	−108.30	−106.70	−105.14	−103.66	−102.25	−99.54	−96.96	−94.47
250	−112.15	−110.53	−108.93	−107.43	−106.00	−103.28	−100.68	−98.18
300	−120.54	−118.81	−117.07	−115.50	−114.02	−111.23	−108.60	−106.07
350	−130.49	−128.00	−125.94	−124.23	−122.67	−119.79	−117.10	−114.54
400		−138.62	−135.60	−133.64	−131.94	−128.93	−126.16	−123.55
450		−153.08	−146.19	−143.72	−141.82	−138.61	−135.74	−133.07
500		−172.70	−157.93	−154.53	−152.30	−148.81	−145.82	−143.06
550		−190.80	−170.97	−166.08	−163.37	−159.51	−156.36	−153.52
600		−207.09	−185.09	−178.37	−175.02	−170.68	−167.35	−164.40
700		−237.05	−214.49	−204.73	−199.88	−194.37	−190.58	−187.40
800		−265.56	−243.83	−232.50	−226.36	−219.62	−215.34	−211.93
900		−293.65	−272.91	−260.90	−253.91	−246.16	−241.46	−237.87
1000		−321.81	−301.92	−289.65	−282.17	−273.73	−268.75	−265.10
				Hexanoate				
25	−80.45	−79.27	−78.16	−77.09	−76.06	−74.07	−72.16	−70.31
50	−81.68	−80.47	−79.32	−78.22	−77.16	−75.13	−73.17	−71.28
75	−83.07	−81.84	−80.68	−79.57	−78.49	−76.43	−74.45	−72.54
100	−84.59	−83.36	−82.19	−81.07	−79.99	−77.92	−75.93	−74.00
125	−86.23	−85.00	−83.83	−82.71	−81.63	−79.55	−77.56	−75.62
150	−87.96	−86.75	−85.58	−84.47	−83.39	−81.31	79.32	−77.38
175	−89.77	−88.59	−87.44	−86.33	−85.25	−83.18	−81.19	−79.26
200	−91.65	−90.51	−89.38	−88.28	−87.22	−85.16	−83.17	−81.24
225	−93.57	−92.50	−91.40	−90.32	−89.26	−87.22	−85.25	−83.33
250	−95.52	−94.55	−93.49	−92.43	−91.39	−89.38	−87.42	85.50
300	−99.36	−98.77	−97.84	−96.85	−95.87	−93.91	−92.00	−90.11
350	−102.47	−102.96	−102.35	−101.49	−100.58	−98.72	−96.87	−95.02
400		−106.87	−106.93	−106.29	−105.50	−103.77	−101.99	−100.20
450		−108.44	−111.41	−111.17	−110.57	−109.03	−107.35	105.62
500			−115.58	−116.08	−115.75	−114.46	−112.91	−111.26
550			−119.27	−120.94	−121.00	−120.05	−118.65	−117.09
600			−122.62	−125.74	−126.31	−125.76	−124.55	−123.10
700				−135.38	−137.10	−137.54	−136.76	−135.55

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Hexanoate — Continued				
800					−148.34	−149.78	−149.47	−148.51
900					−160.30	−162.54	−162.65	−161.89
1000						−175.92	−176.34	−175.65
				Hexanoic Acid				
25	−87.08	−85.72	−84.42	−83.17	−81.95	−79.58	−77.29	−75.04
50	−88.95	−87.58	−86.28	−85.03	−83.81	−81.46	−79.18	−76.96
75	−91.05	−89.68	−88.37	−87.12	−85.90	−83.55	−81.29	−79.08
100	−93.36	−91.99	−90.68	−89.42	−88.20	−85.86	−83.59	−81.39
125	−95.88	−94.50	−93.18	−91.92	−90.70	−88.35	−86.09	−83.89
150	−98.59	−97.20	−95.88	−94.61	−93.38	−91.03	−88.76	−86.56
175	−101.48	−100.09	−98.75	−97.47	−96.24	−93.88	−91.61	−89.40
200	−104.55	−103.14	−101.79	−100.50	−99.26	−96.89	−94.61	−92.40
225	−107.79	−106.38	−105.00	−103.69	−102.44	−100.05	−97.76	−95.55
250	−111.20	−109.78	−108.37	−107.04	−105.77	−103.36	−101.06	−98.84
300	−118.63	−117.10	−115.57	−114.18	−112.87	−110.41	−108.07	−105.83
350	−127.41	−125.22	−123.41	−121.90	−120.53	−117.98	−115.60	−113.32
400		−134.59	−131.94	−130.20	−128.71	−126.04	−123.60	−121.28
450		−147.32	−141.27	−139.10	−137.42	−134.58	−132.05	−129.68
500		−164.54	−151.60	−148.62	−146.65	−143.57	−140.92	−138.49
550		−180.44	−163.07	−158.78	−156.40	−152.99	−150.20	−147.69
600		−194.75	−175.48	−169.58	−166.64	−162.82	−159.87	−157.27
700		−221.06	−201.30	−192.75	−188.49	−183.64	−180.29	−177.49
800		−246.08	−227.05	−217.13	−211.74	−205.81	−202.04	−199.03
900		−270.73	−252.56	−242.03	−235.91	−229.10	−224.96	−221.78
1000		−295.42	−278.00	−267.24	−260.68	−253.27	−248.89	−245.66
				H^+				
25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
100	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
125	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
175	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
200	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
225	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
250	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
300	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
350	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
400		0.00	0.00	0.00	0.00	0.00	0.00	0.00
450		0.00	0.00	0.00	0.00	0.00	0.00	0.00
500			0.00	0.00	0.00	0.00	0.00	0.00
550			0.00	0.00	0.00	0.00	0.00	0.00
600			0.00	0.00	0.00	0.00	0.00	0.00
700				0.00	0.00	0.00	0.00	0.00
800					0.00	0.00	0.00	0.00
900					0.00	0.00	0.00	0.00
1000						0.00	0.00	0.00
				H_2°				
25	4.24	4.54	4.83	5.13	5.43	6.01	6.60	7.18
50	3.85	4.17	4.47	4.78	5.08	5.67	6.26	6.85
75	3.40	3.72	4.04	4.35	4.65	5.25	5.84	6.43
100	2.89	3.21	3.53	3.85	4.16	4.76	5.36	5.95
125	2.32	2.65	2.98	3.29	3.61	4.22	4.81	5.40
150	1.70	2.04	2.37	2.69	3.00	3.62	4.22	4.81
175	1.03	1.37	1.71	2.03	2.35	2.97	3.57	4.17
200	0.32	0.67	1.01	1.34	1.66	2.28	2.89	3.48

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				H_2° — Continued				
225	−0.44	−0.09	0.26	0.59	0.92	1.55	2.16	2.76
250	−1.25	−0.89	−0.53	−0.19	0.14	0.78	1.39	2.00
300	−3.02	−2.63	−2.23	−1.87	−1.53	−0.87	−0.25	0.36
350	−5.18	−4.58	−4.10	−3.71	−3.34	−2.66	−2.02	−1.40
400		−6.89	−6.16	−5.70	−5.30	−4.58	−3.92	−3.29
450		−10.16	−8.43	−7.84	−7.39	−6.62	−5.93	−5.28
500		−14.73	−10.99	−10.16	−9.62	−8.78	−8.06	−7.39
550		−18.91	−13.86	−12.65	−11.99	−11.05	−10.29	−9.60
600		−22.60	−17.00	−15.31	−14.49	−13.43	−12.62	−11.90
700		−29.28	−23.53	−21.06	−19.85	−18.49	−17.56	−16.78
800		−35.52	−29.99	−27.12	−25.58	−23.90	−22.85	−22.01
900		−41.62	−36.34	−33.30	−31.53	−29.60	−28.44	−27.55
1000		−47.69	−42.63	−39.52	−37.63	−35.52	−34.29	−33.38
				$HAsO_4^{-2}$				
25	−170.79	−170.64	−170.47	−170.29	−170.09	−169.68	−169.25	−168.81
50	−170.73	−170.58	−170.42	−170.24	−170.05	−169.66	−169.24	−168.81
75	−170.59	−170.46	−170.30	−170.14	−169.96	−169.59	−169.19	−168.78
100	−170.37	−170.27	−170.14	−169.99	−169.83	−169.48	−169.11	−168.71
125	−170.08	−170.01	−169.91	−169.79	−169.65	−169.33	−168.99	−168.62
150	−169.70	−169.69	−169.63	−169.54	−169.42	−169.15	−168.84	−168.49
175	−169.22	−169.28	−169.28	−169.23	−169.15	−168.93	−168.65	−168.34
200	−168.62	−168.79	−168.86	−168.87	−168.83	−168.67	−168.44	−168.17
225	−167.89	−168.21	−168.37	−168.45	−168.46	−168.38	−168.21	−167.97
250	−166.97	−167.50	−167.80	−167.96	−168.04	−168.05	−167.94	−167.75
300	−164.30	−165.65	−166.38	−166.77	−167.02	−167.26	−167.32	−167.25
350	−159.33	−162.83	−164.53	−165.26	−165.74	−166.30	−166.57	−166.65
400		−159.44	−162.12	−163.38	−164.19	−165.16	−165.68	−165.95
450		−151.39	−158.92	−161.05	−162.31	−163.81	−164.65	−165.14
500			−154.58	−158.15	−160.06	−162.23	−163.45	−164.20
550			−148.88	−154.63	−157.39	−160.40	−162.08	−163.12
600			−142.20	−150.52	−154.29	−158.31	−160.51	−161.87
700				−141.31	−147.02	−153.27	−156.69	−158.81
800					−138.91	−147.23	−151.98	−154.89
900					−130.66	−140.51	−146.52	−150.08
1000						−133.62	−140.59	−144.43
				$H_2AsO_3^-$				
25	−140.33	−140.02	−139.71	−139.40	−139.08	−138.46	−137.83	−137.20
50	−140.99	−140.67	−140.35	−140.04	−139.72	−139.09	−138.47	−137.84
75	−141.65	−141.33	−141.01	−140.69	−140.38	−139.75	−139.13	−138.51
100	−142.30	−141.99	−141.68	−141.36	−141.05	−140.44	−139.82	−139.20
125	−142.95	−142.65	−142.35	−142.04	−141.74	−141.13	−140.52	−139.91
150	−143.58	−143.31	−143.02	−142.73	−142.43	−141.84	−141.24	−140.64
175	−144.20	−143.96	−143.69	−143.41	−143.13	−142.55	−141.97	−141.38
200	−144.79	−144.59	−144.35	−144.09	−143.83	−143.27	−142.71	−142.13
225	−145.34	−145.21	−145.00	−144.77	−144.52	−144.00	−143.45	−142.90
250	−145.84	−145.79	−145.64	−145.44	−145.22	−144.73	−144.21	−143.67
300	−146.51	−146.83	−146.85	−146.75	−146.59	−146.19	−145.73	−145.24
350	−146.10	−147.50	−147.93	−147.98	−147.92	−147.65	−147.27	−146.84
400		−147.66	−148.79	−149.10	−149.19	−149.09	−148.81	−148.45
450		−145.01	−149.29	−150.06	−150.36	−150.49	−150.35	−150.07
500			−149.20	−150.78	−151.41	−151.85	−151.87	−151.69
550			−148.36	−151.24	−152.31	−153.15	−153.36	−153.30
600			−146.93	−151.41	−153.06	−154.37	−154.81	−154.89
700				−151.25	−154.15	−156.61	−157.58	−157.96
800					−155.01	−158.60	−160.15	−160.85
900					−156.02	−160.51	−162.58	−163.54
1000						−162.51	−164.97	−166.03

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$H_2AsO_4^-$				
25	−180.01	−179.60	−179.20	−178.80	−178.40	−177.62	−176.85	−176.08
50	−180.71	−180.29	−179.88	−179.47	−179.07	−178.28	−177.50	−176.73
75	−181.41	−180.99	−180.58	−180.17	−179.77	−178.98	−178.20	−177.43
100	−182.12	−181.70	−181.29	−180.88	−180.49	−179.70	−178.93	−178.16
125	−182.81	−182.41	−182.01	−181.61	−181.22	−180.44	−179.67	−178.91
150	−183.50	−183.12	−182.73	−182.34	−181.96	−181.20	−180.44	−179.69
175	−184.18	−183.82	−183.46	−183.08	−182.71	−181.96	−181.22	−180.48
200	−184.83	−184.52	−184.18	−183.82	−183.46	−182.74	−182.01	−181.28
225	−185.44	−185.19	−184.89	−184.56	−184.22	−183.52	−182.81	−182.10
250	−185.99	−185.84	−185.59	−185.29	−184.98	−184.31	−183.63	−182.93
300	−186.79	−187.01	−186.93	−186.72	−186.47	−185.90	−185.27	−184.62
350	−186.51	−187.83	−188.14	−188.09	−187.93	−187.48	−186.94	−186.34
400		−188.12	−189.14	−189.35	−189.34	−189.06	−188.61	−188.09
450		−185.61	−189.79	−190.45	−190.66	−190.60	−190.29	−189.85
500			−189.86	−191.33	−191.86	−192.11	−191.95	−191.61
550			−189.17	−191.95	−192.92	−193.56	−193.59	−193.36
600			−187.91	−192.28	−193.82	−194.94	−195.20	−195.10
700				−192.46	−195.25	−197.50	−198.28	−198.49
800					−196.47	−199.85	−201.20	−201.72
900					−197.84	−202.12	−203.99	−204.76
1000						−204.50	−206.75	−207.62
				HBr°				
25	−13.14	−12.29	−11.48	−10.70	−9.95	−8.50	−7.10	−5.75
50	−14.23	−13.35	−12.52	−11.72	−10.95	−9.46	−8.03	−6.64
75	−15.34	−14.44	−13.59	−12.77	−11.99	−10.48	−9.03	−7.62
100	−16.46	−15.54	−14.68	−13.85	−13.06	−11.53	−10.06	−8.64
125	−17.58	−16.66	−15.78	−14.95	−14.14	−12.60	−11.12	−9.69
150	−18.72	−17.78	−16.90	−16.06	−15.24	−13.69	−12.20	−10.76
175	−19.86	−18.92	−18.03	−17.17	−16.35	−14.79	−13.29	−11.84
200	−21.02	−20.08	−19.17	−18.30	−17.48	−15.90	−14.39	−12.93
225	−22.19	−21.24	−20.32	−19.44	−18.61	−17.01	−15.50	−14.03
250	−23.39	−22.43	−21.48	−20.60	−19.75	−18.14	−16.61	−15.14
300	−25.88	−24.88	−23.87	−22.94	−22.07	−20.42	−18.87	−17.37
350	−28.87	−27.52	−26.34	−25.34	−24.43	−22.73	−21.15	−19.63
400		−30.62	−28.96	−27.83	−26.85	−25.08	−23.45	−21.91
450		−35.40	−31.80	−30.43	−29.34	−27.47	−25.79	−24.21
500		−42.52	−35.00	−33.16	−31.91	−29.90	−28.15	−26.54
550		−48.69	−38.65	−36.07	−34.57	−32.38	−30.55	−28.89
600		−53.77	−42.65	−39.15	−37.33	−34.90	−32.98	−31.27
700		−62.09	−50.68	−45.67	−43.11	−40.09	−37.94	−36.11
800		−69.04	−58.05	−52.25	−49.04	−45.41	−43.01	−41.07
900		−75.19	−64.69	−58.55	−54.92	−50.78	−48.18	−46.14
1000		−80.84	−70.77	−64.50	−60.62	−56.14	−53.39	−51.32
				HCN°				
25	28.60	29.14	29.65	30.16	30.65	31.61	32.55	33.47
50	27.81	28.37	28.91	29.42	29.93	30.91	31.86	32.80
75	26.96	27.53	28.07	28.60	29.11	30.11	31.07	32.01
100	26.05	26.62	27.17	27.71	28.22	29.22	30.19	31.14
125	25.08	25.66	26.21	26.75	27.27	28.28	29.26	30.21
150	24.06	24.64	25.20	25.74	26.27	27.28	28.26	29.22
175	22.99	23.57	24.14	24.69	25.21	26.23	27.22	28.17
200	21.88	22.46	23.03	23.58	24.11	25.14	26.12	27.08
225	20.73	21.31	21.88	22.44	22.97	24.00	24.99	25.95
250	19.54	20.11	20.69	21.25	21.79	22.82	23.81	24.78
300	17.04	17.59	18.19	18.76	19.31	20.35	21.35	22.33
350	14.29	14.89	15.54	16.13	16.68	17.74	18.76	19.73
400		11.95	12.73	13.35	13.93	15.01	16.03	17.02
450		8.43	9.75	10.44	11.04	12.15	13.19	14.19

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	Pressure, kbar 0.5	1.0	1.5	2.0	3.0	4.0	5.0
				HCN° — Continued				
500		4.17	6.56	7.39	8.04	9.19	10.24	11.25
550		0.08	3.17	4.19	4.91	6.11	7.19	8.21
600		−3.79	−0.41	0.86	1.67	2.93	4.04	5.07
700		−11.29	−7.83	−6.14	−5.13	−3.70	−2.54	−1.47
800		−18.71	−15.37	−13.46	−12.27	−10.68	−9.44	−8.34
900		−26.18	−22.97	−20.97	−19.67	−17.93	−16.64	−15.51
1000		−33.77	−30.67	−28.63	−27.26	−25.43	−24.10	−22.96
				HCO_3^-				
25	−140.28	−139.99	−139.67	−139.35	−139.02	−138.35	−137.65	−136.95
50	−140.86	−140.56	−140.24	−139.91	−139.57	−138.89	−138.19	−137.48
75	−141.43	−141.13	−140.81	−140.48	−140.14	−139.46	−138.76	−138.05
100	−141.99	−141.69	−141.38	−141.05	−140.72	−140.04	−139.35	−138.64
125	−142.54	−142.25	−141.95	−141.63	−141.30	−140.63	−139.95	−139.25
150	−143.07	−142.80	−142.51	−142.21	−141.89	−141.23	−140.56	−139.86
175	−143.58	−143.34	−143.07	−142.78	−142.47	−141.84	−141.17	−140.49
200	−144.05	−143.86	−143.62	−143.35	−143.06	−142.44	−141.79	−141.13
225	−144.48	−144.35	−144.15	−143.90	−143.63	−143.05	−142.42	−141.77
250	−144.84	−144.81	−144.66	−144.45	−144.21	−143.65	−143.05	−142.42
300	−145.24	−145.58	−145.60	−145.49	−145.32	−144.86	−144.32	−143.73
350	−144.52	−145.96	−146.40	−146.44	−146.37	−146.04	−145.59	−145.06
400		−145.83	−146.96	−147.27	−147.34	−147.19	−146.84	−146.39
450		−142.88	−147.15	−147.91	−148.21	−148.29	−148.08	−147.71
500			−146.73	−148.32	−148.94	−149.34	−149.28	−149.03
550			−145.56	−148.44	−149.51	−150.31	−150.45	−150.32
600			−143.79	−148.27	−149.91	−151.19	−151.57	−151.57
700				−147.39	−150.28	−152.72	−153.64	−153.95
800					−150.38	−153.95	−155.47	−156.11
900					−150.59	−155.06	−157.12	−158.03
1000						−156.24	−158.69	−159.71
				HCl°				
25	−22.87	−22.16	−21.49	−20.83	−20.20	−18.97	−17.78	−16.62
50	−23.78	−23.05	−22.35	−21.67	−21.02	−19.76	−18.55	−17.36
75	−24.72	−23.97	−23.26	−22.57	−21.90	−20.63	−19.39	−18.20
100	−25.68	−24.92	−24.19	−23.50	−22.82	−21.53	−20.28	−19.08
125	−26.66	−25.89	−25.15	−24.45	−23.77	−22.46	−21.21	−19.99
150	−27.66	−26.88	−26.13	−25.42	−24.73	−23.42	−22.15	−20.93
175	−28.68	−27.89	−27.13	−26.41	−25.72	−24.39	−23.11	−21.88
200	−29.71	−28.92	−28.15	−27.42	−26.72	−25.38	−24.09	−22.86
225	−30.78	−29.97	−29.18	−28.44	−27.73	−26.38	−25.09	−23.84
250	−31.86	−31.05	−30.24	−29.48	−28.76	−27.39	−26.09	−24.84
300	−34.17	−33.29	−32.41	−31.62	−30.87	−29.46	−28.14	−26.87
350	−37.02	−35.75	−34.70	−33.83	−33.04	−31.58	−30.23	−28.93
400		−38.69	−37.15	−36.15	−35.29	−33.76	−32.36	−31.04
450		−43.39	−39.85	−38.59	−37.62	−35.99	−34.53	−33.18
500		−50.51	−42.93	−41.19	−40.05	−38.27	−36.75	−35.35
550		−56.67	−46.48	−43.97	−42.59	−40.62	−39.01	−37.57
600		−61.70	−50.40	−46.95	−45.24	−43.02	−41.32	−39.82
700		−69.92	−58.32	−53.31	−50.82	−48.00	−46.07	−44.45
800		−76.75	−65.59	−59.77	−56.61	−53.16	−50.97	−49.23
900		−82.80	−72.14	−65.97	−62.38	−58.41	−56.00	−54.16
1000		−88.36	−78.14	−71.83	−67.99	−63.66	−61.11	−59.24
				$HCrO_4^-$				
25	−182.80	−182.29	−181.79	−181.30	−180.82	−179.89	−178.96	−178.06
50	−183.92	−183.39	−182.88	−182.38	−181.90	−180.94	−180.01	−179.09
75	−185.08	−184.54	−184.03	−183.53	−183.04	−182.08	−181.14	−180.22
100	−186.26	−185.73	−185.22	−184.72	−184.23	−183.27	−182.33	−181.41

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$HCrO_4^-$ — Continued				
125	−187.47	−186.95	−186.44	−185.94	−185.46	−184.50	−183.57	−182.65
150	−188.69	−188.19	−187.69	−187.20	−186.72	−185.77	−184.85	−183.94
175	−189.92	−189.44	−188.96	−188.48	−188.01	−187.08	−186.16	−185.26
200	−191.15	−190.71	−190.25	−189.78	−189.32	−188.41	−187.50	−186.61
225	−192.37	−191.98	−191.55	−191.10	−190.66	−189.76	−188.87	−187.99
250	−193.55	−193.25	−192.86	−192.44	−192.01	−191.14	−190.27	−189.40
300	−195.70	−195.72	−195.47	−195.13	−194.75	−193.95	−193.13	−192.29
350	−196.96	−197.96	−198.04	−197.82	−197.53	−196.83	−196.07	−195.28
400		−199.71	−200.47	−200.48	−200.30	−199.75	−199.07	−198.33
450		−198.92	−202.62	−203.04	−203.06	−202.69	−202.12	−201.45
500			−204.30	−205.46	−205.75	−205.65	−205.21	−204.62
550			−205.33	−207.68	−208.37	−208.60	−208.32	−207.83
600			−205.87	−209.68	−210.89	−211.54	−211.45	−211.07
700				−213.34	−215.72	−217.37	−217.72	−217.58
800					−220.50	−223.16	−223.99	−224.11
900					−225.56	−229.04	−230.30	−230.62
1000						−235.14	−236.70	−237.11
				HF°				
25	−71.66	−71.51	−71.34	−71.17	−71.00	−70.64	−70.27	−69.89
50	−72.24	−72.08	−71.91	−71.73	−71.56	−71.20	−70.83	−70.45
75	−72.84	−72.68	−72.50	−72.33	−72.15	−71.79	−71.42	−71.05
100	−73.47	−73.30	−73.13	−72.95	−72.77	−72.41	−72.05	−71.68
125	−74.13	−73.95	−73.78	−73.60	−73.42	−73.06	−72.70	−72.33
150	−74.80	−74.63	−74.45	−74.27	−74.09	−73.73	−73.37	−73.00
175	−75.50	−75.32	−75.15	−74.97	−74.79	−74.43	−74.06	−73.70
200	−76.21	−76.04	−75.86	−75.68	−75.50	−75.14	−74.78	−74.42
225	−76.95	−76.78	−76.60	−76.42	−76.24	−75.88	−75.51	−75.15
250	−77.70	−77.53	−77.35	−77.17	−76.99	−76.63	−76.27	−75.90
300	−79.24	−79.09	−78.91	−78.73	−78.55	−78.19	−77.82	−77.46
350	−80.83	−80.71	−80.53	−80.35	−80.17	−79.81	−79.45	−79.08
400		−82.39	−82.21	−82.03	−81.85	−81.49	−81.12	−80.76
450		−84.13	−83.94	−83.76	−83.58	−83.22	−82.86	−82.50
500		−85.92	−85.73	−85.54	−85.36	−85.00	−84.64	−84.28
550		−87.75	−87.56	−87.37	−87.19	−86.83	−86.47	−86.11
600		−89.63	−89.43	−89.25	−89.06	−88.70	−88.34	−87.98
700		−93.50	−93.30	−93.12	−92.93	−92.57	−92.21	−91.85
800		−97.52	−97.32	−97.13	−96.95	−96.58	−96.22	−95.86
900		−101.67	−101.47	−101.28	−101.10	−100.73	−100.37	−100.01
1000		−105.95	−105.75	−105.56	−105.37	−105.00	−104.64	−104.28
				HF_2^-				
25	−138.16	−137.90	−137.63	−137.36	−137.09	−136.54	−135.99	−135.43
50	−138.68	−138.41	−138.14	−137.87	−137.60	−137.05	−136.50	−135.94
75	−139.15	−138.89	−138.62	−138.35	−138.08	−137.53	−136.99	−136.44
100	−139.58	−139.33	−139.06	−138.80	−138.53	−138.00	−137.46	−136.92
125	−139.97	−139.73	−139.48	−139.22	−138.96	−138.44	−137.91	−137.38
150	−140.32	−140.10	−139.86	−139.61	−139.37	−138.86	−138.34	−137.82
175	−140.61	−140.42	−140.21	−139.98	−139.75	−139.26	−138.76	−138.24
200	−140.86	−140.71	−140.53	−140.32	−140.10	−139.64	−139.15	−138.66
225	−141.03	−140.96	−140.81	−140.63	−140.43	−140.00	−139.53	−139.06
250	−141.13	−141.14	−141.05	−140.91	−140.73	−140.34	−139.90	−139.44
300	−140.92	−141.31	−141.40	−141.36	−141.25	−140.95	−140.58	−140.17
350	−139.55	−141.03	−141.54	−141.65	−141.65	−141.48	−141.20	−140.84
400		−140.18	−141.38	−141.76	−141.91	−141.92	−141.74	−141.46
450		−136.48	−140.79	−141.63	−142.00	−142.25	−142.21	−142.02
500			−139.55	−141.21	−141.91	−142.47	−142.60	−142.52
550			−137.51	−140.45	−141.60	−142.57	−142.90	−142.94
600			−134.82	−139.36	−141.09	−142.54	−143.10	−143.29
700				−136.53	−139.49	−142.11	−143.22	−143.72

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	Pressure, kbar 1.5	2.0	3.0	4.0	5.0
				HF_2^- — Continued				
800					−137.48	−141.23	−142.94	−143.78
900					−135.44	−140.09	−142.34	−143.45
1000						−138.89	−141.54	−142.76
				HO_2^-				
25	−16.10	−16.03	−15.93	−15.83	−15.71	−15.46	−15.17	−14.88
50	−16.22	−16.14	−16.05	−15.95	−15.84	−15.59	−15.32	−15.04
75	−16.28	−16.22	−16.13	−16.04	−15.93	−15.70	−15.44	−15.17
100	−16.31	−16.26	−16.18	−16.10	−16.00	−15.78	−15.54	−15.28
125	−16.30	−16.27	−16.21	−16.13	−16.04	−15.84	−15.61	−15.37
150	−16.25	−16.24	−16.20	−16.14	−16.07	−15.88	−15.67	−15.44
175	−16.15	−16.18	−16.16	−16.12	−16.06	−15.91	−15.72	−15.50
200	−15.99	−16.07	−16.09	−16.08	−16.04	−15.91	−15.75	−15.55
225	−15.77	−15.92	−15.99	−16.00	−15.99	−15.90	−15.76	−15.59
250	−15.45	−15.71	−15.84	−15.90	−15.92	−15.87	−15.76	−15.61
300	−14.42	−15.07	−15.41	−15.58	−15.68	−15.75	−15.72	−15.62
350	−12.22	−13.95	−14.76	−15.11	−15.32	−15.54	−15.61	−15.59
400		−12.48	−13.84	−14.45	−14.82	−15.25	−15.44	−15.51
450		−8.51	−12.50	−13.56	−14.16	−14.85	−15.20	−15.38
500			−10.58	−12.39	−13.32	−14.34	−14.88	−15.18
550			−7.93	−10.90	−12.27	−13.71	−14.47	−14.92
600			−4.75	−9.10	−11.01	−12.95	−13.97	−14.57
700				−4.98	−7.93	−11.02	−12.64	−13.61
800					−4.44	−8.60	−10.88	−12.23
900					−0.91	−5.88	−8.77	−10.43
1000						−3.08	−6.44	−8.24
				HPO_4^{-2}				
25	−260.31	−260.24	−260.16	−260.05	−259.93	−259.65	−259.35	−259.02
50	−260.06	−260.00	−259.91	−259.82	−259.70	−259.45	−259.17	−258.86
75	−259.71	−259.67	−259.60	−259.51	−259.42	−259.19	−258.92	−258.64
100	−259.28	−259.26	−259.22	−259.15	−259.07	−258.87	−258.63	−258.37
125	−258.76	−258.78	−258.77	−258.73	−258.67	−258.51	−258.30	−258.06
150	−258.14	−258.23	−258.26	−258.26	−258.22	−258.10	−257.93	−257.72
175	−257.42	−257.59	−257.68	−257.72	−257.72	−257.65	−257.52	−257.35
200	−256.58	−256.86	−257.02	−257.12	−257.16	−257.16	−257.08	−256.94
225	−255.59	−256.02	−256.28	−256.45	−256.55	−256.63	−256.60	−256.51
250	−254.41	−255.06	−255.46	−255.71	−255.88	−256.05	−256.09	−256.05
300	−251.20	−252.67	−253.51	−254.00	−254.34	−254.76	−254.97	−255.05
350	−245.71	−249.28	−251.12	−251.95	−252.53	−253.27	−253.70	−253.93
400		−245.47	−248.16	−249.52	−250.42	−251.58	−252.27	−252.71
450		−237.33	−244.42	−246.62	−247.98	−249.67	−250.69	−251.35
500			−239.60	−243.17	−245.15	−247.52	−248.93	−249.85
550			−233.49	−239.09	−241.90	−245.10	−246.97	−248.20
600			−226.47	−234.43	−238.21	−242.40	−244.80	−246.36
700				−224.20	−229.74	−236.12	−239.75	−242.07
800					−220.40	−228.75	−233.74	−236.87
900					−210.85	−220.64	−226.90	−230.71
1000						−212.31	−219.56	−223.65
				$H_2PO_4^-$				
25	−270.14	−269.77	−269.41	−269.05	−268.69	−267.98	−267.26	−266.56
50	−270.68	−270.30	−269.93	−269.56	−269.20	−268.48	−267.76	−267.05
75	−271.20	−270.82	−270.45	−270.09	−269.72	−269.01	−268.29	−267.59
100	−271.72	−271.35	−270.98	−270.62	−270.26	−269.55	−268.84	−268.14
125	−272.22	−271.87	−271.51	−271.16	−270.81	−270.10	−269.41	−268.71
150	−272.71	−272.38	−272.04	−271.70	−271.35	−270.67	−269.98	−269.30
175	−273.18	−272.88	−272.56	−272.23	−271.90	−271.23	−270.56	−269.89
200	−273.61	−273.36	−273.07	−272.76	−272.45	−271.80	−271.15	−270.49

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$H_2PO_4^-$ — Continued				
225	−274.00	−273.82	−273.56	−273.29	−272.99	−272.38	−271.74	−271.10
250	−274.32	−274.24	−274.04	−273.80	−273.53	−272.95	−272.34	−271.72
300	−274.63	−274.93	−274.92	−274.77	−274.57	−274.09	−273.55	−272.97
350	−273.83	−275.24	−275.65	−275.66	−275.56	−275.21	−274.76	−274.24
400		−275.05	−276.15	−276.42	−276.47	−276.30	−275.96	−275.52
450		−272.07	−276.27	−277.01	−277.28	−277.35	−277.14	−276.79
500			−275.80	−277.36	−277.96	−278.34	−278.30	−278.06
550			−274.57	−277.42	−278.47	−279.26	−279.42	−279.30
600			−272.76	−277.19	−278.82	−280.10	−280.49	−280.52
700				−276.23	−279.09	−281.53	−282.47	−282.81
800					−279.10	−282.67	−284.21	−284.89
900					−279.22	−283.69	−285.78	−286.73
1000						−284.78	−287.28	−288.33
				$H_2P_2O_7^{-2}$				
25	−480.40	−479.80	−479.21	−478.63	−478.07	−476.96	−475.87	−474.79
50	−481.36	−480.74	−480.14	−479.56	−478.99	−477.86	−476.76	−475.68
75	−482.28	−481.67	−481.07	−480.49	−479.92	−478.80	−477.70	−476.62
100	−483.17	−482.58	−482.00	−481.42	−480.86	−479.75	−478.67	−477.59
125	−484.03	−483.46	−482.90	−482.34	−481.80	−480.71	−479.64	−478.58
150	−484.84	−484.32	−483.78	−483.25	−482.72	−481.66	−480.61	−479.57
175	−485.58	−485.13	−484.64	−484.14	−483.63	−482.62	−481.59	−480.57
200	−486.25	−485.89	−485.46	−485.00	−484.53	−483.56	−482.57	−481.58
225	−486.82	−486.59	−486.24	−485.84	−485.41	−484.50	−483.55	−482.59
250	−487.24	−487.21	−486.97	−486.64	−486.26	−485.42	−484.53	−483.60
300	−487.38	−488.11	−488.24	−488.10	−487.87	−487.22	−486.46	−485.63
350	−485.26	−488.19	−489.17	−489.35	−489.32	−488.94	−488.35	−487.64
400		−487.26	−489.60	−490.31	−490.58	−490.57	−490.19	−489.64
450		−480.71	−489.24	−490.88	−491.60	−492.06	−491.96	−491.59
500			−487.67	−490.94	−492.31	−493.41	−493.65	−493.49
550			−484.55	−490.40	−492.67	−494.58	−495.22	−495.32
600			−480.23	−489.25	−492.67	−495.56	−496.67	−497.05
700				−485.84	−491.72	−496.93	−499.15	−500.17
800					−490.14	−497.63	−501.06	−502.75
900					−488.71	−497.98	−502.51	−504.75
1000						−498.40	−503.74	−506.19
				$H_3PO_4^\circ$				
25	−273.10	−272.54	−272.00	−271.47	−270.96	−269.96	−268.99	−268.04
50	−274.07	−273.49	−272.93	−272.39	−271.87	−270.84	−269.85	−268.89
75	−275.09	−274.49	−273.92	−273.37	−272.84	−271.81	−270.80	−269.83
100	−276.15	−275.54	−274.96	−274.41	−273.87	−272.82	−271.81	−270.83
125	−277.24	−276.62	−276.04	−275.48	−274.93	−273.88	−272.86	−271.87
150	−278.36	−277.74	−277.15	−276.59	−276.04	−274.98	−273.95	−272.96
175	−279.52	−278.90	−278.30	−277.73	−277.17	−276.11	−275.08	−274.08
200	−280.71	−280.08	−279.48	−278.90	−278.34	−277.27	−276.24	−275.23
225	−281.93	−281.30	−280.69	−280.10	−279.54	−278.46	−277.42	−276.41
250	−283.18	−282.55	−281.93	−281.34	−280.77	−279.68	−278.63	−277.62
300	−285.80	−285.16	−284.50	−283.88	−283.30	−282.19	−281.13	−280.11
350	−288.76	−287.95	−287.20	−286.54	−285.94	−284.80	−283.72	−282.69
400		−291.06	−290.04	−289.32	−288.67	−287.50	−286.40	−285.35
450		−295.14	−293.08	−292.22	−291.52	−290.29	−289.16	−288.09
500		−300.56	−296.37	−295.26	−294.47	−293.16	−292.00	−290.91
550		−305.52	−299.96	−298.45	−297.53	−296.12	−294.91	−293.80
600		−309.94	−303.80	−301.78	−300.69	−299.15	−297.90	−296.75
700		−317.94	−311.64	−308.81	−307.30	−305.45	−304.07	−302.86
800		−325.37	−319.30	−316.04	−314.19	−312.00	−310.49	−309.22
900		−332.54	−326.73	−323.29	−321.21	−318.75	−317.12	−315.80
1000		−339.59	−334.01	−330.50	−328.28	−325.63	−323.93	−322.59

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$H_3P_2O_7^-$				
25	−483.60	−483.01	−482.44	−481.88	−481.33	−480.27	−479.23	−478.21
50	−484.90	−484.29	−483.71	−483.14	−482.58	−481.50	−480.44	−479.41
75	−486.26	−485.64	−485.05	−484.47	−483.91	−482.82	−481.76	−480.72
100	−487.66	−487.04	−486.44	−485.87	−485.31	−484.21	−483.15	−482.11
125	−489.08	−488.47	−487.88	−487.31	−486.75	−485.66	−484.60	−483.56
150	−490.54	−489.95	−489.36	−488.79	−488.24	−487.16	−486.10	−485.06
175	−492.01	−491.44	−490.87	−490.31	−489.76	−488.69	−487.64	−486.61
200	−493.50	−492.96	−492.41	−491.86	−491.32	−490.26	−489.22	−488.20
225	−494.98	−494.49	−493.97	−493.44	−492.91	−491.87	−490.84	−489.83
250	−496.44	−496.03	−495.54	−495.03	−494.52	−493.50	−492.49	−491.49
300	−499.18	−499.08	−498.71	−498.27	−497.81	−496.85	−495.88	−494.91
350	−501.13	−501.94	−501.87	−501.55	−501.16	−500.29	−499.38	−498.44
400		−504.38	−504.94	−504.82	−504.54	−503.80	−502.96	−502.07
450		−504.50	−507.78	−508.03	−507.92	−507.36	−506.61	−505.79
500			−510.20	−511.14	−511.28	−510.95	−510.32	−509.57
550			−512.05	−514.08	−514.59	−514.56	−514.08	−513.41
600			−513.47	−516.85	−517.84	−518.19	−517.87	−517.30
700				−522.13	−524.18	−525.45	−525.53	−525.19
800					−530.56	−532.76	−533.27	−533.16
900					−537.27	−540.22	−541.12	−541.18
1000						−547.94	−549.11	−549.25
				HS^-				
25	2.86	3.10	3.35	3.60	3.86	4.38	4.90	5.43
50	2.47	2.72	2.98	3.23	3.49	4.01	4.53	5.06
75	2.12	2.37	2.62	2.88	3.13	3.64	4.16	4.68
100	1.80	2.04	2.29	2.54	2.78	3.29	3.80	4.31
125	1.52	1.74	1.98	2.21	2.45	2.95	3.44	3.95
150	1.27	1.47	1.69	1.91	2.14	2.62	3.10	3.59
175	1.07	1.23	1.42	1.63	1.85	2.30	2.77	3.24
200	0.92	1.03	1.19	1.37	1.57	2.00	2.44	2.91
225	0.83	0.87	0.99	1.14	1.32	1.71	2.13	2.58
250	0.83	0.77	0.83	0.94	1.09	1.44	1.83	2.25
300	1.22	0.76	0.62	0.63	0.70	0.94	1.26	1.63
350	2.79	1.21	0.62	0.46	0.42	0.52	0.75	1.05
400		2.11	0.90	0.47	0.27	0.18	0.29	0.51
450		5.70	1.59	0.70	0.28	−0.07	−0.11	0.01
500			2.89	1.21	0.46	−0.21	−0.43	−0.43
550			4.97	2.05	0.85	−0.25	−0.68	−0.81
600			7.62	3.20	1.44	−0.15	−0.83	−1.12
700				6.08	3.16	0.40	−0.86	−1.49
800					5.27	1.40	−0.50	−1.49
900					7.40	2.67	0.18	−1.11
1000						3.98	1.05	−0.36
				HSO_3^-				
25	−126.13	−125.74	−125.36	−124.98	−124.60	−123.85	−123.11	−122.37
50	−126.97	−126.56	−126.17	−125.78	−125.40	−124.65	−123.90	−123.16
75	−127.80	−127.40	−127.00	−126.62	−126.23	−125.48	−124.73	−123.99
100	−128.64	−128.24	−127.85	−127.46	−127.08	−126.33	−125.59	−124.85
125	−129.47	−129.08	−128.70	−128.32	−127.94	−127.20	−126.47	−125.74
150	−130.29	−129.92	−129.55	−129.18	−128.82	−128.08	−127.36	−126.64
175	−131.10	−130.76	−130.41	−130.05	−129.69	−128.98	−128.26	−127.55
200	−131.88	−131.59	−131.26	−130.92	−130.58	−129.88	−129.18	−128.48
225	−132.63	−132.40	−132.10	−131.79	−131.46	−130.79	−130.11	−129.42
250	−133.32	−133.18	−132.93	−132.65	−132.34	−131.71	−131.03	−130.38
300	−134.42	−134.62	−134.54	−134.34	−134.10	−133.54	−132.94	−132.31
350	−134.47	−135.73	−136.02	−135.97	−135.82	−135.38	−134.85	−134.27
400		−136.30	−137.30	−137.49	−137.48	−137.20	−136.77	−136.26
450		−134.08	−138.22	−138.87	−139.06	−139.00	−138.69	−138.26

1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

t, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				HSO_3^- — Continued				
500			−138.58	−140.02	−140.53	−140.76	−140.60	−140.26
550			−138.20	−140.92	−141.86	−142.46	−142.48	−142.25
600			−137.24	−141.54	−143.04	−144.10	−144.33	−144.23
700				−142.28	−145.02	−147.19	−147.92	−148.11
800					−146.81	−150.08	−151.35	−151.83
900					−148.75	−152.90	−154.67	−155.38
1000						−155.84	−157.96	−158.76
				HSO_4^-				
25	−180.63	−180.22	−179.81	−179.42	−179.02	−178.24	−177.46	−176.69
50	−181.39	−180.96	−180.55	−180.14	−179.74	−178.95	−178.17	−177.40
75	−182.15	−181.73	−181.31	−180.91	−180.50	−179.71	−178.93	−178.16
100	−182.93	−182.51	−182.10	−181.69	−181.29	−180.51	−179.73	−178.96
125	−183.71	−183.30	−182.90	−182.50	−182.10	−181.33	−180.56	−179.79
150	−184.49	−184.10	−183.71	−183.32	−182.93	−182.17	−181.41	−180.65
175	−185.25	−184.90	−184.52	−184.15	−183.77	−183.02	−182.28	−181.53
200	−186.00	−185.69	−185.34	−184.99	−184.62	−183.90	−183.16	−182.43
225	−186.72	−186.47	−186.16	−185.82	−185.48	−184.78	−184.07	−183.35
250	−187.38	−187.22	−186.96	−186.66	−186.34	−185.67	−184.98	−184.28
300	−188.42	−188.63	−188.53	−188.32	−188.07	−187.49	−186.85	−186.19
350	−188.41	−189.70	−189.99	−189.93	−189.77	−189.31	−188.76	−188.15
400		−190.25	−191.26	−191.46	−191.44	−191.14	−190.69	−190.15
450		−188.03	−192.19	−192.83	−193.03	−192.96	−192.63	−192.18
500			−192.55	−194.01	−194.52	−194.74	−194.57	−194.22
550			−192.18	−194.92	−195.88	−196.49	−196.50	−196.26
600			−191.23	−195.58	−197.10	−198.18	−198.41	−198.30
700				−196.42	−199.19	−201.40	−202.15	−202.33
800					−201.11	−204.44	−205.75	−206.24
900					−203.22	−207.44	−209.26	−210.00
1000						−210.59	−212.78	−213.61
				HSO_5^-				
25	−152.37	−151.78	−151.21	−150.66	−150.12	−149.06	−148.02	−147.01
50	−153.67	−153.06	−152.48	−151.91	−151.36	−150.28	−149.23	−148.20
75	−155.01	−154.40	−153.81	−153.24	−152.68	−151.59	−150.54	−149.50
100	−156.40	−155.79	−155.20	−154.62	−154.06	−152.98	−151.92	−150.88
125	−157.82	−157.21	−156.63	−156.06	−155.50	−154.42	−153.36	−152.33
150	−159.27	−158.67	−158.09	−157.53	−156.98	−155.90	−154.85	−153.82
175	−160.73	−160.16	−159.59	−159.04	−158.49	−157.43	−156.38	−155.36
200	−162.20	−161.67	−161.12	−160.58	−160.04	−158.99	−157.95	−156.94
225	−163.67	−163.19	−162.67	−162.14	−161.62	−160.58	−159.56	−158.55
250	−165.12	−164.71	−164.23	−163.73	−163.22	−162.21	−161.20	−160.21
300	−167.84	−167.74	−167.38	−166.94	−166.48	−165.53	−164.57	−163.60
350	−167.76	−170.57	−170.51	−170.19	−169.81	−168.95	−168.04	−167.11
400		−172.98	−173.55	−173.44	−173.16	−172.43	−171.59	−170.72
450		−173.06	−176.36	−176.62	−176.52	−175.96	−175.22	−174.40
500			−178.75	−179.70	−179.85	−179.52	−178.90	−178.16
550			−180.57	−182.61	−183.13	−183.11	−182.63	−181.98
600			−181.95	−185.35	−186.34	−186.70	−186.40	−185.84
700				−190.55	−192.62	−193.91	−194.00	−193.66
800					−198.93	−201.15	−201.68	−201.57
900					−205.57	−208.54	−209.46	−209.53
1000						−216.19	−217.38	−217.53
				H_2S°				
25	−6.67	−6.26	−5.85	−5.45	−5.05	−4.27	−3.49	−2.72
50	−7.47	−7.04	−6.63	−6.22	−5.82	−5.04	−4.26	−3.49
75	−8.33	−7.90	−7.49	−7.08	−6.68	−5.89	−5.11	−4.35
100	−9.26	−8.83	−8.41	−8.00	−7.60	−6.81	−6.04	−5.28

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				H_2S° — Continued				
125	−10.26	−9.82	−9.40	−8.99	−8.58	−7.79	−7.02	−6.26
150	−11.30	−10.87	−10.44	−10.03	−9.62	−8.83	−8.06	−7.30
175	−12.40	−11.97	−11.54	−11.12	−10.72	−9.92	−9.15	−8.39
200	−13.55	−13.11	−12.68	−12.27	−11.86	−11.06	−10.29	−9.53
225	−14.74	−14.31	−13.88	−13.45	−13.04	−12.25	−11.47	−10.71
250	−15.98	−15.55	−15.11	−14.69	−14.28	−13.47	−12.70	−11.93
300	−18.59	−18.17	−17.71	−17.28	−16.86	−16.05	−15.27	−14.50
350	−21.45	−20.98	−20.48	−20.03	−19.60	−18.78	−17.99	−17.22
400		−24.03	−23.41	−22.93	−22.48	−21.64	−20.84	−20.07
450		−27.61	−26.52	−25.97	−25.50	−24.64	−23.83	−23.05
500		−31.88	−29.82	−29.17	−28.65	−27.76	−26.93	−26.14
550		−36.03	−33.35	−32.50	−31.93	−30.99	−30.15	−29.34
600		−40.00	−37.05	−35.99	−35.34	−34.34	−33.47	−32.65
700		−47.77	−44.75	−43.31	−42.47	−41.33	−40.41	−39.56
800		−55.53	−52.61	−50.98	−49.98	−48.69	−47.70	−46.83
900		−63.39	−60.60	−58.88	−57.78	−56.36	−55.33	−54.43
1000		−71.41	−68.72	−66.97	−65.81	−64.31	−63.24	−62.33
				HSe^-				
25	10.50	10.73	10.96	11.20	11.44	11.93	12.44	12.95
50	10.04	10.27	10.50	10.74	10.99	11.48	11.98	12.48
75	9.59	9.82	10.05	10.29	10.53	11.01	11.51	12.00
100	9.16	9.38	9.61	9.84	10.07	10.55	11.03	11.52
125	8.74	8.95	9.17	9.39	9.61	10.08	10.55	11.03
150	8.35	8.54	8.74	8.95	9.16	9.61	10.07	10.53
175	7.99	8.14	8.32	8.51	8.71	9.14	9.58	10.04
200	7.67	7.77	7.92	8.09	8.27	8.67	9.10	9.54
225	7.39	7.43	7.54	7.68	7.84	8.21	8.61	9.03
250	7.19	7.13	7.18	7.28	7.42	7.75	8.13	8.53
300	7.13	6.69	6.55	6.56	6.62	6.85	7.16	7.51
350	8.20	6.66	6.09	5.94	5.90	5.99	6.21	6.50
400		7.12	5.87	5.45	5.26	5.17	5.28	5.49
450		10.35	6.05	5.16	4.74	4.41	4.38	4.49
500			6.82	5.12	4.37	3.72	3.51	3.52
550			8.36	5.37	4.17	3.11	2.70	2.58
600			10.48	5.93	4.16	2.60	1.95	1.68
700				7.56	4.58	1.85	0.64	0.05
800					5.30	1.44	−0.39	−1.32
900					5.93	1.19	−1.20	−2.41
1000						0.89	−1.91	−3.23
				$HSeO_3^-$				
25	−98.34	−97.96	−97.59	−97.22	−96.85	−96.12	−95.39	−94.67
50	−99.15	−98.76	−98.38	−98.01	−97.63	−96.89	−96.17	−95.44
75	−99.98	−99.59	−99.20	−98.83	−98.45	−97.72	−96.99	−96.27
100	−100.81	−100.42	−100.04	−99.67	−99.30	−98.57	−97.84	−97.13
125	−101.64	−101.27	−100.90	−100.53	−100.17	−99.44	−98.73	−98.01
150	102.48	−102.12	−101.76	101.41	101.05	−100.34	−99.63	−98.93
175	−103.30	−102.98	−102.64	−102.29	−101.94	−101.25	−100.56	−99.86
200	−104.11	−103.82	−103.51	−103.18	−102.85	−102.18	−101.50	−100.81
225	−104.88	−104.66	−104.38	−104.08	−103.76	−103.11	−102.45	−101.78
250	−105.60	−105.47	−105.24	−104.97	−104.68	104.06	103.42	−102.77
300	−106.77	−106.99	−106.92	−106.74	−106.51	−105.98	−105.39	−104.78
350	−106.90	−108.18	−108.50	−108.46	−108.32	−107.91	−107.40	−106.85
400		−108.85	−109.88	−110.09	−110.09	−109.84	−109.43	−108.94
450		−106.75	−110.92	−111.58	−111.79	−111.76	−111.48	−111.07
500			−111.40	−112.87	−113.39	−113.65	−113.52	−113.21
550			−111.15	−113.90	−114.86	−115.50	−115.55	−115.35
600			−110.34	−114.67	−116.20	−117.30	−117.56	−117.49
700				−115.75	−118.52	−120.74	−121.50	−121.72

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$HSeO_3^-$ — Continued				
800					−120.67	−124.00	−125.32	−125.83
900					−123.02	−127.23	−129.05	−129.79
1000						−130.61	−132.78	−133.62
				$HSeO_4^-$				
25	−108.10	−107.74	−107.38	−107.02	−106.66	−105.96	−105.25	−104.55
50	−108.95	−108.58	−108.21	−107.85	−107.49	−106.78	−106.07	−105.37
75	−109.75	−109.37	−109.00	−108.64	−108.28	−107.56	−106.86	−106.16
100	−110.48	−110.11	−109.75	−109.38	−109.03	−108.32	−107.62	−106.92
125	−111.17	−110.81	−110.45	−110.10	−109.74	−109.05	−108.35	−107.66
150	−111.81	−111.47	−111.12	−110.77	−110.43	−109.74	−109.06	−108.38
175	−112.39	−112.08	−111.75	−111.42	−111.08	−110.41	−109.74	−109.07
200	−112.92	−112.65	−112.34	−112.03	−111.71	−111.05	−110.40	−109.74
225	−113.38	−113.16	−112.89	−112.60	−112.30	−111.67	−111.03	−110.38
250	−113.75	−113.63	−113.40	−113.14	−112.85	−112.26	−111.64	−111.01
300	−114.13	−114.34	−114.27	−114.10	−113.87	−113.36	−112.79	−112.20
350	−113.38	−114.62	−114.92	−114.89	−114.75	−114.35	−113.86	−113.32
400		−114.26	−115.27	−115.48	−115.48	−115.23	−114.83	−114.36
450		−111.06	−115.18	−115.83	−116.03	−116.00	−115.72	−115.32
500			−114.44	−115.88	−116.39	−116.65	−116.51	−116.20
550			−112.90	−115.60	−116.54	−117.16	−117.20	−117.00
600			−110.71	−114.98	−116.47	−117.54	−117.79	−117.71
700				−113.04	−115.76	−117.92	−118.66	−118.85
800					−114.61	−117.86	−119.12	−119.61
900					−113.39	−117.51	−119.26	−119.97
1000						−117.08	−119.17	−119.97
				$HSiO_3^-$				
25	−242.30	−242.18	−242.04	−241.89	−241.73	−241.40	−241.05	−240.68
50	−242.52	−242.40	−242.26	−242.11	−241.96	−241.63	−241.29	−240.93
75	−242.69	−242.57	−242.44	−242.30	−242.15	−241.83	−241.50	−241.16
100	−242.82	−242.71	−242.58	−242.45	−242.31	−242.01	−241.69	−241.35
125	−242.90	−242.81	−242.70	−242.58	−242.44	−242.16	−241.85	−241.53
150	−242.94	−242.87	−242.78	−242.67	−242.55	−242.29	−241.99	−241.69
175	−242.93	−242.90	−242.83	−242.74	−242.64	−242.39	−242.12	−241.83
200	−242.86	−242.88	−242.85	−242.78	−242.70	−242.48	−242.23	−241.96
225	−242.72	−242.81	−242.83	−242.79	−242.73	−242.55	−242.33	−242.07
250	−242.50	−242.69	−242.76	−242.77	−242.73	−242.60	−242.40	−242.17
300	−241.64	−242.22	−242.49	−242.61	−242.65	−242.63	−242.51	−242.33
350	−239.59	−241.27	−242.01	−242.29	−242.45	−242.57	−242.54	−242.44
400		−239.89	−241.23	−241.78	−242.09	−242.41	−242.51	−242.49
450		−235.87	−240.02	−241.03	−241.57	−242.14	−242.39	−242.48
500			−238.20	−239.99	−240.86	−241.77	−242.20	−242.40
550			−235.62	−238.62	−239.94	−241.26	−241.91	−242.25
600			−232.45	−236.92	−238.80	−240.62	−241.52	−242.02
700				−232.95	−235.95	−238.93	−240.42	−241.27
800					−232.67	−236.76	−238.90	−240.11
900					−229.34	−234.28	−237.01	−238.53
1000						−231.72	−234.90	−236.55
				HVO_4^{-2}				
25	−233.00	−232.80	−232.58	−232.35	−232.12	−231.63	−231.13	−230.61
50	−233.06	−232.85	−232.64	−232.42	−232.19	−231.71	−231.22	−230.72
75	−233.03	−232.85	−232.64	−232.43	−232.21	−231.76	−231.28	−230.79
100	−232.94	−232.78	−232.60	−232.40	−232.20	−231.76	−231.31	−230.84
125	−232.77	−232.65	−232.50	−232.33	−232.14	−231.74	−231.31	−230.87
150	−232.52	−232.46	−232.34	−232.20	−232.04	−231.68	−231.29	−230.87
175	−232.18	−232.19	−232.13	−232.03	−231.91	−231.60	−231.24	−230.84
200	−231.73	−231.84	−231.85	−231.81	−231.72	−231.47	−231.16	−230.80

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				HVO_4^{-2} — Continued				
225	−231.14	−231.40	−231.51	−231.53	−231.49	−231.32	−231.06	−230.74
250	−230.37	−230.84	−231.08	−231.18	−231.21	−231.13	−230.93	−230.66
300	−228.01	−229.30	−229.96	−230.29	−230.48	−230.63	−230.59	−230.44
350	−233.34	−226.79	−228.41	−229.08	−229.51	−229.97	−230.13	−230.13
400		−223.65	−226.32	−227.52	−228.27	−229.13	−229.55	−229.73
450		−215.68	−223.42	−225.50	−226.71	−228.10	−228.83	−229.23
500			−219.37	−222.93	−224.78	−226.84	−227.96	−228.60
550			−213.91	−219.73	−222.45	−225.35	−226.91	−227.85
600			−207.43	−215.93	−219.69	−223.59	−225.67	−226.93
700				−207.31	−213.10	−219.27	−222.56	−224.56
800					−205.69	−213.97	−218.59	−221.36
900					−198.18	−208.04	−213.90	−217.31
1000						−201.97	−208.77	−212.46
				$H_2VO_4^-$				
25	−244.00	−243.66	−243.32	−242.98	−242.65	−241.97	−241.30	−240.63
50	−244.73	−244.38	−244.03	−243.69	−243.35	−242.67	−242.00	−241.33
75	−245.46	−245.11	−244.76	−244.42	−244.08	−243.40	−242.73	−242.07
100	−246.19	−245.85	−245.50	−245.16	−244.83	−244.16	−243.50	−242.83
125	−246.92	−246.59	−246.26	−245.92	−245.59	−244.93	−244.28	−243.62
150	−247.64	−247.33	−247.01	−246.69	−246.37	−245.72	−245.08	−244.43
175	−248.35	−248.07	−247.77	−247.47	−247.15	−246.53	−245.89	−245.26
200	−249.04	−248.80	−248.53	−248.24	−247.94	−247.34	−246.72	−246.10
225	−249.69	−249.51	−249.28	−249.01	−248.74	−248.16	−247.56	−246.96
250	−250.28	−250.20	−250.01	−249.78	−249.53	−248.99	−248.41	−247.82
300	−251.18	−251.45	−251.43	−251.29	−251.11	−250.65	−250.14	−249.59
350	−251.01	−252.35	−252.73	−252.74	−252.65	−252.32	−251.88	−251.39
400		−252.74	−253.83	−254.09	−254.14	−253.98	−253.64	−253.22
450		−250.32	−254.56	−255.28	−255.55	−255.61	−255.40	−255.07
500			−254.72	−256.26	−256.84	−257.20	−257.15	−256.92
550			−254.14	−256.97	−258.00	−258.75	−258.88	−258.76
600			−252.98	−257.41	−259.00	−260.23	−260.59	−260.60
700				−257.79	−260.64	−262.99	−263.87	−264.18
800					−262.07	−265.55	−267.00	−267.61
900					−263.67	−268.05	−270.01	−270.87
1000						−270.66	−272.99	−273.96
				He°				
25	4.66	4.82	4.99	5.16	5.34	5.71	6.08	6.47
50	4.27	4.44	4.62	4.79	4.98	5.34	5.72	6.10
75	3.82	4.00	4.17	4.36	4.54	4.91	5.28	5.66
100	3.31	3.49	3.68	3.86	4.04	4.42	4.79	5.17
125	2.75	2.94	3.12	3.31	3.50	3.87	4.25	4.62
150	2.14	2.33	2.52	2.71	2.90	3.28	3.65	4.03
175	1.48	1.68	1.87	2.07	2.26	2.64	3.02	3.40
200	0.78	0.98	1.19	1.38	1.58	1.96	2.34	2.72
225	0.04	0.25	0.45	0.66	0.86	1.25	1.63	2.01
250	−0.76	−0.54	−0.32	−0.11	0.10	0.49	0.88	1.26
300	−2.51	−2.23	−1.98	−1.75	−1.53	−1.12	−0.72	−0.33
350	−4.56	−4.14	−3.80	−3.53	−3.30	−2.86	−2.45	−2.04
400		−6.39	−5.80	−5.47	−5.20	−4.72	−4.29	−3.88
450		−9.62	−8.02	−7.56	−7.23	−6.70	−6.24	−5.81
500		−14.17	−10.51	−9.81	−9.39	−8.79	−8.30	−7.85
550		−18.30	−13.32	−12.23	−11.69	−10.99	−10.46	−9.99
600		−21.94	−16.40	−14.82	−14.12	−13.30	−12.71	−12.22
700		−28.47	−22.78	−20.42	−19.32	−18.19	−17.49	−16.93
800		−34.55	−29.08	−26.31	−24.87	−23.43	−22.60	−21.98
900		−40.46	−35.25	−32.29	−30.64	−28.93	−27.99	−27.32
1000		−46.33	−41.34	−38.32	−36.53	−34.64	−33.63	−32.95

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Hg^{+2}				
25	39.36	39.15	38.97	38.82	38.69	38.49	38.34	38.21
50	39.57	39.35	39.17	39.01	38.87	38.64	38.46	38.32
75	39.78	39.55	39.36	39.19	39.04	38.80	38.60	38.43
100	39.98	39.74	39.54	39.36	39.21	38.94	38.73	38.54
125	40.18	39.93	39.71	39.52	39.36	39.08	38.85	38.65
150	40.39	40.11	39.88	39.68	39.50	39.21	38.96	38.75
175	40.60	40.30	40.05	39.83	39.64	39.32	39.06	38.83
200	40.83	40.49	40.22	39.98	39.77	39.43	39.15	38.90
225	41.07	40.70	40.39	40.13	39.90	39.53	39.22	38.97
250	41.35	40.92	40.57	40.28	40.03	39.62	39.29	39.02
300	42.04	41.41	40.94	40.59	40.29	39.80	39.41	39.09
350	42.82	42.06	41.32	40.90	40.55	39.96	39.50	39.12
400		41.88	41.67	41.22	40.80	40.11	39.57	39.13
450		40.47	41.95	41.52	41.06	40.26	39.63	39.11
500			42.05	41.81	41.32	40.41	39.68	39.09
550			41.85	42.06	41.59	40.57	39.73	39.05
500			41.31	42.22	41.86	40.76	39.80	39.03
700				42.10	42.40	41.25	40.03	39.04
800					42.94	41.96	40.44	39.22
900					43.56	42.85	41.02	39.58
1000						43.80	41.66	40.11
				Hg_2^{+2}				
25	36.71	36.88	37.07	37.26	37.46	37.86	38.28	38.70
50	37.08	37.26	37.45	37.64	37.84	38.24	38.65	39.07
75	37.43	37.61	37.79	37.99	38.18	38.58	38.98	39.40
100	37.75	37.92	38.10	38.29	38.48	38.88	39.28	39.68
125	38.04	38.21	38.39	38.57	38.76	39.14	39.53	39.93
150	38.33	38.48	38.65	38.82	39.00	39.37	39.76	40.15
175	38.60	38.73	38.89	39.05	39.22	39.58	39.96	40.34
200	38.87	38.97	39.11	39.26	39.42	39.77	40.13	40.50
225	39.14	39.21	39.32	39.46	39.61	39.93	40.28	40.64
250	39.42	39.44	39.53	39.64	39.77	40.08	40.41	40.76
300	40.08	39.91	39.91	39.97	40.07	40.31	40.60	40.92
350	40.87	40.46	40.25	40.27	40.32	40.50	40.73	41.01
400		40.53	40.56	40.53	40.53	40.63	40.81	41.04
450		40.17	40.83	40.76	40.71	40.71	40.83	41.01
500			41.01	40.96	40.86	40.77	40.80	40.93
550			41.08	41.13	41.00	40.80	40.75	40.81
600			40.99	41.26	41.12	40.82	40.67	40.66
700				41.22	41.31	40.85	40.50	40.33
800					41.41	40.93	40.33	39.99
900					41.45	41.01	40.17	39.67
1000						41.03	39.96	39.39
				$Hg(CH_3COO)^+$				
25	−54.76	−54.43	−54.11	−53.79	−53.47	−52.83	−52.20	−51.57
50	−55.32	−54.98	−54.65	−54.32	−54.00	−53.35	−52.72	−52.08
75	−56.06	−55.71	−55.37	−55.04	−54.71	−54.07	−53.43	−52.80
100	−56.93	−56.59	−56.25	−55.91	−55.58	−54.93	−54.30	−53.66
125	−57.94	−57.59	−57.25	−56.92	−56.59	−55.94	−55.30	−54.67
150	−59.05	−58.71	−58.37	−58.04	−57.71	−57.06	−56.43	−55.80
175	−60.27	−59.93	−59.60	−59.27	−58.94	−58.30	−57.66	−57.04
200	−61.58	−61.25	−60.92	−60.60	−60.27	−59.63	−59.00	−58.38
225	−62.97	−62.66	−62.34	−62.02	−61.70	−61.06	−60.43	−59.81
250	−64.43	−64.15	−63.84	−63.52	−63.21	−62.58	−61.96	−61.34
300	−67.55	−67.36	−67.07	−66.77	−66.47	−65.86	−65.25	−64.64
350	−70.85	−70.81	−70.60	−70.32	−70.03	−69.44	−68.85	−68.25
400		−74.64	−74.38	−74.12	−73.85	−73.29	−72.72	−72.14
450		−78.71	−78.40	−78.17	−77.92	−77.40	−76.85	−76.28

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Hg(CH_3COO)^+$ — Continued				
500			−82.65	−82.44	−82.21	−81.73	−81.20	−80.66
550			−87.10	−86.91	−86.71	−86.27	−85.77	−85.25
600			−91.76	−91.58	−91.40	−91.00	−90.54	−90.05
700				−101.50	−101.32	−101.00	−100.62	−100.18
800					−111.90	−111.63	−111.34	−110.96
900					−123.09	−122.85	−122.64	−122.31
1000						−134.63	−134.50	−134.19
				$Hg(CH_3COO)_2^\circ$				
25	−146.58	−145.65	−144.77	−143.92	−143.11	−141.53	−140.01	−138.53
50	−147.80	−146.84	−145.93	−145.06	−144.22	−142.60	−141.04	−139.53
75	−149.39	−148.42	−147.49	−146.61	−145.75	−144.11	−142.53	−141.00
100	−151.29	−150.31	−149.37	−148.47	−147.61	−145.95	−144.36	−142.82
125	−153.47	−152.47	−151.53	−150.63	−149.76	−148.09	−146.48	−144.93
150	−155.88	−154.89	−153.94	−153.03	−152.15	−150.48	−148.87	−147.31
175	−158.52	−157.53	−156.57	−155.66	−154.78	−153.10	−151.48	−149.92
200	−161.37	−160.38	−159.42	−158.51	−157.63	−155.93	−154.32	−152.75
225	−164.40	−163.43	−162.47	−161.55	−160.67	−158.97	−157.35	−155.78
250	−167.61	−166.67	−165.70	−164.78	−163.89	−162.19	−160.57	−158.99
300	−174.52	−173.67	−172.69	−171.76	−170.87	−169.16	−167.53	−165.95
350	−182.04	−181.31	−180.32	−179.38	−178.49	−176.77	−175.13	−173.55
400		−189.56	−188.54	−187.59	−186.69	−184.96	−183.32	−181.73
450		−198.47	−197.30	−196.34	−195.42	−193.69	−192.04	−190.45
500		−208.05	−206.59	−205.59	−204.66	−202.92	−201.26	−199.66
550		−218.02	−216.37	−215.31	−214.37	−212.61	−210.94	−209.34
600		−228.34	−226.61	−225.48	−224.51	−222.74	−221.06	−219.45
700		−250.04	−248.29	−247.05	−246.03	−244.20	−242.51	−240.89
800		−273.10	−271.38	−270.08	−269.01	−267.14	−265.43	−263.80
900		−297.43	−295.74	−294.42	−293.31	−291.40	−289.67	−288.03
1000		−322.92	−321.26	−319.93	−318.80	−316.87	−315.13	−313.49
				$Hg(CH_3COO)_3^-$				
25	−239.02	−237.43	−235.92	−234.49	−233.11	−230.46	−227.93	−225.49
50	−240.67	−239.02	−237.47	−236.00	−234.58	−231.86	−229.27	−226.76
75	−242.91	−241.24	−239.67	−238.18	−236.74	−233.98	−231.35	−228.81
100	−245.66	−243.98	−242.40	−240.89	−239.44	−236.67	−234.01	−231.45
125	−248.84	−247.16	−245.58	−244.06	−242.61	−239.82	−237.16	−234.58
150	−252.40	−250.74	−249.16	−247.64	−246.19	−243.40	−240.73	−238.14
175	−256.31	−254.68	−253.10	−251.59	−250.14	−247.35	−244.68	−242.09
200	−260.53	−258.94	−257.38	−255.88	−254.43	−251.65	−248.98	−246.40
225	−265.02	−263.50	−261.96	−260.48	−259.04	−256.27	−253.61	−251.03
250	−269.75	−268.34	−266.84	−265.37	−263.95	−261.20	−258.55	−255.98
300	−279.75	−278.75	−277.36	−275.96	−274.58	−271.88	−269.27	−266.72
350	−289.81	−289.89	−288.80	−287.51	−286.19	−283.58	−281.02	−278.50
400		−301.45	−300.98	−299.89	−298.69	−296.19	−293.70	−291.23
450		−311.48	−313.71	−312.99	−311.96	−309.63	−307.23	−304.82
500			−326.75	−326.71	−325.92	−323.83	−321.54	−319.20
550			−339.89	−340.93	−340.51	−338.72	−336.57	−334.31
600			−353.23	−355.61	−355.66	−354.24	−352.26	−350.09
700				−386.45	−387.56	−387.06	−385.46	−383.52
800					−421.62	−422.04	−420.87	−419.15
900					−457.93	−459.09	−458.31	−456.76
1000						−498.15	−497.64	−496.17
				Ho^{+3}				
25	−161.40	−161.87	−162.28	−162.64	−162.97	−163.56	−164.07	−164.52
50	−160.01	−160.50	−160.93	−161.31	−161.67	−162.29	−162.84	−163.34
75	−158.57	−159.08	−159.53	−159.93	−160.30	−160.96	−161.55	−162.08
100	−157.08	−157.62	−158.09	−158.51	−158.90	−159.59	−160.21	−160.76

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Ho^{+3} — Continued				
125	−155.55	−156.11	−156.61	−157.06	−157.46	−158.19	−158.83	−159.42
150	−153.96	−154.56	−155.10	−155.57	−156.00	−156.76	−157.44	−158.05
175	−152.31	−152.97	−153.54	−154.04	−154.50	−155.31	−156.02	−156.66
200	−150.59	−151.31	−151.94	−152.49	−152.97	−153.83	−154.58	−155.25
225	−148.79	−149.60	−150.29	−150.89	−151.42	−152.33	−153.12	−153.83
250	−146.91	−147.82	−148.60	−149.25	−149.82	−150.81	−151.65	−152.39
300	−142.80	−144.07	−145.08	−145.85	−146.53	−147.69	−148.65	−149.48
350	−138.77	−139.97	−141.47	−142.34	−143.12	−144.46	−145.57	−146.52
400		−138.04	−137.90	−138.76	−139.62	−141.15	−142.42	−143.50
450		−140.56	−134.57	−135.15	−136.05	−137.75	−139.19	−140.41
500			−131.85	−131.58	−132.41	−134.26	−135.89	−137.26
550			−130.17	−128.15	−128.72	−130.67	−132.49	−134.03
600			−129.68	−124.97	−124.99	−126.96	−128.97	−130.69
700				−119.78	−117.48	−119.05	−121.50	−123.64
800					−109.81	−110.41	−113.36	−115.96
900					−101.58	−101.05	−104.57	−107.61
1000						−91.25	−95.36	−98.64
				Isoleucine				
25	−82.20	−80.97	−79.79	−78.65	−77.54	−75.38	−73.28	−71.23
50	−83.61	−82.38	−81.20	−80.06	−78.96	−76.81	−74.74	−72.71
75	−85.20	−83.96	−82.78	−81.65	−80.54	−78.40	−76.34	−74.32
100	−86.95	−85.71	−84.52	−83.39	−82.28	−80.15	−78.09	−76.08
125	−88.85	−87.60	−86.41	−85.27	−84.17	−82.03	−79.98	−77.97
150	−90.88	−89.64	−88.44	−87.30	−86.19	−84.05	−82.00	−80.00
175	−93.06	−91.81	−90.61	−89.46	−88.35	−86.20	−84.14	−82.14
200	−95.36	−94.11	−92.90	−91.74	−90.62	−88.48	−86.41	−84.41
225	−97.79	−96.54	−95.31	−94.14	−93.02	−90.86	−88.79	−86.78
250	−100.34	−99.09	−97.84	−96.66	−95.53	−93.36	−91.28	−89.27
300	−105.85	−104.58	−103.25	−102.03	−100.87	−98.66	−96.57	−94.54
350	−112.28	−110.63	−109.12	−107.82	−106.62	−104.36	−102.24	−100.19
400		−117.54	−115.49	−114.04	−112.76	−110.43	−108.26	−106.19
450		−126.65	−122.41	−120.69	−119.29	−116.85	−114.62	−112.52
500		−138.71	−130.03	−127.78	−126.20	−123.60	−121.30	−119.15
550		−149.96	−138.42	−135.33	−133.47	−130.66	−128.28	−126.08
600		−160.22	−147.45	−143.32	−141.11	−138.03	−135.54	−133.29
700		−179.35	−166.27	−160.42	−157.36	−153.62	−150.88	−148.49
800		−197.78	−185.16	−178.44	−174.64	−170.21	−167.19	−164.67
900		−216.07	−204.02	−196.90	−192.63	−187.63	−184.37	−181.75
1000		−234.51	−222.93	−215.67	−211.12	−205.73	−202.32	−199.66
				I^-				
25	−12.41	−11.98	−11.56	−11.14	−10.73	−9.89	−9.07	−8.25
50	−13.02	−12.58	−12.15	−11.72	−11.30	−10.46	−9.63	−8.80
75	−13.58	−13.14	−12.71	−12.28	−11.86	−11.02	−10.18	−9.35
100	−14.10	−13.67	−13.24	−12.81	−12.39	−11.55	−10.72	−9.90
125	−14.57	−14.15	−13.73	−13.31	−12.90	−12.07	−11.25	−10.43
150	−14.99	−14.59	−14.19	−13.78	−13.37	−12.56	−11.75	−10.94
175	−15.36	−14.99	−14.61	−14.22	−13.82	−13.03	−12.23	−11.43
200	−15.67	−15.35	−14.99	−14.62	−14.24	−13.47	−12.69	−11.90
225	−15.90	−15.65	−15.33	−14.99	−14.63	−13.89	−13.13	−12.36
250	−16.04	−15.90	−15.63	−15.32	−14.99	−14.28	−13.55	−12.80
300	−15.92	−16.16	−16.08	−15.87	−15.60	−14.99	−14.32	−13.61
350	−14.59	−15.95	−16.29	−16.24	−16.07	−15.59	−15.01	−14.36
400		−15.17	−16.19	−16.40	−16.39	−16.09	−15.61	−15.04
450		−11.50	−15.64	−16.31	−16.52	−16.46	−16.12	−15.64
500			−14.43	−15.92	−16.45	−16.71	−16.53	−16.16
550			−12.39	−15.17	−16.16	−16.81	−16.84	−16.59
600			−9.71	−14.08	−15.64	−16.78	−17.04	−16.93
700				−11.20	−13.99	−16.30	−17.10	−17.31

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				I^- — Continued				
800					−11.88	−15.32	−16.73	−17.27
900					−9.70	−14.03	−15.98	−16.79
1000						−12.65	−15.00	−15.92
				I_3^-				
25	−12.30	−11.64	−11.00	−10.38	−9.78	−8.60	−7.46	−6.34
50	−13.74	−13.06	−12.40	−11.77	−11.15	−9.96	−8.79	−7.66
75	−15.21	−14.52	−13.86	−13.22	−12.59	−11.38	−10.21	−9.07
100	−16.70	−16.01	−15.34	−14.70	−14.07	−12.86	−11.69	−10.54
125	−18.20	−17.52	−16.85	−16.21	−15.59	−14.37	−13.20	−12.05
150	−19.72	−19.04	−18.38	−17.75	−17.13	−15.92	−14.75	−13.60
175	−21.23	−20.58	−19.93	−19.30	−18.69	−17.49	−16.32	−15.18
200	−22.75	−22.13	−21.50	−20.88	−20.27	−19.08	−17.92	−16.79
225	−24.25	−23.68	−23.07	−22.46	−21.87	−20.70	−19.55	−18.42
250	−25.72	−25.22	−24.64	−24.06	−23.48	−22.33	−21.19	−20.07
300	−28.47	−28.26	−27.79	−27.27	−26.73	−25.63	−24.53	−23.44
350	−30.47	−31.10	−30.90	−30.48	−30.00	−28.98	−27.94	−26.88
400		−33.52	−33.89	−33.65	−33.27	−32.37	−31.39	−30.37
450		−33.84	−36.65	−36.75	−36.52	−35.77	−34.87	−33.91
500			−39.01	−39.72	−39.73	−39.18	−38.39	−37.49
550			−40.84	−42.53	−42.86	−42.59	−41.92	−41.10
600			−42.25	−45.16	−45.91	−45.98	−45.47	−44.73
700				−50.11	−51.83	−52.72	−52.56	−52.02
800					−57.70	−59.43	−59.65	−59.32
900					−63.80	−66.20	−66.77	−66.60
1000						−73.15	−73.96	−73.86
				IO^-				
25	−9.20	−9.21	−9.19	−9.15	−9.10	−8.97	−8.81	−8.62
50	−9.11	−9.12	−9.10	−9.07	−9.03	−8.91	−8.77	−8.60
75	−8.92	−8.93	−8.93	−8.91	−8.87	−8.77	−8.64	−8.49
100	−8.64	−8.67	−8.68	−8.66	−8.64	−8.55	−8.44	−8.30
125	−8.28	−8.34	−8.36	−8.36	−8.34	−8.28	−8.18	−8.06
150	−7.85	−7.93	−7.97	−7.99	−7.99	−7.95	−7.87	−7.76
175	−7.33	−7.45	−7.53	−7.57	−7.58	−7.57	−7.51	−7.42
200	−6.73	−6.90	−7.01	−7.08	−7.12	−7.14	−7.10	−7.03
225	−6.03	−6.28	−6.44	−6.54	−6.60	−6.66	−6.66	−6.61
250	−5.21	−5.56	−5.79	−5.94	−6.03	−6.14	−6.17	−6.15
300	−3.09	−3.84	−4.29	−4.55	−4.74	−4.96	−5.08	−5.12
350	0.26	−1.55	−2.48	−2.92	−3.22	−3.61	−3.83	−3.95
400		1.07	−0.33	−1.02	−1.49	−2.08	−2.44	−2.65
450		5.98	2.30	1.17	0.48	−0.38	−0.90	−1.23
500			5.54	3.71	2.70	1.50	0.79	0.33
550			9.49	6.62	5.20	3.57	2.64	2.03
600			13.98	9.88	7.96	5.84	4.64	3.87
700				17.03	14.19	10.97	9.15	8.00
800					21.04	16.82	14.32	12.77
900					28.15	23.18	20.06	18.17
1000						29.81	26.20	24.16
				IO_3^-				
25	−30.60	−30.30	−29.99	−29.68	−29.38	−28.76	−28.14	−27.52
50	−31.29	−30.98	−30.67	−30.36	−30.05	−29.43	−28.81	−28.19
75	−31.96	−31.65	−31.34	−31.03	−30.72	−30.10	−29.49	−28.88
100	−32.61	−32.31	−32.00	−31.70	−31.39	−30.78	−30.17	−29.57
125	−33.24	−32.95	−32.65	−32.35	−32.05	−31.46	−30.86	−30.26
150	−33.85	−33.58	−33.29	−33.00	−32.71	−32.13	−31.54	−30.95
175	−34.42	−34.18	−33.92	−33.64	−33.36	−32.80	−32.22	−31.64
200	−34.96	−34.76	−34.52	−34.27	−34.01	−33.46	−32.90	−32.34

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				IO_3^- — Continued				
225	−35.45	−35.31	−35.11	−34.88	−34.64	−34.12	−33.58	−33.03
250	−35.86	−35.82	−35.67	−35.47	−35.25	−34.77	−34.26	−33.72
300	−36.37	−36.68	−36.70	−36.60	−36.44	−36.05	−35.59	−35.10
350	−35.76	−37.15	−37.56	−37.61	−37.55	−37.28	−36.91	−36.48
400		−37.05	−38.18	−38.49	−38.57	−38.47	−38.20	−37.84
450		−34.12	−38.40	−39.17	−39.47	−39.59	−39.45	−39.17
500			−38.02	−39.59	−40.21	−40.64	−40.66	−40.48
550			−36.85	−39.72	−40.79	−41.61	−41.81	−41.75
600			−35.08	−39.55	−41.18	−42.48	−42.91	−42.98
700				−38.63	−41.51	−43.94	−44.89	−45.27
800					−41.54	−45.10	−46.62	−47.30
900					−41.64	−46.09	−48.13	−49.06
1000						−47.12	−49.53	−50.57
				IO_4^-				
25	−14.00	−13.39	−12.79	−12.22	−11.65	−10.55	−9.48	−8.43
50	−15.33	−14.70	−14.09	−13.50	−12.92	−11.80	−10.71	−9.65
75	−16.68	−16.04	−15.42	−14.83	−14.25	−13.12	−12.02	−10.95
100	−18.04	−17.40	−16.79	−16.19	−15.61	−14.47	−13.38	−12.30
125	−19.41	−18.78	−18.17	−17.57	−16.99	−15.86	−14.76	−13.69
150	−20.79	−20.17	−19.56	−18.97	−18.39	−17.27	−16.18	−15.11
175	−22.16	−21.56	−20.97	−20.39	−19.81	−18.70	−17.61	−16.55
200	−23.52	−22.96	−22.38	−21.81	−21.25	−20.15	−19.07	−18.01
225	−24.86	−24.35	−23.80	−23.24	−22.70	−21.61	−20.55	−19.50
250	−26.17	−25.73	−25.21	−24.68	−24.15	−23.09	−22.04	−21.00
300	−28.57	−28.43	−28.03	−27.56	−27.08	−26.07	−25.06	−24.05
350	−30.14	−30.89	−30.78	−30.42	−30.00	−29.09	−28.13	−27.16
400		−32.88	−33.38	−33.23	−32.92	−32.12	−31.23	−30.31
450		−32.58	−35.73	−35.93	−35.78	−35.16	−34.36	−33.50
500			−37.62	−38.49	−38.59	−38.19	−37.50	−36.71
550			−38.92	−40.85	−41.30	−41.19	−40.65	−39.94
600			−39.77	−43.00	−43.91	−44.18	−43.79	−43.18
700				−46.95	−48.90	−50.05	−50.05	−49.65
800					−53.80	−55.85	−56.27	−56.08
900					−58.89	−61.67	−62.47	−62.45
1000						−67.64	−68.71	−68.76
				In^{+3}				
25	−23.40	−23.88	−24.29	−24.66	−25.00	−25.59	−26.11	−26.57
50	−21.79	−22.29	−22.72	−23.12	−23.47	−24.11	−24.67	−25.18
75	−20.13	−20.65	−21.10	−21.51	−21.89	−22.56	−23.16	−23.70
100	−18.42	−18.96	−19.44	−19.87	−20.27	−20.97	−21.60	−22.16
125	−16.66	−17.23	−17.74	−18.19	−18.61	−19.35	−20.00	−20.60
150	−14.83	−15.46	−16.00	−16.48	−16.92	−17.70	−18.38	−19.01
175	−12.95	−13.62	−14.21	−14.73	−15.20	−16.02	−16.74	−17.39
200	−11.00	−11.74	−12.38	−12.94	−13.44	−14.32	−15.08	−15.76
225	−8.96	−9.79	−10.50	−11.11	−11.65	−12.59	−13.40	−14.12
250	−6.83	−7.77	−8.57	−9.24	−9.83	−10.84	−11.70	−12.46
300	−2.23	−3.54	−4.58	−5.37	−6.07	−7.25	−8.24	−9.10
350	2.23	1.05	−0.50	−1.38	−2.19	−3.56	−4.70	−5.68
400		3.27	3.54	2.68	1.79	0.22	−1.08	−2.20
450		0.47	7.28	6.75	5.84	4.10	2.61	1.35
500			10.32	10.76	9.95	8.06	6.39	4.97
550			12.19	14.61	14.11	12.13	10.27	8.68
600			12.70	18.16	18.29	16.33	14.27	12.49
700				23.95	26.68	25.22	22.72	20.52
800					35.22	34.89	31.89	29.21
900					44.37	45.32	41.74	38.60
1000						56.24	52.03	48.65

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				K^+				
25	−67.51	−67.39	−67.26	−67.12	−66.97	−66.64	−66.30	−65.95
50	−68.12	−67.99	−67.86	−67.71	−67.56	−67.24	−66.90	−66.56
75	−68.73	−68.60	−68.46	−68.32	−68.17	−67.85	−67.51	−67.17
100	−69.35	−69.22	−69.08	−68.94	−68.79	−68.47	−68.14	−67.80
125	−69.98	−69.85	−69.71	−69.57	−69.41	−69.10	−68.77	−68.44
150	−70.61	−70.48	−70.35	−70.20	−70.05	−69.74	−69.42	−69.08
175	−71.24	−71.12	−70.99	−70.85	−70.70	−70.39	−70.07	−69.74
200	−71.88	−71.77	−71.64	−71.50	−71.35	−71.05	−70.73	−70.40
225	−72.52	−72.41	−72.29	−72.15	−72.01	−71.71	−71.40	−71.07
250	−73.15	−73.06	−72.95	−72.82	−72.68	−72.38	−72.07	−71.75
300	−74.40	−74.37	−74.27	−74.15	−74.02	−73.74	−73.44	−73.13
350	−75.59	−75.65	−75.61	−75.50	−75.39	−75.12	−74.83	−74.53
400		−77.01	−76.95	−76.87	−76.76	−76.52	−76.25	−75.96
450		−78.33	−78.30	−78.24	−78.15	−77.94	−77.68	−77.40
500			−79.65	−79.62	−79.55	−79.36	−79.13	−78.86
550			−80.99	−80.99	−80.95	−80.80	−80.59	−80.34
600			−82.34	−82.38	−82.36	−82.25	−82.06	−81.83
700				−85.19	−85.19	−85.15	−85.02	−84.83
800					−88.05	−88.06	−88.00	−87.85
900					−90.95	−90.99	−90.99	−90.89
1000						−93.96	−94.02	−93.93
				$KAlO_2^\circ$				
25	−264.38	−264.01	−263.65	−263.30	−262.95	−262.25	−261.56	−260.88
50	−265.28	−264.90	−264.52	−264.16	−263.80	−263.09	−262.40	−261.71
75	−266.18	−265.79	−265.41	−265.04	−264.67	−263.96	−263.26	−262.57
100	−267.09	−266.69	−266.31	−265.93	−265.57	−264.85	−264.14	−263.45
125	−268.00	−267.60	−267.21	−266.83	−266.46	−265.74	−265.04	−264.34
150	−268.91	−268.51	−268.12	−267.74	−267.37	−266.64	−265.94	−265.24
175	−269.83	−269.43	−269.04	−268.65	−268.28	−267.55	−266.84	−266.15
200	−270.75	−270.35	−269.95	−269.57	−269.20	−268.47	−267.76	−267.06
225	−271.67	−271.28	−270.88	−270.49	−270.12	−269.38	−268.67	−267.97
250	−272.60	−272.21	−271.80	−271.42	−271.04	−270.30	−269.59	−268.89
300	−274.45	−274.08	−273.67	−273.28	−272.89	−272.15	−271.44	−270.74
350	−276.35	−275.99	−275.55	−275.15	−274.76	−274.02	−273.29	−272.59
400		−277.96	−277.46	−277.04	−276.65	−275.89	−275.16	−274.46
450		−280.14	−279.40	−278.95	−278.54	−277.77	−277.04	−276.33
500		−282.61	−281.39	−280.88	−280.45	−279.67	−278.93	−278.21
550		−284.97	−283.44	−282.84	−282.38	−281.57	−280.82	−280.10
600		−287.20	−285.54	−284.83	−284.33	−283.49	−282.72	−281.99
700		−291.45	−289.75	−288.85	−288.26	−287.35	−286.55	−285.81
800		−295.54	−293.89	−292.90	−292.22	−291.23	−290.41	−289.65
900		−299.55	−297.96	−296.92	−296.20	−295.14	−294.30	−293.53
1000		−303.50	−301.97	−300.91	−300.16	−299.06	−298.20	−297.42
				KBr°				
25	−90.01	−89.50	−89.00	−88.51	−88.04	−87.11	−86.21	−85.31
50	−91.19	−90.66	−90.15	−89.65	−89.16	−88.21	−87.29	−86.39
75	−92.37	−91.82	−91.30	−90.79	−90.30	−89.34	−88.41	−87.50
100	−93.54	−92.98	−92.46	−91.94	−91.45	−90.48	−89.55	−88.63
125	−94.70	−94.15	−93.62	−93.10	−92.60	−91.63	−90.69	−89.77
150	−95.87	−95.31	−94.78	−94.26	−93.76	−92.78	−91.84	−90.92
175	−97.03	−96.48	−95.94	−95.42	−94.92	−93.94	−93.00	−92.07
200	−98.20	−97.65	−97.11	−96.59	−96.08	−95.10	−94.15	−93.23
225	−99.36	−98.82	−98.27	−97.75	−97.24	−96.26	−95.31	−94.39
250	−100.51	−99.99	−99.44	−98.92	−98.41	−97.43	−96.48	−95.55
300	−102.81	−102.33	−101.79	−101.26	−100.75	−99.77	−98.81	−97.89
350	−105.08	−104.69	−104.14	−103.61	−103.10	−102.11	−101.16	−100.23
400		−107.05	−106.50	−105.97	−105.45	−104.46	−103.51	−102.58
450		−109.44	−108.86	−108.33	−107.81	−106.82	−105.86	−104.93

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

				Pressure, kbar				
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				KBr° — Continued				
500		−111.87	−111.24	−110.70	−110.18	−109.18	−108.22	−107.29
550		−114.28	−113.62	−113.07	−112.55	−111.55	−110.59	−109.66
600		−116.69	−116.01	−115.45	−114.93	−113.92	−112.96	−112.03
700		−121.49	−120.81	−120.23	−119.70	−118.69	−117.72	−116.78
800		−126.30	−125.62	−125.03	−124.48	−123.46	−122.49	−121.55
900		−131.10	−130.43	−129.83	−129.28	−128.26	−127.28	−126.34
1000		−135.91	−135.24	−134.64	−134.09	−133.06	−132.09	−131.14
				$K(CH_3COO)^\circ$				
25	−155.42	−154.73	−154.07	−153.43	−152.80	−151.60	−150.43	−149.28
50	−156.67	−155.95	−155.27	−154.61	−153.97	−152.74	−151.54	−150.38
75	−158.01	−157.28	−156.59	−155.92	−155.27	−154.02	−152.81	−151.63
100	−159.44	−158.70	−158.00	−157.33	−156.67	−155.41	−154.19	−153.01
125	−160.95	−160.21	−159.50	−158.81	−158.16	−156.88	−155.66	−154.47
150	−162.52	−161.78	−161.06	−160.38	−159.71	−158.44	−157.21	−156.01
175	−164.16	−163.41	−162.70	−162.01	−161.34	−160.06	−158.83	−157.63
200	−165.85	−165.11	−164.39	−163.70	−163.03	−161.74	−160.51	−159.31
225	−167.59	−166.87	−166.14	−165.45	−164.78	−163.49	−162.25	−161.05
250	−169.38	−168.67	−167.95	−167.25	−166.58	−165.29	−164.04	−162.84
300	−173.09	−172.45	−171.71	−171.01	−170.33	−169.03	−167.79	−166.58
350	−176.97	−176.41	−175.66	−174.95	−174.27	−172.97	−171.72	−170.50
400		−180.58	−179.79	−179.07	−178.38	−177.07	−175.82	−174.60
450		−185.02	−184.09	−183.35	−182.65	−181.33	−180.07	−178.85
500		−189.78	−188.56	−187.78	−187.07	−185.74	−184.47	−183.25
550		−194.60	−193.19	−192.36	−191.63	−190.28	−189.01	−187.78
600		−199.46	−197.97	−197.07	−196.32	−194.95	−193.67	−192.44
700		−209.39	−207.88	−206.87	−206.06	−204.65	−203.35	−202.11
800		−219.64	−218.16	−217.09	−216.24	−214.78	−213.46	−212.21
900		−230.21	−228.77	−227.67	−226.79	−225.29	−223.96	−222.70
1000		−241.10	−239.68	−238.58	−237.67	−236.15	−234.80	−233.54
				$K(CH_3COO)_2^-$				
25	−242.99	−241.66	−240.40	−239.20	−238.03	−235.81	−233.67	−231.60
50	−244.64	−243.27	−241.97	−240.73	−239.54	−237.25	−235.06	−232.94
75	−246.51	−245.12	−243.81	−242.55	−241.34	−239.02	−236.80	−234.66
100	−248.57	−247.17	−245.85	−244.58	−243.36	−241.03	−238.79	−236.63
125	−250.79	−249.39	−248.06	−246.79	−245.57	−243.23	−240.98	−238.81
150	−253.15	−251.76	−250.43	−249.16	−247.94	−245.59	−243.34	−241.16
175	−255.63	−254.26	−252.94	−251.67	−250.45	−248.11	−245.86	−243.68
200	−258.21	−256.88	−255.57	−254.31	−253.10	−250.76	−248.51	−246.33
225	−260.87	−259.61	−258.32	−257.07	−255.86	−253.54	−251.30	−249.12
250	−263.61	−262.43	−261.17	−259.94	−258.74	−256.43	−254.20	−252.03
300	−269.14	−268.30	−267.14	−265.97	−264.80	−262.54	−260.34	−258.19
350	−274.26	−274.33	−273.41	−272.33	−271.22	−269.03	−266.87	−264.75
400		−280.27	−279.88	−278.97	−277.95	−275.86	−273.76	−271.67
450		−284.55	−286.42	−285.82	−284.94	−282.99	−280.96	−278.93
500			−292.85	−292.81	−292.15	−290.39	−288.46	−286.48
550			−299.03	−299.90	−299.54	−298.03	−296.22	−294.31
600			−305.06	−307.06	−307.09	−305.89	−304.22	−302.39
700				−321.72	−322.64	−322.21	−320.86	−319.22
800					−338.93	−339.27	−338.28	−336.82
900					−356.13	−357.09	−356.42	−355.11
1000						−375.71	−375.27	−374.02
				KCl°				
25	−96.50	−96.03	−95.57	−95.13	−94.69	−93.84	−93.00	−92.17
50	−97.49	−97.00	−96.53	−96.07	−95.62	−94.75	−93.90	−93.06
75	−98.48	−97.99	−97.51	−97.04	−96.59	−95.71	−94.85	−94.00
100	−99.49	−98.98	−98.50	−98.03	−97.57	−96.68	−95.82	−94.97

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				KCl° — Continued				
125	−100.49	−99.99	−99.50	−99.02	−98.56	−97.67	−96.80	−95.95
150	−101.50	−100.99	−100.50	−100.02	−99.56	−98.66	−97.79	−96.94
175	−102.50	−102.00	−101.50	−101.02	−100.56	−99.66	−98.78	−97.93
200	−103.51	−103.00	−102.51	−102.03	−101.56	−100.66	−99.78	−98.93
225	−104.51	−104.01	−103.51	−103.03	−102.56	−101.66	−100.78	−99.92
250	−105.51	−105.02	−104.52	−104.04	−103.57	−102.66	−101.78	−100.92
300	−107.49	−107.04	−106.53	−106.05	−105.57	−104.66	−103.78	−102.92
350	−109.48	−109.08	−108.55	−108.06	−107.58	−106.66	−105.78	−104.92
400		−111.14	−110.58	−110.07	−109.59	−108.67	−107.78	−106.91
450		−113.32	−112.62	−112.09	−111.60	−110.67	−109.78	−108.91
500		−115.67	−114.68	−114.12	−113.62	−112.67	−111.77	−110.90
550		−117.95	−116.77	−116.15	−115.63	−114.67	−113.77	−112.89
600		−120.14	−118.88	−118.20	−117.65	−116.68	−115.76	−114.88
700		−124.38	−123.10	−122.30	−121.70	−120.68	−119.75	−118.86
800		−128.50	−127.25	−126.40	−125.75	−124.68	−123.73	−122.83
900		−132.55	−131.34	−130.46	−129.78	−128.67	−127.71	−126.80
1000		−136.56	−135.37	−134.48	−133.78	−132.65	−131.68	−130.77
				$KHSO_4^\circ$				
25	−246.55	−245.93	−245.33	−244.76	−244.19	−243.10	−242.03	−240.99
50	−248.00	−247.35	−246.74	−246.14	−245.57	−244.45	−243.36	−242.30
75	−249.51	−248.85	−248.22	−247.62	−247.03	−245.90	−244.80	−243.73
100	−251.07	−250.41	−249.78	−249.17	−248.57	−247.43	−246.33	−245.25
125	−252.69	−252.02	−251.38	−250.77	−250.17	−249.02	−247.91	−246.83
150	−254.35	−253.68	−253.04	−252.42	−251.83	−250.67	−249.56	−248.47
175	−256.06	−255.39	−254.75	−254.13	−253.52	−252.37	−251.25	−250.16
200	−257.80	−257.14	−256.49	−255.87	−255.27	−254.11	−252.99	−251.90
225	−259.57	−258.93	−258.28	−257.65	−257.05	−255.89	−254.76	−253.67
250	−261.38	−260.75	−260.10	−259.47	−258.87	−257.70	−256.58	−255.49
300	−265.07	−264.50	−263.85	−263.22	−262.61	−261.45	−260.32	−259.22
350	−268.84	−268.38	−267.73	−267.10	−266.49	−265.32	−264.19	−263.09
400		−272.38	−271.72	−271.09	−270.48	−269.31	−268.18	−267.08
450		−276.48	−275.82	−275.19	−274.58	−273.40	−272.27	−271.17
500		−280.70	−280.02	−279.39	−278.78	−277.60	−276.47	−275.37
550		−285.00	−284.32	−283.68	−283.07	−281.89	−280.76	−279.65
600		−289.39	−288.70	−288.06	−287.45	−286.27	−285.13	−284.03
700		−298.40	−297.71	−297.07	−296.45	−295.27	−294.13	−293.03
800		−307.70	−307.01	−306.36	−305.74	−304.56	−303.42	−302.32
900		−317.26	−316.58	−315.93	−315.31	−314.12	−312.98	−311.88
1000		−327.07	−326.38	−325.73	−325.11	−323.92	−322.78	−321.68
				KI°				
25	−77.74	−77.09	−76.46	−75.86	−75.27	−74.13	−73.02	−71.93
50	−78.98	−78.30	−77.66	−77.04	−76.43	−75.26	−74.13	−73.03
75	−80.21	−79.53	−78.87	−78.24	−77.62	−76.44	−75.30	−74.18
100	−81.45	−80.75	−80.09	−79.45	−78.83	−77.63	−76.48	−75.36
125	−82.68	−81.98	−81.31	−80.67	−80.04	−78.84	−77.68	−76.56
150	−83.91	−83.21	−82.54	−81.89	−81.27	−80.06	−78.90	−77.76
175	−85.15	−84.45	−83.77	−83.12	−82.49	−81.28	−80.12	−78.98
200	−86.38	−85.69	−85.01	−84.36	−83.73	−82.51	−81.34	−80.21
225	−87.61	−86.93	−86.25	−85.60	−84.96	−83.75	−82.57	−81.44
250	−88.84	−88.18	−87.49	−86.84	−86.21	−84.99	−83.81	−82.67
300	−91.27	−90.68	−89.99	−89.33	−88.70	−87.48	−86.30	−85.15
350	−93.68	−93.19	−92.50	−91.84	−91.21	−89.98	−88.80	−87.65
400		−95.72	−95.03	−94.36	−93.72	−92.49	−91.31	−90.17
450		−98.29	−97.56	−96.90	−96.25	−95.02	−93.84	−92.69
500		−100.89	−100.11	−99.44	−98.80	−97.56	−96.37	−95.22
550		−103.48	−102.68	−101.99	−101.35	−100.11	−98.92	−97.77
600		−106.07	−105.25	−104.56	−103.91	−102.66	−101.48	−100.32
700		−111.25	−110.43	−109.72	−109.05	−107.80	−106.61	−105.45

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				KI° — Continued				
800		−116.45	−115.63	−114.90	−114.23	−112.97	−111.77	−110.62
900		−121.65	−120.84	−120.11	−119.43	−118.17	−116.97	−115.81
1000		−126.88	−126.07	−125.34	−124.66	−123.38	−122.18	−121.02
				KOH°				
25	−103.88	−103.70	−103.52	−103.34	−103.15	−102.76	−102.36	−101.96
50	−104.58	−104.40	−104.21	−104.02	−103.83	−103.44	−103.04	−102.64
75	−105.28	−105.09	−104.90	−104.71	−104.52	−104.12	−103.73	−103.33
100	−105.98	−105.79	−105.60	−105.41	−105.21	−104.82	−104.42	−104.03
125	−106.69	−106.49	−106.30	−106.10	−105.91	−105.51	−105.12	−104.72
150	−107.39	−107.20	−107.00	−106.80	−106.61	−106.21	−105.82	−105.42
175	−108.10	−107.90	−107.70	−107.50	−107.31	−106.91	−106.52	−106.12
200	−108.80	−108.61	−108.41	−108.21	−108.01	−107.61	−107.22	−106.82
225	−109.51	−109.31	−109.11	−108.91	−108.71	−108.31	−107.92	−107.52
250	−110.22	−110.02	−109.82	−109.61	−109.41	−109.01	−108.62	−108.22
300	−111.64	−111.45	−111.23	−111.02	−110.82	−110.42	−110.02	−109.62
350	−113.12	−112.89	−112.66	−112.44	−112.23	−111.82	−111.42	−111.02
400		−114.39	−114.10	−113.87	−113.65	−113.23	−112.82	−112.42
450		−116.10	−115.57	−115.30	−115.07	−114.64	−114.23	−113.82
500		−118.09	−117.08	−116.75	−116.50	−116.06	−115.64	−115.23
550		−119.97	−118.64	−118.23	−117.94	−117.47	−117.04	−116.63
600		−121.71	−120.24	−119.72	−119.40	−118.90	−118.46	−118.04
700		−124.95	−123.45	−122.74	−122.33	−121.76	−121.29	−120.85
800		−128.02	−126.58	−125.77	−125.27	−124.63	−124.13	−123.68
900		−130.99	−129.60	−128.75	−128.21	−127.50	−126.97	−126.51
1000		−133.89	−132.56	−131.69	−131.12	−130.36	−129.82	−129.36
				KSO_4^-				
25	−246.64	−246.30	−245.97	−245.63	−245.30	−244.63	−243.96	−243.30
50	−247.51	−247.16	−246.81	−246.47	−246.13	−245.46	−244.79	−244.13
75	−248.36	−248.01	−247.66	−247.32	−246.98	−246.31	−245.65	−244.99
100	−249.20	−248.85	−248.51	−248.17	−247.84	−247.17	−246.51	−245.86
125	−250.02	−249.69	−249.35	−249.02	−248.69	−248.04	−247.38	−246.73
150	−250.83	−250.51	−250.19	−249.87	−249.55	−248.90	−248.26	−247.62
175	−251.61	−251.32	−251.02	−250.71	−250.40	−249.77	−249.14	−248.51
200	−252.36	−252.11	−251.84	−251.55	−251.25	−250.64	−250.02	−249.40
225	−253.07	−252.88	−252.64	−252.37	−252.09	−251.51	−250.91	−250.30
250	−253.72	−253.62	−253.42	−253.18	−252.92	−252.37	−251.79	−251.20
300	−254.71	−254.94	−254.91	−254.75	−254.55	−254.09	−253.56	−253.01
350	−254.65	−255.92	−256.25	−256.24	−256.13	−255.78	−255.33	−254.83
400		−256.32	−257.36	−257.60	−257.63	−257.43	−257.07	−256.64
450		−253.94	−258.11	−258.79	−259.02	−259.04	−258.80	−258.44
500			−258.27	−259.74	−260.28	−260.58	−260.49	−260.23
550			−257.67	−260.41	−261.38	−262.06	−262.15	−261.99
600			−256.49	−260.80	−262.33	−263.46	−263.75	−263.72
700				−261.04	−263.80	−266.02	−266.81	−267.05
800					−265.01	−268.32	−269.65	−270.18
900					−266.32	−270.51	−272.32	−273.09
1000						−272.77	−274.93	−275.78
				Kr°				
25	3.55	3.95	4.33	4.71	5.09	5.82	6.55	7.26
50	3.12	3.53	3.93	4.32	4.70	5.45	6.19	6.91
75	2.59	3.01	3.42	3.82	4.21	4.97	5.71	6.43
100	1.98	2.41	2.82	3.22	3.62	4.38	5.13	5.86
125	1.29	1.73	2.15	2.55	2.95	3.72	4.47	5.20
150	0.54	0.98	1.40	1.81	2.21	2.99	3.74	4.48
175	−0.29	0.16	0.59	1.00	1.41	2.19	2.95	3.69
200	−1.17	−0.72	−0.28	0.14	0.54	1.33	2.09	2.84

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Kr° — Continued				
225	−2.12	−1.66	−1.22	−0.79	−0.38	0.42	1.18	1.93
250	−3.12	−2.66	−2.20	−1.77	−1.35	−0.55	0.22	0.97
300	−5.34	−4.84	−4.35	−3.89	−3.46	−2.63	−1.85	−1.09
350	−8.00	−7.29	−6.70	−6.21	−5.75	−4.90	−4.10	−3.33
400		−10.16	−9.30	−8.73	−8.23	−7.34	−6.52	−5.73
450		−14.10	−12.16	−11.45	−10.90	−9.95	−9.10	−8.29
500		−19.50	−15.35	−14.38	−13.73	−12.71	−11.82	−10.99
550		−24.49	−18.92	−17.53	−16.75	−15.62	−14.68	−13.83
600		−28.97	−22.79	−20.89	−19.93	−18.67	−17.68	−16.80
700		−37.23	−30.89	−28.14	−26.76	−25.16	−24.05	−23.10
800		−45.10	−39.00	−35.80	−34.06	−32.12	−30.87	−29.86
900		−52.88	−47.05	−43.67	−41.68	−39.46	−38.09	−37.03
1000		−60.70	−55.11	−51.65	−49.53	−47.11	−45.66	−44.58
				Leucine				
25	−82.00	−80.75	−79.55	−78.38	−77.25	−75.05	−72.91	−70.82
50	−83.39	−82.13	−80.93	−79.77	−78.64	−76.45	−74.34	−72.27
75	−84.95	−83.69	−82.48	−81.33	−80.20	−78.02	−75.92	−73.87
100	−86.68	−85.42	−84.21	−83.05	−81.92	−79.75	−77.65	−75.61
125	−88.57	−87.30	−86.09	−84.92	−83.80	−81.62	−79.53	−77.49
150	−90.60	−89.33	−88.11	−86.94	−85.82	−83.64	−81.54	−79.50
175	−92.77	−91.50	−90.27	−89.10	−87.97	−85.79	−83.69	−81.65
200	−95.07	−93.80	−92.56	−91.39	−90.25	−88.06	−85.96	−83.92
225	−97.50	−96.23	−94.98	−93.79	−92.65	−90.45	−88.35	−86.30
250	−100.05	−98.79	−97.52	−96.32	−95.17	−92.96	−90.85	−88.80
300	−105.59	−104.30	−102.96	−101.72	−100.54	−98.30	−96.17	−94.11
350	−112.01	−110.38	−108.87	−107.55	−106.33	−104.04	−101.88	−99.80
400		−117.31	−115.27	−113.82	−112.53	−110.17	−107.96	−105.86
450		−126.38	−122.25	−120.52	−119.12	−116.65	−114.39	−112.26
500		−138.29	−129.90	−127.67	−126.09	−123.47	−121.15	−118.97
550		−149.44	−138.32	−135.29	−133.44	−130.62	−128.21	−125.99
600		−159.66	−147.37	−143.35	−141.16	−138.09	−135.57	−133.30
700		−178.84	−166.25	−160.59	−157.59	−153.88	−151.12	−148.72
800		−197.42	−185.28	−178.77	−175.07	−170.70	−167.68	−165.15
900		−215.94	−204.32	−197.44	−193.29	−188.37	−185.13	−182.50
1000		−234.64	−223.49	−216.47	−212.05	−206.76	−203.36	−200.70
				La^{+3}				
25	−164.00	−164.43	−164.81	−165.15	−165.45	−165.99	−166.46	−166.87
50	−162.66	−163.12	−163.51	−163.87	−164.19	−164.76	−165.27	−165.72
75	−161.27	−161.74	−162.15	−162.52	−162.86	−163.47	−164.00	−164.49
100	−159.83	−160.32	−160.75	−161.14	−161.50	−162.13	−162.69	−163.20
125	−158.34	−158.85	−159.31	−159.72	−160.09	−160.75	−161.34	−161.87
150	−156.78	−157.34	−157.83	−158.26	−158.65	−159.35	−159.96	−160.52
175	−155.17	−155.78	−156.30	−156.76	−157.18	−157.92	−158.56	−159.14
200	−153.50	−154.16	−154.73	−155.23	−155.68	−156.46	−157.14	−157.75
225	−151.74	−152.48	−153.11	−153.65	−154.14	−154.97	−155.69	−156.33
250	−149.90	−150.73	−151.44	−152.04	−152.56	−153.46	−154.22	−154.90
300	−145.88	−147.05	−147.98	−148.69	−149.31	−150.35	−151.23	−151.99
350	−141.79	−143.01	−144.40	−145.20	−145.92	−147.14	−148.15	−149.01
400		−140.72	−140.80	−141.63	−142.43	−143.83	−144.98	−145.96
450		−141.80	−137.35	−138.00	−138.85	−140.42	−141.74	−142.85
500			−134.33	−134.35	−135.19	−136.92	−138.41	−139.66
550			−132.07	−130.78	−131.44	−133.31	−134.98	−136.38
600			−130.68	−127.37	−127.64	−129.57	−131.43	−133.00
700				−121.40	−119.89	−121.62	−123.91	−125.87
800					−111.92	−112.97	−115.75	−118.13
900					−103.45	−103.66	−106.98	−109.76
1000						−93.94	−97.81	−100.80

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Li^+				
25	−69.93	−69.94	−69.93	−69.91	−69.89	−69.82	−69.73	−69.64
50	−70.02	−70.02	−70.02	−70.02	−70.00	−69.96	−69.90	−69.84
75	−70.12	−70.14	−70.15	−70.14	−70.14	−70.11	−70.08	−70.03
100	−70.26	−70.28	−70.29	−70.30	−70.29	−70.28	−70.26	−70.23
125	−70.41	−70.44	−70.46	−70.47	−70.47	−70.47	−70.46	−70.44
150	−70.58	−70.62	−70.64	−70.66	−70.67	−70.69	−70.68	−70.67
175	−70.77	−70.81	−70.85	−70.88	−70.89	−70.92	−70.92	−70.92
200	−70.96	−71.02	−71.07	−71.11	−71.13	−71.17	−71.19	−71.19
225	−71.16	−71.24	−71.31	−71.35	−71.39	−71.43	−71.46	−71.48
250	−71.36	−71.47	−71.55	−71.61	−71.65	−71.72	−71.76	−71.79
300	−71.74	−71.94	−72.08	−72.16	−72.23	−72.33	−72.40	−72.45
350	−72.09	−72.40	−72.65	−72.76	−72.86	−73.00	−73.10	−73.18
400		−73.19	−73.27	−73.41	−73.53	−73.72	−73.86	−73.96
450		−74.40	−73.95	−74.09	−74.24	−74.48	−74.66	−74.80
500			−74.71	−74.82	−74.99	−75.28	−75.51	−75.68
550			−75.60	−75.58	−75.76	−76.12	−76.39	−76.59
600			−76.62	−76.41	−76.57	−76.97	−77.30	−77.54
700				−78.30	−78.26	−78.72	−79.17	−79.51
800					−80.07	−80.51	−81.09	−81.53
900					−81.95	−82.32	−83.05	−83.58
1000						−84.22	−85.07	−85.66
				$Li(CH_3COO)^\circ$				
25	−158.61	−158.04	−157.50	−156.97	−156.45	−155.45	−154.46	−153.50
50	−159.18	−158.59	−158.03	−157.49	−156.96	−155.93	−154.93	−153.95
75	−159.89	−159.30	−158.72	−158.17	−157.63	−156.59	−155.58	−154.59
100	−160.73	−160.12	−159.54	−158.98	−158.44	−157.39	−156.37	−155.38
125	−161.67	−161.06	−160.47	−159.91	−159.36	−158.31	−157.29	−156.29
150	−162.70	−162.09	−161.51	−160.94	−160.39	−159.33	−158.30	−157.30
175	−163.83	−163.22	−162.63	−162.06	−161.51	−160.44	−159.41	−158.41
200	−165.04	−164.43	−163.84	−163.27	−162.71	−161.64	−160.61	−159.61
225	−166.32	−165.72	−165.13	−164.55	−164.00	−162.92	−161.89	−160.89
250	−167.67	−167.09	−166.49	−165.91	−165.36	−164.28	−163.25	−162.24
300	−170.57	−170.03	−169.43	−168.85	−168.29	−167.21	−166.17	−165.16
350	−173.72	−173.24	−172.62	−172.04	−171.47	−170.39	−169.34	−168.33
400		−176.72	−176.06	−175.47	−174.90	−173.80	−172.76	−171.74
450		−180.54	−179.74	−179.12	−178.54	−177.44	−176.39	−175.37
500		−184.72	−183.63	−182.98	−182.39	−181.28	−180.22	−179.20
550		−189.03	−187.75	−187.04	−186.43	−185.30	−184.24	−183.21
600		−193.42	−192.06	−191.28	−190.65	−189.51	−188.43	−187.40
700		−202.55	−201.17	−200.28	−199.59	−198.40	−197.31	−196.27
800		−212.17	−210.82	−209.87	−209.13	−207.90	−206.79	−205.74
900		−222.26	−220.95	−219.97	−219.20	−217.93	−216.81	−215.75
1000		−232.80	−231.51	−230.53	−229.74	−228.44	−227.31	−226.25
				$Li(CH_3COO)_2^-$				
25	−246.81	−245.62	−244.49	−243.41	−242.36	−240.35	−238.42	−236.54
50	−247.63	−246.41	−245.25	−244.14	−243.06	−241.00	−239.02	−237.10
75	−248.76	−247.52	−246.35	−245.22	−244.14	−242.05	−240.05	−238.11
100	−250.14	−248.90	−247.72	−246.59	−245.50	−243.41	−241.39	−239.44
125	−251.74	−250.51	−249.33	−248.20	−247.11	−245.02	−243.00	−241.04
150	−253.53	−252.31	−251.15	−250.03	−248.94	−246.85	−244.84	−242.88
175	−255.47	−254.30	−253.15	−252.04	−250.96	−248.88	−246.88	−244.92
200	−257.56	−256.44	−255.32	−254.22	−253.16	−251.10	−249.10	−247.16
225	−259.76	−258.72	−257.63	−256.57	−255.52	−253.48	−251.50	−249.57
250	−262.05	−261.13	−260.09	−259.05	−258.03	−256.02	−254.06	−252.15
300	−266.69	−266.22	−265.36	−264.41	−263.45	−261.53	−259.63	−257.75
350	−270.69	−271.47	−271.01	−270.21	−269.35	−267.55	−265.73	−263.90
400		−276.67	−276.91	−276.37	−275.66	−274.03	−272.31	−270.55
450		−279.50	−282.88	−282.80	−282.30	−280.91	−279.31	−277.64

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Li(CH_3COO)_2^-$ — Continued				
500			−288.67	−289.41	−289.23	−288.14	−286.71	−285.14
550			−294.08	−296.12	−296.38	−295.69	−294.45	−293.00
600			−299.26	−302.89	−303.73	−303.52	−302.50	−301.19
700				−316.92	−319.00	−319.93	−319.45	−318.44
800					−335.23	−337.30	−337.40	−336.70
900					−352.68	−355.64	−356.27	−355.84
1000						−375.06	−376.08	−375.75
				$LiCl^\circ$				
25	−99.25	−98.92	−98.59	−98.27	−97.94	−97.31	−96.67	−96.05
50	−99.60	−99.25	−98.91	−98.58	−98.25	−97.60	−96.97	−96.33
75	−99.99	−99.63	−99.29	−98.95	−98.61	−97.96	−97.32	−96.68
100	−100.41	−100.05	−99.69	−99.35	−99.02	−98.36	−97.71	−97.07
125	−100.86	−100.49	−100.14	−99.79	−99.45	−98.79	−98.14	−97.50
150	−101.34	−100.97	−100.61	−100.26	−99.92	−99.25	−98.60	−97.96
175	−101.85	−101.48	−101.12	−100.76	−100.42	−99.75	−99.10	−98.45
200	−102.39	−102.02	−101.65	−101.29	−100.95	−100.27	−99.61	−98.97
225	−102.96	−102.58	−102.21	−101.85	−101.50	−100.82	−100.16	−99.51
250	−103.55	−103.18	−102.79	−102.43	−102.07	−101.39	−100.72	−100.08
300	−104.84	−104.45	−104.04	−103.66	−103.30	−102.60	−101.93	−101.27
350	−106.38	−105.86	−105.39	−104.99	−104.61	−103.89	−103.21	−102.55
400		−107.51	−106.87	−106.41	−106.01	−105.26	−104.57	−103.90
450		−109.85	−108.48	−107.94	−107.49	−106.71	−106.00	−105.31
500		−113.11	−110.29	−109.57	−109.07	−108.24	−107.50	−106.80
550		−116.07	−112.32	−111.32	−110.73	−109.83	−109.06	−108.35
600		−118.67	−114.52	−113.19	−112.48	−111.49	−110.69	−109.95
700		−123.34	−119.09	−117.20	−116.21	−115.01	−114.12	−113.34
800		−127.68	−123.58	−121.40	−120.17	−118.74	−117.76	−116.94
900		−131.87	−127.95	−125.65	−124.26	−122.64	−121.59	−120.73
1000		−136.02	−132.26	−129.91	−128.43	−126.69	−125.58	−124.71
				Lu^{+3}				
25	−159.40	−159.91	−160.35	−160.75	−161.12	−161.76	−162.32	−162.83
50	−157.79	−158.32	−158.79	−159.21	−159.59	−160.28	−160.89	−161.45
75	−156.13	−156.68	−157.17	−157.61	−158.01	−158.74	−159.38	−159.97
100	−154.43	−155.00	−155.51	−155.97	−156.39	−157.15	−157.83	−158.45
125	−152.67	−153.28	−153.82	−154.30	−154.74	−155.54	−156.24	−156.89
150	−150.86	−151.52	−152.09	−152.60	−153.06	−153.90	−154.63	−155.31
175	−148.99	−149.70	−150.31	−150.86	−151.35	−152.23	−153.00	−153.70
200	−147.06	−147.83	−148.50	−149.08	−149.61	−150.54	−151.35	−152.09
225	−145.04	−145.89	−146.63	−147.27	−147.84	−148.83	−149.69	−150.45
250	−142.93	−143.90	−144.72	−145.42	−146.03	−147.09	−148.00	−148.81
300	−138.38	−139.71	−140.77	−141.59	−142.31	−143.54	−144.58	−145.48
350	−133.96	−135.18	−136.74	−137.65	−138.48	−139.90	−141.08	−142.10
400		−132.93	−132.75	−133.64	−134.55	−136.16	−137.51	−138.66
450		−135.46	−129.03	−129.62	−130.55	−132.34	−133.86	−135.16
500			−125.98	−125.65	−126.50	−128.43	−130.14	−131.60
550			−124.05	−121.83	−122.39	−124.42	−126.32	−127.95
600			−123.41	−118.30	−118.26	−120.29	−122.39	−124.20
700				−112.49	−109.97	−111.54	−114.08	−116.31
800					−101.53	−102.04	−105.08	−107.78
900					−92.52	−91.80	−95.42	−98.57
1000						−81.11	−85.33	−88.73
				Methanamine				
25	5.04	5.54	6.03	6.51	6.99	7.94	8.89	9.82
50	4.24	4.74	5.22	5.70	6.18	7.11	8.03	8.95
75	3.36	3.86	4.35	4.82	5.29	6.22	7.13	8.03
100	2.42	2.92	3.40	3.88	4.34	5.26	6.17	7.06

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
Methanamine — Continued								
125	1.41	1.90	2.39	2.86	3.33	4.25	5.14	6.03
150	0.33	0.83	1.32	1.79	2.26	3.17	4.07	4.95
175	−0.80	−0.31	0.18	0.66	1.13	2.04	2.93	3.81
200	−1.99	−1.50	−1.01	−0.53	−0.06	0.85	1.74	2.62
225	−3.24	−2.75	−2.25	−1.77	−1.30	−0.39	0.50	1.38
250	−4.53	−4.05	−3.55	−3.07	−2.59	−1.68	−0.79	0.09
300	−7.29	−6.81	−6.29	−5.80	−5.32	−4.40	−3.50	−2.63
350	−10.35	−9.80	−9.23	−8.72	−8.23	−7.30	−6.39	−5.51
400		−13.08	−12.37	−11.82	−11.31	−10.36	−9.45	−8.56
450		−17.02	−15.72	−15.10	−14.56	−13.57	−12.65	−11.75
500		−21.79	−19.31	−18.55	−17.96	−16.94	−15.99	−15.09
550		−26.40	−23.17	−22.18	−21.52	−20.44	−19.47	−18.56
600		−30.79	−27.24	−25.98	−25.22	−24.07	−23.08	−22.15
700		−39.37	−35.73	−34.01	−33.04	−31.71	−30.65	−29.68
800		−47.93	−44.42	−42.47	−41.29	−39.79	−38.65	−37.65
900		−56.62	−53.25	−51.20	−49.90	−48.24	−47.04	−46.02
1000		−65.48	−62.25	−60.15	−58.78	−57.02	−55.78	−54.75
Methane								
25	−8.23	−7.80	−7.37	−6.95	−6.54	−5.74	−4.95	−4.18
50	−8.82	−8.37	−7.93	−7.50	−7.08	−6.26	−5.46	−4.67
75	−9.52	−9.05	−8.60	−8.17	−7.74	−6.91	−6.10	−5.31
100	−10.32	−9.84	−9.38	−8.94	−8.51	−7.67	−6.85	−6.06
125	−11.20	−10.71	−10.25	−9.80	−9.36	−8.52	−7.70	−6.90
150	−12.16	−11.67	−11.20	−10.74	−10.30	−9.45	−8.62	−7.82
175	−13.19	−12.70	−12.22	−11.76	−11.31	−10.45	−9.62	−8.81
200	−14.30	−13.80	−13.31	−12.84	−12.39	−11.52	−10.68	−9.87
225	−15.48	−14.96	−14.46	−13.99	−13.53	−12.65	−11.81	−10.99
250	−16.73	−16.20	−15.69	−15.20	−14.74	−13.85	−13.00	−12.17
300	−19.47	−18.89	−18.32	−17.81	−17.32	−16.40	−15.54	−14.70
350	−22.81	−21.91	−21.22	−20.64	−20.13	−19.17	−18.28	−17.43
400		−25.46	−24.39	−23.72	−23.15	−22.14	−21.21	−20.34
450		−30.49	−27.90	−27.03	−26.38	−25.29	−24.33	−23.43
500		−37.50	−31.83	−30.60	−29.82	−28.62	−27.61	−26.68
550		−43.90	−36.25	−34.44	−33.47	−32.13	−31.05	−30.09
600		−49.56	−41.07	−38.54	−37.32	−35.79	−34.64	−33.64
700		−59.82	−51.10	−47.39	−45.58	−43.59	−42.26	−41.17
800		−69.42	−61.04	−56.71	−54.40	−51.93	−50.41	−49.22
900		−78.80	−70.80	−66.20	−63.56	−60.69	−59.01	−57.75
1000		−88.14	−80.47	−75.77	−72.94	−69.80	−68.01	−66.72
Methanol								
25	−42.05	−41.60	−41.15	−40.70	−40.25	−39.37	−38.49	−37.61
50	−42.89	−42.44	−42.00	−41.55	−41.12	−40.25	−39.39	−38.54
75	−43.81	−43.36	−42.92	−42.48	−42.05	−41.19	−40.35	−39.51
100	−44.81	−44.35	−43.91	−43.47	−43.04	−42.19	−41.36	−40.53
125	−45.87	−45.41	−44.97	−44.53	−44.10	−43.26	−42.43	−41.61
150	−46.99	−46.54	−46.09	−45.65	−45.23	−44.38	−43.56	−42.74
175	−48.17	−47.72	−47.27	−46.84	−46.41	−45.57	−44.74	−43.93
200	−49.42	−48.97	−48.51	−48.08	−47.65	−46.80	−45.98	−45.17
225	−50.72	−50.27	−49.81	−49.37	−48.94	−48.10	−47.27	−46.46
250	−52.07	−51.62	−51.16	−50.72	−50.28	−49.44	−48.61	−47.80
300	−54.96	−54.50	−54.02	−53.56	−53.12	−52.26	−51.43	−50.62
350	−58.19	−57.62	−57.08	−56.60	−56.14	−55.27	−54.43	−53.61
400		−61.06	−60.35	−59.82	−59.34	−58.44	−57.60	−56.77
450		−65.26	−63.84	−63.22	−62.71	−61.78	−60.91	−60.08
500		−70.45	−67.60	−66.82	−66.24	−65.26	−64.37	−63.53
550		−75.42	−71.66	−70.60	−69.94	−68.89	−67.97	−67.11
600		−80.11	−75.95	−74.56	−73.79	−72.66	−71.71	−70.83
700		−89.15	−84.89	−82.95	−81.90	−80.56	−79.53	−78.61

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Methanol — Continued				
800		−98.10	−93.99	−91.77	−90.49	−88.92	−87.80	−86.84
900		−107.13	−103.20	−100.85	−99.41	−97.67	−96.47	−95.48
1000		−116.31	−112.53	−110.14	−108.61	−106.74	−105.50	−104.49
				Methionine				
25	−120.20	−118.97	−117.80	−116.66	−115.55	−113.39	−111.30	−109.26
50	−121.92	−120.68	−119.50	−118.37	−117.26	−115.12	−113.05	−111.03
75	−123.76	−122.53	−121.35	−120.21	−119.10	−116.97	−114.91	−112.90
100	−125.74	−124.50	−123.31	−122.17	−121.07	−118.93	−116.88	−114.87
125	−127.83	−126.58	−125.39	−124.25	−123.14	−121.01	−118.95	−116.95
150	−130.04	−128.79	−127.59	−126.44	−125.33	−123.19	−121.13	−119.13
175	−132.36	−131.10	−129.89	−128.73	−127.61	−125.46	−123.40	−121.40
200	−134.78	−133.52	−132.29	−131.12	−130.00	−127.84	−125.77	−123.76
225	−137.32	−136.04	−134.79	−133.61	−132.47	−130.30	−128.22	−126.21
250	−139.96	−138.67	−137.39	−136.19	−135.04	−132.85	−130.76	−128.74
300	−145.66	−144.28	−142.89	−141.63	−140.44	−138.20	−136.08	−134.04
350	−152.45	−150.45	−148.81	−147.43	−146.18	−143.87	−141.70	−139.63
400		−157.61	−155.19	−153.62	−152.26	−149.83	−147.61	−145.50
450		−167.72	−162.18	−160.20	−158.68	−156.09	−153.79	−151.63
500		−181.83	−169.95	−167.23	−165.44	−162.63	−160.22	−158.00
550		−194.60	−178.65	−174.72	−172.55	−169.44	−166.91	−164.62
600		−205.79	−188.09	−182.69	−180.00	−176.52	−173.83	−171.46
700		−225.72	−207.57	−199.73	−195.83	−191.40	−188.35	−185.79
800		−244.08	−226.60	−217.49	−212.56	−207.14	−203.69	−200.95
900		−261.73	−245.05	−235.39	−229.77	−223.54	−219.76	−216.86
1000		−279.10	−263.10	−253.23	−247.22	−240.43	−236.43	−233.48
				Monochloroacetate				
25	−92.86	−92.26	−91.68	−91.11	−90.55	−89.44	−88.34	−87.26
50	−93.75	−93.15	−92.57	−92.00	−91.43	−90.33	−89.25	−88.18
75	−94.67	−94.07	−93.49	−92.92	−92.36	−91.26	−90.19	−89.13
100	−95.60	−95.01	−94.43	−93.87	−93.32	−92.23	−91.16	−90.11
125	−96.55	−95.97	−95.40	−94.85	−94.30	−93.23	−92.17	−91.13
150	−97.51	−96.95	−96.40	−95.85	−95.31	−94.25	−93.21	−92.17
175	−98.46	−97.94	−97.40	−96.87	−96.34	−95.30	−94.27	−93.25
200	−99.41	−98.93	−98.42	−97.90	−97.39	−96.37	−95.35	−94.35
225	−100.33	−99.92	−99.44	−98.95	−98.45	−97.46	−96.46	−95.47
250	−101.22	−100.89	−100.46	−100.00	−99.53	−98.57	−97.59	−96.62
300	−102.73	−102.77	−102.49	−102.12	−101.71	−100.83	−99.91	−98.98
350	−103.25	−104.35	−104.45	−104.22	−103.90	−103.13	−102.29	−101.41
400		−105.44	−106.25	−106.26	−106.08	−105.47	−104.72	−103.90
450		−103.81	−107.74	−108.19	−108.21	−107.82	−107.19	−106.45
500			−108.70	−109.95	−110.27	−110.16	−109.68	−109.04
550			108.96	111.47	112.23	112.49	112.19	111.65
600			−108.68	−112.76	−114.07	−114.79	−114.69	−114.28
700				−114.94	−117.48	−119.29	−119.68	−119.55
800					−120.80	−123.70	−124.63	−124.78
900					−124.38	−128.15	−129.56	−129.95
1000						−132.81	−134.57	−135.04
				Monochloroacetic Acid				
25	−55.12	−54.29	−53.48	−52.70	−51.93	−50.42	−48.95	−47.51
50	−56.61	−55.78	−54.97	−54.19	−53.42	−51.94	−50.49	−49.07
75	−58.20	−57.36	−56.55	−55.77	−55.00	−53.52	−52.08	−50.67
100	−59.87	−59.02	−58.21	−57.43	−56.66	−55.19	−53.75	−52.35
125	−61.62	−60.77	−59.95	−59.17	−58.40	−56.92	−55.49	−54.09
150	−63.45	−62.59	−61.77	−60.98	−60.21	−58.73	−57.30	−55.90
175	−65.36	−64.50	−63.66	−62.87	−62.10	−60.61	−59.17	−57.77
200	−67.34	−66.47	−65.63	−64.82	−64.04	−62.55	−61.11	−59.70

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
Monochloroacetic Acid — Continued								
225	−69.41	−68.53	−67.66	−66.85	−66.06	−64.55	−63.10	−61.70
250	−71.55	−70.66	−69.77	−68.94	−68.14	−66.62	−65.16	−63.74
300	−76.16	−75.17	−74.19	−73.31	−72.48	−70.92	−69.43	−68.00
350	−81.62	−80.10	−78.92	−77.95	−77.06	−75.44	−73.92	−72.47
400		−85.81	−83.99	−82.85	−81.89	−80.17	−78.61	−77.12
450		−93.90	−89.53	−88.06	−86.96	−85.11	−83.48	−81.96
500		−105.23	−95.68	−93.60	−92.28	−90.25	−88.54	−86.96
550		−115.43	−102.56	−99.50	−97.86	−95.59	−93.77	−92.14
600		−124.32	−110.02	−105.75	−103.70	−101.12	−99.17	−97.47
700		−140.03	−125.36	−119.10	−116.05	−112.70	−110.46	−108.61
800		−154.36	−140.24	−132.95	−129.05	−124.89	−122.33	−120.33
900		−168.04	−154.57	−146.82	−142.37	−137.55	−134.71	−132.59
1000		−181.42	−168.50	−160.59	−155.82	−150.54	−147.52	−145.35
Monochloroacetyl Chloride								
25	−96.77	−96.04	−95.34	−94.66	−94.00	−92.71	−91.46	−90.23
50	−98.12	−97.37	−96.66	−95.96	−95.29	−93.99	−92.73	−91.50
75	−99.55	−98.79	−98.07	−97.37	−96.69	−95.38	−94.11	−92.88
100	−101.07	−100.30	−99.57	−98.87	−98.18	−96.86	−95.59	−94.35
125	−102.66	−101.89	−101.15	−100.44	−99.75	−98.43	−97.15	−95.91
150	−104.34	−103.56	−102.81	−102.09	−101.40	−100.07	−98.78	−97.54
175	−106.08	−105.29	−104.54	−103.82	−103.12	−101.78	−100.49	−99.24
200	−107.89	−107.10	−106.34	−105.61	−104.90	−103.55	−102.26	−101.00
225	−109.78	−108.98	−108.20	−107.46	−106.75	−105.39	−104.09	−102.83
250	−111.73	−110.93	−110.13	−109.38	−108.66	−107.29	−105.98	−104.71
300	−115.90	−115.05	−114.19	−113.40	−112.66	−111.25	−109.92	−108.64
350	−120.71	−119.52	−118.51	−117.66	−116.88	−115.43	−114.07	−112.77
400		−124.58	−123.13	−122.16	−121.32	−119.80	−118.41	−117.09
450		−131.36	−128.12	−126.92	−125.98	−124.37	−122.93	−121.58
500		−140.44	−133.58	−131.95	−130.86	−129.13	−127.63	−126.24
550		−148.79	−139.60	−137.28	−135.97	−134.06	−132.49	−131.06
600		−156.25	−146.06	−142.90	−141.29	−139.17	−137.50	−136.03
700		−169.83	−159.38	−154.82	−152.52	−149.86	−147.99	−146.40
800		−182.58	−172.51	−167.23	−164.34	−161.10	−159.01	−157.31
900		−194.99	−185.37	−179.77	−176.49	−172.80	−170.51	−168.73
1000		−207.29	−198.07	−192.35	−188.84	−184.83	−182.41	−180.60
Mg^{+2}								
25	−108.50	−108.74	−108.94	−109.12	−109.27	−109.51	−109.71	−109.88
50	−107.68	−107.92	−108.13	−108.31	−108.47	−108.74	−108.97	−109.16
75	−106.84	−107.10	−107.32	−107.51	−107.68	−107.97	−108.22	−108.43
100	−106.01	−106.28	−106.51	−106.72	−106.90	−107.21	−107.47	−107.69
125	−105.17	−105.46	−105.71	−105.92	−106.12	−106.45	−106.73	−106.97
150	−104.32	−104.64	−104.90	−105.14	−105.34	−105.70	−105.99	−106.25
175	−103.45	−103.80	−104.10	−104.35	−104.57	−104.95	−105.27	−105.55
200	−102.56	−102.95	−103.28	−103.56	−103.81	−104.22	−104.56	−104.86
225	−101.64	−102.09	−102.46	−102.77	−103.04	−103.49	−103.86	−104.18
250	−100.68	−101.20	−101.62	−101.97	−102.27	−102.76	−103.17	−103.51
300	−98.59	−99.35	−99.93	−100.35	−100.72	−101.32	−101.80	−102.20
350	−96.58	−97.34	−98.23	−98.72	−99.16	−99.88	−100.45	−100.93
400		−96.73	−96.61	−97.10	−97.59	−98.44	−99.12	−99.67
450		−98.87	−95.19	−95.52	−96.04	−97.00	−97.79	−98.44
500			−94.19	−94.01	−94.49	−95.56	−96.46	−97.21
550			−93.86	−92.62	−92.95	−94.09	−95.13	−95.99
600			−94.29	−91.43	−91.43	−92.60	−93.76	−94.74
700				−89.89	−88.48	−89.43	−90.88	−92.12
800					−85.56	−85.94	−87.72	−89.27
900					−82.44	−82.13	−84.29	−86.12
1000						−78.18	−80.73	−82.71

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Mg(CH_3COO)^+$				
25	−198.52	−198.22	−197.92	−197.62	−197.32	−196.71	−196.11	−195.51
50	−198.28	−197.97	−197.66	−197.35	−197.05	−196.44	−195.84	−195.23
75	−198.18	−197.86	−197.55	−197.25	−196.94	−196.33	−195.73	−195.13
100	−198.20	−197.89	−197.58	−197.27	−196.97	−196.36	−195.76	−195.17
125	−198.32	−198.01	−197.71	−197.41	−197.11	−196.51	−195.92	−195.32
150	−198.53	−198.24	−197.94	−197.64	−197.35	−196.76	−196.17	−195.59
175	−198.82	−198.54	−198.26	−197.97	−197.68	−197.10	−196.52	−195.94
200	−199.17	−198.92	−198.65	−198.38	−198.10	−197.53	−196.96	−196.39
225	−199.59	−199.37	−199.12	−198.86	−198.59	−198.04	−197.49	−196.92
250	−200.05	−199.88	−199.66	−199.41	−199.16	−198.63	−198.08	−197.53
300	−201.07	−201.06	−200.91	−200.70	−200.48	−200.00	−199.49	−198.97
350	−202.33	−202.41	−202.41	−202.23	−202.04	−201.62	−201.16	−200.67
400		−204.64	−204.17	−203.99	−203.83	−203.47	−203.06	−202.61
450		−208.37	−206.22	−205.98	−205.83	−205.52	−205.17	−204.76
500			−208.66	−208.18	−208.02	−207.77	−207.47	−207.11
550			−211.60	−210.62	−210.39	−210.18	−209.94	−209.64
600			−215.05	−213.32	−212.94	−212.74	−212.57	−212.32
700				−219.58	−218.54	−218.25	−218.22	−218.10
800					−224.71	−224.16	−224.29	−224.32
900					−231.30	−230.44	−230.75	−230.92
1000						−237.11	−237.61	−237.85
				$Mg(CH_3COO)_2^\circ$				
25	−287.83	−286.93	−286.07	−285.25	−284.46	−282.92	−281.44	−280.00
50	−287.99	−287.06	−286.17	−285.33	−284.51	−282.94	−281.42	−279.95
75	−288.46	−287.52	−286.62	−285.76	−284.93	−283.33	−281.79	−280.31
100	−289.21	−288.25	−287.34	−286.47	−285.63	−284.02	−282.47	−280.97
125	−290.18	−289.21	−288.30	−287.42	−286.58	−284.95	−283.40	−281.89
150	−291.36	−290.40	−289.47	−288.59	−287.74	−286.11	−284.55	−283.03
175	−292.74	−291.78	−290.85	−289.96	−289.11	−287.47	−285.90	−284.38
200	−294.29	−293.34	−292.41	−291.52	−290.66	−289.02	−287.44	−285.92
225	−296.01	−295.07	−294.13	−293.24	−292.38	−290.73	−289.16	−287.63
250	−297.88	−296.96	−296.02	−295.13	−294.27	−292.61	−291.03	−289.50
300	−302.03	−301.20	−300.25	−299.35	−298.48	−296.82	−295.23	−293.70
350	−306.70	−305.99	−305.03	−304.12	−303.25	−301.58	−299.99	−298.45
400		−311.32	−310.32	−309.40	−308.52	−306.84	−305.25	−303.70
450		−317.23	−316.08	−315.14	−314.26	−312.57	−310.97	−309.42
500		−323.74	−322.30	−321.33	−320.43	−318.73	−317.12	−315.56
550		−330.57	−328.95	−327.92	−327.00	−325.29	−323.67	−322.11
600		−337.70	−336.00	−334.90	−333.95	−332.22	−330.60	−329.03
700		−352.85	−351.13	−349.92	−348.92	−347.14	−345.49	−343.92
800		−369.16	−367.47	−366.20	−365.15	−363.32	−361.66	−360.08
900		−386.55	−384.89	−383.60	−382.52	−380.65	−378.97	−377.38
1000		−404.95	−403.32	−402.01	−400.91	−399.02	−397.33	−395.74
				$MgCO_3^\circ$				
25	−238.76	−238.94	−239.09	−239.22	−239.33	−239.50	−239.63	−239.73
50	−238.14	−238.32	−238.48	−238.61	−238.72	−238.91	−239.06	−239.19
75	−237.48	−237.67	−237.82	−237.96	−238.08	−238.28	−238.44	−238.58
100	−236.80	−236.99	−237.14	−237.28	−237.40	−237.61	−237.78	−237.92
125	−236.10	−236.28	−236.44	−236.58	−236.70	−236.91	−237.09	237.24
150	−235.38	−235.56	−235.72	−235.86	−235.99	−236.20	−236.38	−236.54
175	−234.65	−234.83	−234.99	−235.13	−235.25	−235.47	−235.65	−235.81
200	−233.90	−234.08	−234.24	−234.38	−234.50	−234.72	−234.91	−235.07
225	−233.15	−233.32	−233.48	−233.62	−233.74	−233.96	−234.15	−234.31
250	−232.38	−232.55	−232.71	−232.85	−232.97	−233.19	−233.38	−233.54
300	−230.84	−230.98	−231.13	−231.27	−231.39	−231.61	−231.80	−231.97
350	−229.31	−229.38	−229.52	−229.65	−229.77	−229.99	−230.18	−230.35
400		−227.77	−227.88	−228.01	−228.12	−228.34	−228.52	−228.69
450		−226.26	−226.23	−226.33	−226.44	−226.65	−226.83	−227.00

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$MgCO_3^\circ$ — Continued				
500		−224.89	−224.57	−224.64	−224.74	−224.93	−225.12	−225.28
550		−223.42	−222.91	−222.93	−223.01	−223.19	−223.37	−223.53
600		−221.85	−221.25	−221.20	−221.26	−221.43	−221.60	−221.76
700		−218.48	−217.87	−217.71	−217.71	−217.83	−217.99	−218.14
800		−214.92	−214.34	−214.12	−214.08	−214.16	−214.29	−214.44
900		−211.22	−210.68	−210.43	−210.36	−210.40	−210.52	−210.66
1000		−207.41	−206.90	−206.64	−206.55	−206.57	−206.68	−206.82
				$MgCl^+$				
25	−139.70	−139.68	−139.63	−139.57	−139.50	−139.33	−139.14	−138.93
50	−139.23	−139.20	−139.16	−139.10	−139.04	−138.88	−138.70	−138.50
75	−138.83	−138.81	−138.77	−138.71	−138.65	−138.50	−138.33	−138.14
100	−138.49	−138.47	−138.44	−138.39	−138.33	−138.19	−138.03	−137.85
125	−138.20	−138.19	−138.16	−138.12	−138.07	−137.94	−137.79	−137.62
150	−137.95	−137.95	−137.94	−137.91	−137.86	−137.74	−137.60	−137.44
175	−137.73	−137.76	−137.76	−137.74	−137.70	−137.60	−137.47	−137.32
200	−137.54	−137.60	−137.61	−137.60	−137.58	−137.50	−137.38	−137.24
225	−137.38	−137.46	−137.50	−137.51	−137.50	−137.44	−137.34	−137.21
250	−137.22	−137.35	−137.42	−137.45	−137.45	−137.41	−137.33	−137.22
300	−136.92	−137.20	−137.35	−137.42	−137.46	−137.48	−137.44	−137.36
350	−136.83	−137.08	−137.40	−137.50	−137.58	−137.66	−137.68	−137.64
400		−137.95	−137.63	−137.71	−137.82	−137.97	−138.04	−138.04
450		−140.75	−138.09	−138.06	−138.17	−138.38	−138.50	−138.56
500			−138.94	−138.56	−138.63	−138.88	−139.07	−139.18
550			−140.33	−139.23	−139.19	−139.47	−139.72	−139.89
600			−142.31	−140.13	−139.85	−140.12	−140.44	−140.68
700				−142.69	−141.49	−141.57	−142.03	−142.41
800					−143.45	−143.12	−143.75	−144.30
900					−145.54	−144.74	−145.58	−146.27
1000						−146.51	−147.55	−148.33
				MgF^+				
25	−177.69	−177.80	−177.88	−177.94	−177.98	−178.02	−178.03	−178.00
50	−177.03	−177.14	−177.23	−177.29	−177.34	−177.40	−177.42	−177.42
75	−176.43	−176.55	−176.64	−176.71	−176.77	−176.84	−176.88	−176.89
100	−175.88	−176.01	−176.11	−176.19	−176.25	−176.34	−176.39	−176.42
125	−175.38	−175.52	−175.63	−175.72	−175.79	−175.89	−175.96	−175.99
150	−174.92	−175.08	−175.20	−175.30	−175.38	−175.49	−175.57	−175.62
175	−174.49	−174.66	−174.80	−174.92	−175.01	−175.14	−175.23	−175.29
200	−174.08	−174.28	−174.44	−174.57	−174.67	−174.83	−174.94	−175.01
225	−173.69	−173.92	−174.11	−174.26	−174.37	−174.55	−174.68	−174.77
250	−173.30	−173.58	−173.80	−173.97	−174.11	−174.31	−174.46	−174.57
300	−172.54	−172.96	−173.27	−173.48	−173.66	−173.93	−174.13	−174.27
350	−172.08	−172.37	−172.86	−173.10	−173.32	−173.66	−173.92	−174.11
400		−173.00	−172.64	−172.85	−173.09	−173.50	−173.82	−174.06
450		−176.22	−172.71	−172.74	−172.97	−173.44	−173.82	−174.12
500			−173.27	−172.80	−172.96	−173.46	−173.91	−174.27
550			−174.53	−173.07	−173.06	−173.57	−174.08	−174.50
600			−176.58	−173.61	−173.27	−173.73	−174.31	−174.80
700				−175.63	−174.02	−174.16	−174.89	−175.53
800					−175.10	−174.64	−175.54	−176.36
900					−176.26	−175.14	−176.24	−177.24
1000						−175.73	−177.06	−178.16
				$MgHCO_3^+$				
25	−250.20	−250.13	−250.04	−249.94	−249.83	−249.58	−249.32	−249.05
50	−250.19	−250.11	−250.02	−249.92	−249.81	−249.57	−249.32	−249.06
75	−250.28	−250.20	−250.11	−250.01	−249.91	−249.68	−249.43	−249.18
100	−250.46	−250.38	−250.30	−250.20	−250.10	−249.88	−249.64	−249.39

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$MgHCO_3^+$ — Continued				
125	−250.71	−250.65	−250.56	−250.47	−250.37	−250.16	−249.93	−249.69
150	−251.03	−250.98	−250.90	−250.82	−250.72	−250.52	−250.29	−250.06
175	−251.41	−251.37	−251.31	−251.23	−251.14	−250.94	−250.73	−250.50
200	−251.84	−251.82	−251.77	−251.70	−251.62	−251.44	−251.23	−251.01
225	−252.32	−252.32	−252.28	−252.23	−252.15	−251.99	−251.79	−251.58
250	−252.82	−252.86	−252.84	−252.80	−252.74	−252.59	−252.41	−252.21
300	−253.91	−254.06	−254.11	−254.10	−254.07	−253.95	−253.80	−253.62
350	−255.11	−255.36	−255.55	−255.57	−255.56	−255.50	−255.39	−255.24
400		−257.27	−257.16	−257.20	−257.23	−257.22	−257.14	−257.03
450		−260.02	−258.97	−258.99	−259.04	−259.09	−259.06	−258.98
500			−261.02	−260.93	−260.99	−261.09	−261.12	−261.08
550			−263.37	−263.03	−263.07	−263.22	−263.30	−263.31
600			−266.03	−265.29	−265.27	−265.46	−265.60	−265.66
700				−270.40	−270.01	−270.22	−270.49	−270.65
800					−275.17	−275.27	−275.70	−275.98
900					−280.66	−280.60	−281.19	−281.58
1000						−286.24	−286.98	−287.43
				Mn^{+2}				
25	−54.50	−54.69	−54.84	−54.96	−55.06	−55.22	−55.32	−55.40
50	−54.06	−54.25	−54.41	−54.54	−54.65	−54.83	−54.97	−55.07
75	−53.61	−53.81	−53.98	−54.12	−54.25	−54.44	−54.60	−54.72
100	−53.16	−53.38	−53.56	−53.71	−53.84	−54.06	−54.23	−54.37
125	−52.70	−52.93	−53.13	−53.29	−53.44	−53.67	−53.86	−54.01
150	−52.23	−52.49	−52.70	−52.88	−53.04	−53.29	−53.50	−53.67
175	−51.74	−52.03	−52.27	−52.47	−52.64	−52.92	−53.14	−53.33
200	−51.22	−51.55	−51.82	−52.05	−52.24	−52.55	−52.80	−53.00
225	−50.68	−51.06	−51.37	−51.62	−51.83	−52.18	−52.45	−52.68
250	−50.09	−50.54	−50.90	−51.18	−51.42	−51.81	−52.11	−52.36
300	−48.75	−49.43	−49.93	−50.28	−50.59	−51.07	−51.45	−51.75
350	−47.39	−48.14	−48.94	−49.36	−49.73	−50.32	−50.79	−51.15
400		−48.01	−47.99	−48.43	−48.86	−49.57	−50.13	−50.57
450		−50.02	−47.18	−47.52	−47.98	−48.81	−49.47	−50.00
500			−46.68	−46.64	−47.09	−48.03	−48.80	−49.43
550			−46.70	−45.84	−46.19	−47.22	−48.12	−48.84
600			−47.29	−45.18	−45.30	−46.38	−47.40	−48.23
700				−44.52	−43.53	−44.50	−45.81	−46.89
800					−41.75	−42.31	−43.94	−45.30
900					−39.78	−39.82	−41.81	−43.43
1000						−37.20	−39.54	−41.30
				$MnCl^+$				
25	−86.29	−86.21	−86.11	−86.00	−85.89	−85.63	−85.36	−85.08
50	−86.62	−86.53	−86.43	−86.33	−86.21	−85.96	−85.70	−85.43
75	−87.01	−86.92	−86.82	−86.71	−86.60	−86.35	−86.10	−85.83
100	−87.44	−87.35	−87.25	−87.15	−87.03	−86.79	−86.54	−86.28
125	−87.91	−87.83	−87.73	−87.63	−87.52	−87.28	−87.04	−86.78
150	−88.42	−88.34	−88.25	−88.15	−88.04	−87.81	−87.57	−87.32
175	−88.96	−88.89	−88.80	−88.71	−88.60	−88.38	−88.15	−87.90
200	−89.53	−89.47	−89.39	−89.30	−89.20	−88.99	−88.76	−88.51
225	−90.11	−90.07	−90.00	−89.92	−89.83	−89.62	−89.40	−89.17
250	−90.72	−90.70	−90.65	−90.57	−90.49	−90.29	−90.08	−89.85
300	−91.95	−92.02	−92.00	−91.95	−91.88	−91.71	−91.52	−91.30
350	−93.18	−93.37	−93.45	−93.42	−93.38	−93.24	−93.07	−92.87
400		−94.99	−94.98	−94.98	−94.96	−94.86	−94.71	−94.54
450		−96.82	−96.59	−96.61	−96.62	−96.56	−96.44	−96.29
500			−98.29	−98.32	−98.34	−98.33	−98.25	−98.13
550			−100.09	−100.08	−100.14	−100.18	−100.14	−100.04
600			−101.99	−101.93	−101.98	−102.08	−102.08	−102.02
700				−105.87	−105.85	−106.02	−106.13	−106.14

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$MnCl^+$ — Continued				
800					−109.93	−110.13	−110.35	−110.44
900					−114.20	−114.40	−114.73	−114.89
1000						−118.85	−119.28	−119.47
				MnO_4^-				
25	−106.90	−106.41	−105.93	−105.47	−105.01	−104.10	−103.22	−102.34
50	−108.04	−107.54	−107.05	−106.57	−106.10	−105.19	−104.29	−103.41
75	−109.18	−108.68	−108.18	−107.70	−107.23	−106.31	−105.41	−104.52
100	−110.33	−109.82	−109.33	−108.85	−108.38	−107.46	−106.56	−105.67
125	−111.47	−110.97	−110.48	−110.01	−109.54	−108.62	−107.73	−106.85
150	−112.60	−112.12	−111.64	−111.17	−110.71	−109.80	−108.91	−108.04
175	−113.72	−113.26	−112.80	−112.34	−111.89	−110.99	−110.11	−109.24
200	−114.82	−114.40	−113.96	−113.51	−113.07	−112.19	−111.32	−110.46
225	−115.89	−115.52	−115.11	−114.68	−114.25	−113.40	−112.54	−111.69
250	−116.91	−116.62	−116.25	−115.85	−115.44	−114.61	−113.77	−112.94
300	−118.69	−118.72	−118.49	−118.16	−117.80	−117.04	−116.25	−115.45
350	−119.55	−120.53	−120.62	−120.42	−120.14	−119.47	−118.74	−117.98
400		−121.81	−122.57	−122.59	−122.43	−121.90	−121.25	−120.54
450		−120.54	−124.19	−124.62	−124.64	−124.30	−123.76	−123.12
500			−125.31	−126.46	−126.76	−126.67	−126.25	−125.70
550			−125.74	−128.06	−128.75	−129.00	−128.74	−128.27
600			−125.66	−129.42	−130.62	−131.27	−131.19	−130.83
700				−131.68	−134.02	−135.66	−136.01	−135.90
800					−137.26	−139.89	−140.71	−140.84
900					−140.64	−144.08	−145.32	−145.65
1000						−148.38	−149.92	−150.33
				MnO_4^{-2}				
25	−119.70	−119.38	−119.06	−118.73	−118.41	−117.74	−117.07	−116.39
50	−120.00	−119.67	−119.35	−119.03	−118.70	−118.04	−117.37	−116.70
75	−120.20	−119.89	−119.57	−119.26	−118.94	−118.29	−117.64	−116.98
100	−120.31	−120.02	−119.73	−119.43	−119.12	−118.49	−117.86	−117.22
125	−120.34	−120.09	−119.82	−119.54	−119.25	−118.66	−118.04	−117.42
150	−120.28	−120.08	−119.85	−119.60	−119.33	−118.77	−118.19	−117.59
175	−120.11	−119.99	−119.81	−119.60	−119.36	−118.85	−118.30	−117.73
200	−119.83	−119.81	−119.70	−119.53	−119.34	−118.88	−118.38	−117.84
225	−119.41	−119.53	−119.51	−119.41	−119.26	−118.87	−118.42	−117.92
250	−118.80	−119.13	−119.23	−119.21	−119.12	−118.82	−118.43	−117.97
300	−116.75	−117.88	−118.39	−118.59	−118.66	−118.58	−118.34	−117.99
350	−112.33	−115.66	−117.10	−117.64	−117.93	−118.15	−118.10	−117.90
400		−112.62	−115.22	−116.29	−116.91	−117.52	−117.72	−117.69
450		−104.37	−112.49	−114.47	−115.54	−116.67	−117.17	−117.35
500			−108.54	−112.06	−113.79	−115.58	−116.45	−116.87
550			−103.07	−108.99	−111.60	−114.24	−115.54	−116.24
600			−96.47	−105.27	−108.97	−112.61	−114.42	−115.43
700				−96.66	−102.57	−108.51	−111.52	−113.24
800					−95.28	−103.42	−107.72	−110.18
900					−87.86	−97.67	−103.17	−106.25
1000						−91.74	−98.15	−101.50
				$MnSO_4^\circ$				
25	−235.64	−235.57	−235.49	−235.39	−235.29	−235.06	−234.82	−234.56
50	−235.75	−235.67	−235.58	−235.49	−235.39	−235.16	−234.93	−234.68
75	−235.82	−235.74	−235.66	−235.56	−235.46	−235.24	−235.01	−234.77
100	−235.88	−235.80	−235.71	−235.61	−235.51	−235.29	−235.06	−234.82
125	−235.92	−235.84	−235.74	−235.65	−235.54	−235.33	−235.10	−234.87
150	−235.94	−235.86	−235.77	−235.67	−235.57	−235.35	−235.12	−234.89
175	−235.96	−235.87	−235.78	−235.68	−235.58	−235.36	−235.14	−234.90
200	−235.96	−235.87	−235.78	−235.68	−235.58	−235.36	−235.14	−234.91

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$MnSO_4^\circ$ — Continued				
225	−235.95	−235.87	−235.77	−235.67	−235.57	−235.35	−235.13	−234.90
250	−235.94	−235.85	−235.75	−235.65	−235.55	−235.33	−235.11	−234.88
300	−235.89	−235.80	−235.70	−235.59	−235.49	−235.27	−235.04	−234.81
350	−235.84	−235.73	−235.61	−235.51	−235.40	−235.17	−234.95	−234.72
400		−235.66	−235.51	−235.39	−235.28	−235.05	−234.83	−234.59
450		−235.70	−235.40	−235.27	−235.14	−234.91	−234.68	−234.45
500		−235.88	−235.29	−235.12	−234.99	−234.75	−234.51	−234.27
550		−235.97	−235.20	−234.97	−234.82	−234.56	−234.32	−234.08
600		−235.95	−235.10	−234.81	−234.63	−234.36	−234.11	−233.87
700		−235.73	−234.86	−234.46	−234.23	−233.91	−233.64	−233.39
800		−235.34	−234.50	−234.04	−233.76	−233.40	−233.11	−232.85
900		−234.83	−234.02	−233.53	−233.22	−232.82	−232.52	−232.26
1000		−234.22	−233.44	−232.94	−232.62	−232.19	−231.88	−231.62
				MoO_4^{-2}				
25	−199.90	−199.55	−199.19	−198.84	−198.48	−197.76	−197.03	−196.31
50	−200.02	−199.66	−199.31	−198.95	−198.59	−197.88	−197.16	−196.43
75	−200.06	−199.72	−199.37	−199.02	−198.67	−197.97	−197.26	−196.55
100	−200.03	−199.71	−199.39	−199.05	−198.72	−198.03	−197.34	−196.65
125	−199.93	−199.65	−199.35	−199.04	−198.72	−198.07	−197.40	−196.73
150	−199.75	−199.52	−199.26	−198.98	−198.69	−198.07	−197.44	−196.79
175	−199.48	−199.33	−199.12	−198.88	−198.61	−198.05	−197.45	−196.82
200	−199.09	−199.05	−198.91	−198.72	−198.50	−197.99	−197.43	−196.84
225	−198.57	−198.67	−198.63	−198.50	−198.33	−197.90	−197.39	−196.84
250	−197.87	−198.19	−198.27	−198.23	−198.12	−197.77	−197.33	−196.83
300	−195.65	−196.79	−197.29	−197.48	−197.53	−197.41	−197.13	−196.74
350	−191.11	−194.44	−195.90	−196.42	−196.70	−196.89	−196.81	−196.56
400		−191.42	−193.95	−195.00	−195.61	−196.20	−196.36	−196.30
450		−183.46	−191.19	−193.13	−194.20	−195.31	−195.79	−195.94
500			−187.26	−190.71	−192.42	−194.20	−195.06	−195.46
550			−181.92	−187.65	−190.23	−192.86	−194.16	−194.84
600			−175.52	−183.99	−187.63	−191.26	−193.07	−194.08
700				−175.63	−181.34	−187.25	−190.27	−192.01
800					−174.24	−182.28	−186.62	−189.12
900					−167.05	−176.69	−182.26	−185.40
1000						−170.97	−177.48	−180.89
				N-Butane				
25	0.04	0.99	1.90	2.77	3.62	5.23	6.79	8.30
50	−1.09	−0.10	0.84	1.74	2.60	4.27	5.86	7.41
75	−2.44	−1.42	−0.47	0.45	1.33	3.02	4.64	6.21
100	−3.97	−2.94	−1.97	−1.04	−0.14	1.57	3.21	4.79
125	−5.67	−4.62	−3.63	−2.69	−1.79	−0.06	1.60	3.19
150	−7.52	−6.46	−5.46	−4.50	−3.59	−1.84	−0.18	1.43
175	−9.51	−8.44	−7.42	−6.46	−5.53	−3.77	−2.09	−0.47
200	−11.63	−10.55	−9.52	−8.54	−7.60	−5.82	−4.13	−2.50
225	−13.89	−12.80	−11.74	−10.75	−9.80	−8.00	−6.29	−4.65
250	−16.29	−15.18	−14.09	−13.07	−12.11	−10.29	−8.57	−6.91
300	−21.55	−20.34	−19.14	−18.07	−17.07	−15.19	−13.44	−11.75
350	−27.91	−26.12	−24.69	−23.51	−22.44	−20.49	−18.69	−16.98
400		−32.91	−30.76	−29.39	−28.22	−26.17	−24.30	−22.55
450		−42.51	−37.47	−35.73	−34.40	−32.20	−30.26	−28.45
500		−55.89	−44.99	−42.55	−40.98	−38.56	−36.52	−34.66
550		−68.11	−53.43	−49.88	−47.95	−45.26	−43.10	−41.17
600		−78.92	−62.63	−57.71	−55.31	−52.26	−49.96	−47.95
700		−98.48	−81.76	−74.59	−71.06	−67.14	−64.49	−62.31
800		−116.79	−100.70	−92.35	−87.86	−83.02	−80.01	−77.65
900		−134.66	−119.29	−110.44	−105.32	−99.72	−96.40	−93.90
1000		−152.44	−137.71	−128.66	−123.18	−117.07	−113.53	−110.99

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				N-Butylbenzene				
25	36.11	37.80	39.41	40.96	42.47	45.39	48.21	50.97
50	34.37	36.07	37.68	39.23	40.74	43.64	46.44	49.17
75	32.32	34.03	35.64	37.20	38.70	41.60	44.39	47.10
100	30.00	31.70	33.32	34.88	36.38	39.28	42.07	44.77
125	27.40	29.12	30.74	32.30	33.81	36.71	39.49	42.20
150	24.57	26.28	27.92	29.48	30.99	33.89	36.68	39.39
175	21.50	23.21	24.86	26.43	27.95	30.86	33.65	36.36
200	18.21	19.92	21.58	23.17	24.69	27.61	30.41	33.12
225	14.70	16.42	18.10	19.69	21.23	24.16	26.96	29.68
250	10.99	12.70	14.41	16.02	17.57	20.51	23.33	26.05
300	2.88	4.63	6.44	8.11	9.69	12.69	15.53	18.27
350	−6.58	−4.35	−2.30	−0.53	1.11	4.18	7.06	9.83
400		−14.61	−11.84	−9.87	−8.13	−4.96	−2.02	0.78
450		−27.94	−22.25	−19.92	−18.02	−14.70	−11.69	−8.84
500		−45.30	−33.71	−30.67	−28.53	−25.00	−21.89	−18.99
550		−61.70	−46.31	−42.15	−39.65	−35.85	−32.62	−29.64
600		−76.89	−59.87	−54.34	−51.36	−47.20	−43.83	−40.78
700		−105.74	−88.29	−80.49	−76.37	−71.34	−67.62	−64.40
800		−134.01	−117.19	−108.21	−103.12	−97.16	−93.09	−89.69
900		−162.44	−146.36	−136.86	−131.15	−124.43	−120.04	−116.50
000		−191.36	−175.92	−166.22	−160.14	−152.90	−148.30	−144.72
				N-Heptane				
25	6.47	7.97	9.38	10.73	12.02	14.49	16.84	19.12
50	4.78	6.33	7.79	9.18	10.51	13.05	15.48	17.82
75	2.78	4.36	5.85	7.27	8.62	11.21	13.68	16.06
100	0.50	2.12	3.63	5.06	6.44	9.06	11.56	13.97
125	−2.01	−0.38	1.16	2.61	4.00	6.65	9.18	11.61
150	−4.74	−3.09	−1.53	−0.06	1.34	4.02	6.57	9.01
175	−7.67	−6.01	−4.43	−2.94	−1.52	1.19	3.75	6.22
200	−10.80	−9.12	−7.52	−6.01	−4.57	−1.84	0.75	3.23
225	−14.13	−12.43	−10.79	−9.25	−7.79	−5.03	−2.43	0.07
250	−17.64	−15.92	−14.24	−12.67	−11.19	−8.40	−5.77	−3.25
300	−25.36	−23.49	−21.65	−20.00	−18.46	−15.58	−12.90	−10.34
350	−34.71	−31.98	−29.78	−27.97	−26.33	−23.34	−20.59	−17.98
400		−41.95	−38.67	−36.57	−34.79	−31.64	−28.80	−26.12
450		−56.12	−48.50	−45.85	−43.82	−40.45	−37.49	−34.74
500		−75.93	−59.52	−55.83	−53.44	−49.75	−46.64	−43.80
550		−93.97	−71.92	−66.55	−63.62	−59.51	−56.22	−53.29
600		−109.90	−85.42	−78.01	−74.37	−69.73	−66.23	−63.17
700		−138.60	−113.49	−102.69	−97.36	−91.42	−87.40	−84.08
800		−165.39	−141.21	−128.65	−121.89	−114.56	−110.00	−106.41
900		−191.45	−168.37	−155.04	−147.33	−138.88	−133.84	−130.05
1000		−217.34	−195.21	−181.59	−173.33	−164.10	−158.75	−154.89
				N-Heptylbenzene				
25	42.64	44.87	47.00	49.04	51.02	54.84	58.52	62.11
50	40.33	42.58	44.71	46.75	48.73	52.54	56.20	59.76
75	37.61	39.86	41.99	44.04	46.02	49.82	53.47	57.02
100	34.49	36.75	38.89	40.94	42.92	46.73	50.38	53.92
125	31.01	33.28	35.43	37.49	39.48	43.28	46.93	50.47
150	27.20	29.48	31.64	33.71	35.70	39.51	43.17	46.71
175	23.07	25.35	27.53	29.61	31.61	35.44	39.10	42.65
200	18.64	20.92	23.12	25.21	27.23	31.07	34.74	38.30
225	13.91	16.19	18.42	20.54	22.56	26.43	30.11	33.67
250	8.88	11.17	13.45	15.59	17.63	21.52	25.22	28.80
300	−2.11	0.26	2.68	4.91	7.01	10.97	14.71	18.32
350	−15.07	−11.93	−9.15	−6.77	−4.58	−0.51	3.30	6.94
400		−25.95	−22.08	−19.42	−17.08	−12.86	−8.97	−5.27
450		−44.50	−36.27	−33.04	−30.47	−26.02	−22.02	−18.25

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

				Pressure, kbar				
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				N-Heptylbenzene — Continued				
500		−69.03	−51.94	−47.67	−44.72	−39.97	−35.82	−31.97
550		−92.04	−69.26	−63.31	−59.83	−54.65	−50.32	−46.37
600		−113.17	−87.95	−79.94	−75.74	−70.04	−65.50	−61.43
700		−152.97	−127.12	−115.69	−109.80	−102.78	−97.73	−93.40
800		−191.69	−166.78	−153.59	−146.25	−137.84	−132.24	−127.65
900		−230.47	−206.66	−192.70	−184.41	−174.87	−168.79	−164.00
1000		−269.79	−246.94	−232.69	−223.84	−213.53	−207.14	−202.27
				N-Hexane				
25	4.42	5.74	6.98	8.17	9.31	11.50	13.59	15.61
50	2.93	4.30	5.58	6.81	7.98	10.23	12.38	14.45
75	1.16	2.55	3.86	5.11	6.31	8.60	10.79	12.89
100	−0.86	0.56	1.89	3.16	4.38	6.70	8.91	11.04
125	−3.08	−1.65	−0.30	0.99	2.22	4.56	6.79	8.94
150	−5.51	−4.05	−2.69	−1.39	−0.14	2.22	4.47	6.64
175	−8.11	−6.65	−5.26	−3.94	−2.69	−0.30	1.97	4.16
200	−10.89	−9.41	−8.00	−6.67	−5.40	−2.98	−0.70	1.50
225	−13.85	−12.35	−10.91	−9.55	−8.27	−5.83	−3.52	−1.31
250	−16.98	−15.46	−13.97	−12.59	−11.28	−8.82	−6.49	−4.26
300	−23.84	−22.19	−20.57	−19.11	−17.75	−15.21	−12.84	−10.57
350	−32.15	−29.74	−27.80	−26.21	−24.76	−22.12	−19.69	−17.38
400		−38.61	−35.72	−33.87	−32.30	−29.52	−27.00	−24.63
450		−51.19	−44.47	−42.13	−40.34	−37.36	−34.74	−32.31
500		−68.74	−54.28	−51.02	−48.91	−45.65	−42.90	−40.39
550		−84.74	−65.30	−60.57	−57.98	−54.36	−51.45	−48.85
600		−98.89	−77.31	−70.77	−67.56	−63.47	−60.37	−57.67
700		−124.42	−102.28	−92.75	−88.06	−82.81	−79.26	−76.32
800		−148.27	−126.96	−115.88	−109.92	−103.45	−99.42	−96.25
900		−171.51	−151.15	−139.41	−132.61	−125.15	−120.70	−117.35
1000		−194.61	−175.09	−163.09	−155.80	−147.66	−142.94	−139.53
				N-Hexylbenzene				
25	40.39	42.44	44.40	46.28	48.10	51.62	55.01	58.32
50	38.27	40.34	42.29	44.17	45.99	49.50	52.87	56.15
75	35.77	37.84	39.80	41.69	43.51	47.01	50.37	53.64
100	32.92	35.00	36.96	38.85	40.67	44.17	47.53	50.80
125	29.74	31.82	33.80	35.69	37.51	41.02	44.38	47.64
150	26.25	28.34	30.33	32.22	34.06	37.57	40.93	44.20
175	22.47	24.57	26.57	28.48	30.32	33.84	37.21	40.48
200	18.42	20.51	22.54	24.46	26.31	29.84	33.22	36.50
225	14.10	16.19	18.24	20.18	22.04	25.60	28.99	32.27
250	9.51	11.61	13.69	15.66	17.54	21.11	24.52	27.81
300	−0.52	1.64	3.86	5.90	7.83	11.47	14.91	18.23
350	−12.32	−9.48	−6.94	−4.76	−2.75	0.98	4.48	7.83
400		−22.25	−18.74	−16.31	−14.17	−10.30	−6.72	−3.32
450		−39.05	−31.67	−28.74	−26.39	−22.32	−18.65	−15.19
500		−61.19	−45.94	−42.08	−39.40	−35.05	−31.25	−27.71
550		−82.00	−61.68	−56.33	−53.17	−48.46	−44.49	−40.87
600		−101.15	−78.67	−71.48	−67.69	−62.50	−58.35	−54.62
700		−137.30	−114.25	−104.03	−98.73	−92.37	−87.77	−83.81
800		−172.54	−150.33	−138.54	−131.95	−124.36	−119.27	−115.07
900		−207.87	−186.64	−174.16	−166.73	−158.13	−152.62	−148.24
1000		−243.72	−223.34	−210.61	−202.68	−193.39	−187.60	183.16
				N-Octane				
25	8.58	10.26	11.84	13.34	14.78	17.54	20.16	22.69
50	6.78	8.52	10.15	11.70	13.18	16.02	18.72	21.32
75	4.62	6.40	8.06	9.64	11.16	14.05	16.80	19.44
100	2.17	3.98	5.67	7.27	8.81	11.73	14.52	17.20

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				N-Octane — Continued				
125	−0.54	1.29	3.00	4.62	6.18	9.14	11.95	14.65
150	−3.49	−1.65	0.09	1.73	3.30	6.29	9.12	11.85
175	−6.67	−4.81	−3.05	−1.39	0.20	3.22	6.07	8.82
200	−10.06	−8.19	−6.40	−4.71	−3.11	−0.06	2.82	5.59
225	−13.67	−11.77	−9.95	−8.24	−6.61	−3.53	−0.63	2.16
250	−17.49	−15.57	−13.69	−11.95	−10.30	−7.19	−4.26	−1.45
300	−25.85	−23.80	−21.75	−19.91	−18.20	−15.00	−12.01	−9.16
350	−35.98	−33.01	−30.59	−28.58	−26.77	−23.45	−20.39	−17.48
400		−43.84	−40.27	−37.95	−35.98	−32.49	−29.33	−26.36
450		−59.13	−50.95	−48.05	−45.82	−42.09	−38.80	−35.75
500		−80.45	−62.92	−58.91	−56.29	−52.22	−48.78	−45.64
550		−99.90	−76.37	−70.58	−67.39	−62.88	−59.24	−55.99
600		−117.12	−91.01	−83.04	−79.09	−74.02	−70.16	−66.78
700		−148.25	−121.46	−109.89	−104.15	−97.68	−93.28	−89.62
800		−177.38	−151.59	−138.15	−130.88	−122.94	−117.95	−114.01
900		−205.79	−181.16	−166.91	−158.63	−149.49	−144.00	−139.84
1000		−234.06	−210.44	−195.88	−187.01	−177.06	−171.23	−167.00
				N-Octylbenzene				
25	44.69	47.11	49.40	51.61	53.75	57.87	61.83	65.69
50	42.19	44.62	46.93	49.13	51.27	55.37	59.32	63.16
75	39.24	41.68	43.99	46.20	48.33	52.43	56.37	60.20
100	35.86	38.31	40.62	42.84	44.98	49.08	53.02	56.84
125	32.09	34.55	36.87	39.10	41.24	45.35	49.29	53.11
150	27.95	30.42	32.70	34.99	37.14	41.26	45.21	49.03
175	23.47	25.94	28.30	30.54	32.70	36.84	40.79	44.62
200	18.65	21.12	23.51	25.77	27.94	32.10	36.06	39.89
225	13.51	15.99	18.41	20.69	22.88	27.06	31.04	34.88
250	8.05	10.54	13.00	15.32	17.53	21.73	25.73	29.58
300	−3.91	−1.33	1.31	3.71	5.99	10.27	14.32	18.21
350	−18.03	−14.59	−11.55	−8.97	−6.60	−2.20	1.91	5.85
400		−29.86	−25.63	−22.73	−20.19	−15.62	−11.41	−7.41
450		−50.15	−41.07	−37.55	−34.75	−29.93	−25.59	−21.52
500		−77.06	−58.14	−53.46	−50.25	−45.08	−40.59	−36.42
550		−102.28	−77.04	−70.48	−66.68	−61.05	−56.35	−52.07
600		−125.39	−97.44	−88.60	−84.00	−77.78	−72.85	−68.44
700		−168.84	−140.18	−127.56	−121.07	−113.38	−107.89	−103.19
800		−211.05	−183.44	−168.85	−160.75	−151.53	−145.42	−140.43
900		−253.27	−226.89	−211.44	−202.29	−191.81	−185.17	−179.96
1000		−296.06	−270.75	−254.97	−245.20	−233.86	−226.88	−221.59
				N-Pentane				
25	2.13	3.27	4.35	5.37	6.37	8.27	10.09	11.85
50	0.80	1.98	3.09	4.15	5.17	7.13	9.00	10.81
75	−0.79	0.42	1.55	2.64	3.68	5.67	7.57	9.41
100	−2.58	−1.35	−0.20	0.90	1.95	3.97	5.89	7.75
125	−4.56	−3.32	−2.15	−1.04	0.03	2.07	4.01	5.89
150	−6.71	−5.46	−4.27	−3.14	−2.07	−0.01	1.95	3.84
175	−9.03	−7.76	−6.55	−5.41	−4.32	−2.25	−0.27	1.63
200	−11.50	−10.21	−8.99	−7.83	−6.73	−4.63	−2.64	−0.72
225	−14.12	−12.82	−11.57	−10.39	−9.27	−7.15	−5.14	−3.21
250	−16.89	−15.57	−14.28	−13.09	−11.95	−9.80	−7.78	−5.83
300	−22.98	−21.55	−20.13	−18.86	−17.68	−15.47	−13.40	−11.43
350	−30.37	−28.24	−26.54	−25.15	−23.89	−21.59	−19.47	−17.45
400		−36.11	−33.56	−31.94	−30.56	−28.14	−25.94	−23.88
450		−47.30	−41.32	−39.25	−37.69	−35.08	−32.80	−30.68
500		−62.96	−50.01	−47.13	−45.27	−42.42	−40.01	−37.82
550		−77.21	−59.80	−55.59	−53.31	−50.12	−47.58	−45.30
600		−89.79	−70.46	−64.63	−61.79	−58.18	−55.47	−53.10
700		−112.46	−92.63	−84.11	−79.94	−75.29	−72.17	−69.60

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

				Pressure, kbar				
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				N-Pentane — Continued				
800		−133.61	−114.51	−104.61	−99.29	−93.56	−90.00	−87.22
900		−154.17	−135.95	−125.44	−119.37	−112.75	−108.82	−105.87
1000		−174.61	−157.13	−146.40	−139.89	−132.65	−128.48	−125.48
				N-Pentylbenzene				
25	38.21	40.08	41.86	43.58	45.25	48.47	51.57	54.60
50	36.28	38.16	39.95	41.66	43.33	46.53	49.62	52.62
75	34.01	35.89	37.68	39.40	41.06	44.26	47.34	50.33
100	31.42	33.31	35.10	36.82	38.49	41.68	44.76	47.75
125	28.53	30.43	32.23	33.95	35.62	38.82	41.90	44.88
150	25.37	27.27	29.08	30.81	32.48	35.69	38.77	41.75
175	21.95	23.85	25.67	27.41	29.09	32.31	35.39	38.38
200	18.27	20.18	22.02	23.77	25.46	28.69	31.77	34.77
225	14.36	16.26	18.13	19.90	21.59	24.84	27.94	30.93
250	10.21	12.11	14.01	15.80	17.51	20.77	23.88	26.89
300	1.14	3.09	5.11	6.96	8.72	12.04	15.18	18.21
350	−9.49	−6.95	−4.66	−2.69	−0.86	2.54	5.73	8.79
400		−18.47	−15.33	−13.13	−11.19	−7.67	−4.41	−1.31
450		−33.54	−27.00	−24.37	−22.25	−18.55	−15.21	−12.05
500		−53.29	−39.86	−36.41	−34.00	−30.07	−26.61	−23.39
550		−71.89	−54.04	−49.28	−46.45	−42.19	−38.60	−35.30
600		−89.06	−69.31	−62.95	−59.56	−54.89	−51.13	−47.74
700		−121.56	−101.31	−92.30	−87.59	−81.89	−77.74	−74.14
800		−153.32	−133.80	−123.41	−117.58	−110.80	−106.22	−102.42
900		−185.20	−166.54	−155.55	−148.98	−141.32	−136.37	−132.41
1000		−217.58	−199.67	−188.46	−181.45	−173.19	−167.99	−163.98
				N-Propylbenzene				
25	34.17	35.68	37.12	38.51	39.86	42.48	45.02	47.49
50	32.62	34.13	35.57	36.96	38.31	40.91	43.43	45.88
75	30.80	32.32	33.76	35.15	36.50	39.09	41.60	44.04
100	28.73	30.26	31.70	33.09	34.44	37.03	39.53	41.96
125	26.44	27.96	29.41	30.81	32.15	34.75	37.25	39.68
150	23.93	25.45	26.91	28.31	29.66	32.26	34.76	37.18
175	21.21	22.74	24.21	25.61	26.96	29.57	32.07	34.50
200	18.30	19.83	21.31	22.72	24.08	26.69	29.20	31.63
225	15.21	16.73	18.22	19.65	21.02	23.64	26.15	28.58
250	11.93	13.44	14.96	16.40	17.78	20.42	22.94	25.38
300	4.79	6.32	7.93	9.41	10.82	13.50	16.04	18.49
350	−3.51	−1.59	0.22	1.79	3.25	5.98	8.56	11.03
400		−10.59	−8.18	−6.45	−4.91	−2.09	0.53	3.04
450		−22.18	−17.34	−15.30	−13.63	−10.69	−8.00	−5.46
500		−37.16	−27.40	−24.77	−22.89	−19.78	−17.01	−14.42
550		−51.36	−38.43	−34.87	−32.69	−29.34	−26.48	−23.83
600		−64.57	−50.28	−45.57	−42.99	−39.35	−36.37	−33.66
700		−89.76	−75.12	−68.51	−64.99	−60.62	−57.35	−54.50
800		−114.55	−100.43	−92.84	−88.51	−83.37	−79.80	−76.80
900		−139.54	−126.03	−118.01	−113.16	−107.38	−103.55	−100.43
1000		−164.98	−152.01	−143.83	−138.67	−132.46	−128.45	−125.30
				N_2°				
25	4.35	4.74	5.12	5.50	5.87	6.60	7.32	8.03
50	3.72	4.13	4.53	4.91	5.30	6.04	6.77	7.49
75	3.00	3.42	3.83	4.22	4.61	5.36	6.10	6.82
100	2.20	2.62	3.04	3.44	3.83	4.59	5.34	6.06
125	1.32	1.75	2.18	2.58	2.98	3.75	4.49	5.22
150	0.37	0.82	1.24	1.65	2.06	2.83	3.58	4.32
175	−0.64	−0.19	0.25	0.66	1.07	1.85	2.61	3.35
200	−1.72	−1.26	−0.81	−0.39	0.02	0.82	1.58	2.32

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				N_2° — Continued				
225	−2.86	−2.39	−1.93	−1.50	−1.08	−0.28	0.49	1.24
250	−4.07	−3.58	−3.10	−2.66	−2.23	−1.42	−0.64	0.11
300	−6.72	−6.16	−5.62	−5.15	−4.70	−3.86	−3.06	−2.29
350	−9.97	−9.05	−8.38	−7.84	−7.36	−6.47	−5.65	−4.87
400		−12.48	−11.40	−10.75	−10.21	−9.27	−8.41	−7.60
450		−17.48	−14.75	−13.89	−13.26	−12.23	−11.33	−10.49
500		−24.61	−18.52	−17.26	−16.49	−15.35	−14.39	−13.52
550		−31.05	−22.80	−20.90	−19.93	−18.62	−17.60	−16.69
600		−36.65	−27.47	−24.80	−23.55	−22.04	−20.94	−19.99
700		−46.58	−37.17	−33.20	−31.31	−29.30	−28.00	−26.95
800		−55.71	−46.66	−42.02	−39.58	−37.04	−35.54	−34.38
900		−64.50	−55.86	−50.93	−48.13	−45.16	−43.47	−42.24
1000		−73.15	−64.87	−59.83	−56.82	−53.56	−51.76	−50.50
				NH_3°				
25	−6.38	−6.09	−5.79	−5.49	−5.19	−4.58	−3.97	−3.36
50	−7.05	−6.75	−6.45	−6.15	−5.86	−5.26	−4.66	−4.06
75	−7.75	−7.45	−7.15	−6.85	−6.56	−5.97	−5.38	−4.79
100	−8.48	−8.18	−7.89	−7.59	−7.29	−6.71	−6.12	−5.54
125	−9.26	−8.95	−8.66	−8.36	−8.06	−7.48	−6.90	−6.32
150	−10.06	−9.76	−9.46	−9.16	−8.87	−8.28	−7.71	−7.13
175	−10.89	−10.59	−10.29	−9.99	−9.70	−9.12	−8.54	−7.97
200	−11.75	−11.45	−11.15	−10.85	−10.56	−9.98	−9.40	−8.83
225	−12.64	−12.34	−12.04	−11.74	−11.45	−10.87	−10.29	−9.72
250	−13.55	−13.26	−12.96	−12.66	−12.36	−11.78	−11.21	−10.64
300	−15.46	−15.18	−14.87	−14.56	−14.27	−13.68	−13.11	−12.54
350	−17.50	−17.21	−16.88	−16.57	−16.26	−15.67	−15.10	−14.53
400		−19.38	−18.99	−18.66	−18.35	−17.75	−17.17	−16.60
450		−21.83	−21.20	−20.84	−20.51	−19.91	−19.32	−18.75
500		−24.64	−23.52	−23.11	−22.76	−22.14	−21.54	−20.97
550		−27.39	−25.97	−25.46	−25.09	−24.44	−23.84	−23.25
600		−30.07	−28.52	−27.90	−27.48	−26.81	−26.19	−25.61
700		−35.38	−33.79	−32.98	−32.48	−31.73	−31.09	−30.49
800		−40.73	−39.19	−38.29	−37.70	−36.88	−36.21	−35.60
900		−46.17	−44.69	−43.75	−43.11	−42.23	−41.53	−40.90
1000		−51.72	−50.29	−49.33	−48.67	−47.74	−47.03	−46.40
				NH_4^+				
25	−18.99	−18.77	−18.55	−18.32	−18.09	−17.62	−17.14	−16.66
50	−19.67	−19.45	−19.23	−19.00	−18.77	−18.31	−17.85	−17.39
75	−20.38	−20.16	−19.94	−19.71	−19.49	−19.04	−18.58	−18.13
100	−21.12	−20.90	−20.68	−20.46	−20.23	−19.79	−19.34	−18.89
125	−21.89	−21.67	−21.45	−21.22	−21.00	−20.56	−20.12	−19.68
150	−22.67	−22.46	−22.24	−22.02	−21.80	−21.36	−20.93	−20.49
175	−23.48	−23.27	−23.05	−22.84	−22.62	−22.19	−21.76	−21.32
200	−24.31	−24.10	−23.89	−23.68	−23.46	−23.03	−22.61	−22.18
225	−25.15	−24.95	−24.75	−24.54	−24.32	−23.90	−23.48	−23.05
250	−26.00	−25.82	−25.62	−25.41	−25.21	−24.79	−24.37	−23.95
300	−27.73	−27.60	−27.42	−27.22	−27.02	−26.61	−26.20	−25.79
350	−29.44	−29.42	−29.28	−29.09	−28.90	−28.51	−28.11	−27.71
400		−31.33	−31.18	−31.02	−30.84	−30.47	−30.08	−29.68
450		−33.24	−33.14	−32.99	−32.83	−32.48	−32.10	−31.72
500			−35.13	−35.01	−34.87	−34.54	−34.18	−33.81
550			−37.15	−37.07	−36.94	−36.64	−36.31	−35.95
600			−39.20	−39.16	−39.06	−38.79	−38.47	−38.13
700				−43.48	−43.40	−43.19	−42.92	−42.61
800					−47.88	−47.73	−47.51	−47.23
900					−52.51	−52.38	−52.22	−51.97
1000						−57.17	−57.05	−56.81

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				NO_2^-				
25	−7.70	−7.41	−7.11	−6.81	−6.51	−5.91	−5.31	−4.71
50	−8.41	−8.11	−7.81	−7.51	−7.21	−6.60	−6.00	−5.40
75	−9.09	−8.79	−8.49	−8.19	−7.89	−7.29	−6.69	−6.09
100	−9.75	−9.45	−9.15	−8.86	−8.56	−7.97	−7.38	−6.78
125	−10.37	−10.08	−9.80	−9.51	−9.22	−8.63	−8.05	−7.47
150	−10.96	−10.69	−10.42	−10.14	−9.86	−9.29	−8.72	−8.15
175	−11.51	−11.28	−11.02	−10.76	−10.49	−9.94	−9.38	−8.82
200	−12.02	−11.83	−11.60	−11.36	−11.10	−10.57	−10.03	−9.48
225	−12.47	−12.35	−12.15	−11.93	−11.70	−11.20	−10.67	−10.14
250	−12.86	−12.82	−12.68	−12.49	−12.28	−11.81	−11.31	−10.79
300	−13.27	−13.59	−13.61	−13.52	−13.37	−12.99	−12.55	−12.08
350	−12.57	−13.95	−14.37	−14.42	−14.37	−14.11	−13.75	−13.33
400		−13.73	−14.86	−15.17	−15.26	−15.17	−14.91	−14.56
450		−10.65	−14.94	−15.71	−16.01	−16.15	−16.01	−15.75
500			−14.40	−15.98	−16.60	−17.04	−17.06	−16.90
550			−13.07	−15.94	−17.00	−17.83	−18.04	−17.99
600			−11.12	−15.59	−17.22	−18.52	−18.95	−19.03
700				−14.27	−17.15	−19.58	−20.53	−20.91
800					−16.74	−20.29	−21.81	−22.49
900					−16.36	−20.81	−22.83	−23.77
1000						−21.32	−23.72	−24.75
				NO_3^-				
25	−26.51	−26.17	−25.83	−25.49	−25.15	−24.47	−23.79	−23.12
50	−27.37	−27.01	−26.64	−26.29	−25.93	−25.22	−24.51	−23.81
75	−28.21	−27.84	−27.47	−27.10	−26.74	−26.01	−25.29	−24.57
100	−29.04	−28.66	−28.29	−27.92	−27.55	−26.82	−26.09	−25.37
125	−29.84	−29.48	−29.11	−28.74	−28.37	−27.64	−26.92	−26.19
150	−30.62	−30.27	−29.91	−29.55	−29.19	−28.47	−27.75	−27.02
175	−31.38	−31.05	−30.71	−30.36	−30.01	−29.30	−28.58	−27.86
200	−32.10	−31.81	−31.49	−31.16	−30.82	−30.12	−29.42	−28.71
225	−32.77	−32.55	−32.26	−31.95	−31.62	−30.95	−30.26	−29.56
250	−33.38	−33.24	−33.00	−32.72	−32.41	−31.77	−31.10	−30.41
300	−34.29	−34.49	−34.40	−34.20	−33.96	−33.39	−32.77	−32.12
350	−34.13	−35.37	−35.65	−35.59	−35.43	−34.98	−34.43	−33.83
400		−35.67	−36.66	−36.85	−36.83	−36.53	−36.07	−35.53
450		−33.19	−37.30	−37.92	−38.11	−38.02	−37.68	−37.22
500			−37.34	−38.76	−39.25	−39.44	−39.25	−38.88
550			−36.62	−39.31	−40.23	−40.79	−40.78	−40.51
600			−35.31	−39.57	−41.04	−42.06	−42.25	−42.11
700				−39.53	−42.23	−44.34	−45.02	−45.15
800					−43.14	−46.34	−47.55	−47.97
900					−44.14	−48.21	−49.91	−50.56
1000						−50.13	−52.17	−52.91
				Na^+				
25	−62.59	−62.59	−62.58	−62.55	−62.51	−62.42	−62.30	−62.16
50	−62.95	−62.94	−62.92	−62.89	−62.85	−62.74	−62.62	−62.48
75	−63.33	−63.32	−63.29	−63.26	−63.21	−63.11	−62.98	−62.85
100	−63.74	−63.72	−63.70	−63.66	−63.61	−63.51	−63.38	−63.25
125	−64.16	−64.15	−64.12	−64.08	−64.04	−63.94	−63.81	−63.68
150	−64.60	−64.59	−64.57	−64.53	−64.49	−64.39	−64.27	−64.14
175	−65.06	−65.05	−65.04	−65.01	−64.97	−64.87	−64.75	−64.62
200	−65.53	−65.53	−65.52	−65.49	−65.46	−65.37	−65.25	−65.13
225	−66.01	−66.03	−66.02	−66.00	−65.97	−65.89	−65.78	−65.66
250	−66.49	−66.53	−66.54	−66.53	−66.50	−66.42	−66.32	−66.21
300	−67.45	−67.56	−67.61	−67.61	−67.60	−67.55	−67.46	−67.36
350	−68.38	−68.60	−68.72	−68.75	−68.76	−68.74	−68.67	−68.58
400		−69.83	−69.89	−69.94	−69.97	−69.98	−69.94	−69.87
450		−71.18	−71.09	−71.17	−71.22	−71.27	−71.25	−71.20

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Na^+ — Continued				
500			−72.34	−72.43	−72.51	−72.60	−72.62	−72.59
550			−73.64	−73.72	−73.83	−73.97	−74.02	−74.02
600			−75.00	−75.06	−75.18	−75.36	−75.46	−75.49
700				−77.89	−77.96	−78.23	−78.42	−78.51
800					−80.86	−81.18	−81.46	−81.63
900					−83.88	−84.20	−84.59	−84.82
1000						−87.32	−87.80	−88.06
				$NaAlO_2^\circ$				
25	−260.28	−260.06	−259.83	−259.58	−259.32	−258.79	−258.24	−257.67
50	−260.60	−260.37	−260.13	−259.88	−259.63	−259.11	−258.57	−258.03
75	−260.99	−260.75	−260.51	−260.27	−260.01	−259.50	−258.97	−258.44
100	−261.44	−261.21	−260.96	−260.72	−260.46	−259.95	−259.43	−258.90
125	−261.96	−261.72	−261.47	−261.23	−260.97	−260.46	−259.95	−259.43
150	−262.53	−262.29	−262.04	−261.79	−261.54	−261.03	−260.52	−260.00
175	−263.15	−262.91	−262.66	−262.41	−262.16	−261.65	−261.13	−260.62
200	−263.82	−263.58	−263.33	−263.07	−262.82	−262.31	−261.80	−261.28
225	−264.54	−264.30	−264.04	−263.79	−263.53	−263.02	−262.51	−261.99
250	−265.31	−265.06	−264.80	−264.54	−264.28	−263.77	−263.26	−262.75
300	−266.98	−266.72	−266.44	−266.18	−265.91	−265.39	−264.88	−264.37
350	−268.92	−268.57	−268.26	−267.97	−267.70	−267.17	−266.65	−266.13
400		−270.67	−270.23	−269.92	−269.63	−269.08	−268.55	−268.03
450		−273.30	−272.38	−272.01	−271.69	−271.12	−270.58	−270.05
500		−276.62	−274.74	−274.25	−273.89	−273.29	−272.73	−272.20
550		−279.81	−277.31	−276.63	−276.22	−275.57	−274.99	−274.45
600		−282.83	−280.06	−279.16	−278.67	−277.96	−277.36	−276.81
700		−288.69	−285.85	−284.58	−283.90	−283.05	−282.40	−281.81
800		−294.54	−291.81	−290.34	−289.50	−288.50	−287.79	−287.18
900		−300.50	−297.89	−296.34	−295.40	−294.27	−293.51	−292.88
000		−306.62	−304.10	−302.52	−301.52	−300.31	−299.52	−298.88
				$NaBr^\circ$				
25	−85.61	−85.23	−84.86	−84.50	−84.14	−83.43	−82.72	−82.03
50	−86.47	−86.08	−85.70	−85.32	−84.95	−84.23	−83.52	−82.82
75	−87.35	−86.95	−86.56	−86.18	−85.80	−85.07	−84.36	−83.65
100	−88.25	−87.84	−87.44	−87.06	−86.68	−85.94	−85.22	−84.52
125	−89.16	−88.75	−88.35	−87.96	−87.58	−86.84	−86.12	−85.41
150	−90.09	−89.68	−89.27	−88.88	−88.50	−87.75	−87.03	−86.32
175	−91.04	−90.62	−90.21	−89.82	−89.43	−88.68	−87.96	−87.24
200	−92.01	−91.59	−91.17	−90.77	−90.39	−89.63	−88.90	−88.19
225	−92.99	−92.57	−92.15	−91.74	−91.35	−90.60	−89.86	−89.15
250	−93.98	−93.56	−93.14	−92.73	−92.34	−91.57	−90.84	−90.12
300	−96.04	−95.62	−95.17	−94.75	−94.35	−93.57	−92.83	−92.10
350	−98.29	−97.77	−97.27	−96.83	−96.41	−95.62	−94.87	−94.14
400		−100.12	−99.46	−98.97	−98.54	−97.72	−96.95	−96.21
450		−103.03	−101.75	−101.19	−100.72	−99.87	−99.09	−98.33
500		−106.73	−104.19	−103.48	−102.95	−102.06	−101.26	−100.50
550		−110.15	−106.81	−105.86	−105.25	−104.30	−103.47	−102.69
600		−113.25	−109.56	−108.32	−107.61	−106.59	−105.73	−104.93
700		−118.95	−115.17	−113.44	−112.49	−111.28	−110.34	−109.51
800		−124.30	−120.66	−118.67	−117.52	−116.11	−115.10	−114.23
900		−129.49	−126.00	−123.91	−122.62	−121.05	−119.96	−119.07
1000		−134.60	−131.24	−129.11	−127.74	−126.06	−124.93	−124.02
				$Na(CH_3COO)^\circ$				
25	−150.72	−150.16	−149.62	−149.09	−148.57	−147.57	−146.59	−145.64
50	−151.65	−151.06	−150.51	−149.96	−149.44	−148.41	−147.42	−146.44
75	−152.70	−152.10	−151.53	−150.98	−150.45	−149.41	−148.41	−147.43
100	−153.86	−153.25	−152.68	−152.12	−151.58	−150.54	−149.52	−148.54

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				$Na(CH_3COO)^\circ$ — Continued				
125	−155.11	−154.50	−153.92	−153.36	−152.81	−151.76	−150.75	−149.75
150	−156.44	−155.83	−155.25	−154.68	−154.14	−153.08	−152.06	−151.07
175	−157.85	−157.25	−156.66	−156.09	−155.54	−154.48	−153.46	−152.46
200	−159.34	−158.73	−158.14	−157.57	−157.02	−155.96	−154.93	−153.93
225	−160.88	−160.29	−159.70	−159.13	−158.57	−157.51	−156.48	−155.48
250	−162.49	−161.92	−161.32	−160.75	−160.19	−159.12	−158.09	−157.09
300	−165.88	−165.35	−164.75	−164.17	−163.61	−162.54	−161.51	−160.50
350	−169.50	−169.03	−168.41	−167.82	−167.26	−166.18	−165.14	−164.14
400		−172.94	−172.28	−171.69	−171.12	−170.03	−168.99	−167.98
450		−177.16	−176.36	−175.75	−175.17	−174.08	−173.03	−172.01
500		−181.73	−180.64	−179.99	−179.40	−178.30	−177.24	−176.23
550		−186.39	−185.12	−184.41	−183.81	−182.69	−181.63	−180.60
600		−191.13	−189.77	−189.00	−188.37	−187.23	−186.16	−185.14
700		−200.89	−199.51	−198.62	−197.94	−196.75	−195.67	−194.63
800		−211.06	−209.71	−208.77	−208.03	−206.80	−205.70	−204.65
900		−221.64	−220.33	−219.36	−218.59	−217.32	−216.20	−215.15
1000		−232.61	−231.33	−230.35	−229.56	−228.27	−227.14	−226.09
				$Na(CH_3COO)_2^-$				
25	−238.47	−237.28	−236.16	−235.08	−234.04	−232.03	−230.11	−228.24
50	−239.73	−238.51	−237.35	−236.24	−235.18	−233.12	−231.15	−229.24
75	−241.27	−240.03	−238.85	−237.73	−236.65	−234.57	−232.58	−230.64
100	−243.03	−241.78	−240.60	−239.47	−238.39	−236.29	−234.29	−232.34
125	−244.98	−243.74	−242.56	−241.43	−240.34	−238.24	−236.23	−234.28
150	−247.10	−245.88	−244.70	−243.58	−242.49	−240.39	−238.38	−236.43
175	−249.36	−248.17	−247.01	−245.89	−244.81	−242.72	−240.71	−238.76
200	−251.76	−250.61	−249.47	−248.36	−247.29	−245.21	−243.21	−241.26
225	−254.25	−253.17	−252.06	−250.97	−249.91	−247.85	−245.86	−243.92
250	−256.83	−255.85	−254.77	−253.71	−252.67	−250.63	−248.66	−246.73
300	−262.05	−261.47	−260.53	−259.54	−258.54	−256.58	−254.64	−252.74
350	−266.73	−267.24	−266.63	−265.76	−264.85	−262.98	−261.11	−259.25
400		−272.89	−272.95	−272.31	−271.52	−269.79	−267.99	−266.19
450		−276.32	−279.34	−279.11	−278.50	−276.96	−275.27	−273.53
500			−285.55	−286.06	−285.73	−284.44	−282.88	−281.23
550			−291.40	−293.09	−293.17	−292.22	−290.81	−289.25
600			−297.02	−300.19	−300.78	−300.25	−299.03	−297.58
700				−314.78	−316.53	−317.00	−316.22	−315.01
800					−333.14	−334.63	−334.33	−333.38
900					−350.86	−353.16	−353.30	−352.54
1000						−372.67	−373.11	−372.43
				$NaCl^\circ$				
25	−92.91	−92.62	−92.34	−92.06	−91.77	−91.21	−90.65	−90.09
50	−93.62	−93.32	−93.03	−92.73	−92.44	−91.87	−91.30	−90.74
75	−94.35	−94.04	−93.74	−93.44	−93.15	−92.57	−92.00	−91.44
100	−95.09	−94.78	−94.48	−94.18	−93.88	−93.30	−92.73	−92.16
125	−95.86	−95.54	−95.23	−94.93	−94.63	−94.05	−93.47	−92.91
150	−96.64	−96.32	−96.01	−95.70	−95.41	−94.82	−94.24	−93.67
175	−97.43	−97.12	−96.80	−96.50	−96.20	−95.61	−95.03	−94.46
200	−98.24	−97.93	−97.61	−97.30	−97.00	−96.41	−95.83	−95.26
225	−99.07	−98.75	−98.44	−98.13	−97.82	−97.23	−96.65	−96.08
250	−99.90	−99.60	−99.28	−98.97	−98.66	−98.07	−97.48	−96.91
300	−101.62	−101.33	−101.00	−100.68	−100.38	−99.78	−99.19	−98.62
350	−103.41	−103.12	−102.78	−102.45	−102.14	−101.54	−100.95	−100.37
400		−105.00	−104.61	−104.28	−103.96	−103.35	−102.75	−102.18
450		−107.08	−106.51	−106.15	−105.82	−105.20	−104.60	−104.02
500		−109.41	−108.47	−108.07	−107.73	−107.09	−106.49	−105.90
550		−111.69	−110.52	−110.04	−109.68	−109.02	−108.41	−107.83
600		−113.90	−112.63	−112.07	−111.67	−111.00	−110.38	−109.78
700		−118.24	−116.94	−116.24	−115.77	−115.04	−114.40	−113.79

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$NaCl^\circ$ — Continued				
800		−122.57	−121.30	−120.52	−120.00	−119.21	−118.54	−117.93
900		−126.91	−125.69	−124.88	−124.32	−123.48	−122.80	−122.17
1000		−131.30	−130.12	−129.30	−128.71	−127.84	−127.15	−126.52
				NaF°				
25	−128.57	−128.48	−128.37	−128.25	−128.13	−127.86	−127.58	−127.28
50	−128.88	−128.78	−128.67	−128.55	−128.42	−128.16	−127.89	−127.60
75	−129.22	−129.11	−129.00	−128.88	−128.75	−128.49	−128.22	−127.94
100	−129.57	−129.46	−129.35	−129.23	−129.10	−128.84	−128.57	−128.29
125	−129.95	−129.84	−129.72	−129.60	−129.48	−129.21	−128.95	−128.67
150	−130.35	−130.24	−130.12	−129.99	−129.87	−129.61	−129.34	−129.07
175	−130.76	−130.65	−130.53	−130.41	−130.28	−130.02	−129.75	−129.48
200	−131.20	−131.08	−130.96	−130.84	−130.71	−130.45	−130.18	−129.91
225	−131.65	−131.53	−131.41	−131.29	−131.16	−130.90	−130.63	−130.36
250	−132.11	−132.00	−131.88	−131.75	−131.62	−131.36	−131.10	−130.82
300	−133.10	−132.99	−132.86	−132.73	−132.60	−132.33	−132.07	−131.80
350	−134.17	−134.04	−133.90	−133.76	−133.63	−133.36	−133.09	−132.82
400		−135.17	−135.00	−134.85	−134.71	−134.44	−134.17	−133.90
450		−136.48	−136.16	−136.00	−135.85	−135.57	−135.30	−135.02
500		−138.00	−137.39	−137.19	−137.04	−136.75	−136.47	−136.19
550		−139.49	−138.70	−138.44	−138.27	−137.97	−137.68	−137.40
600		−140.94	−140.06	−139.74	−139.54	−139.23	−138.93	−138.65
700		−143.81	−142.91	−142.48	−142.22	−141.86	−141.55	−141.26
800		−146.70	−145.83	−145.34	−145.04	−144.63	−144.30	−144.01
900		−149.65	−148.81	−148.30	−147.97	−147.52	−147.18	−146.87
1000		−152.66	−151.86	−151.34	−150.99	−150.52	−150.17	−149.86
				$NaHSiO_3^\circ$				
25	−307.14	−306.93	−306.71	−306.49	−306.26	−305.81	−305.35	−304.89
50	−307.65	−307.42	−307.20	−306.97	−306.74	−306.28	−305.83	−305.37
75	−308.16	−307.93	−307.70	−307.47	−307.24	−306.79	−306.33	−305.87
100	−308.70	−308.46	−308.23	−308.00	−307.77	−307.30	−306.85	−306.39
125	−309.24	−309.00	−308.77	−308.53	−308.30	−307.84	−307.38	−306.92
150	−309.80	−309.56	−309.32	−309.09	−308.85	−308.39	−307.93	−307.48
175	−310.37	−310.13	−309.89	−309.65	−309.42	−308.96	−308.50	−308.04
200	−310.95	−310.71	−310.47	−310.23	−310.00	−309.53	−309.07	−308.62
225	−311.54	−311.30	−311.06	−310.82	−310.59	−310.12	−309.66	−309.20
250	−312.14	−311.91	−311.66	−311.42	−311.19	−310.72	−310.26	−309.80
300	−313.37	−313.15	−312.90	−312.66	−312.42	−311.95	−311.49	−311.03
350	−314.67	−314.45	−314.19	−313.94	−313.70	−313.23	−312.76	−312.30
400		−315.82	−315.52	−315.26	−315.01	−314.53	−314.07	−313.61
450		−317.34	−316.90	−316.62	−316.36	−315.88	−315.41	−314.94
500		−319.06	−318.33	−318.02	−317.75	−317.25	−316.78	−316.31
550		−320.74	−319.82	−319.46	−319.17	−318.66	−318.18	−317.71
600		−322.37	−321.37	−320.94	−320.63	−320.10	−319.61	−319.14
700		−325.56	−324.54	−323.99	−323.63	−323.05	−322.55	−322.07
800		−328.73	−327.74	−327.14	−326.73	−326.11	−325.59	−325.10
900		−331.93	−330.98	−330.35	−329.90	−329.25	−328.71	−328.21
1000		−335.16	−334.24	−333.60	−333.14	−332.46	−331.91	−331.41
				NaI°				
25	−72.90	−72.40	−71.91	−71.44	−70.97	−70.06	−69.17	−68.30
50	−73.87	−73.35	−72.84	−72.36	−71.88	−70.95	−70.05	−69.16
75	−74.86	−74.33	−73.81	−73.32	−72.84	−71.90	−70.99	−70.09
100	−75.87	−75.33	−74.81	−74.31	−73.82	−72.88	−71.96	−71.06
125	−76.90	−76.35	−75.83	−75.33	−74.84	−73.89	−72.97	−72.07
150	−77.94	−77.40	−76.87	−76.37	−75.87	−74.92	−74.00	−73.09
175	−79.00	−78.46	−77.93	−77.43	−76.93	−75.97	−75.05	−74.14
200	−80.08	−79.54	−79.01	−78.50	−78.01	−77.05	−76.12	−75.21

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				NaI° — Continued				
225	−81.16	−80.64	−80.11	−79.59	−79.10	−78.14	−77.21	−76.30
250	−82.26	−81.75	−81.22	−80.70	−80.21	−79.24	−78.31	−77.40
300	−84.48	−84.01	−83.48	−82.97	−82.47	−81.50	−80.57	−79.66
350	−86.71	−86.33	−85.80	−85.28	−84.78	−83.81	−82.88	−81.97
400		−88.70	−88.17	−87.65	−87.15	−86.18	−85.24	−84.33
450		−91.12	−90.58	−90.06	−89.56	−88.59	−87.65	−86.74
500		−93.59	−93.03	−92.51	−92.01	−91.04	−90.10	−89.19
550		−96.09	−95.53	−95.01	−94.50	−93.53	−92.59	−91.68
600		−98.63	−98.07	−97.54	−97.03	−96.06	−95.12	−94.21
700		−103.80	−103.24	−102.71	−102.20	−101.22	−100.28	−99.37
800		−109.10	−108.53	−108.00	−107.49	−106.51	−105.57	−104.65
900		−114.50	−113.94	−113.40	−112.89	−111.91	−110.97	−110.05
1000		−120.01	−119.44	−118.91	−118.40	−117.42	−116.47	−115.56
				NaOH°				
25	−99.10	−99.09	−99.06	−99.02	−98.97	−98.85	−98.71	−98.55
50	−99.28	−99.26	−99.23	−99.19	−99.14	−99.03	−98.90	−98.75
75	−99.53	−99.50	−99.47	−99.43	−99.38	−99.26	−99.13	−98.99
100	−99.83	−99.80	−99.76	−99.72	−99.66	−99.54	−99.41	−99.27
125	−100.20	−100.16	−100.11	−100.06	−100.00	−99.87	−99.74	−99.60
150	−100.62	−100.56	−100.50	−100.44	−100.38	−100.25	−100.11	−99.96
175	−101.09	−101.02	−100.95	−100.88	−100.81	−100.66	−100.52	−100.37
200	−101.63	−101.53	−101.44	−101.36	−101.28	−101.12	−100.97	−100.81
225	−102.23	−102.09	−101.98	−101.88	−101.79	−101.62	−101.45	−101.29
250	−102.91	−102.72	−102.57	−102.45	−102.34	−102.15	−101.97	−101.80
300	−104.60	−104.18	−103.92	−103.73	−103.58	−103.33	−103.11	−102.92
350	−107.37	−106.06	−105.51	−105.21	−104.99	−104.65	−104.39	−104.16
400		−108.85	−107.44	−106.91	−106.57	−106.12	−105.79	−105.51
450		−114.69	−109.86	−108.88	−108.36	−107.73	−107.31	−106.98
500		−124.77	−112.98	−111.18	−110.37	−109.49	−108.96	−108.56
550		−133.23	−116.96	−113.84	−112.61	−111.40	−110.72	−110.25
600		−139.81	−121.62	−116.88	−115.08	−113.46	−112.61	−112.05
700		−149.89	−131.20	−123.78	−120.65	−117.98	−116.74	−115.97
800		−157.76	−139.81	−130.99	−126.72	−122.97	−121.29	−120.31
900		−164.41	−147.33	−137.91	−132.89	−128.25	−126.20	−125.06
1000		−170.35	−154.02	−144.38	−138.92	−133.67	−131.37	−130.17
				Nd^{+3}				
25	−160.60	−161.09	−161.52	−161.91	−162.26	−162.90	−163.47	−163.99
50	−159.32	−159.82	−160.27	−160.67	−161.04	−161.70	−162.30	−162.85
75	−157.98	−158.49	−158.95	−159.37	−159.75	−160.44	−161.06	−161.63
100	−156.57	−157.11	−157.59	−158.02	−158.42	−159.13	−159.78	−160.37
125	−155.11	−155.67	−156.17	−156.63	−157.04	−157.79	−158.46	−159.07
150	−153.58	−154.19	−154.72	−155.19	−155.63	−156.41	−157.10	−157.74
175	−151.99	−152.64	−153.21	−153.72	−154.18	−154.99	−155.72	−156.38
200	−150.32	−151.03	−151.65	−152.20	−152.68	−153.55	−154.31	−155.00
225	−148.57	−149.36	−150.04	−150.63	−151.16	−152.08	−152.88	−153.59
250	−146.72	−147.61	−148.37	−149.02	−149.59	−150.57	−151.42	−152.17
300	−142.68	−143.92	−144.90	−145.66	−146.32	−147.46	−148.43	−149.26
350	−138.60	−139.84	−141.30	−142.15	−142.92	−144.24	−145.33	−146.28
400		−137.67	−137.68	−138.54	−139.40	−140.90	−142.15	−143.22
450		−139.28	−134.23	−134.88	−135.78	−137.45	−138.86	−140.07
500			−131.28	−131.21	−132.06	−133.89	−135.48	−136.83
550			−129.18	−127.61	−128.26	−130.21	−131.99	−133.50
600			−128.06	−124.21	−124.40	−126.39	−128.37	−130.05
700				−118.34	−116.53	−118.25	−120.66	−122.73
800					−108.43	−109.34	−112.24	−114.76
900					−99.75	−99.71	−103.16	−106.09
1000						−89.62	−93.63	−96.79

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Ne°				
25	4.56	4.81	5.06	5.31	5.55	6.05	6.56	7.06
50	4.11	4.36	4.62	4.88	5.13	5.64	6.14	6.64
75	3.58	3.85	4.11	4.37	4.63	5.14	5.64	6.14
100	3.00	3.27	3.53	3.80	4.06	4.57	5.08	5.58
125	2.35	2.63	2.90	3.17	3.43	3.95	4.46	4.97
150	1.66	1.94	2.22	2.49	2.76	3.28	3.79	4.30
175	0.92	1.21	1.49	1.77	2.03	2.56	3.08	3.59
200	0.13	0.42	0.71	0.99	1.27	1.80	2.32	2.83
225	−0.71	−0.40	−0.11	0.18	0.46	1.00	1.52	2.04
250	−1.60	−1.28	−0.97	−0.67	−0.39	0.16	0.69	1.20
300	−3.55	−3.18	−2.82	−2.50	−2.20	−1.64	−1.09	−0.57
350	−5.95	−5.31	−4.85	−4.49	−4.17	−3.57	−3.01	−2.47
400		−7.83	−7.08	−6.64	−6.27	−5.63	−5.04	−4.49
450		−11.51	−9.55	−8.95	−8.52	−7.81	−7.20	−6.62
500		−16.75	−12.33	−11.45	−10.91	−10.12	−9.46	−8.86
550		−21.48	−15.49	−14.13	−13.45	−12.54	−11.83	−11.21
600		−25.60	−18.94	−17.01	−16.13	−15.07	−14.31	−13.65
700		−32.94	−26.09	−23.22	−21.87	−20.45	−19.54	−18.81
800		−39.69	−33.11	−29.75	−27.99	−26.19	−25.13	−24.32
900		−46.20	−39.92	−36.35	−34.33	−32.21	−31.02	−30.16
000		−52.62	−46.61	−42.95	−40.78	−38.45	−37.17	−36.29
				Ni^{+2}				
25	−10.90	−11.22	−11.50	−11.74	−11.95	−12.32	−12.63	−12.90
50	−10.12	−10.45	−10.74	−11.00	−11.23	−11.63	−11.97	−12.27
75	−9.32	−9.67	−9.97	−10.24	−10.48	−10.90	−11.27	−11.59
100	−8.51	−8.88	−9.19	−9.47	−9.72	−10.17	−10.55	−10.90
125	−7.68	−8.07	−8.40	−8.69	−8.96	−9.43	−9.83	−10.20
150	−6.83	−7.24	−7.60	−7.91	−8.19	−8.68	−9.11	−9.49
175	−5.96	−6.40	−6.78	−7.11	−7.41	−7.93	−8.38	−8.78
200	−5.05	−5.53	−5.95	−6.30	−6.62	−7.18	−7.65	−8.07
225	−4.10	−4.64	−5.09	−5.48	−5.83	−6.42	−6.92	−7.36
250	−3.11	−3.71	−4.22	−4.64	−5.02	−5.65	−6.19	−6.65
300	−0.93	−1.76	−2.42	−2.92	−3.36	−4.10	−4.71	−5.24
350	1.22	0.39	−0.59	−1.16	−1.66	−2.52	−3.23	−3.83
400		1.21	1.20	0.63	0.06	−0.92	−1.73	−2.41
450		−0.55	2.83	2.41	1.81	0.71	−0.20	−0.98
500			4.09	4.15	3.58	2.38	1.34	0.47
550			4.74	5.79	5.37	4.08	2.92	1.95
600			4.69	7.28	7.16	5.84	4.55	3.46
700				9.51	10.73	9.60	8.02	6.67
800					14.34	13.75	11.84	10.19
900					18.21	18.27	15.99	14.06
1000						22.99	20.33	18.25
				$Ni(CH_3COO)^{+}$				
25	−101.12	−100.91	−100.70	−100.48	−100.26	−99.81	−99.35	−98.88
50	−100.90	−100.69	−100.47	−100.25	−100.02	−99.57	−99.11	−98.65
75	−100.80	−100.58	−100.36	−100.14	−99.92	−99.47	−99.02	−98.56
100	−100.80	−100.59	−100.37	−100.15	−99.93	−99.49	−99.04	−98.59
125	−100.88	−100.68	−100.47	−100.25	−100.04	−99.60	−99.16	−98.71
150	−101.04	−100.85	−100.65	−100.44	−100.23	−99.80	−99.37	−98.93
175	−101.27	−101.09	−100.90	−100.70	−100.50	−100.08	−99.66	−99.22
200	−101.55	−101.40	−101.22	−101.03	−100.84	−100.44	−100.02	−99.60
225	−101.88	−101.76	−101.60	−101.43	−101.25	−100.86	−100.45	−100.04
250	−102.24	−102.17	−102.04	−101.88	−101.71	−101.34	−100.95	−100.55
300	−103.05	−103.12	−103.06	−102.94	−102.80	−102.49	−102.13	−101.76
350	−104.52	−104.20	−104.30	−104.21	−104.10	−103.84	−103.53	−103.19
400		−106.10	−105.75	−105.66	−105.59	−105.38	−105.12	−104.82
450		−109.38	−107.46	−107.31	−107.25	−107.11	−106.90	−106.64

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Ni(CH_3COO)^+$ — Continued				
500			−109.51	−109.15	−109.08	−108.98	−108.83	−108.62
550			−112.01	−111.19	−111.05	−111.01	−110.92	−110.75
600			−114.97	−113.45	−113.18	−113.15	−113.13	−113.02
700				−118.74	−117.85	−117.75	−117.87	−117.89
800					−123.02	−122.68	−122.96	−123.12
900					−128.53	−127.89	−128.36	−128.66
1000						−133.44	−134.08	−134.46
				$Ni(CH_3COO)_2^\circ$				
25	−190.61	−189.82	−189.06	−188.33	−187.62	−186.25	−184.93	−183.64
50	−190.79	−189.97	−189.19	−188.43	−187.71	−186.30	−184.95	−183.64
75	−191.24	−190.40	−189.61	−188.84	−188.11	−186.68	−185.32	−183.99
100	−191.92	−191.08	−190.27	−189.50	−188.75	−187.32	−185.94	−184.60
125	−192.81	−191.95	−191.14	−190.36	−189.61	−188.17	−186.78	−185.43
150	−193.87	−193.02	−192.20	−191.42	−190.66	−189.21	−187.82	−186.46
175	−195.10	−194.25	−193.43	−192.64	−191.88	−190.43	−189.03	−187.67
200	−196.48	−195.64	−194.81	−194.02	−193.26	−191.80	−190.40	−189.04
225	−198.01	−197.17	−196.35	−195.56	−194.79	−193.33	−191.92	−190.55
250	−199.66	−198.85	−198.02	−197.23	−196.46	−194.99	−193.58	−192.21
300	−203.33	−202.59	−201.76	−200.96	−200.19	−198.71	−197.29	−195.92
350	−207.46	−206.82	−205.97	−205.16	−204.39	−202.91	−201.49	−200.11
400		−211.52	−210.63	−209.81	−209.03	−207.54	−206.11	−204.73
450		−216.73	−215.70	−214.86	−214.07	−212.57	−211.14	−209.76
500		−222.49	−221.16	−220.29	−219.49	−217.98	−216.54	−215.15
550		−228.52	−227.01	−226.08	−225.26	−223.73	−222.29	−220.89
600		−234.79	−233.20	−232.20	−231.36	−229.81	−228.36	−226.96
700		−248.10	−246.48	−245.37	−244.47	−242.88	−241.41	−240.00
800		−262.39	−260.80	−259.63	−258.68	−257.04	−255.55	−254.14
900		−277.60	−276.05	−274.86	−273.87	−272.20	−270.69	−269.27
1000		−293.68	−292.16	−290.96	−289.96	−288.25	−286.74	−285.31
				$Ni(CH_3COO)_3^-$				
25	−279.69	−278.25	−276.88	−275.57	−274.31	−271.89	−269.57	−267.32
50	−280.00	−278.51	−277.11	−275.77	−274.48	−272.00	−269.62	−267.32
75	−280.75	−279.24	−277.83	−276.47	−275.16	−272.65	−270.25	−267.92
100	−281.86	−280.35	−278.93	−277.57	−276.25	−273.73	−271.31	−268.97
125	−283.27	−281.78	−280.36	−279.00	−277.69	−275.17	−272.74	−270.40
150	−284.96	−283.49	−282.08	−280.73	−279.43	−276.91	−274.49	−272.15
175	−286.88	−285.46	−284.07	−282.74	−281.44	−278.94	−276.53	−274.19
200	−289.00	−287.65	−286.29	−284.98	−283.70	−281.22	−278.83	−276.50
225	−291.29	−290.04	−288.73	−287.45	−286.19	−283.75	−281.37	−279.06
250	−293.72	−292.61	−291.37	−290.12	−288.89	−286.49	−284.14	−281.85
300	−298.75	−298.20	−297.16	−296.02	−294.87	−292.58	−290.30	−288.06
350	−303.34	−304.10	−303.54	−302.58	−301.54	−299.39	−297.22	−295.04
400		−310.45	−310.39	−309.68	−308.81	−306.86	−304.81	−302.72
450		−315.13	−317.51	−317.24	−316.59	−314.91	−313.01	−311.03
500			−324.70	−325.16	−324.83	−323.47	−321.77	−319.91
550			−331.80	−333.35	−333.44	−332.50	−331.02	−329.31
600			−338.94	−341.79	−342.39	−341.95	−340.73	−339.18
700				−359.70	−361.28	−361.96	−361.35	−360.16
800					−381.62	−383.34	−383.38	−382.59
900					−403.58	−406.06	−406.73	−406.26
1000						−430.24	−431.39	−431.06
				$NiCl^+$				
25	−40.92	−40.99	−41.03	−41.06	−41.07	−41.05	−41.00	−40.92
50	−40.50	−40.58	−40.62	−40.65	−40.67	−40.66	−40.63	−40.57
75	−40.10	−40.18	−40.23	−40.27	−40.29	−40.29	−40.27	−40.23
100	−39.72	−39.80	−39.86	−39.90	−39.92	−39.94	−39.93	−39.90

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
$NiCl^+$ — Continued								
125	−39.34	−39.44	−39.50	−39.55	−39.58	−39.61	−39.61	−39.59
150	−38.97	−39.08	−39.16	−39.21	−39.25	−39.30	−39.31	−39.30
175	−38.61	−38.73	−38.82	−38.89	−38.94	−39.00	−39.02	−39.02
200	−38.24	−38.39	−38.49	−38.58	−38.64	−38.71	−38.75	−38.76
225	−37.87	−38.04	−38.17	−38.27	−38.34	−38.44	−38.49	−38.51
250	−37.48	−37.70	−37.85	−37.97	−38.06	−38.18	−38.25	−38.28
300	−36.65	−36.99	−37.23	−37.39	−37.51	−37.69	−37.80	−37.86
350	−35.91	−36.24	−36.65	−36.83	−36.99	−37.23	−37.39	−37.50
400		−36.30	−36.13	−36.32	−36.50	−36.80	−37.02	−37.17
450		−37.97	−35.77	−35.85	−36.05	−36.41	−36.68	−36.88
500			−35.67	−35.46	−35.63	−36.04	−36.37	−36.62
550			−35.99	−35.16	−35.24	−35.68	−36.08	−36.39
600			−36.77	−35.00	−34.88	−35.33	−35.79	−36.16
700				−35.22	−34.30	−34.60	−35.21	−35.71
800					−33.81	−33.77	−34.55	−35.21
900					−33.29	−32.84	−33.81	−34.63
1000						−31.90	−33.07	−33.96
Octanoate								
25	−76.34	−74.80	−73.34	−71.95	−70.61	−68.05	−65.59	−63.22
50	−77.94	−76.34	−74.84	−73.41	−72.04	−69.41	−66.89	−64.45
75	−79.75	−78.13	−76.61	−75.16	−73.76	−71.09	−68.54	−66.07
100	−81.73	−80.11	−78.57	−77.11	−75.70	−73.01	−70.44	−67.95
125	−83.87	−82.25	−80.71	−79.24	−77.83	−75.12	−72.54	−70.04
150	−86.14	−84.53	−82.99	−81.52	−80.11	−77.40	−74.81	−72.30
175	−88.53	−86.94	−85.41	−83.95	−82.53	−79.82	−77.23	−74.72
200	−91.01	−89.47	−87.95	−86.49	−85.08	−82.38	−79.79	−77.28
225	−93.58	−92.10	−90.60	−89.15	−87.75	−85.06	−82.47	−79.97
250	−96.19	−94.81	−93.34	−91.91	−90.53	−87.85	−85.27	−82.77
300	−101.48	−100.46	−99.09	−97.72	−96.37	−93.74	−91.19	−88.71
350	−106.28	−106.23	−105.12	−103.84	−102.55	−100.00	−97.49	−95.04
400		−111.89	−111.33	−110.23	−109.03	−106.58	−104.14	−101.72
450		−115.78	−117.59	−116.81	−115.76	−113.46	−111.09	−108.73
500			−123.70	−123.52	−122.69	−120.59	−118.32	−116.02
550			−129.53	−130.30	−129.79	−127.94	−125.80	−123.57
600			−135.18	−137.13	−137.02	−135.51	−133.51	−131.36
700				−151.09	−151.92	−151.20	−149.54	−147.58
800					−167.51	−167.60	−166.31	−164.55
900					−183.98	−184.72	−183.77	−182.16
1000						−202.63	−201.91	−200.36
Octanoic Acid								
25	−83.40	−81.68	−80.04	−78.46	−76.92	−73.96	−71.09	−68.30
50	−85.64	−83.91	−82.27	−80.69	−79.16	−76.20	−73.36	−70.59
75	−88.20	−86.46	−84.81	−83.23	−81.70	−78.75	−75.91	−73.15
100	−91.04	−89.29	−87.64	−86.05	−84.52	−81.57	−78.73	−75.98
125	−94.15	−92.39	−90.73	−89.14	−87.60	−84.64	−81.80	−79.05
150	−97.51	−95.74	−94.07	−92.47	−90.92	−87.96	−85.12	−82.36
175	−101.10	−99.33	−97.64	−96.03	−94.47	−91.50	−88.65	−85.89
200	−104.93	−103.15	−101.44	−99.81	−98.25	−95.26	−92.40	−89.63
225	−108.99	−107.20	−105.46	−103.81	−102.23	−99.21	−96.34	−93.57
250	−113.28	−111.47	−109.68	−108.00	−106.41	−103.37	−100.48	−97.69
300	−122.63	−120.69	−118.75	−116.99	−115.34	−112.23	−109.30	−106.48
350	−133.75	−130.95	−128.65	−126.74	−125.00	−121.78	−118.79	−115.93
400		−142.83	−139.45	−137.24	−135.35	−131.99	−128.90	−125.99
450		−159.03	−151.29	−148.53	−146.40	−142.81	−139.61	−136.63
500		−181.03	−164.43	−160.62	−158.12	−154.22	−150.88	−147.82
550		−201.34	−179.05	−173.56	−170.52	−166.20	−162.69	−159.52
600		−219.60	−194.88	−187.33	−183.57	−178.72	−174.99	−171.71
700		−253.22	−227.85	−216.89	−211.45	−205.28	−201.04	−197.50

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				Octanoic Acid — Continued				
800		−285.21	−260.79	−248.06	−241.16	−233.61	−228.82	−225.01
900		−316.75	−293.43	−279.93	−272.09	−263.40	−258.14	−254.13
1000		−348.38	−326.02	−312.23	−303.83	−294.36	−288.79	−284.71
				O_2°				
25	3.95	4.31	4.67	5.01	5.36	6.04	6.70	7.37
50	3.25	3.62	3.99	4.35	4.70	5.39	6.07	6.73
75	2.45	2.84	3.21	3.57	3.93	4.63	5.31	5.99
100	1.57	1.96	2.34	2.71	3.08	3.78	4.47	5.15
125	0.61	1.01	1.40	1.78	2.14	2.86	3.55	4.23
150	−0.42	−0.01	0.39	0.77	1.14	1.86	2.56	3.25
175	−1.51	−1.09	−0.69	−0.30	0.08	0.81	1.51	2.20
200	−2.67	−2.24	−1.82	−1.43	−1.04	−0.31	0.41	1.10
225	−3.89	−3.45	−3.02	−2.61	−2.22	−1.48	−0.76	−0.06
250	−5.19	−4.73	−4.28	−3.86	−3.46	−2.70	−1.97	−1.26
300	−8.03	−7.48	−6.96	−6.51	−6.08	−5.29	−4.54	−3.82
350	−11.54	−10.56	−9.89	−9.37	−8.90	−8.06	−7.29	−6.55
400		−14.24	−13.10	−12.45	−11.92	−11.01	−10.20	−9.43
450		−19.68	−16.66	−15.77	−15.14	−14.13	−13.27	−12.47
500		−27.52	−20.69	−19.35	−18.56	−17.41	−16.49	−15.66
550		−34.55	−25.27	−23.20	−22.18	−20.86	−19.85	−18.97
600		−40.62	−30.29	−27.33	−26.00	−24.45	−23.35	−22.43
700		−51.28	−40.67	−36.24	−34.18	−32.06	−30.75	−29.71
800		−60.96	−50.76	−45.57	−42.88	−40.17	−38.61	−37.46
900		−70.20	−60.47	−54.95	−51.86	−48.65	−46.89	−45.65
1000		−79.25	−69.93	−64.29	−60.95	−57.41	−55.52	−54.24
				OH^-				
25	−37.59	−37.64	−37.67	−37.68	−37.68	−37.66	−37.62	−37.56
50	−37.50	−37.54	−37.56	−37.57	−37.57	−37.55	−37.50	−37.44
75	−37.36	−37.40	−37.42	−37.44	−37.44	−37.42	−37.38	−37.33
100	−37.17	−37.23	−37.26	−37.28	−37.29	−37.28	−37.25	−37.20
125	−36.95	−37.02	−37.06	−37.09	−37.11	−37.12	−37.10	−37.06
150	−36.67	−36.77	−36.84	−36.89	−36.92	−36.94	−36.94	−36.92
175	−36.35	−36.49	−36.58	−36.65	−36.70	−36.75	−36.77	−36.76
200	−35.97	−36.16	−36.29	−36.39	−36.46	−36.54	−36.58	−36.59
225	−35.51	−35.78	−35.96	−36.09	−36.19	−36.31	−36.38	−36.41
250	−34.96	−35.33	−35.59	−35.76	−35.89	−36.07	−36.17	−36.22
300	−33.44	−34.23	−34.70	−35.00	−35.21	−35.51	−35.70	−35.82
350	−30.80	−32.62	−33.60	−34.07	−34.41	−34.87	−35.17	−35.37
400		−30.89	−32.24	−32.96	−33.46	−34.14	−34.57	−34.87
450		−27.21	−30.51	−31.64	−32.36	−33.30	−33.90	−34.32
500			−28.28	−30.05	−31.08	−32.35	−33.15	−33.70
550			−25.46	−28.16	−29.59	−31.28	−32.31	−33.01
600			−22.24	−26.01	−27.89	−30.07	−31.37	−32.24
700				−21.32	−23.98	−27.22	−29.14	−30.40
800					−19.66	−23.83	−26.44	−28.11
900					−15.25	−20.09	−23.33	−25.35
1000						−16.23	−19.98	−22.16
				Pentanoate				
25	−82.60	−81.61	−80.66	−79.75	−78.87	−77.16	−75.52	−73.93
50	−83.63	−82.61	−81.64	−80.70	−79.80	−78.06	−76.38	−74.75
75	−84.80	−83.76	−82.77	−81.83	−80.91	−79.15	−77.46	−75.81
100	−86.06	−85.02	−84.03	−83.08	−82.17	−80.40	−78.70	−77.04
125	−87.41	−86.38	−85.40	−84.45	−83.53	−81.76	−80.06	−78.40
150	−88.84	−87.83	−86.85	−85.91	−84.99	−83.23	−81.53	−79.87
175	−90.33	−89.34	−88.38	−87.45	−86.54	−84.79	−83.09	−81.44
200	−91.86	−90.92	−89.98	−89.06	−88.17	−86.43	−84.74	−83.10

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pentanoate — Continued				
225	−93.42	−92.55	−91.64	−90.74	−89.86	−88.14	−86.47	−84.84
250	−94.98	−94.22	−93.35	−92.48	−91.62	−89.93	−88.27	−86.65
300	−97.98	−97.61	−96.89	−96.10	−95.29	−93.68	−92.07	−90.48
350	−100.15	−100.89	−100.53	−99.88	−99.15	−97.64	−96.10	−94.56
400		−103.83	−104.16	−103.75	−103.16	−101.79	−100.34	−98.86
450		−104.22	−107.64	−107.65	−107.26	−106.10	−104.76	−103.35
500			−110.72	−111.51	−111.42	−110.53	−109.33	−108.01
550			−113.23	−115.27	−115.60	−115.07	−114.04	−112.82
600			−115.33	−118.91	−119.78	−119.70	−118.87	−117.77
700				−126.11	−128.19	−129.17	−128.82	−127.98
800					−136.90	−138.95	−139.11	−138.54
900					−146.21	−149.11	−149.74	−149.40
1000						−159.80	−160.75	−160.50
				Pentanoic Acid				
25	−89.21	−88.04	−86.91	−85.82	−84.76	−82.70	−80.70	−78.74
50	−90.89	−89.71	−88.58	−87.50	−86.44	−84.39	−82.41	−80.47
75	−92.76	−91.57	−90.45	−89.36	−88.30	−86.26	−84.29	−82.36
100	−94.81	−93.62	−92.49	−91.40	−90.34	−88.30	−86.33	−84.41
125	−97.03	−95.83	−94.70	−93.60	−92.54	−90.50	−88.53	−86.62
150	−99.41	−98.21	−97.06	−95.96	−94.90	−92.85	−90.88	−88.97
175	−101.94	−100.73	−99.58	−98.47	−97.40	−95.35	−93.38	−91.46
200	−104.62	−103.41	−102.23	−101.12	−100.04	−97.98	−96.00	−94.08
225	−107.44	−106.22	−105.03	−103.90	−102.82	−100.74	−98.75	−96.82
250	−110.41	−109.18	−107.96	−106.81	−105.72	−103.62	−101.62	−99.69
300	−116.85	−115.54	−114.22	−113.01	−111.88	−109.74	−107.71	−105.76
350	−124.50	−122.57	−121.01	−119.70	−118.51	−116.30	−114.23	−112.25
400		−130.66	−128.37	−126.87	−125.58	−123.27	−121.15	−119.13
450		−141.61	−136.42	−134.55	−133.10	−130.64	−128.44	−126.38
500		−156.42	−145.32	−142.75	−141.05	−138.38	−136.09	−133.97
550		−170.09	−155.19	−151.50	−149.44	−146.49	−144.08	−141.90
600		−182.38	−165.85	−160.78	−158.25	−154.95	−152.40	−150.13
700		−204.97	−188.02	−180.68	−177.01	−172.83	−169.94	−167.50
800		−226.43	−210.11	−201.59	−196.95	−191.85	−188.59	−185.98
900		−247.55	−231.96	−222.93	−217.66	−211.80	−208.22	−205.48
1000		−268.69	−253.74	−244.51	−238.87	−232.49	−228.71	−225.91
				Phenol				
25	−12.59	−11.58	−10.61	−9.67	−8.75	−6.95	−5.21	−3.49
50	−13.81	−12.80	−11.83	−10.89	−9.98	−8.20	−6.47	−4.78
75	−15.17	−14.16	−13.19	−12.25	−11.34	−9.57	−7.86	−6.18
100	−16.67	−15.66	−14.69	−13.75	−12.84	−11.07	−9.36	−7.69
125	−18.30	−17.28	−16.31	−15.37	−14.45	−12.69	−10.98	−9.32
150	−20.04	−19.02	−18.04	−17.10	−16.19	−14.42	−12.72	−11.05
175	−21.89	−20.87	−19.89	−18.94	−18.03	−16.26	−14.55	−12.89
200	−23.85	−22.84	−21.84	−20.89	−19.97	−18.20	−16.49	−14.83
225	−25.92	−24.90	−23.90	−22.94	−22.01	−20.23	−18.52	−16.86
250	−28.09	−27.07	−26.05	−25.08	−24.15	−22.36	−20.64	−18.98
300	−32.76	−31.73	−30.65	−29.65	−28.69	−26.88	−25.15	−23.47
350	−38.15	−36.84	−35.62	−34.57	−33.58	−31.72	−29.97	−28.28
400		−42.64	−41.00	−39.83	−38.79	−36.88	−35.09	−33.38
450		−50.16	−46.84	−45.45	−44.32	−42.32	−40.49	−38.75
500		−59.97	−53.23	−51.44	−50.16	−48.04	−46.16	−44.39
550		−69.17	−60.23	−57.79	−56.31	−54.03	−52.07	−50.27
600		−77.63	−67.75	−64.51	−62.75	−60.26	−58.23	−56.38
700		−93.53	−83.40	−78.85	−76.43	−73.44	−71.21	−69.26
800		−108.95	−99.19	−93.95	−90.97	−87.45	−85.01	−82.95
900		−124.33	−114.99	−109.46	−106.12	−102.15	−99.53	−97.40
1000		−139.86	−130.90	−125.25	−121.69	−117.43	−114.68	−112.53

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Phenylalanine				
25	−49.50	−48.08	−46.72	−45.41	−44.14	−41.66	−39.27	−36.92
50	−50.92	−49.49	−48.14	−46.83	−45.56	−43.10	−40.72	−38.40
75	−52.51	−51.08	−49.72	−48.41	−47.14	−44.69	−42.33	−40.02
100	−54.26	−52.83	−51.46	−50.15	−48.88	−46.44	−44.08	−41.78
125	−56.16	−54.72	−53.36	−52.04	−50.77	−48.33	−45.97	−43.68
150	−58.20	−56.76	−55.39	−54.08	−52.80	−50.35	−47.99	−45.70
175	−60.38	−58.94	−57.56	−56.24	−54.96	−52.51	−50.15	−47.85
200	−62.68	−61.25	−59.85	−58.52	−57.24	−54.78	−52.42	−50.12
225	−65.11	−63.68	−62.27	−60.93	−59.64	−57.17	−54.80	−52.51
250	−67.66	−66.24	−64.81	−63.45	−62.16	−59.67	−57.30	−55.00
300	−73.17	−71.73	−70.23	−68.83	−67.51	−64.99	−62.59	−60.28
350	−79.57	−77.80	−76.11	−74.64	−73.27	−70.70	−68.27	−65.94
400		−84.72	−82.49	−80.87	−79.43	−76.78	−74.31	−71.95
450		−93.86	−89.43	−87.53	−85.97	−83.21	−80.68	−78.29
500		−105.95	−97.06	−94.63	−92.89	−89.97	−87.37	−84.94
550		−117.22	−105.47	−102.20	−100.18	−97.05	−94.36	−91.88
600		−127.50	−114.52	−110.21	−107.83	−104.44	−101.64	−99.10
700		−146.68	−133.38	−127.35	−124.11	−120.06	−117.01	−114.33
800		−165.15	−152.32	−145.40	−141.43	−136.68	−133.35	−130.55
900		−183.48	−171.21	−163.90	−159.46	−154.13	−150.57	−147.66
1000		−201.95	−190.16	−182.71	−177.99	−172.27	−168.55	−165.61
				Propane				
25	−1.96	−1.19	−0.44	0.27	0.96	2.30	3.59	4.84
50	−2.90	−2.10	−1.33	−0.60	0.12	1.49	2.81	4.09
75	−4.03	−3.20	−2.42	−1.67	−0.94	0.45	1.79	3.09
100	−5.30	−4.46	−3.67	−2.91	−2.17	−0.76	0.59	1.90
125	−6.71	−5.86	−5.06	−4.29	−3.54	−2.12	−0.76	0.56
150	−8.25	−7.39	−6.57	−5.80	−5.05	−3.61	−2.23	−0.90
175	−9.91	−9.04	−8.21	−7.42	−6.66	−5.21	−3.83	−2.49
200	−11.68	−10.80	−9.96	−9.16	−8.39	−6.93	−5.53	−4.18
225	−13.57	−12.68	−11.81	−11.00	−10.22	−8.74	−7.34	−5.98
250	−15.57	−14.66	−13.77	−12.94	−12.15	−10.65	−9.23	−7.87
300	−19.95	−18.96	−17.99	−17.11	−16.28	−14.74	−13.29	−11.91
350	−25.27	−23.79	−22.61	−21.64	−20.77	−19.17	−17.68	−16.26
400		−29.46	−27.68	−26.55	−25.59	−23.90	−22.36	−20.92
450		−37.47	−33.28	−31.84	−30.75	−28.93	−27.33	−25.84
500		−48.63	−39.55	−37.54	−36.24	−34.25	−32.57	−31.03
550		−58.82	−46.60	−43.66	−42.06	−39.84	−38.06	−36.46
600		−67.84	−54.28	−50.20	−48.21	−45.69	−43.79	−42.13
700		−84.17	−70.26	−64.29	−61.36	−58.11	−55.93	−54.12
800		−99.47	−86.07	−79.13	−75.40	−71.39	−68.90	−66.94
900		−114.40	−101.61	−94.24	−89.99	−85.34	−82.59	−80.52
1000		−129.26	−117.00	−109.47	−104.91	−99.84	−96.91	−94.80
				Propanoate				
25	−86.77	−86.13	−85.52	−84.92	−84.34	−83.20	−82.09	−81.00
50	−87.47	−86.81	−86.18	−85.57	−84.98	−83.82	−82.69	−81.58
75	−88.23	−87.57	−86.94	−86.32	−85.72	−84.56	−83.42	−82.31
100	−89.06	−88.40	−87.77	−87.16	−86.56	−85.39	−84.26	−83.15
125	−89.94	−89.29	−88.67	−88.06	−87.46	−86.30	−85.18	−84.07
150	−90.87	−90.24	−89.63	−89.03	−88.44	−87.29	−86.17	−85.07
175	−91.83	−91.23	−90.64	−90.05	−89.48	−88.34	−87.23	−86.14
200	−92.81	−92.26	−91.70	−91.13	−90.57	−89.45	−88.36	−87.28
225	−93.80	−93.32	−92.79	−92.25	−91.70	−90.62	−89.54	−88.47
250	−94.77	−94.40	−93.92	−93.41	−92.89	−91.83	−90.78	−89.73
300	−96.51	−96.54	−96.23	−95.82	−95.36	−94.40	−93.40	−92.39
350	−97.32	−98.48	−98.58	−98.31	−97.95	−97.12	−96.20	−95.25
400		−100.05	−100.85	−100.84	−100.63	−99.96	−99.15	−98.27
450		−98.94	−102.89	−103.35	−103.35	−102.91	−102.23	−101.43

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Propanoate — Continued				
500			−104.48	−105.75	−106.07	−105.94	−105.42	−104.73
550			−105.43	−108.00	−108.77	−109.03	−108.70	−108.12
600			−105.91	−110.07	−111.42	−112.16	−112.05	−111.61
700				−114.03	−116.62	−118.51	−118.93	−118.80
800					−121.98	−124.99	−126.00	−126.18
900					−127.82	−131.73	−133.26	−133.70
1000						−138.88	−140.79	−141.33
				Propanoic Acid				
25	−93.43	−92.63	−91.86	−91.11	−90.37	−88.93	−87.51	−86.12
50	−94.73	−93.93	−93.16	−92.41	−91.67	−90.24	−88.85	−87.49
75	−96.13	−95.33	−94.56	−93.81	−93.08	−91.66	−90.28	−88.92
100	−97.64	−96.84	−96.06	−95.32	−94.59	−93.17	−91.79	−90.44
125	−99.25	−98.44	−97.67	−96.92	−96.19	−94.77	−93.40	−92.05
150	−100.96	−100.14	−99.36	−98.61	−97.88	−96.46	−95.09	−93.74
175	−102.75	−101.94	−101.15	−100.39	−99.65	−98.23	−96.86	−95.52
200	−104.63	−103.82	−103.02	−102.25	−101.51	−100.09	−98.71	−97.37
225	−106.60	−105.78	−104.97	−104.20	−103.45	−102.01	−100.63	−99.29
250	−108.66	−107.83	−107.00	−106.22	−105.46	−104.02	−102.63	−101.28
300	−113.08	−112.20	−111.30	−110.48	−109.70	−108.23	−106.82	−105.46
350	−118.23	−116.98	−115.93	−115.04	−114.22	−112.70	−111.27	−109.89
400		−122.43	−120.91	−119.89	−119.01	−117.43	−115.96	−114.56
450		−129.74	−126.31	−125.05	−124.07	−122.39	−120.87	−119.44
500		−139.55	−132.25	−130.54	−129.39	−127.57	−125.99	−124.53
550		−148.60	−138.81	−136.36	−134.98	−132.98	−131.32	−129.81
600		−156.72	−145.87	−142.52	−140.83	−138.59	−136.84	−135.28
700		−171.62	−160.49	−155.65	−153.22	−150.41	−148.44	−146.76
800		−185.72	−175.00	−169.39	−166.32	−162.91	−160.70	−158.91
900		−199.54	−189.30	−183.35	−179.87	−175.96	−173.54	−171.67
1000		−213.32	−203.50	−197.43	−193.70	−189.45	−186.90	−185.00
				PO_4^{-3}				
25	−243.50	−243.85	−244.14	−244.39	−244.60	−244.95	−245.22	−245.44
50	−242.07	−242.44	−242.76	−243.04	−243.27	−243.67	−243.99	−244.26
75	−240.45	−240.86	−241.21	−241.52	−241.78	−242.23	−242.60	−242.91
100	−238.66	−239.13	−239.52	−239.86	−240.16	−240.67	−241.08	−241.43
125	−236.70	−237.24	−237.69	−238.08	−238.42	−238.99	−239.46	−239.86
150	−234.56	−235.20	−235.73	−236.18	−236.56	−237.21	−237.74	−238.19
175	−232.22	−233.00	−233.62	−234.15	−234.60	−235.34	−235.94	−236.44
200	−229.67	−230.62	−231.37	−231.99	−232.51	−233.37	−234.05	−234.62
225	−226.86	−228.04	−228.96	−229.70	−230.32	−231.31	−232.09	−232.74
250	−223.72	−225.25	−226.39	−227.27	−228.00	−229.15	−230.05	−230.78
300	−216.09	−218.88	−220.73	−221.99	−223.00	−224.56	−225.74	−226.68
350	−205.27	−210.90	−214.34	−216.11	−217.50	−219.58	−221.13	−222.34
400		−203.17	−207.11	−209.61	−211.48	−214.22	−216.20	−217.73
450		−191.38	−198.84	−202.39	−204.90	−208.45	−210.96	−212.86
500			−189.27	−194.35	−197.70	−202.26	−205.38	−207.71
550			−178.34	−185.46	−189.84	−195.60	−199.43	−202.24
600			−166.69	−175.82	−181.31	−188.44	−193.09	−196.44
700				−155.69	−162.57	−172.55	−179.09	−183.68
800					−142.41	−154.69	−163.31	−169.21
900					−121.59	−135.35	−145.97	−152.98
1000						−115.36	−127.60	−135.12
				Pb^{+2}				
25	−5.71	−5.88	−6.01	−6.12	−6.21	−6.34	−6.43	−6.49
50	−5.80	−5.98	−6.12	−6.24	−6.33	−6.49	−6.60	−6.68
75	−5.88	−6.06	−6.21	−6.34	−6.44	−6.61	−6.74	−6.84
100	−5.94	−6.14	−6.29	−6.43	−6.54	−6.73	−6.87	−6.98

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pb^{+2} — Continued				
125	−5.99	−6.20	−6.37	−6.51	−6.63	−6.83	−6.99	−7.12
150	−6.02	−6.24	−6.43	−6.58	−6.72	−6.94	−7.11	−7.25
175	−6.03	−6.28	−6.48	−6.65	−6.80	−7.03	−7.22	−7.38
200	−6.01	−6.29	−6.52	−6.71	−6.87	−7.13	−7.33	−7.50
225	−5.96	−6.28	−6.54	−6.75	−6.93	−7.22	−7.44	−7.63
250	−5.88	−6.25	−6.55	−6.78	−6.98	−7.30	−7.55	−7.75
300	−5.53	−6.10	−6.51	−6.81	−7.06	−7.45	−7.76	−8.00
350	−5.04	−5.76	−6.43	−6.79	−7.09	−7.58	−7.95	−8.25
400		−6.12	−6.33	−6.73	−7.09	−7.68	−8.13	−8.48
450		−7.46	−6.25	−6.64	−7.06	−7.75	−8.28	−8.71
500			−6.29	−6.54	−6.99	−7.79	−8.42	−8.92
550			−6.55	−6.44	−6.88	−7.79	−8.52	−9.10
600			−7.06	−6.38	−6.74	−7.74	−8.59	−9.26
700				−6.56	−6.37	−7.46	−8.56	−9.43
800					−5.93	−6.89	−8.28	−9.38
900					−5.32	−6.08	−7.77	−9.07
1000						−5.15	−7.12	−8.52
				$Pb(CH_3COO)^+$				
25	−97.25	−96.87	−96.50	−96.14	−95.77	−95.06	−94.36	−93.66
50	−98.22	−97.83	−97.44	−97.07	−96.70	−95.97	−95.26	−94.56
75	−99.31	−98.90	−98.51	−98.13	−97.76	−97.03	−96.31	−95.61
100	−100.49	−100.09	−99.69	−99.31	−98.93	−98.20	−97.48	−96.77
125	−101.77	−101.36	−100.96	−100.58	−100.20	−99.46	−98.74	−98.03
150	−103.13	−102.72	−102.32	−101.93	−101.55	−100.81	−100.09	−99.38
175	−104.56	−104.15	−103.75	−103.36	−102.98	−102.24	−101.51	−100.80
200	−106.06	−105.65	−105.25	−104.86	−104.48	−103.73	−103.01	−102.30
225	−107.62	−107.22	−106.82	−106.43	−106.05	−105.30	−104.57	−103.86
250	−109.24	−108.86	−108.45	−108.06	−107.68	−106.93	−106.20	−105.49
300	−112.64	−112.29	−111.89	−111.50	−111.11	−110.36	−109.64	−108.92
350	−116.22	−115.95	−115.54	−115.15	−114.76	−114.02	−113.29	−112.57
400		−119.79	−119.39	−119.00	−118.61	−117.86	−117.14	−116.42
450		−123.82	−123.42	−123.02	−122.64	−121.89	−121.16	−120.45
500			−127.61	−127.22	−126.84	−126.09	−125.36	−124.65
550			−131.96	−131.57	−131.19	−130.44	−129.72	−129.00
600			−136.46	−136.07	−135.69	−134.94	−134.22	−133.51
700				−145.48	−145.10	−144.35	−143.63	−142.92
800					−155.00	−154.26	−153.54	−152.83
900					−165.35	−164.61	−163.89	−163.18
1000						−175.38	−174.66	−173.95
				$Pb(CH_3COO)_2^\circ$				
25	−186.89	−185.91	−184.97	−184.08	−183.21	−181.54	−179.94	−178.38
50	−188.79	−187.77	−186.81	−185.89	−185.00	−183.29	−181.64	−180.05
75	−190.96	−189.92	−188.94	−188.01	−187.10	−185.36	−183.70	−182.08
100	−193.35	−192.30	−191.31	−190.37	−189.45	−187.70	−186.02	−184.39
125	−195.94	−194.89	−193.89	−192.93	−192.01	−190.24	−188.55	−186.91
150	−198.71	−197.65	−196.64	−195.68	−194.76	−192.98	−191.28	−189.63
175	−201.63	−200.58	−199.57	−198.60	−197.67	−195.89	−194.18	−192.53
200	−204.70	−203.66	−202.64	−201.67	−200.74	−198.95	−197.24	−195.58
225	−207.91	−206.89	−205.87	−204.89	−203.96	−202.16	−200.45	−198.79
250	−211.25	−210.25	−209.22	−208.25	−207.31	−205.51	−203.79	−202.13
300	−218.26	−217.35	−216.32	−215.34	−214.40	−212.59	−210.86	−209.19
350	−225.71	−224.93	−223.89	−222.90	−221.95	−220.13	−218.40	−216.73
400		−232.97	−231.88	−230.88	−229.93	−228.10	−226.37	−224.69
450		−241.51	−240.28	−239.26	−238.30	−236.47	−234.72	−233.04
500		−250.59	−249.07	−248.01	−247.04	−245.19	−243.44	−241.75
550		−259.94	−258.23	−257.12	−256.12	−254.26	−252.50	−250.81
600		−269.51	−267.72	−266.54	−265.52	−263.64	−261.88	−260.18
700		−289.40	−287.59	−286.30	−285.22	−283.30	−281.51	−279.80

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				$Pb(CH_3COO)_2^\circ$ — Continued				
800		−310.26	−308.47	−307.12	−305.99	−304.02	−302.22	−300.50
900		−332.01	−330.26	−328.89	−327.73	−325.72	−323.89	−322.17
1000		−354.61	−352.89	−351.50	−350.32	−348.29	−346.45	−344.72
				$PbCl^+$				
25	−39.05	−38.95	−38.83	−38.71	−38.58	−38.30	−38.00	−37.69
50	−39.76	−39.65	−39.53	−39.40	−39.27	−38.99	−38.70	−38.41
75	−40.47	−40.36	−40.24	−40.12	−39.98	−39.71	−39.42	−39.13
100	−41.21	−41.09	−40.97	−40.85	−40.71	−40.44	−40.16	−39.87
125	−41.95	−41.84	−41.72	−41.59	−41.46	−41.19	−40.91	−40.62
150	−42.70	−42.59	−42.47	−42.35	−42.22	−41.95	−41.67	−41.39
175	−43.47	−43.36	−43.24	−43.12	−42.99	−42.72	−42.45	−42.17
200	−44.24	−44.14	−44.02	−43.90	−43.77	−43.51	−43.24	−42.96
225	−45.02	−44.93	−44.81	−44.69	−44.57	−44.31	−44.04	−43.76
250	−45.81	−45.72	−45.61	−45.50	−45.38	−45.12	−44.85	−44.58
300	−47.38	−47.33	−47.24	−47.13	−47.02	−46.77	−46.51	−46.24
350	−48.92	−48.95	−48.89	−48.80	−48.69	−48.45	−48.20	−47.94
400		−50.63	−50.58	−50.49	−50.39	−50.17	−49.93	−49.68
450		−52.28	−52.27	−52.21	−52.13	−51.92	−51.69	−51.45
500			−53.99	−53.95	−53.88	−53.70	−53.48	−53.25
550			−55.70	−55.70	−55.65	−55.50	−55.30	−55.07
600			−57.44	−57.47	−57.45	−57.32	−57.14	−56.92
700				−61.09	−61.08	−61.01	−60.87	−60.68
800					−64.79	−64.76	−64.67	−64.51
900					−68.58	−68.58	−68.53	−68.40
1000						−72.47	−72.45	−72.33
				$PbCl_2^\circ$				
25	−71.20	−70.79	−70.39	−69.99	−69.60	−68.84	−68.09	−67.34
50	−72.38	−71.95	−71.54	−71.13	−70.73	−69.96	−69.19	−68.44
75	−73.57	−73.13	−72.71	−72.29	−71.89	−71.11	−70.34	−69.58
100	−74.76	−74.32	−73.89	−73.48	−73.07	−72.28	−71.51	−70.75
125	−75.97	−75.52	−75.09	−74.67	−74.26	−73.47	−72.69	−71.93
150	−77.18	−76.73	−76.30	−75.88	−75.47	−74.67	−73.89	−73.13
175	−78.41	−77.96	−77.52	−77.10	−76.69	−75.89	−75.11	−74.34
200	−79.64	−79.19	−78.75	−78.33	−77.92	−77.11	−76.33	−75.57
225	−80.88	−80.44	−80.00	−79.57	−79.16	−78.35	−77.57	−76.80
250	−82.12	−81.69	−81.25	−80.82	−80.41	−79.60	−78.81	−78.05
300	−84.63	−84.23	−83.78	−83.35	−82.93	−82.12	−81.33	−80.57
350	−87.18	−86.82	−86.35	−85.92	−85.49	−84.68	−83.89	−83.12
400		−89.46	−88.96	−88.52	−88.09	−87.26	−86.47	−85.70
450		−92.26	−91.62	−91.15	−90.71	−89.88	−89.08	−88.31
500		−95.25	−94.32	−93.82	−93.37	−92.53	−91.72	−90.94
550		−98.20	−97.08	−96.52	−96.05	−95.20	−94.39	−93.61
600		−101.09	−99.88	−99.26	−98.77	−97.89	−97.08	−96.29
700		−106.78	−105.56	−104.82	−104.27	−103.35	−102.52	−101.72
800		−112.45	−111.25	−110.46	−109.86	−108.90	−108.05	−107.24
900		−118.12	−116.96	−116.14	−115.51	−114.51	−113.64	−112.83
1000		−123.82	−122.69	−121.86	−121.21	−120.18	−119.31	−118.49
				$PbCl_3^-$				
25	−102.15	−101.39	−100.66	−99.95	−99.26	−97.93	−96.64	−95.38
50	−103.62	−102.83	−102.08	−101.35	−100.65	−99.29	−97.97	−96.69
75	−105.07	−104.27	−103.51	−102.77	−102.06	−100.69	−99.36	−98.07
100	−106.50	−105.70	−104.94	−104.20	−103.49	−102.11	−100.77	−99.47
125	−107.93	−107.13	−106.37	−105.63	−104.92	−103.54	−102.20	−100.90
150	−109.33	−108.55	−107.79	−107.06	−106.35	−104.97	−103.64	−102.34
175	−110.72	−109.96	−109.21	−108.48	−107.78	−106.41	−105.08	−103.78
200	−112.08	−111.35	−110.62	−109.90	−109.21	−107.84	−106.52	−105.23

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$PbCl_3^-$ — Continued				
225	−113.41	−112.73	−112.02	−111.32	−110.63	−109.28	−107.97	−106.68
250	−114.69	−114.09	−113.40	−112.72	−112.05	−110.72	−109.42	−108.14
300	−117.01	−116.70	−116.12	−115.49	−114.86	−113.58	−112.32	−111.06
350	−118.53	−119.05	−118.73	−118.20	−117.63	−116.43	−115.21	−113.99
400		−120.94	−121.17	−120.82	−120.34	−119.25	−118.09	−116.91
450		−120.75	−123.34	−123.31	−122.98	−122.03	−120.96	−119.83
500			−125.06	−125.63	−125.52	−124.77	−123.80	−122.73
550			−126.23	−127.74	−127.94	−127.46	−126.61	−125.62
600			−126.96	−129.64	−130.25	−130.10	−129.39	−128.48
700				−133.02	−134.56	−135.20	−134.83	−134.12
800					−138.68	−140.12	−140.13	−139.61
900					−142.89	−144.98	−145.32	−144.95
1000						−149.88	−150.46	−150.15
				$PbCl_4^{-2}$				
25	−133.26	−132.10	−130.99	−129.93	−128.90	−126.91	−124.99	−123.13
50	−134.76	−133.56	−132.43	−131.34	−130.29	−128.26	−126.30	−124.40
75	−136.27	−135.07	−133.93	−132.83	−131.77	−129.72	−127.75	−125.83
100	−137.79	−136.60	−135.46	−134.36	−133.30	−131.25	−129.28	−127.36
125	−139.30	−138.13	−137.01	−135.92	−134.87	−132.83	−130.87	−128.95
150	−140.81	−139.68	−138.57	−137.51	−136.47	−134.45	−132.49	−130.58
175	−142.28	−141.21	−140.14	−139.10	−138.08	−136.09	−134.16	−132.26
200	−143.70	−142.72	−141.71	−140.70	−139.71	−137.76	−135.85	−133.97
225	−145.05	−144.20	−143.26	−142.30	−141.34	−139.44	−137.56	−135.71
250	−146.28	−145.63	−144.78	−143.88	−142.97	−141.13	−139.30	−137.48
300	−148.15	−148.25	−147.72	−147.00	−146.22	−144.55	−142.82	−141.08
350	−147.87	−150.18	−150.43	−150.00	−149.40	−147.96	−146.39	−144.76
400		−151.04	−152.72	−152.79	−152.47	−151.36	−149.98	−148.48
450		−146.32	−154.29	−155.27	−155.37	−154.70	−153.57	−152.23
500			−154.73	−157.32	−158.05	−157.97	−157.14	−156.00
550			−153.67	−158.84	−160.44	−161.13	−160.67	−159.75
600			−151.47	−159.81	−162.54	−164.17	−164.14	−163.47
700				−160.77	−165.99	−169.85	−170.84	−170.75
800					−169.03	−175.12	−177.22	−177.73
900					−172.40	−180.26	−183.36	−184.36
1000						−185.63	−189.46	−190.65
				Pd^{+2}				
25	42.20	41.97	41.78	41.62	41.49	41.26	41.09	40.96
50	42.77	42.53	42.33	42.16	42.01	41.77	41.57	41.40
75	43.35	43.10	42.89	42.71	42.55	42.28	42.06	41.88
100	43.93	43.67	43.45	43.26	43.09	42.80	42.56	42.36
125	44.53	44.25	44.01	43.81	43.63	43.32	43.06	42.84
150	45.14	44.83	44.58	44.36	44.16	43.83	43.56	43.33
175	45.77	45.43	45.15	44.91	44.70	44.35	44.05	43.80
200	46.42	46.05	45.74	45.47	45.25	44.86	44.54	44.27
225	47.11	46.69	46.34	46.05	45.79	45.37	45.03	44.74
250	47.84	47.35	46.95	46.63	46.35	45.89	45.51	45.20
300	49.48	48.76	48.22	47.82	47.48	46.92	46.48	46.11
350	51.13	50.35	49.51	49.05	48.64	47.97	47.44	47.00
400		50.79	50.76	50.28	49.82	49.03	48.40	47.89
450		49.08	51.89	51.51	51.01	50.10	49.37	48.77
500			52.70	52.70	52.21	51.20	50.35	49.66
550			53.01	53.82	53.43	52.32	51.36	50.57
600			52.73	54.80	54.65	53.50	52.40	51.50
700				56.13	57.08	56.03	54.66	53.51
800					59.54	58.90	57.20	55.77
900					62.19	62.07	60.02	58.33
1000						65.39	62.98	61.16

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$PdCl^+$				
25	2.50	2.52	2.56	2.62	2.69	2.85	3.03	3.24
50	2.64	2.67	2.71	2.76	2.83	2.98	3.15	3.34
75	2.74	2.76	2.80	2.85	2.91	3.05	3.22	3.40
100	2.79	2.81	2.84	2.89	2.95	3.08	3.24	3.41
125	2.81	2.82	2.85	2.89	2.94	3.07	3.22	3.38
150	2.80	2.80	2.82	2.86	2.90	3.02	3.16	3.32
175	2.77	2.76	2.77	2.79	2.83	2.94	3.07	3.21
200	2.72	2.69	2.68	2.70	2.73	2.82	2.94	3.08
225	2.66	2.60	2.57	2.58	2.60	2.67	2.78	2.91
250	2.59	2.49	2.45	2.43	2.44	2.50	2.59	2.71
300	2.47	2.25	2.13	2.09	2.07	2.08	2.14	2.23
350	2.29	2.00	1.74	1.66	1.61	1.57	1.59	1.65
400		1.15	1.25	1.15	1.07	0.98	0.95	0.97
450		−0.67	0.62	0.57	0.47	0.31	0.23	0.22
500			−0.20	−0.10	−0.21	−0.42	−0.55	−0.61
550			−1.30	−0.87	−0.94	−1.20	−1.39	−1.49
600			−2.71	−1.76	−1.73	−2.03	−2.28	−2.43
700				−3.99	−3.49	−3.76	−4.15	−4.43
800					−5.46	−5.57	−6.12	−6.53
900					−7.53	−7.43	−8.15	−8.68
1000						−9.42	−10.30	−10.90
				$PdCl_2^\circ$				
25	−35.20	−34.93	−34.66	−34.38	−34.11	−33.57	−33.03	−32.49
50	−35.27	−34.98	−34.70	−34.42	−34.15	−33.60	−33.05	−32.51
75	−35.44	−35.14	−34.86	−34.57	−34.29	−33.74	−33.19	−32.65
100	−35.69	−35.39	−35.10	−34.81	−34.53	−33.97	−33.42	−32.88
125	−36.03	−35.72	−35.43	−35.13	−34.85	−34.29	−33.73	−33.19
150	−36.43	−36.12	−35.82	−35.53	−35.24	−34.67	−34.12	−33.57
175	−36.90	−36.59	−36.29	−35.99	−35.69	−35.12	−34.57	−34.02
200	−37.44	−37.12	−36.81	−36.51	−36.21	−35.64	−35.08	−34.52
225	−38.04	−37.72	−37.40	−37.09	−36.79	−36.21	−35.64	−35.09
250	−38.71	−38.37	−38.04	−37.73	−37.42	−36.84	−36.27	−35.71
300	−40.24	−39.87	−39.50	−39.16	−38.85	−38.24	−37.66	−37.10
350	−42.21	−41.63	−41.18	−40.81	−40.47	−39.84	−39.24	−38.67
400		−43.78	−43.09	−42.65	−42.28	−41.61	−41.00	−40.41
450		−46.95	−45.26	−44.70	−44.27	−43.55	−42.91	−42.31
500		−51.46	−47.76	−46.95	−46.44	−45.65	−44.98	−44.36
550		−55.61	−50.61	−49.42	−48.79	−47.91	−47.19	−46.54
600		−59.31	−53.76	−52.10	−51.31	−50.30	−49.54	−48.86
700		−66.12	−60.42	−57.98	−56.80	−55.50	−54.61	−53.88
800		−72.62	−67.13	−64.30	−62.78	−61.16	−60.16	−59.36
900		−79.08	−73.84	−70.84	−69.11	−67.23	−66.11	−65.27
1000		−85.62	−80.60	−77.53	−75.67	−73.61	−72.43	−71.57
				$PdCl_3^-$				
25	−69.80	−69.28	−68.78	−68.29	−67.80	−66.84	−65.90	−64.97
50	−69.79	−69.26	−68.75	−68.25	−67.75	−66.78	−65.83	−64.90
75	−69.91	−69.38	−68.87	−68.36	−67.87	−66.90	−65.95	−65.01
100	−70.13	−69.61	−69.10	−68.60	−68.11	−67.15	−66.20	−65.27
125	−70.43	−69.93	−69.43	−68.94	−68.46	−67.51	−66.57	−65.65
150	−70.80	−70.32	−69.85	−69.37	−68.90	−67.97	−67.05	−66.13
175	−71.21	−70.78	−70.33	−69.88	−69.42	−68.51	−67.61	−66.71
200	−71.66	−71.29	−70.88	−70.45	−70.02	−69.14	−68.26	−67.37
225	−72.13	−71.84	−71.48	−71.08	−70.68	−69.84	−68.98	−68.12
250	−72.58	−72.42	−72.12	−71.77	−71.39	−70.60	−69.78	−68.94
300	−73.28	−73.57	−73.49	−73.26	−72.97	−72.30	−71.56	−70.78
350	−73.09	−74.52	−74.94	−74.88	−74.71	−74.19	−73.56	−72.86
400		−75.54	−76.38	−76.58	−76.57	−76.26	−75.76	−75.16
450		−74.68	−77.68	−78.30	−78.51	−78.47	−78.13	−77.64

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$PdCl_3^-$ — Continued				
500			−78.67	−79.96	−80.49	−80.79	−80.65	−80.28
550			−79.24	−81.54	−82.48	−83.19	−83.28	−83.06
600			−79.56	−83.03	−84.45	−85.65	−86.00	−85.96
700				−86.11	−88.40	−90.69	−91.66	−92.00
800					−92.60	−95.87	−97.51	−98.26
900					−97.31	−101.29	−103.57	−104.65
1000						−107.16	−109.94	−111.17
				$PdCl_4^{-2}$				
25	−104.00	−103.24	−102.51	−101.79	−101.09	−99.72	−98.38	−97.06
50	−103.55	−102.77	−102.02	−101.30	−100.59	−99.20	−97.85	−96.51
75	−103.21	−102.45	−101.70	−100.98	−100.27	−98.89	−97.54	−96.21
100	−102.97	−102.23	−101.50	−100.80	−100.10	−98.73	−97.39	−96.07
125	−102.80	−102.10	−101.40	−100.72	−100.04	−98.70	−97.38	−96.08
150	−102.67	−102.03	−101.38	−100.72	−100.07	−98.77	−97.48	−96.20
175	−102.56	−102.01	−101.41	−100.80	−100.18	−98.94	−97.68	−96.44
200	−102.44	−102.01	−101.49	−100.94	−100.36	−99.18	−97.98	−96.76
225	−102.27	−102.01	−101.60	−101.12	−100.60	−99.50	−98.35	−97.18
250	−102.01	−102.00	−101.72	−101.33	−100.88	−99.88	−98.80	−97.68
300	−100.88	−101.79	−101.96	−101.81	−101.54	−100.79	−99.89	−98.90
350	−97.86	−100.93	−102.13	−102.32	−102.29	−101.88	−101.20	−100.37
400		−100.27	−102.09	−102.79	−103.08	−103.09	−102.69	−102.06
450		−96.33	−101.63	−103.11	−103.84	−104.39	−104.32	−103.93
500			−100.49	−103.17	−104.51	−105.73	−106.06	−105.94
550			−98.50	−102.92	−105.02	−107.06	−107.86	−108.05
600			−96.06	−102.39	−105.36	−108.35	−109.69	−110.23
700				−101.30	−105.65	−110.71	−113.29	−114.62
800					−105.93	−112.76	−116.72	−118.89
900					−106.70	−114.77	−120.03	−122.91
1000						−117.19	−123.49	−126.68
				$PdOH^+$				
25	−13.00	−13.09	−13.15	−13.19	−13.21	−13.22	−13.19	−13.14
50	−12.69	−12.78	−12.85	−12.89	−12.92	−12.94	−12.94	−12.91
75	−12.43	−12.52	−12.59	−12.64	−12.67	−12.71	−12.71	−12.70
100	−12.19	−12.29	−12.37	−12.42	−12.46	−12.51	−12.53	−12.52
125	−11.99	−12.10	−12.18	−12.24	−12.29	−12.34	−12.37	−12.37
150	−11.80	−11.92	−12.02	−12.09	−12.14	−12.21	−12.25	−12.26
175	−11.64	−11.77	−11.88	−11.96	−12.02	−12.10	−12.15	−12.17
200	−11.48	−11.64	−11.76	−11.85	−11.92	−12.03	−12.09	−12.12
225	−11.33	−11.52	−11.66	−11.77	−11.85	−11.97	−12.05	−12.09
250	−11.18	−11.41	−11.57	−11.70	−11.80	−11.94	−12.03	−12.09
300	−10.86	−11.20	−11.45	−11.61	−11.74	−11.94	−12.07	−12.15
350	−10.63	−10.99	−11.39	−11.59	−11.75	−12.01	−12.18	−12.31
400		−11.51	−11.43	−11.63	−11.83	−12.14	−12.37	−12.53
450		−13.37	−11.63	−11.76	−11.96	−12.34	−12.62	−12.83
500			−12.07	−11.96	−12.16	−12.59	−12.93	−13.19
550			−12.88	−12.28	−12.41	−12.88	−13.28	−13.59
600			−14.09	−12.74	−12.72	−13.20	−13.67	−14.04
700				−14.18	−13.50	−13.89	−14.51	−15.01
800					−14.46	−14.59	−15.37	−16.02
900					−15.48	−15.29	−16.26	−17.04
1000						−16.06	−17.21	−18.07
				PdO°				
25	−11.50	−11.65	−11.77	−11.87	−11.95	−12.08	−12.17	−12.23
50	−11.25	−11.40	−11.53	−11.63	−11.72	−11.86	−11.96	−12.05
75	−11.00	−11.15	−11.28	−11.38	−11.47	−11.62	−11.74	−11.83
100	−10.76	−10.90	−11.03	−11.13	−11.23	−11.38	−11.50	−11.60
125	−10.52	−10.66	−10.79	−10.89	−10.98	−11.14	−11.26	−11.36

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				PdO° — Continued				
150	−10.29	−10.43	−10.55	−10.65	−10.74	−10.89	−11.02	−11.13
175	−10.07	−10.20	−10.32	−10.42	−10.51	−10.66	−10.78	−10.89
200	−9.86	−9.98	−10.09	−10.19	−10.27	−10.42	−10.55	−10.65
225	−9.67	−9.77	−9.88	−9.97	−10.05	−10.19	−10.32	−10.42
250	−9.50	−9.58	−9.67	−9.75	−9.83	−9.97	−10.09	−10.19
300	−9.26	−9.24	−9.29	−9.35	−9.41	−9.53	−9.64	−9.74
350	−9.39	−9.03	−8.97	−8.99	−9.03	−9.12	−9.21	−9.30
400		−9.11	−8.75	−8.69	−8.69	−8.74	−8.80	−8.88
450		−10.25	−8.68	−8.46	−8.39	−8.38	−8.42	−8.47
500		−12.88	−8.83	−8.32	−8.15	−8.05	−8.05	−8.08
550		−14.92	−9.27	−8.29	−7.97	−7.76	−7.70	−7.71
600		−16.26	−9.94	−8.38	−7.86	−7.50	−7.39	−7.36
700		−17.81	−11.31	−8.80	−7.80	−7.07	−6.82	−6.72
800		−18.51	−12.27	−9.27	−7.87	−6.75	−6.34	−6.17
900		−18.72	−12.79	−9.57	−7.91	−6.47	−5.93	−5.70
1000		−18.63	−12.97	−9.67	−7.84	−6.19	−5.57	−5.32
				Pr^{+3}				
25	−162.60	−163.08	−163.50	−163.88	−164.22	−164.84	−165.39	−165.90
50	−161.30	−161.79	−162.23	−162.62	−162.98	−163.63	−164.21	−164.74
75	−159.94	−160.44	−160.89	−161.29	−161.66	−162.34	−162.94	−163.49
100	−158.50	−159.03	−159.49	−159.91	−160.30	−161.00	−161.62	−162.20
125	−157.00	−157.56	−158.04	−158.48	−158.89	−159.62	−160.27	−160.86
150	−155.44	−156.03	−156.55	−157.01	−157.43	−158.19	−158.87	−159.49
175	−153.80	−154.44	−155.00	−155.49	−155.94	−156.74	−157.44	−158.08
200	−152.09	−152.78	−153.39	−153.92	−154.40	−155.24	−155.98	−156.65
225	−150.29	−151.06	−151.73	−152.30	−152.82	−153.72	−154.50	−155.20
250	−148.38	−149.26	−150.01	−150.64	−151.19	−152.16	−152.98	−153.72
300	−144.23	−145.45	−146.42	−147.16	−147.81	−148.93	−149.87	−150.69
350	−140.01	−141.24	−142.68	−143.52	−144.28	−145.57	−146.64	−147.57
400		−138.90	−138.92	−139.77	−140.61	−142.08	−143.31	−144.36
450		−140.24	−135.31	−135.95	−136.84	−138.48	−139.87	−141.05
500			−132.17	−132.11	−132.96	−134.77	−136.33	−137.65
550			−129.85	−128.34	−128.99	−130.92	−132.66	−134.15
600			−128.48	−124.73	−124.94	−126.92	−128.86	−130.52
700				−118.43	−116.68	−118.40	−120.77	−122.82
800					−108.15	−109.09	−111.95	−114.44
900					−99.03	−99.04	−102.45	−105.35
1000						−88.51	−92.49	−95.60
				Ra^{+2}				
25	−134.20	−134.31	−134.39	−134.45	−134.49	−134.54	−134.54	−134.52
50	−134.51	−134.63	−134.71	−134.78	−134.83	−134.89	−134.91	−134.92
75	−134.81	−134.93	−135.02	−135.09	−135.14	−135.22	−135.26	−135.28
100	−135.08	−135.21	−135.31	−135.39	−135.45	−135.54	−135.59	−135.62
125	−135.34	−135.48	−135.59	−135.68	−135.75	−135.85	−135.92	−135.96
150	−135.59	−135.74	−135.86	−135.96	−136.04	−136.16	−136.23	−136.28
175	−135.81	−135.99	−136.12	−136.23	−136.32	−136.46	−136.55	−136.61
200	−136.01	−136.21	−136.37	−136.49	−136.60	−136.75	−136.86	−136.93
225	−136.18	−136.41	−136.60	−136.74	−136.86	−137.04	−137.16	−137.25
250	−136.31	−136.59	−136.81	−136.98	−137.12	−137.32	−137.46	−137.57
300	−136.41	−136.87	−137.20	−137.42	−137.59	−137.87	−138.06	−138.20
350	−136.33	−136.98	−137.52	−137.80	−138.03	−138.38	−138.63	−138.82
400		−137.60	−137.82	−138.15	−138.43	−138.87	−139.19	−139.43
450		−138.81	−138.11	−138.46	−138.79	−139.33	−139.72	−140.02
500			−138.45	−138.73	−139.12	−139.76	−140.24	−140.60
550			−138.91	−138.99	−139.39	−140.14	−140.72	−141.15
600			−139.51	−139.26	−139.63	−140.48	−141.16	−141.67
700				−139.98	−140.00	−140.98	−141.89	−142.58
800					−140.27	−141.23	−142.40	−143.29

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pressure, kbar				
				Ra^{+2} — Continued				
900					−140.41	−141.26	−142.70	−143.77
1000						−141.19	−142.88	−144.03
				Rb^{+}				
25	−67.80	−67.62	−67.43	−67.23	−67.02	−66.59	−66.13	−65.67
50	−68.52	−68.34	−68.14	−67.94	−67.74	−67.31	−66.87	−66.42
75	−69.24	−69.05	−68.86	−68.66	−68.46	−68.04	−67.60	−67.16
100	−69.96	−69.77	−69.58	−69.38	−69.18	−68.76	−68.34	−67.90
125	−70.68	−70.50	−70.31	−70.11	−69.91	−69.50	−69.07	−68.64
150	−71.41	−71.23	−71.04	−70.84	−70.64	−70.24	−69.82	−69.39
175	−72.14	−71.96	−71.78	−71.58	−71.38	−70.98	−70.56	−70.14
200	−72.87	−72.70	−72.51	−72.32	−72.13	−71.73	−71.31	−70.89
225	−73.59	−73.44	−73.26	−73.07	−72.88	−72.48	−72.07	−71.65
250	−74.32	−74.17	−74.00	−73.82	−73.63	−73.23	−72.83	−72.42
300	−75.75	−75.65	−75.50	−75.32	−75.14	−74.76	−74.37	−73.96
350	−77.12	−77.12	−77.00	−76.84	−76.67	−76.30	−75.92	−75.52
400		−78.63	−78.51	−78.37	−78.21	−77.86	−77.48	−77.10
450		−80.10	−80.02	−79.90	−79.75	−79.42	−79.06	−78.69
500			−81.53	−81.43	−81.30	−81.00	−80.66	−80.29
550			−83.02	−82.96	−82.86	−82.58	−82.26	−81.91
600			−84.52	−84.50	−84.42	−84.17	−83.87	−83.53
700				−87.60	−87.54	−87.36	−87.10	−86.80
800					−90.68	−90.55	−90.35	−90.08
900					−93.86	−93.76	−93.61	−93.37
1000						−97.00	−96.89	−96.66
				$RbBr^{\circ}$				
25	−91.01	−90.44	−89.89	−89.35	−88.83	−87.81	−86.82	−85.85
50	−92.35	−91.76	−91.19	−90.64	−90.10	−89.06	−88.06	−87.07
75	−93.66	−93.06	−92.48	−91.92	−91.38	−90.33	−89.31	−88.31
100	−94.96	−94.34	−93.76	−93.20	−92.65	−91.59	−90.56	−89.56
125	−96.23	−95.62	−95.03	−94.46	−93.91	−92.84	−91.81	−90.81
150	−97.50	−96.88	−96.29	−95.72	−95.17	−94.09	−93.06	−92.05
175	−98.75	−98.14	−97.54	−96.97	−96.41	−95.34	−94.30	−93.29
200	−100.00	−99.39	−98.79	−98.21	−97.65	−96.58	−95.54	−94.52
225	−101.23	−100.63	−100.03	−99.45	−98.89	−97.81	−96.77	−95.75
250	−102.44	−101.86	−101.26	−100.68	−100.12	−99.04	−97.99	−96.98
300	−104.84	−104.31	−103.70	−103.12	−102.56	−101.47	−100.42	−99.40
350	−107.17	−106.73	−106.12	−105.54	−104.97	−103.88	−102.83	−101.81
400		−109.15	−108.53	−107.94	−107.37	−106.28	−105.22	−104.20
450		−111.59	−110.91	−110.32	−109.75	−108.65	−107.60	−106.57
500		−114.07	−113.29	−112.69	−112.11	−111.01	−109.95	−108.93
550		−116.50	−115.67	−115.04	−114.46	−113.35	−112.29	−111.26
600		−118.89	−118.03	−117.38	−116.79	−115.68	−114.62	−113.59
700		−123.59	−122.72	−122.03	−121.42	−120.29	−119.22	−118.19
800		−128.20	−127.34	−126.63	−126.00	−124.86	−123.78	−122.75
900		−132.74	−131.89	−131.17	−130.53	−129.37	−128.29	−127.25
1000		−137.22	−136.38	−135.66	−135.01	−133.85	−132.76	−131.72
				$RbCl^{\circ}$				
25	−97.87	−97.34	−96.83	−96.34	−95.85	−94.90	−93.97	−93.06
50	−99.07	−98.52	−97.99	−97.48	−96.99	−96.02	−95.07	−94.15
75	−100.24	−99.68	−99.15	−98.63	−98.12	−97.14	−96.19	−95.26
100	−101.39	−100.83	−100.29	−99.76	−99.25	−98.27	−97.31	−96.37
125	−102.53	−101.96	−101.42	−100.89	−100.38	−99.38	−98.42	−97.48
150	−103.66	−103.09	−102.54	−102.01	−101.49	−100.50	−99.53	−98.59
175	−104.77	−104.21	−103.65	−103.12	−102.60	−101.60	−100.63	−99.69
200	−105.88	−105.31	−104.76	−104.22	−103.71	−102.70	−101.73	−100.79
225	−106.97	−106.41	−105.86	−105.32	−104.80	−103.80	−102.82	−101.88

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				RbCl° — Continued				
250	−108.05	−107.51	−106.95	−106.41	−105.89	−104.88	−103.91	−102.96
300	−110.17	−109.68	−109.11	−108.57	−108.05	−107.04	−106.06	−105.11
350	−112.24	−111.83	−111.26	−110.72	−110.19	−109.18	−108.20	−107.25
400		−113.97	−113.39	−112.84	−112.31	−111.29	−110.31	−109.36
450		−116.13	−115.50	−114.94	−114.41	−113.39	−112.41	−111.45
500		−118.33	−117.60	−117.03	−116.50	−115.47	−114.49	−113.53
550		−120.49	−119.70	−119.11	−118.57	−117.54	−116.55	−115.60
600		−122.61	−121.79	−121.18	−120.63	−119.59	−118.60	−117.64
700		−126.75	−125.93	−125.28	−124.71	−123.66	−122.66	−121.70
800		−130.81	−129.99	−129.33	−128.74	−127.67	−126.67	−125.70
900		−134.80	−134.00	−133.32	−132.72	−131.64	−130.63	−129.66
1000		−138.73	−137.94	−137.26	−136.66	−135.57	−134.56	−133.59
				RbF°				
25	−136.45	−136.22	−135.99	−135.75	−135.52	−135.04	−134.56	−134.07
50	−137.23	−136.99	−136.75	−136.51	−136.27	−135.78	−135.30	−134.82
75	−137.98	−137.74	−137.49	−137.25	−137.01	−136.52	−136.04	−135.56
100	−138.72	−138.47	−138.23	−137.98	−137.74	−137.25	−136.77	−136.29
125	−139.45	−139.20	−138.95	−138.71	−138.46	−137.98	−137.49	−137.01
150	−140.18	−139.92	−139.67	−139.43	−139.18	−138.69	−138.21	−137.73
175	−140.89	−140.64	−140.39	−140.14	−139.89	−139.40	−138.92	−138.44
200	−141.60	−141.35	−141.09	−140.84	−140.60	−140.11	−139.63	−139.15
225	−142.30	−142.05	−141.80	−141.55	−141.30	−140.81	−140.33	−139.85
250	−142.99	−142.75	−142.49	−142.24	−141.99	−141.51	−141.02	−140.54
300	−144.35	−144.13	−143.87	−143.62	−143.37	−142.88	−142.40	−141.92
350	−145.67	−145.50	−145.24	−144.99	−144.74	−144.25	−143.77	−143.29
400		−146.85	−146.59	−146.34	−146.09	−145.60	−145.12	−144.64
450		−148.20	−147.93	−147.68	−147.43	−146.94	−146.45	−145.97
500		−149.54	−149.26	−149.01	−148.76	−148.26	−147.78	−147.30
550		−150.86	−150.58	−150.32	−150.07	−149.58	−149.09	−148.62
600		−152.17	−151.89	−151.63	−151.38	−150.88	−150.40	−149.92
700		−154.77	−154.48	−154.22	−153.96	−153.47	−152.98	−152.50
800		−157.32	−157.04	−156.77	−156.51	−156.02	−155.53	−155.05
900		−159.84	−159.56	−159.29	−159.04	−158.54	−158.05	−157.57
1000		−162.34	−162.05	−161.79	−161.53	−161.03	−160.54	−160.06
				RbI°				
25	−79.10	−78.39	−77.70	−77.04	−76.40	−75.15	−73.95	−72.77
50	−80.49	−79.75	−79.05	−78.37	−77.71	−76.43	−75.20	−74.01
75	−81.86	−81.11	−80.39	−79.70	−79.03	−77.74	−76.50	−75.28
100	−83.22	−82.46	−81.73	−81.03	−80.36	−79.05	−77.80	−76.58
125	−84.56	−83.79	−83.06	−82.36	−81.68	−80.37	−79.11	−77.88
150	−85.89	−85.12	−84.39	−83.68	−83.00	−81.68	−80.41	−79.18
175	−87.21	−86.44	−85.70	−85.00	−84.31	−82.99	−81.72	−80.48
200	−88.52	−87.76	−87.02	−86.31	−85.62	−84.29	−83.02	−81.78
225	−89.82	−89.07	−88.33	−87.61	−86.92	−85.59	−84.32	−83.08
250	−91.10	−90.38	−89.63	−88.91	−88.22	−86.89	−85.61	−84.37
300	−93.63	−92.97	−92.22	−91.50	−90.81	−89.47	−88.19	−86.95
350	−96.09	−95.55	−94.80	−94.08	−93.38	−92.04	−90.76	−89.51
400		−98.12	−97.36	−96.63	−95.93	−94.59	−93.31	−92.06
450		−100.69	−99.91	−99.18	−98.48	−97.13	−95.84	−94.59
500		−103.28	−102.45	−101.71	−101.01	−99.66	−98.37	−97.12
550		−105.85	−104.98	−104.23	−103.53	−102.18	−100.88	−99.63
600		−108.39	−107.50	−106.75	−106.03	−104.68	−103.38	−102.13
700		−113.41	−112.52	−111.74	−111.02	−109.66	−108.36	−107.10
800		−118.37	−117.49	−116.70	−115.97	−114.60	−113.29	−112.03
900		−123.29	−122.41	−121.62	−120.88	−119.50	−118.20	−116.93
1000		−128.17	−127.29	−126.50	−125.76	−124.37	−123.06	−121.80

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				ReO_4^-				
25	−166.00	−165.44	−164.90	−164.37	−163.85	−162.84	−161.85	−160.88
50	−167.20	−166.63	−166.07	−165.53	−165.00	−163.97	−162.97	−161.99
75	−168.41	−167.83	−167.27	−166.72	−166.19	−165.15	−164.15	−163.15
100	−169.62	−169.04	−168.48	−167.93	−167.40	−166.36	−165.35	−164.36
125	−170.83	−170.25	−169.70	−169.16	−168.63	−167.59	−166.59	−165.60
150	−172.03	−171.47	−170.92	−170.39	−169.86	−168.84	−167.84	−166.85
175	−173.22	−172.69	−172.15	−171.63	−171.11	−170.10	−169.10	−168.12
200	−174.40	−173.90	−173.38	−172.87	−172.36	−171.36	−170.38	−169.41
225	−175.54	−175.10	−174.61	−174.11	−173.62	−172.64	−171.67	−170.71
250	−176.64	−176.28	−175.83	−175.36	−174.88	−173.92	−172.97	−172.02
300	−178.59	−178.54	−178.22	−177.82	−177.40	−176.51	−175.60	−174.68
350	−179.64	−180.53	−180.52	−180.24	−179.89	−179.10	−178.24	−177.37
400		−182.00	−182.65	−182.58	−182.34	−181.68	−180.91	−180.08
450		−180.99	−184.46	−184.79	−184.73	−184.25	−183.57	−182.82
500			−185.78	−186.82	−187.03	−186.79	−186.24	−185.56
550			−186.45	−188.62	−189.21	−189.29	−188.89	−188.30
600			−186.62	−190.19	−191.27	−191.75	−191.52	−191.03
700				−192.89	−195.08	−196.51	−196.71	−196.45
800					−198.74	−201.14	−201.78	−201.77
900					−202.56	−205.74	−206.79	−206.96
1000						−210.46	−211.80	−212.04
				Rn°				
25	2.79	3.42	4.02	4.61	5.18	6.29	7.36	8.41
50	2.31	2.96	3.59	4.19	4.78	5.91	7.00	8.07
75	1.69	2.36	3.00	3.61	4.21	5.35	6.46	7.54
100	0.96	1.64	2.28	2.90	3.51	4.67	5.78	6.87
125	0.12	0.81	1.46	2.09	2.69	3.86	4.99	6.09
150	−0.81	−0.12	0.54	1.17	1.79	2.96	4.10	5.20
175	−1.83	−1.14	−0.47	0.17	0.79	1.97	3.11	4.22
200	−2.94	−2.24	−1.56	−0.92	−0.30	0.90	2.04	3.15
225	−4.12	−3.42	−2.74	−2.09	−1.46	−0.26	0.89	2.01
250	−5.39	−4.69	−3.99	−3.33	−2.70	−1.49	−0.33	0.79
300	−8.16	−7.45	−6.71	−6.03	−5.38	−4.14	−2.97	−1.84
350	−11.46	−10.56	−9.72	−9.00	−8.32	−7.06	−5.86	−4.72
400		−14.16	−13.03	−12.23	−11.51	−10.20	−8.99	−7.83
450		−18.96	−16.67	−15.72	−14.94	−13.57	−12.33	−11.14
500		−25.34	−20.71	−19.48	−18.60	−17.15	−15.86	−14.66
550		−31.32	−25.19	−23.51	−22.49	−20.93	−19.59	−18.36
600		−36.81	−30.03	−27.81	−26.60	−24.89	−23.50	−22.24
700		−47.14	−40.19	−37.06	−35.40	−33.35	−31.82	−30.48
800		−57.19	−50.49	−46.89	−44.85	−42.42	−40.75	−39.34
900		−67.26	−60.85	−57.05	−54.75	−52.02	−50.22	−48.76
1000		−77.47	−71.31	−67.44	−64.99	−62.06	−60.17	−58.70
				Serine				
25	−122.10	−121.39	−120.70	−120.02	−119.35	−118.05	−116.76	−115.50
50	−123.29	−122.58	−121.89	−121.21	−120.55	−119.26	−118.00	−116.76
75	−124.54	−123.83	−123.13	−122.46	−121.80	−120.52	−119.27	−118.05
100	−125.85	−125.13	−124.44	−123.76	−123.11	−121.83	−120.59	−119.37
125	−127.21	−126.49	−125.79	−125.12	−124.46	−123.18	−121.94	−120.73
150	−128.63	−127.90	−127.20	−126.52	−125.86	−124.59	−123.35	−122.13
175	−130.09	−129.36	−128.66	−127.98	−127.31	−126.03	−124.79	−123.58
200	−131.61	−130.88	−130.16	−129.48	−128.81	−127.52	−126.28	−125.07
225	−133.18	−132.44	−131.72	−131.02	−130.35	−129.06	−127.81	−126.59
250	−134.80	−134.06	−133.32	−132.61	−131.93	−130.63	−129.38	−128.16
300	−138.26	−137.46	−136.66	−135.92	−135.22	−133.89	−132.62	−131.39
350	−142.29	−141.16	−140.21	−139.41	−138.68	−137.30	−136.01	−134.77
400		−145.38	−144.00	−143.08	−142.29	−140.86	−139.54	−138.27
450		−151.21	−148.10	−146.96	−146.07	−144.56	−143.19	−141.89

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Sat.	0.5	1.0	Pressure, kbar 1.5	2.0	3.0	4.0	5.0
Serine — Continued								
500		−159.25	−152.61	−151.06	−150.03	−148.39	−146.96	−145.64
550		−166.53	−157.63	−155.41	−154.16	−152.35	−150.86	−149.49
600		−172.91	−163.04	−160.00	−158.46	−156.45	−154.86	−153.46
700		−184.26	−174.14	−169.74	−167.54	−164.99	−163.21	−161.70
800		−194.68	−184.93	−179.83	−177.05	−173.95	−171.95	−170.34
900		−204.65	−195.34	−189.94	−186.78	−183.23	−181.04	−179.35
1000		−214.42	−205.49	−199.97	−196.59	−192.73	−190.42	−188.70
				S_2^{-2}				
25	19.00	19.24	19.48	19.73	20.00	20.53	21.09	21.65
50	18.89	19.13	19.37	19.62	19.88	20.41	20.95	21.50
75	18.88	19.11	19.34	19.58	19.83	20.34	20.86	21.40
100	18.97	19.17	19.38	19.61	19.84	20.33	20.83	21.35
125	19.15	19.31	19.50	19.70	19.91	20.37	20.85	21.34
150	19.43	19.54	19.68	19.85	20.04	20.46	20.91	21.38
175	19.82	19.85	19.94	20.07	20.23	20.60	21.01	21.45
200	20.33	20.26	20.28	20.36	20.48	20.78	21.15	21.56
225	21.00	20.78	20.70	20.72	20.78	21.02	21.33	21.70
250	21.85	21.42	21.22	21.15	21.15	21.30	21.55	21.87
300	24.41	23.17	22.55	22.26	22.10	22.01	22.11	22.32
350	29.34	25.92	24.35	23.71	23.33	22.93	22.83	22.89
400		29.39	26.74	25.57	24.86	24.07	23.71	23.59
450		37.85	29.98	27.92	26.76	25.44	24.77	24.44
500			34.43	30.87	29.05	27.06	26.02	25.44
550			40.33	34.48	31.79	28.96	27.47	26.60
600			47.33	38.73	34.98	31.15	29.14	27.95
700				48.35	42.52	36.41	33.20	31.28
800					50.98	42.74	38.21	35.53
900					59.63	49.78	44.02	40.70
1000						57.04	50.35	46.76
				SO_2^0				
25	−71.98	−71.53	−71.09	−70.66	−70.24	−69.41	−68.60	−67.81
50	−72.99	−72.52	−72.07	−71.63	−71.20	−70.35	−69.53	−68.73
75	−74.09	−73.60	−73.14	−72.69	−72.25	−71.40	−70.57	−69.76
100	−75.25	−74.76	−74.29	−73.83	−73.39	−72.53	−71.69	−70.87
125	−76.47	−75.97	−75.50	−75.04	−74.59	−73.72	−72.88	−72.06
150	−77.75	−77.25	−76.77	−76.30	−75.85	−74.98	−74.13	−73.31
175	−79.09	−78.58	−78.09	−77.62	−77.17	−76.29	−75.44	−74.61
200	−80.48	−79.97	−79.47	−79.00	−78.54	−77.65	−76.79	−75.96
225	−81.92	−81.41	−80.90	−80.42	−79.95	−79.06	−78.20	−77.36
250	−83.41	−82.89	−82.38	−81.88	−81.41	−80.51	−79.64	−78.80
300	−86.58	−86.03	−85.47	−84.95	−84.47	−83.54	−82.66	−81.81
350	−90.20	−89.42	−88.76	−88.20	−87.69	−86.73	−85.83	−84.97
400		−93.21	−92.26	−91.62	−91.07	−90.07	−89.14	−88.26
450		−98.13	−96.01	−95.22	−94.60	−93.54	−92.59	−91.69
500		−104.59	−100.08	−99.02	−98.30	−97.15	−96.16	−95.24
550		−110.57	−104.54	−103.01	−102.15	−100.89	−99.85	−98.90
600		−115.98	−109.29	−107.21	−106.16	−104.76	−103.65	−102.67
700		−125.95	−119.09	−116.09	−114.58	−112.82	−111.59	−110.53
800		−135.41	−128.80	−125.33	−123.42	−121.29	−119.91	−118.78
900		−144.67	−138.36	−134.68	−132.52	−130.09	−128.57	−127.39
1000		−153.90	−147.84	−144.09	−141.78	−139.13	−137.53	−136.33
				SO_3^{-2}				
25	−116.30	−116.23	−116.14	−116.02	−115.89	−115.60	−115.28	−114.93
50	−116.05	−115.99	−115.91	−115.81	−115.69	−115.43	−115.13	−114.81
75	−115.69	−115.65	−115.58	−115.50	−115.40	−115.16	−114.89	−114.59
100	−115.21	−115.20	−115.16	−115.09	−115.01	−114.81	−114.57	−114.30

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				SO_3^{-2} — Continued				
125	−114.63	−114.66	−114.65	−114.61	−114.56	−114.39	−114.18	−113.94
150	−113.93	−114.02	−114.06	−114.06	−114.03	−113.91	−113.73	−113.52
175	−113.11	−113.29	−113.38	−113.42	−113.43	−113.36	−113.23	−113.05
200	−112.16	−112.44	−112.61	−112.71	−112.76	−112.76	−112.68	−112.54
225	−111.04	−111.47	−111.74	−111.91	−112.02	−112.10	−112.07	−111.98
250	−109.72	−110.37	−110.77	−111.03	−111.20	−111.38	−111.42	−111.38
300	−106.19	−107.66	−108.50	−109.00	−109.34	−109.76	−109.97	−110.05
350	−100.33	−103.90	−105.74	−106.58	−107.16	−107.91	−108.33	−108.57
400		−99.66	−102.37	−103.73	−104.64	−105.80	−106.50	−106.93
450		−91.01	−98.18	−100.38	−101.75	−103.44	−104.46	−105.12
500			−92.85	−96.44	−98.43	−100.80	−102.21	−103.13
550			−86.19	−91.83	−94.65	−97.86	−99.73	−100.95
600			−78.58	−86.61	−90.41	−94.61	−97.01	−98.56
700				−75.15	−80.73	−87.12	−90.75	−93.07
800					−70.07	−78.45	−83.44	−86.56
900					−59.12	−68.95	−75.20	−79.00
1000						−59.13	−66.37	−70.46
				SO_4^{-2}				
25	−177.93	−177.76	−177.56	−177.33	−177.09	−176.56	−176.00	−175.41
50	−177.98	−177.80	−177.58	−177.34	−177.09	−176.54	−175.95	−175.34
75	−177.94	−177.76	−177.54	−177.30	−177.05	−176.50	−175.91	−175.28
100	−177.81	−177.64	−177.44	−177.21	−176.97	−176.43	−175.84	−175.23
125	−177.59	−177.46	−177.28	−177.07	−176.84	−176.32	−175.76	−175.15
150	−177.28	−177.20	−177.06	−176.88	−176.67	−176.18	−175.64	−175.05
175	−176.86	−176.86	−176.77	−176.63	−176.44	−176.00	−175.49	−174.93
200	−176.33	−176.42	−176.41	−176.31	−176.17	−175.79	−175.32	−174.79
225	−175.65	−175.89	−175.96	−175.94	−175.84	−175.53	−175.11	−174.62
250	−174.78	−175.24	−175.44	−175.49	−175.46	−175.23	−174.87	−174.42
300	−172.21	−173.48	−174.10	−174.38	−174.51	−174.51	−174.30	−173.96
350	−167.30	−170.73	−172.31	−172.93	−173.29	−173.60	−173.59	−173.40
400		−167.33	−169.95	−171.10	−171.78	−172.49	−172.74	−172.73
450		−159.05	−166.77	−168.80	−169.94	−171.17	−171.73	−171.93
500			−162.42	−165.93	−167.71	−169.62	−170.55	−171.00
550			−156.64	−162.41	−165.06	−167.80	−169.18	−169.92
600			−149.81	−158.27	−161.96	−165.71	−167.60	−168.66
700				−148.93	−154.65	−160.66	−163.77	−165.57
800					−146.48	−154.60	−159.03	−161.60
900					−138.15	−147.86	−153.52	−156.73
1000						−140.92	−147.53	−151.01
				$S_2O_3^{-2}$				
25	−124.90	−124.58	−124.26	−123.94	−123.63	−123.02	−122.41	−121.81
50	−125.25	−124.90	−124.56	−124.23	−123.90	−123.25	−122.61	−121.97
75	−125.50	−125.15	−124.81	−124.48	−124.14	−123.48	−122.83	−122.18
100	−125.68	−125.34	−125.01	−124.68	−124.35	−123.70	−123.05	−122.40
125	−125.77	−125.46	−125.15	−124.84	−124.52	−123.89	−123.25	−122.61
150	−125.77	−125.51	−125.23	−124.94	−124.65	−124.04	−123.43	−122.80
175	−125.67	−125.48	−125.25	−125.00	−124.73	−124.16	−123.57	−122.97
200	−125.45	−125.37	−125.20	−124.99	−124.76	−124.24	−123.69	−123.12
225	−125.09	−125.15	−125.07	−124.93	−124.74	−124.29	−123.78	−123.24
250	−124.56	−124.82	−124.86	−124.79	−124.66	−124.30	−123.85	−123.35
300	−122.66	−123.72	−124.16	−124.31	−124.33	−124.18	−123.87	−123.48
350	−118.38	−121.65	−123.02	−123.50	−123.75	−123.88	−123.77	−123.51
400		−118.74	−121.29	−122.31	−122.87	−123.39	−123.52	−123.43
450		−110.56	−118.72	−120.64	−121.66	−122.69	−123.12	−123.23
500			−114.91	−118.39	−120.06	−121.76	−122.55	−122.90
550			−109.58	−115.47	−118.04	−120.57	−121.79	−122.42
600			−103.10	−111.91	−115.57	−119.11	−120.84	−121.77
700				−103.62	−109.51	−115.37	−118.27	−119.91

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, C°	Sat.	0.5	1.0	Pressure, kbar 1.5	2.0	3.0	4.0	5.0
				SO_3^{-2} — Continued				
800					−102.59	−110.64	−114.83	−117.21
900					−95.54	−105.28	−110.67	−113.65
1000						−99.76	−106.05	−109.29
				$S_2O_4^{-2}$				
25	−143.50	−143.09	−142.68	−142.28	−141.87	−141.07	−140.26	−139.46
50	−144.00	−143.59	−143.17	−142.77	−142.36	−141.55	−140.75	−139.94
75	−144.42	−144.01	−143.61	−143.21	−142.81	−142.01	−141.21	−140.42
100	−144.76	−144.37	−143.99	−143.60	−143.21	−142.43	−141.65	−140.87
125	−145.02	−144.67	−144.31	−143.94	−143.57	−142.81	−142.05	−141.29
150	−145.20	−144.90	−144.57	−144.23	−143.88	−143.16	−142.43	−141.69
175	−145.29	−145.06	−144.78	−144.47	−144.15	−143.48	−142.78	−142.06
200	−145.26	−145.13	−144.92	−144.66	−144.37	−143.75	−143.09	−142.41
225	−145.10	−145.11	−144.98	−144.79	−144.55	−144.00	−143.38	−142.73
250	−144.76	−144.98	−144.97	−144.85	−144.67	−144.20	−143.64	−143.04
300	−143.29	−144.29	−144.68	−144.77	−144.74	−144.48	−144.07	−143.57
350	−139.45	−142.66	−143.95	−144.38	−144.57	−144.60	−144.37	−144.01
400		−140.11	−142.65	−143.61	−144.12	−144.53	−144.54	−144.34
450		−132.15	−140.50	−142.38	−143.34	−144.26	−144.56	−144.56
500			−137.10	−140.57	−142.19	−143.76	−144.43	−144.66
550			−132.15	−138.10	−140.61	−143.02	−144.12	−144.62
600			−126.02	−134.97	−138.61	−142.02	−143.61	−144.42
700				−127.54	−133.49	−139.23	−141.98	−143.48
800					−127.53	−135.50	−139.53	−141.75
900					−121.49	−131.19	−136.39	−139.20
1000						−126.75	−132.83	−135.89
				$S_2O_5^{-2}$				
25	−189.00	−188.56	−188.12	−187.68	−187.25	−186.39	−185.53	−184.68
50	−189.58	−189.13	−188.68	−188.24	−187.81	−186.95	−186.09	−185.24
75	−190.08	−189.63	−189.20	−188.76	−188.33	−187.48	−186.63	−185.78
100	−190.50	−190.08	−189.66	−189.24	−188.82	−187.98	−187.14	−186.31
125	−190.85	−190.46	−190.07	−189.66	−189.26	−188.45	−187.63	−186.82
150	−191.12	−190.78	−190.42	−190.04	−189.66	−188.88	−188.10	−187.30
175	−191.30	−191.03	−190.72	−190.38	−190.02	−189.29	−188.53	−187.76
200	−191.37	−191.20	−190.95	−190.66	−190.34	−189.66	−188.94	−188.20
225	−191.31	−191.28	−191.11	−190.88	−190.61	−189.99	−189.32	−188.62
250	−191.07	−191.25	−191.20	−191.04	−190.82	−190.29	−189.67	−189.01
300	−189.81	−190.77	−191.11	−191.16	−191.10	−190.77	−190.30	−189.74
350	−186.19	−189.36	−190.60	−190.98	−191.13	−191.09	−190.80	−190.38
400		−187.00	−189.51	−190.43	−190.89	−191.23	−191.18	−190.92
450		−179.18	−187.58	−189.42	−190.34	−191.18	−191.41	−191.35
500			−184.39	−187.84	−189.41	−190.91	−191.50	−191.66
550			−179.65	−185.59	−188.07	−190.40	−191.41	−191.84
600			−173.71	−182.70	−186.30	−189.63	−191.14	−191.87
700				−175.72	−181.67	−187.32	−189.99	−191.40
800					−176.21	−184.11	−188.04	−190.16
900					−170.69	−180.33	−185.42	−188.13
1000						−176.45	−182.40	−185.36
				$S_2O_6^{-2}$				
25	−231.00	−230.50	−230.01	−229.53	−229.05	−228.10	−227.16	−226.23
50	−231.71	−231.20	−230.70	−230.21	−229.73	−228.77	−227.83	−226.90
75	−232.34	−231.84	−231.35	−230.86	−230.38	−229.43	−228.50	−227.57
100	−232.91	−232.42	−231.94	−231.47	−231.00	−230.07	−229.15	−228.23
125	−233.40	−232.95	−232.50	−232.04	−231.59	−230.68	−229.77	−228.87
150	−233.82	−233.42	−233.00	−232.57	−232.13	−231.26	−230.38	−229.50
175	−234.16	−233.82	−233.45	−233.05	−232.65	−231.81	−230.96	−230.10
200	−234.39	−234.15	−233.84	−233.49	−233.12	−232.33	−231.52	−230.69

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species *other than* H_2O *as a function of* temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$S_2O_6^{-2}$ — Continued				
225	−234.49	−234.39	−234.16	−233.87	−233.54	−232.82	−232.06	−231.26
250	−234.43	−234.53	−234.41	−234.20	−233.92	−233.28	−232.57	−231.81
300	−233.52	−234.40	−234.67	−234.65	−234.53	−234.09	−233.52	−232.86
350	−230.27	−233.36	−234.51	−234.82	−234.91	−234.75	−234.36	−233.83
400		−231.33	−233.79	−234.63	−235.03	−235.24	−235.08	−234.71
450		−223.74	−232.22	−234.00	−234.84	−235.55	−235.67	−235.50
500			−229.40	−232.79	−234.30	−235.65	−236.12	−236.17
550			−225.00	−230.93	−233.34	−235.52	−236.41	−236.72
600			−219.39	−228.42	−231.97	−235.15	−236.52	−237.13
700				−222.20	−228.15	−233.66	−236.17	−237.44
800					−223.53	−231.30	−235.06	−237.03
900					−218.89	−228.43	−233.32	−235.86
1000						−225.47	−231.21	−233.99
				$S_2O_8^{-2}$				
25	−266.50	−265.59	−264.72	−263.88	−263.07	−261.48	−259.94	−258.44
50	−267.94	−267.01	−266.12	−265.26	−264.43	−262.81	−261.25	−259.72
75	−269.34	−268.40	−267.51	−266.65	−265.81	−264.19	−262.61	−261.08
100	−270.70	−269.77	−268.89	−268.03	−267.20	−265.58	−264.01	−262.47
125	−272.02	−271.12	−270.25	−269.40	−268.58	−266.97	−265.41	−263.88
150	−273.29	−272.43	−271.58	−270.76	−269.95	−268.36	−266.82	−265.30
175	−274.50	−273.70	−272.89	−272.09	−271.30	−269.75	−268.23	−266.73
200	−275.63	−274.92	−274.16	−273.40	−272.64	−271.12	−269.63	−268.15
225	−276.66	−276.08	−275.39	−274.67	−273.95	−272.49	−271.03	−269.58
250	−277.55	−277.16	−276.57	−275.92	−275.24	−273.84	−272.43	−271.01
300	−278.66	−279.00	−278.74	−278.27	−277.71	−276.49	−275.19	−273.85
350	−277.56	−280.06	−280.58	−280.40	−280.04	−279.05	−277.90	−276.68
400		−279.98	−281.93	−282.25	−282.17	−281.51	−280.56	−279.46
450		−274.24	−282.48	−283.72	−284.05	−283.84	−283.14	−282.21
500			−281.82	−284.68	−285.64	−286.02	−285.63	−284.89
550			−279.61	−285.04	−286.89	−288.03	−288.01	−287.50
600			−276.18	−284.79	−287.77	−289.86	−290.26	−290.01
700				−283.14	−288.61	−292.94	−294.37	−294.70
800					−288.84	−295.40	−297.95	−298.88
900					−289.20	−297.54	−301.10	−302.52
1000						−299.74	−304.03	−305.65
				S_3^{-2}				
25	17.60	17.94	18.28	18.62	18.97	19.67	20.37	21.07
50	17.26	17.60	17.94	18.29	18.63	19.33	20.02	20.72
75	17.01	17.34	17.67	18.01	18.35	19.03	19.71	20.40
100	16.84	17.15	17.47	17.79	18.12	18.78	19.44	20.12
125	16.76	17.03	17.32	17.63	17.93	18.56	19.21	19.86
150	16.77	16.99	17.24	17.52	17.80	18.39	19.01	19.64
175	16.88	17.03	17.23	17.46	17.72	18.27	18.85	19.45
200	17.10	17.15	17.28	17.47	17.69	18.18	18.72	19.29
225	17.47	17.37	17.42	17.54	17.71	18.13	18.62	19.16
250	18.02	17.71	17.64	17.68	17.79	18.12	18.56	19.05
300	19.94	18.84	18.35	18.18	18.13	18.25	18.53	18.91
350	24.23	20.93	19.52	19.01	18.73	18.56	18.64	18.89
400		23.86	21.27	20.22	19.63	19.06	18.91	18.98
450		32.05	23.87	21.91	20.86	19.78	19.33	19.19
500			27.70	24.19	22.48	20.74	19.92	19.54
550			33.05	27.13	24.53	21.95	20.69	20.04
600			39.56	30.72	27.03	23.44	21.67	20.71
700				39.06	33.15	27.24	24.30	22.63
800					40.14	32.04	27.80	25.38
900					47.25	37.47	32.03	29.01
1000						43.06	36.72	33.44

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$S_3O_6^{-2}$				
25	−229.00	−228.46	−227.94	−227.43	−226.92	−225.91	−224.92	−223.94
50	−229.79	−229.24	−228.71	−228.19	−227.67	−226.66	−225.66	−224.68
75	−230.50	−229.96	−229.43	−228.91	−228.40	−227.40	−226.41	−225.42
100	−231.15	−230.63	−230.11	−229.61	−229.10	−228.11	−227.13	−226.16
125	−231.73	−231.24	−230.75	−230.26	−229.77	−228.81	−227.85	−226.89
150	−232.25	−231.80	−231.34	−230.88	−230.41	−229.47	−228.54	−227.60
175	−232.67	−232.30	−231.88	−231.45	−231.01	−230.11	−229.21	−228.29
200	−233.00	−232.72	−232.37	−231.98	−231.57	−230.73	−229.86	−228.97
225	−233.20	−233.06	−232.79	−232.46	−232.10	−231.31	−230.48	−229.63
250	−233.24	−233.30	−233.14	−232.88	−232.57	−231.87	−231.09	−230.28
300	−232.55	−233.38	−233.60	−233.54	−233.38	−232.87	−232.23	−231.52
350	−229.52	−232.56	−233.65	−233.92	−233.97	−233.74	−233.28	−232.69
400		−230.73	−233.15	−233.95	−234.31	−234.44	−234.20	−233.77
450		−223.30	−231.81	−233.54	−234.34	−234.97	−235.01	−234.77
500			−229.20	−232.56	−234.02	−235.29	−235.68	−235.66
550			−225.02	−230.93	−233.30	−235.39	−236.19	−236.43
600			−219.62	−228.66	−232.17	−235.25	−236.53	−237.06
700				−222.91	−228.84	−234.25	−236.66	−237.85
800					−224.73	−232.41	−236.06	−237.93
900					−220.62	−230.07	−234.85	−237.29
1000						−227.67	−233.28	−235.95
				S_4^{-2}				
25	16.50	16.94	17.38	17.81	18.24	19.09	19.95	20.79
50	15.93	16.38	16.82	17.25	17.69	18.54	19.40	20.24
75	15.44	15.88	16.31	16.74	17.17	18.02	18.86	19.70
100	15.02	15.44	15.86	16.28	16.69	17.53	18.35	19.18
125	14.68	15.07	15.46	15.86	16.26	17.06	17.87	18.68
150	14.42	14.75	15.11	15.49	15.87	16.64	17.42	18.21
175	14.25	14.51	14.83	15.16	15.51	16.24	16.99	17.76
200	14.19	14.36	14.60	14.89	15.21	15.88	16.59	17.33
225	14.26	14.29	14.45	14.68	14.95	15.56	16.22	16.92
250	14.51	14.33	14.37	14.53	14.74	15.27	15.88	16.53
300	15.79	14.83	14.48	14.42	14.48	14.80	15.27	15.83
350	19.43	16.26	15.01	14.63	14.47	14.50	14.79	15.21
400		18.63	16.12	15.20	14.73	14.38	14.43	14.69
450		26.47	18.07	16.23	15.30	14.46	14.21	14.27
500			21.28	17.83	16.25	14.75	14.15	13.98
550			26.04	20.10	17.62	15.28	14.26	13.82
600			32.00	23.02	19.41	16.07	14.56	13.82
700				30.04	24.09	18.42	15.75	14.33
800					29.59	21.69	17.75	15.61
900					35.16	25.51	20.41	17.69
1000						29.45	23.48	20.52
				$S_4O_6^{-2}$				
25	−248.70	−247.84	−247.01	−246.21	−245.44	−243.92	−242.46	−241.02
50	−250.22	−249.34	−248.49	−247.68	−246.88	−245.34	−243.85	−242.40
75	−251.71	−250.82	−249.97	−249.15	−248.35	−246.81	−245.31	−243.85
100	−253.16	−252.28	−251.44	−250.63	−249.83	−248.29	−246.80	−245.33
125	−254.57	−253.72	−252.90	−252.09	−251.31	−249.78	−248.30	−246.84
150	−255.94	−255.13	−254.33	−253.55	−252.78	−251.28	−249.81	−248.36
175	−257.26	−256.51	−255.74	−254.99	−254.24	−252.76	−251.32	−249.89
200	−258.50	−257.84	−257.12	−256.40	−255.68	−254.25	−252.83	−251.42
225	−259.65	−259.11	−258.46	−257.79	−257.10	−255.72	−254.34	−252.96
250	−260.66	−260.30	−259.76	−259.14	−258.50	−257.18	−255.84	−254.49
300	−262.03	−262.39	−262.17	−261.73	−261.21	−260.06	−258.83	−257.56
350	−261.23	−263.72	−264.26	−264.12	−263.78	−262.87	−261.79	−260.62
400		−263.90	−265.87	−266.22	−266.17	−265.58	−264.69	−263.66
450		−258.45	−266.70	−267.96	−268.32	−268.17	−267.52	−266.66

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$S_4O_6^{-2}$ — Continued				
500			−266.34	−269.20	−270.19	−270.62	−270.28	−269.60
550			−264.43	−269.86	−271.72	−272.91	−272.93	−272.48
600			−261.32	−269.92	−272.90	−275.02	−275.47	−275.27
700				−268.89	−274.37	−278.70	−280.17	−280.54
800					−275.24	−281.80	−284.36	−285.32
900					−276.28	−284.61	−288.16	−289.60
1000						−287.49	−291.76	−293.40
				S_5^{-2}				
25	15.70	16.24	16.77	17.29	17.81	18.82	19.82	20.81
50	14.90	15.45	15.99	16.52	17.04	18.06	19.07	20.06
75	14.17	14.72	15.25	15.77	16.29	17.31	18.31	19.30
100	13.50	14.03	14.55	15.07	15.57	16.58	17.57	18.55
125	12.90	13.40	13.90	14.39	14.89	15.87	16.84	17.81
150	12.37	12.82	13.29	13.76	14.23	15.18	16.13	17.08
175	11.92	12.31	12.73	13.17	13.61	14.52	15.44	16.37
200	11.58	11.86	12.23	12.62	13.03	13.89	14.77	15.67
225	11.36	11.51	11.79	12.12	12.49	13.29	14.13	14.99
250	11.30	11.25	11.41	11.68	11.99	12.71	13.50	14.33
300	11.94	11.12	10.91	10.98	11.15	11.67	12.32	13.05
350	14.93	11.90	10.81	10.55	10.52	10.76	11.24	11.84
400		13.69	11.27	10.48	10.14	10.02	10.26	10.71
450		21.09	12.57	10.85	10.06	9.45	9.42	9.67
500			15.13	11.78	10.33	9.08	8.70	8.74
550			19.27	13.36	11.00	8.93	8.15	7.92
600			24.62	15.59	12.09	9.02	7.76	7.24
700				21.24	15.32	9.92	7.53	6.36
800					19.32	11.66	8.03	6.17
900					23.32	13.89	9.14	6.72
1000						16.18	10.59	7.94
				$S_5O_6^{-2}$				
25	−229.00	−228.38	−227.79	−227.20	−226.63	−225.50	−224.39	−223.30
50	−229.97	−229.34	−228.73	−228.13	−227.55	−226.41	−225.29	−224.19
75	−230.87	−230.24	−229.64	−229.05	−228.46	−227.33	−226.21	−225.11
100	−231.72	−231.11	−230.51	−229.93	−229.36	−228.23	−227.13	−226.03
125	−232.51	−231.93	−231.35	−230.79	−230.23	−229.12	−228.03	−226.95
150	−233.23	−232.69	−232.15	−231.61	−231.07	−229.99	−228.92	−227.86
175	−233.87	−233.41	−232.91	−232.39	−231.88	−230.84	−229.80	−228.76
200	−234.42	−234.05	−233.61	−233.14	−232.66	−231.67	−230.66	−229.65
225	−234.86	−234.62	−234.26	−233.84	−233.40	−232.47	−231.50	−230.52
250	−235.13	−235.09	−234.84	−234.49	−234.10	−233.25	−232.33	−231.39
300	−234.95	−235.66	−235.78	−235.63	−235.38	−234.71	−233.93	−233.08
350	−232.45	−235.37	−236.33	−236.50	−236.45	−236.05	−235.44	−234.71
400		−234.01	−236.34	−237.04	−237.29	−237.25	−236.85	−236.28
450		−226.98	−235.52	−237.14	−237.84	−238.28	−238.16	−237.76
500			−233.44	−236.70	−238.06	−239.13	−239.34	−239.16
550			−229.78	−235.63	−237.88	−239.76	−240.38	−240.45
600			−224.89	−233.91	−237.31	−240.17	−241.26	−241.61
700				−229.27	−235.14	−240.32	−242.51	−243.50
800					−232.23	−239.69	−243.08	−244.73
900					−229.37	−238.61	−243.10	−245.30
1000						−237.50	−242.80	−245.22
				Sc^{+3}				
25	−140.20	−140.67	−141.09	−141.45	−141.79	−142.37	−142.89	−143.35
50	−138.64	−139.13	−139.57	−139.96	−140.31	−140.94	−141.50	−142.00
75	−137.03	−137.54	−137.99	−138.40	−138.77	−139.44	−140.03	−140.57
100	−135.37	−135.91	−136.38	−136.81	−137.20	−137.90	−138.52	−139.08

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Sc^{+3} — Continued				
125	−133.65	−134.22	−134.73	−135.18	−135.59	−136.32	−136.97	−137.56
150	−131.88	−132.49	−133.03	−133.51	−133.94	−134.72	−135.40	−136.02
175	−130.04	−130.71	−131.29	−131.81	−132.27	−133.09	−133.80	−134.45
200	−128.13	−128.87	−129.51	−130.06	−130.56	−131.43	−132.19	−132.87
225	−126.14	−126.96	−127.67	−128.28	−128.82	−129.75	−130.55	−131.27
250	−124.05	−124.99	−125.78	−126.45	−127.04	−128.04	−128.90	−129.65
300	−119.54	−120.85	−121.89	−122.67	−123.37	−124.55	−125.53	−126.38
350	−115.17	−116.35	−117.89	−118.77	−119.57	−120.94	−122.08	−123.05
400		−114.22	−113.95	−114.80	−115.68	−117.25	−118.55	−119.65
450		−117.10	−110.29	−110.82	−111.72	−113.46	−114.94	−116.19
500			−107.33	−106.89	−107.70	−109.58	−111.24	−112.66
550			−105.55	−103.12	−103.62	−105.59	−107.45	−109.03
600			−105.12	−99.65	−99.52	−101.48	−103.54	−105.31
700				−94.03	−91.29	−92.75	−95.25	−97.44
800					−82.91	−83.24	−86.24	−88.91
900					−73.93	−72.96	−76.55	−79.68
1000						−62.21	−66.40	−69.78
				SeO_3^{-2}				
25	−88.40	−88.21	−88.00	−87.79	−87.56	−87.09	−86.60	−86.10
50	−88.41	−88.22	−88.02	−87.81	−87.59	−87.13	−86.65	−86.17
75	−88.31	−88.14	−87.95	−87.75	−87.54	−87.10	−86.64	−86.17
100	−88.12	−87.97	−87.80	−87.62	−87.42	−87.01	−86.57	−86.12
125	−87.83	−87.72	−87.58	−87.42	−87.24	−86.86	−86.45	−86.02
150	−87.44	−87.38	−87.28	−87.15	−87.00	−86.66	−86.28	−85.88
175	−86.93	−86.95	−86.90	−86.82	−86.70	−86.41	−86.07	−85.70
200	−86.29	−86.42	−86.45	−86.41	−86.34	−86.11	−85.81	−85.48
225	−85.51	−85.78	−85.90	−85.93	−85.91	−85.76	−85.52	−85.22
250	−84.52	−85.01	−85.26	−85.38	−85.42	−85.35	−85.18	−84.93
300	−81.70	−83.00	−83.67	−84.02	−84.22	−84.39	−84.37	−84.24
350	−76.51	−79.97	−81.61	−82.29	−82.73	−83.21	−83.40	−83.42
400		−76.28	−78.95	−80.16	−80.92	−81.81	−82.25	−82.45
450		−67.74	−75.44	−77.54	−78.75	−80.17	−80.93	−81.34
500			−70.75	−74.32	−76.18	−78.26	−79.40	−80.07
550			−64.62	−70.43	−73.15	−76.08	−77.67	−78.63
600			−57.44	−65.91	−69.67	−73.60	−75.71	−76.99
700				−55.76	−61.53	−67.72	−71.05	−73.07
800					−52.47	−60.75	−65.40	−68.20
900					−43.18	−53.04	−58.93	−62.37
1000						−45.07	−51.91	−55.63
				SeO_4^{-2}				
25	−105.50	−105.26	−105.01	−104.75	−104.48	−103.94	−103.38	−102.81
50	−105.77	−105.53	−105.28	−105.02	−104.76	−104.22	−103.67	−103.11
75	−105.94	−105.71	−105.47	−105.22	−104.97	−104.45	−103.92	−103.37
100	−106.02	−105.82	−105.60	−105.36	−105.13	−104.63	−104.12	−103.59
125	−106.02	−105.85	−105.66	−105.45	−105.23	−104.76	−104.27	−103.77
150	−105.92	−105.81	−105.65	−105.48	−105.28	−104.85	−104.39	−103.91
175	−105.73	−105.69	−105.58	−105.44	−105.28	−104.90	−104.47	−104.02
200	−105.41	−105.47	−105.44	−105.35	−105.22	−104.90	−104.52	−104.10
225	−104.95	−105.15	−105.21	−105.18	−105.11	−104.86	−104.52	−104.14
250	−104.30	−104.71	−104.90	−104.95	−104.93	−104.77	−104.50	−104.16
300	−102.19	−103.39	−103.98	−104.26	−104.40	−104.46	−104.34	−104.11
350	−97.70	−101.08	−102.61	−103.23	−103.59	−103.95	−104.03	−103.95
400		−97.98	−100.66	−101.80	−102.49	−103.24	−103.57	−103.66
450		−89.70	−97.85	−99.90	−101.05	−102.32	−102.95	−103.25
500			−93.82	−97.41	−99.21	−101.15	−102.15	−102.69
550			−88.28	−94.25	−96.94	−99.71	−101.15	−101.98
600			−81.62	−90.45	−94.22	−98.00	−99.95	−101.09
700				−81.69	−87.64	−93.73	−96.87	−98.72

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				SeO_4^{-2} — Continued				
800					−80.18	−88.44	−92.88	−95.49
900					−72.57	−82.49	−88.14	−91.36
1000						−76.36	−82.92	−86.41
				SiF_6^{-2}				
25	−525.70	−525.21	−524.72	−524.25	−523.78	−522.84	−521.91	−520.99
50	−526.39	−525.89	−525.40	−524.91	−524.44	−523.50	−522.57	−521.64
75	−527.00	−526.50	−526.02	−525.54	−525.07	−524.14	−523.21	−522.29
100	−527.54	−527.07	−526.60	−526.13	−525.67	−524.75	−523.84	−522.93
125	−528.02	−527.57	−527.13	−526.68	−526.23	−525.34	−524.45	−523.56
150	−528.41	−528.02	−527.61	−527.18	−526.76	−525.89	−525.03	−524.16
175	−528.72	−528.40	−528.03	−527.64	−527.24	−526.42	−525.59	−524.74
200	−528.93	−528.70	−528.39	−528.05	−527.69	−526.92	−526.12	−525.31
225	−529.00	−528.91	−528.69	−528.41	−528.09	−527.39	−526.63	−525.85
250	−528.91	−529.03	−528.92	−528.71	−528.44	−527.82	−527.12	−526.38
300	−527.95	−528.84	−529.12	−529.12	−529.00	−528.58	−528.02	−527.38
350	−524.64	−527.74	−528.91	−529.23	−529.33	−529.18	−528.80	−528.29
400		−525.66	−528.13	−528.98	−529.39	−529.62	−529.47	−529.12
450		−518.03	−526.50	−528.29	−529.15	−529.87	−530.01	−529.85
500			−523.62	−527.02	−528.54	−529.91	−530.40	−530.47
550			−519.17	−525.10	−527.52	−529.73	−530.63	−530.96
600			−513.51	−522.53	−526.09	−529.29	−530.68	−531.31
700				−516.19	−522.14	−527.67	−530.20	−531.50
800					−517.39	−525.18	−528.96	−530.96
900					−512.61	−522.16	−527.09	−529.66
1000						−519.06	−524.84	−527.64
				SiO_2^o				
25	−199.19	−198.99	−198.79	−198.59	−198.38	−197.95	−197.51	−197.07
50	−199.58	−199.41	−199.23	−199.05	−198.86	−198.49	−198.11	−197.73
75	−199.91	−199.75	−199.59	−199.42	−199.25	−198.91	−198.57	−198.22
100	−200.23	−200.08	−199.92	−199.76	−199.60	−199.29	−198.97	−198.65
125	−200.55	−200.40	−200.25	−200.10	−199.95	−199.65	−199.35	−199.05
150	−200.88	−200.74	−200.60	−200.46	−200.31	−200.02	−199.73	−199.44
175	−201.23	−201.10	−200.96	−200.83	−200.69	−200.41	−200.13	−199.85
200	−201.60	−201.48	−201.35	−201.22	−201.09	−200.82	−200.55	−200.28
225	−202.00	−201.88	−201.76	−201.63	−201.50	−201.24	−200.98	−200.72
250	−202.40	−202.31	−202.19	−202.07	−201.95	−201.70	−201.44	−201.19
300	−203.25	−203.21	−203.12	−203.02	−202.90	−202.67	−202.43	−202.19
350	−204.03	−204.17	−204.13	−204.05	−203.95	−203.74	−203.51	−203.28
400		−205.08	−205.20	−205.16	−205.09	−204.90	−204.69	−204.47
450		−205.56	−206.29	−206.33	−206.29	−206.14	−205.95	−205.75
500		−205.39	−207.37	−207.56	−207.57	−207.47	−207.30	−207.11
550		−205.60	−208.39	−208.82	−208.91	−208.86	−208.72	−208.55
600		−206.25	−209.38	−210.10	−210.29	−210.33	−210.22	−210.07
700		−208.37	−211.59	−212.79	−213.23	−213.45	−213.42	−213.31
800		−211.22	−214.31	−215.76	−216.40	−216.82	−216.87	−216.80
900		−214.59	−217.52	−219.08	−219.86	−220.44	−220.56	−220.51
1000		−218.36	−221.16	−222.76	−223.61	−224.31	−224.47	−224.44
				Sm^{+2}				
25	−123.00	−123.06	−123.09	−123.09	−123.09	−123.04	−122.96	−122.85
50	−122.85	−122.91	−122.94	−122.96	−122.96	−122.92	−122.86	−122.77
75	−122.71	−122.77	−122.81	−122.83	−122.84	−122.82	−122.77	−122.70
100	−122.57	−122.65	−122.70	−122.73	−122.74	−122.74	−122.70	−122.64
125	−122.44	−122.53	−122.59	−122.63	−122.65	−122.67	−122.65	−122.60
150	−122.30	−122.41	−122.49	−122.54	−122.58	−122.61	−122.60	−122.57
175	−122.16	−122.30	−122.40	−122.47	−122.51	−122.57	−122.58	−122.56
200	−122.00	−122.17	−122.30	−122.39	−122.45	−122.53	−122.56	−122.56

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Sm^{+2} — Continued				
225	−121.82	−122.04	−122.20	−122.31	−122.40	−122.51	−122.56	−122.57
250	−121.60	−121.89	−122.09	−122.24	−122.35	−122.49	−122.57	−122.60
300	−121.03	−121.54	−121.87	−122.08	−122.24	−122.47	−122.61	−122.69
350	−120.38	−121.04	−121.64	−121.92	−122.14	−122.47	−122.68	−122.82
400		−121.46	−121.45	−121.76	−122.04	−122.48	−122.78	−122.99
450		−123.38	−121.37	−121.63	−121.95	−122.50	−122.89	−123.18
500			−121.50	−121.52	−121.86	−122.52	−123.02	−123.38
550			−122.00	−121.47	−121.77	−122.53	−123.14	−123.60
600			−122.91	−121.53	−121.68	−122.52	−123.25	−123.80
700				−122.16	−121.52	−122.37	−123.37	−124.15
800					−121.39	−122.00	−123.30	−124.33
900					−121.16	−121.43	−123.06	−124.32
1000						−120.79	−122.75	−124.12
				Sm^{+3}				
25	−159.10	−159.57	−159.99	−160.36	−160.69	−161.28	−161.80	−162.26
50	−157.79	−158.28	−158.72	−159.11	−159.46	−160.10	−160.66	−161.17
75	−156.42	−156.93	−157.38	−157.79	−158.16	−158.83	−159.42	−159.96
100	−154.98	−155.52	−155.99	−156.42	−156.81	−157.51	−158.13	−158.70
125	−153.49	−154.05	−154.55	−155.00	−155.41	−156.14	−156.79	−157.39
150	−151.93	−152.54	−153.07	−153.54	−153.97	−154.74	−155.42	−156.04
175	−150.30	−150.96	−151.53	−152.04	−152.50	−153.31	−154.02	−154.66
200	−148.60	−149.32	−149.94	−150.49	−150.98	−151.84	−152.59	−153.26
225	−146.82	−147.61	−148.30	−148.89	−149.42	−150.34	−151.13	−151.84
250	−144.93	−145.84	−146.61	−147.25	−147.82	−148.81	−149.65	−150.39
300	−140.82	−142.07	−143.07	−143.83	−144.50	−145.65	−146.61	−147.44
350	−136.70	−137.93	−139.41	−140.27	−141.04	−142.36	−143.46	−144.41
400		−135.76	−135.73	−136.60	−137.46	−138.97	−140.22	−141.29
450		−137.56	−132.25	−132.88	−133.78	−135.46	−136.88	−138.09
500			−129.28	−129.15	−130.00	−131.85	−133.44	−134.80
550			−127.21	−125.52	−126.15	−128.11	−129.89	−131.41
600			−126.19	−122.09	−122.23	−124.23	−126.21	−127.90
700				−116.22	−114.28	−115.96	−118.38	−120.47
800					−106.08	−106.91	−109.82	−112.36
900					−97.30	−97.12	−100.60	−103.56
1000						−86.87	−90.92	−94.11
				Sn^{+2}				
25	−6.63	−6.80	−6.93	−7.04	−7.13	−7.25	−7.34	−7.39
50	−6.53	−6.70	−6.84	−6.96	−7.05	−7.20	−7.31	−7.39
75	−6.41	−6.59	−6.74	−6.86	−6.97	−7.14	−7.26	−7.36
100	−6.27	−6.47	−6.63	−6.76	−6.88	−7.06	−7.20	−7.31
125	−6.12	−6.34	−6.51	−6.66	−6.78	−6.98	−7.14	−7.27
150	−5.96	−6.19	−6.38	−6.54	−6.68	−6.90	−7.08	−7.22
175	−5.77	−6.03	−6.24	−6.42	−6.57	−6.82	−7.01	−7.17
200	−5.55	−5.85	−6.09	−6.29	−6.46	−6.73	−6.95	−7.12
225	−5.30	−5.64	−5.92	−6.15	−6.34	−6.64	−6.88	−7.07
250	−5.00	−5.41	−5.73	−5.99	−6.20	−6.55	−6.81	−7.02
300	−4.23	−4.85	−5.31	−5.64	−5.91	−6.34	−6.67	−6.93
350	−3.37	−4.11	−4.85	−5.24	−5.57	−6.11	−6.52	−6.85
400		−4.33	−4.40	−4.82	−5.21	−5.86	−6.36	−6.75
450		−6.23	−4.03	−4.38	−4.82	−5.58	−6.18	−6.65
500			−3.89	−3.95	−4.40	−5.27	−5.98	−6.53
550			−4.13	−3.57	−3.95	−4.92	−5.74	−6.40
600			−4.82	−3.27	−3.48	−4.52	−5.47	−6.22
700				−3.18	−2.50	−3.52	−4.74	−5.73
800					−1.47	−2.19	−3.72	−4.97
900					−0.23	−0.56	−2.42	−3.91
1000						1.22	−0.97	−2.59

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Sr^{+2}				
25	−134.76	−134.95	−135.09	−135.21	−135.30	−135.43	−135.51	−135.56
50	−134.56	−134.75	−134.90	−135.02	−135.12	−135.27	−135.37	−135.43
75	−134.35	−134.55	−134.71	−134.83	−134.94	−135.10	−135.21	−135.29
100	−134.13	−134.34	−134.50	−134.64	−134.75	−134.93	−135.05	−135.14
125	−133.90	−134.12	−134.30	−134.44	−134.56	−134.75	−134.89	−134.99
150	−133.65	−133.89	−134.08	−134.24	−134.37	−134.58	−134.73	−134.84
175	−133.38	−133.64	−133.86	−134.03	−134.17	−134.40	−134.57	−134.69
200	−133.09	−133.38	−133.62	−133.81	−133.97	−134.22	−134.41	−134.55
225	−132.77	−133.10	−133.37	−133.58	−133.76	−134.04	−134.25	−134.40
250	−132.40	−132.79	−133.10	−133.35	−133.55	−133.86	−134.09	−134.26
300	−131.51	−132.10	−132.53	−132.84	−133.09	−133.48	−133.76	−133.98
350	−130.49	−131.23	−131.92	−132.29	−132.60	−133.08	−133.44	−133.71
400		−131.12	−131.30	−131.71	−132.08	−132.66	−133.10	−133.44
450		−132.19	−130.73	−131.11	−131.53	−132.22	−132.75	−133.16
500			−130.31	−130.51	−130.95	−131.76	−132.38	−132.87
550			−130.14	−129.92	−130.35	−131.26	−131.99	−132.56
600			−130.29	−129.39	−129.71	−130.71	−131.56	−132.22
700				−128.70	−128.38	−129.44	−130.55	−131.42
800					−126.99	−127.88	−129.28	−130.39
900					−125.44	−126.08	−127.79	−129.11
1000						−124.16	−126.17	−127.60
				$SrCO_3^\circ$				
25	−264.86	−265.01	−265.13	−265.22	−265.30	−265.42	−265.50	−265.56
50	−265.05	−265.20	−265.32	−265.42	−265.50	−265.64	−265.74	−265.81
75	−265.19	−265.34	−265.46	−265.57	−265.66	−265.80	−265.91	−266.00
100	−265.30	−265.45	−265.58	−265.68	−265.77	−265.92	−266.04	−266.14
125	−265.39	−265.54	−265.66	−265.77	−265.86	−266.02	−266.14	−266.24
150	−265.46	−265.60	−265.73	−265.84	−265.93	−266.09	−266.21	−266.32
175	−265.50	−265.65	−265.77	−265.88	−265.98	−266.13	−266.26	−266.37
200	−265.53	−265.68	−265.80	−265.91	−266.00	−266.16	−266.29	−266.40
225	−265.55	−265.69	−265.81	−265.92	−266.01	−266.17	−266.30	−266.41
250	−265.55	−265.68	−265.81	−265.91	−266.01	−266.17	−266.30	−266.41
300	−265.53	−265.64	−265.76	−265.86	−265.95	−266.11	−266.25	−266.36
350	−265.51	−265.55	−265.66	−265.76	−265.85	−266.01	−266.14	−266.25
400		−265.45	−265.52	−265.61	−265.70	−265.86	−265.99	−266.10
450		−265.43	−265.36	−265.43	−265.51	−265.66	−265.79	−265.90
500		−265.54	−265.18	−265.22	−265.29	−265.43	−265.55	−265.66
550		−265.55	−265.00	−264.98	−265.03	−265.16	−265.28	−265.39
600		−265.43	−264.81	−264.72	−264.75	−264.86	−264.97	−265.08
700		−264.97	−264.33	−264.13	−264.10	−264.17	−264.27	−264.37
800		−264.29	−263.68	−263.42	−263.35	−263.37	−263.45	−263.54
900		−263.44	−262.86	−262.59	−262.48	−262.46	−262.53	−262.61
1000		−262.46	−261.91	−261.63	−261.50	−261.46	−261.52	−261.60
				$SrCl^+$				
25	−165.80	−165.72	−165.63	−165.52	−165.41	−165.16	−164.90	−164.62
50	−166.09	−166.01	−165.91	−165.80	−165.69	−165.45	−165.19	−164.93
75	−166.40	−166.32	−166.22	−166.12	−166.01	−165.77	−165.52	−165.26
100	−166.74	−166.66	−166.56	−166.46	−166.35	−166.12	−165.87	−165.62
125	−167.09	−167.01	−166.92	−166.82	−166.72	−166.49	−166.25	−166.00
150	−167.47	−167.39	−167.31	−167.21	−167.11	−166.88	−166.65	−166.40
175	−167.85	−167.79	−167.71	−167.61	−167.52	−167.30	−167.07	−166.83
200	−168.25	−168.19	−168.12	−168.04	−167.94	−167.74	−167.51	−167.28
225	−168.65	−168.61	−168.55	−168.47	−168.39	−168.19	−167.97	−167.74
250	−169.05	−169.04	−168.99	−168.93	−168.85	−168.66	−168.45	−168.23
300	−169.84	−169.92	−169.91	−169.87	−169.80	−169.64	−169.46	−169.25
350	−170.58	−170.78	−170.87	−170.85	−170.81	−170.68	−170.52	−170.33
400		−171.88	−171.87	−171.88	−171.86	−171.77	−171.64	−171.47
450		−173.17	−172.91	−172.94	−172.94	−172.90	−172.80	−172.66

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$SrCl^+$ — Continued				
500			−174.00	−174.03	−174.06	−174.07	−174.00	−173.89
550			−175.16	−175.15	−175.21	−175.26	−175.24	−175.15
600			−176.40	−176.32	−176.38	−176.49	−176.51	−176.45
700				−178.82	−178.79	−178.98	−179.10	−179.13
800					−181.31	−181.52	−181.76	−181.87
900					−183.91	−184.12	−184.47	−184.65
1000						−186.80	−187.26	−187.48
				SrF^+				
25	−202.29	−202.36	−202.40	−202.42	−202.43	−202.41	−202.35	−202.28
50	−202.15	−202.22	−202.26	−202.29	−202.30	−202.30	−202.26	−202.20
75	−202.04	−202.12	−202.16	−202.19	−202.21	−202.22	−202.19	−202.15
100	−201.96	−202.04	−202.09	−202.13	−202.15	−202.16	−202.15	−202.11
125	−201.90	−201.99	−202.05	−202.09	−202.12	−202.14	−202.13	−202.11
150	−201.86	−201.96	−202.03	−202.07	−202.11	−202.14	−202.15	−202.13
175	−201.83	−201.94	−202.02	−202.08	−202.12	−202.17	−202.18	−202.17
200	−201.82	−201.94	−202.04	−202.11	−202.16	−202.22	−202.24	−202.24
225	−201.80	−201.95	−202.06	−202.15	−202.21	−202.28	−202.32	−202.33
250	−201.79	−201.97	−202.10	−202.20	−202.27	−202.37	−202.42	−202.44
300	−201.72	−202.02	−202.22	−202.35	−202.45	−202.59	−202.68	−202.73
350	−201.69	−202.04	−202.39	−202.55	−202.68	−202.88	−203.00	−203.08
400		−202.62	−202.62	−202.80	−202.96	−203.22	−203.39	−203.50
450		−204.12	−202.97	−203.11	−203.29	−203.60	−203.82	−203.98
500			−203.48	−203.48	−203.67	−204.03	−204.30	−204.50
550			−204.24	−203.92	−204.08	−204.49	−204.82	−205.07
600			−205.28	−204.46	−204.53	−204.97	−205.37	−205.66
700				−205.93	−205.54	−205.98	−206.51	−206.92
800					−206.70	−206.98	−207.67	−208.22
900					−207.91	−207.99	−208.85	−209.51
1000						−209.06	−210.08	−210.81
				Threonine				
25	−120.00	−119.10	−118.23	−117.39	−116.56	−114.95	−113.37	−111.82
50	−121.38	−120.48	−119.61	−118.77	−117.95	−116.35	−114.79	−113.27
75	−122.86	−121.96	−121.09	−120.25	−119.43	−117.83	−116.29	−114.78
100	−124.44	−123.53	−122.65	−121.81	−120.99	−119.40	−117.86	−116.36
125	−126.10	−125.18	−124.31	−123.46	−122.64	−121.05	−119.52	−118.02
150	−127.85	−126.93	−126.05	−125.20	−124.37	−122.78	−121.24	−119.74
175	−129.67	−128.75	−127.86	−127.01	−126.18	−124.58	−123.04	−121.54
200	−131.58	−130.65	−129.75	−128.89	−128.06	−126.46	−124.91	−123.41
225	−133.57	−132.64	−131.72	−130.85	−130.01	−128.40	−126.85	−125.34
250	−135.64	−134.70	−133.76	−132.87	−132.02	−130.40	−128.84	−127.33
300	−140.08	−139.07	−138.06	−137.13	−136.26	−134.60	−133.02	−131.49
350	−145.30	−143.86	−142.67	−141.66	−140.74	−139.03	−137.42	−135.87
400		−149.37	−147.62	−146.47	−145.47	−143.68	−142.03	−140.46
450		−156.98	−153.01	−151.57	−150.46	−148.55	−146.85	−145.24
500		−167.44	−158.97	−157.00	−155.70	−153.64	−151.86	−150.21
550		−176.96	−165.60	−162.77	−161.19	−158.92	−157.05	−155.35
600		−185.36	−172.76	−168.89	−166.94	−164.40	−162.42	−160.66
700		−200.46	−187.53	−181.92	−179.12	−175.90	−173.67	−171.78
800		−214.46	−202.01	−195.50	−191.96	−188.04	−185.53	−183.51
900		−227.98	−216.09	−209.20	−205.17	−200.68	−197.92	−195.80
1000		−241.33	−229.93	−222.88	−218.58	−213.69	−210.77	−208.61
				Trichloroacetate				
25	−102.14	−101.30	−100.50	−99.72	−98.96	−97.47	−96.03	−94.62
50	−103.78	−102.93	−102.12	−101.33	−100.56	−99.07	−97.62	−96.21
75	−105.46	−104.60	−103.78	−102.99	−102.22	−100.73	−99.28	−97.86
100	−107.16	−106.30	−105.49	−104.69	−103.92	−102.43	−100.98	−99.57

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Trichloroacetate — Continued				
125	−108.89	−108.04	−107.22	−106.43	−105.66	−104.18	−102.73	−101.32
150	−110.63	−109.80	−108.99	−108.20	−107.44	−105.96	−104.52	−103.11
175	−112.39	−111.58	−110.78	−110.00	−109.24	−107.77	−106.34	−104.93
200	−114.16	−113.38	−112.59	−111.82	−111.07	−109.61	−108.18	−106.79
225	−115.92	−115.19	−114.42	−113.66	−112.92	−111.47	−110.06	−108.67
250	−117.67	−117.00	−116.26	−115.53	−114.80	−113.36	−111.96	−110.59
300	−121.02	−120.62	−119.97	−119.29	−118.59	−117.21	−115.84	−114.49
350	−123.76	−124.11	−123.68	−123.08	−122.44	−121.13	−119.80	−118.48
400		−127.29	−127.33	−126.88	−126.32	−125.10	−123.83	−122.55
450		−128.75	−130.81	−130.65	−130.22	−129.13	−127.93	−126.69
500			−133.99	−134.33	−134.09	−133.18	−132.07	−130.88
550			−136.76	−137.91	−137.94	−137.25	−136.25	−135.13
600			−139.21	−141.36	−141.75	−141.34	−140.47	−139.42
700				−148.09	−149.27	−149.55	−148.97	−148.09
800					−156.83	−157.81	−157.55	−156.84
900					−164.66	−166.19	−166.23	−165.66
1000						−174.79	−175.03	−174.51
				Trichloroacetic Acid				
25	−57.17	−56.10	−55.06	−54.06	−53.08	−51.18	−49.34	−47.53
50	−59.14	−58.06	−57.02	−56.02	−55.05	−53.16	−51.34	−49.55
75	−61.21	−60.13	−59.09	−58.09	−57.12	−55.23	−53.41	−51.64
100	−63.39	−62.29	−61.25	−60.25	−59.27	−57.39	−55.57	−53.80
125	−65.66	−64.55	−63.50	−62.49	−61.51	−59.63	−57.81	−56.04
150	−68.02	−66.90	−65.84	−64.83	−63.84	−61.95	−60.13	−58.36
175	−70.47	−69.34	−68.27	−67.24	−66.25	−64.35	−62.52	−60.74
200	−73.01	−71.87	−70.78	−69.74	−68.74	−66.82	−64.98	−63.20
225	−75.65	−74.49	−73.37	−72.31	−71.30	−69.36	−67.51	−65.72
250	−78.40	−77.21	−76.05	−74.96	−73.93	−71.97	−70.11	−68.31
300	−84.30	−82.95	−81.65	−80.30	−79.41	−77.39	−75.49	−73.67
350	−91.46	−89.26	−87.64	−86.35	−85.19	−83.07	−81.11	−79.25
400		−96.69	−94.10	−92.54	−91.25	−89.00	−86.96	−85.05
450		−107.68	−101.18	−99.12	−97.62	−95.16	−93.03	−91.06
500		−123.57	−109.14	−106.14	−104.31	−101.57	−99.31	−97.26
550		−137.67	−118.15	−113.65	−111.33	−108.22	−105.80	−103.66
600		−149.70	−127.99	−121.65	−118.69	−115.11	−112.49	−110.25
700		−170.44	−148.16	−138.76	−134.29	−129.52	−126.45	−123.98
800		−188.87	−167.44	−156.45	−150.68	−144.67	−141.11	−138.40
900		−206.13	−185.68	−174.01	−167.38	−160.36	−156.37	−153.48
1000		−222.75	−203.16	−191.23	−184.10	−176.39	−172.12	−169.17
				Trichloroacetyl Chloride				
25	−100.90	−99.93	−99.00	−98.10	−97.23	−95.55	−93.92	−92.33
50	−102.72	−101.73	−100.79	−99.88	−99.00	−97.30	−95.66	−94.06
75	−104.65	−103.64	−102.69	−101.77	−100.88	−99.17	−97.52	−95.92
100	−106.67	−105.65	−104.69	−103.76	−102.87	−101.15	−99.49	−97.88
125	−108.78	−107.76	−106.78	−105.85	−104.95	−103.22	−101.55	−99.94
150	−110.98	−109.95	−108.96	−108.02	−107.11	−105.37	−103.70	−102.08
175	−113.27	−112.22	−111.22	−110.27	−109.35	−107.60	−105.92	−104.29
200	−115.64	−114.58	−113.57	−112.60	−111.67	−109.90	−108.21	−106.58
225	−118.10	−117.03	−115.99	−115.01	−114.07	−112.28	−110.58	−108.93
250	−120.66	−119.56	−118.49	−117.49	−116.53	−114.73	−113.01	−111.36
300	−126.12	−124.91	−123.73	−122.66	−121.67	−119.81	−118.06	−116.38
350	−132.62	−130.76	−129.31	−128.14	−127.08	−125.14	−123.34	−121.63
400		−137.54	−135.31	−133.93	−132.76	−130.71	−128.85	−127.09
450		−147.21	−141.85	−140.06	−138.72	−136.51	−134.56	−132.76
500		−160.86	−149.12	−146.58	−144.97	−142.53	−140.48	−138.62
550		−173.11	−157.27	−153.51	−151.52	−148.78	−146.60	−144.66
600		−183.71	−166.11	−160.87	−158.36	−155.24	−152.91	−150.88
700		−202.32	−184.26	−176.57	−172.84	−168.76	−166.06	−163.85

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Trichloroacetyl Chloride — Continued				
800		−219.17	−201.79	−192.82	−188.04	−182.97	−179.87	−177.47
900		−235.15	−218.56	−209.04	−203.58	−197.69	−194.25	−191.70
1000		−250.70	−234.80	−225.07	−219.21	−212.76	−209.10	−206.49
				Toluene				
25	30.26	31.40	32.49	33.56	34.59	36.61	38.56	40.48
50	29.06	30.20	31.29	32.35	33.38	35.38	37.32	39.21
75	27.66	28.81	29.90	30.96	31.99	33.98	35.90	37.78
100	26.09	27.24	28.33	29.39	30.42	32.40	34.32	36.19
125	24.35	25.50	26.60	27.66	28.68	30.67	32.58	34.45
150	22.45	23.60	24.71	25.77	26.80	28.78	30.69	32.56
175	20.41	21.56	22.67	23.73	24.76	26.75	28.67	30.53
200	18.23	19.38	20.49	21.56	22.60	24.59	26.50	28.37
225	15.92	17.06	18.18	19.26	20.30	22.29	24.21	26.08
250	13.47	14.60	15.74	16.83	17.88	19.88	21.80	23.67
300	8.18	9.30	10.50	11.61	12.68	14.71	16.64	18.52
350	2.10	3.45	4.77	5.94	7.03	9.10	11.06	12.95
400		−3.15	−1.45	−0.18	0.97	3.09	5.08	6.99
450		−11.45	−8.19	−6.72	−5.49	−3.30	−1.27	0.66
500		−21.95	−15.55	−13.71	−12.35	−10.04	−7.96	−6.00
550		−31.98	−23.57	−21.13	−19.58	−17.12	−14.98	−12.99
600		−41.43	−32.15	−28.98	−27.17	−24.53	−22.31	−20.28
700		−59.64	−50.13	−45.75	−43.34	−40.23	−37.84	−35.71
800		−77.71	−68.54	−63.53	−60.61	−57.01	−54.42	−52.20
900		−96.02	−87.24	−81.96	−78.70	−74.70	−71.94	−69.65
1000		−114.73	−106.29	−100.91	−97.45	−93.17	−90.30	−87.99
				Tryptophan				
25	−26.90	−25.23	−23.63	−22.09	−20.59	−17.69	−14.89	−12.15
50	−27.92	−26.24	−24.64	−23.11	−21.61	−18.73	−15.95	−13.24
75	−29.13	−27.44	−25.85	−24.31	−22.82	−19.95	−17.18	−14.48
100	−30.50	−28.82	−27.22	−25.69	−24.20	−21.33	−18.57	−15.88
125	−32.04	−30.36	−28.76	−27.23	−25.74	−22.87	−20.12	−17.44
150	−33.73	−32.06	−30.45	−28.92	−27.43	−24.56	−21.81	−19.13
175	−35.56	−33.89	−32.29	−30.75	−29.26	−26.39	−23.64	−20.96
200	−37.52	−35.87	−34.26	−32.71	−31.22	−28.35	−25.60	−22.93
225	−39.60	−37.97	−36.35	−34.80	−33.31	−30.44	−27.69	−25.01
250	−41.80	−40.20	−38.57	−37.02	−35.52	−32.65	−29.89	−27.22
300	−46.54	−45.04	−43.37	−41.80	−40.29	−37.40	−34.63	−31.95
350	−51.87	−50.37	−48.62	−47.01	−45.48	−42.57	−39.79	−37.10
400		−56.32	−54.32	−52.64	−51.08	−48.13	−45.33	−42.63
450		−63.50	−60.48	−58.67	−57.05	−54.05	−51.23	−48.52
500		−72.24	−67.15	−65.10	−63.39	−60.32	−57.46	−54.73
550		−80.78	−74.35	−71.91	−70.08	−66.91	−64.01	−61.26
600		−89.02	−82.02	−79.10	−77.10	−73.80	−70.86	−68.08
700		−105.32	−98.17	−94.45	−92.05	−88.45	−85.39	−82.55
800		−121.84	−114.92	−110.78	−108.04	−104.12	−100.93	−98.03
900		−138.82	−132.15	−127.83	−124.87	−120.68	−117.38	−114.43
1000		−156.31	−149.87	−145.48	−142.39	−138.02	−134.65	−131.68
				Tyrosine				
25	−87.30	−85.87	−84.50	−83.18	−81.89	−79.39	−76.98	−74.61
50	−88.51	−87.08	−85.71	−84.39	−83.10	−80.63	−78.23	−75.89
75	−89.86	−88.42	−87.05	−85.73	−84.45	−81.98	−79.59	−77.27
100	−91.33	−89.89	−88.52	−87.20	−85.92	−83.45	−81.07	−78.76
125	−92.93	−91.48	−90.11	−88.79	−87.51	−85.04	−82.67	−80.35
150	−94.63	−93.19	−91.81	−90.49	−89.20	−86.74	−84.36	−82.05
175	−96.44	−95.00	−93.62	−92.29	−91.00	−88.53	−86.16	−83.85
200	−98.35	−96.92	−95.52	−94.19	−92.90	−90.43	−88.05	−85.74

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Tyrosine — Continued				
225	−100.36	−98.93	−97.53	−96.19	−94.89	−92.41	−90.03	−87.72
250	−102.46	−101.05	−99.63	−98.28	−96.98	−94.49	−92.10	−89.79
300	−106.97	−105.58	−104.10	−102.72	−101.40	−98.89	−96.49	−94.16
350	−112.15	−110.56	−108.95	−107.51	−106.15	−103.60	−101.17	−98.84
400		−116.21	−114.18	−112.63	−111.22	−108.60	−106.15	−103.79
450		−123.54	−119.85	−118.09	−116.59	−113.89	−111.39	−109.01
500		−133.13	−126.06	−123.89	−122.25	−119.44	−116.89	−114.47
550		−142.10	−132.87	−130.06	−128.22	−125.24	−122.62	−120.17
600		−150.34	−140.17	−136.58	−134.46	−131.29	−128.59	−126.09
700		−165.79	−155.38	−150.49	−147.73	−144.05	−141.16	−138.56
800		−180.75	−170.70	−165.13	−161.82	−157.61	−154.51	−151.82
900		−195.64	−186.01	−180.15	−176.47	−171.84	−168.55	−165.78
1000		−210.66	−201.40	−195.43	−191.54	−186.61	−183.21	−180.41
				Tb^{+3}				
25	−159.50	−159.95	−160.35	−160.70	−161.02	−161.57	−162.06	−162.49
50	−158.11	−158.58	−159.00	−159.37	−159.71	−160.31	−160.84	−161.31
75	−156.66	−157.15	−157.59	−157.97	−158.33	−158.96	−159.52	−160.03
100	−155.15	−155.67	−156.12	−156.53	−156.91	−157.57	−158.16	−158.69
125	−153.59	−154.14	−154.62	−155.05	−155.44	−156.14	−156.76	−157.32
150	−151.96	−152.55	−153.07	−153.52	−153.94	−154.67	−155.32	−155.91
175	−150.27	−150.91	−151.47	−151.96	−152.40	−153.18	−153.86	−154.47
200	−148.51	−149.21	−149.82	−150.35	−150.82	−151.65	−152.37	−153.02
225	−146.66	−147.44	−148.12	−148.69	−149.21	−150.10	−150.86	−151.54
250	−144.71	−145.60	−146.36	−147.00	−147.55	−148.51	−149.32	−150.04
300	−140.47	−141.72	−142.71	−143.47	−144.13	−145.25	−146.18	−146.99
350	−136.27	−137.47	−138.95	−139.80	−140.56	−141.87	−142.95	−143.87
400		−135.33	−135.20	−136.04	−136.89	−138.38	−139.62	−140.67
450		−137.52	−131.66	−132.24	−133.13	−134.79	−136.20	−137.39
500			−128.71	−128.46	−129.28	−131.10	−132.69	−134.04
550			−126.76	−124.80	−125.37	−127.29	−129.07	−130.58
600			−125.95	−121.37	−121.40	−123.35	−125.33	−127.01
700				−115.61	−113.38	−114.95	−117.36	−119.46
800					−105.14	−105.77	−108.68	−111.24
900					−96.32	−95.85	−99.33	−102.32
1000						−85.45	−89.52	−92.74
				Tl^{+}				
25	−7.74	−7.52	−7.30	−7.07	−6.84	−6.37	−5.90	−5.43
50	−8.49	−8.26	−8.03	−7.80	−7.56	−7.09	−6.62	−6.15
75	−9.23	−9.00	−8.76	−8.53	−8.30	−7.83	−7.36	−6.89
100	−9.98	−9.74	−9.51	−9.27	−9.04	−8.57	−8.10	−7.63
125	−10.73	−10.49	−10.25	−10.02	−9.78	−9.31	−8.85	−8.38
150	−11.48	−11.24	−11.00	−10.77	−10.53	−10.07	−9.60	−9.14
175	−12.22	−11.99	−11.76	−11.53	−11.29	−10.83	−10.36	−9.90
200	−12.97	−12.75	−12.52	−12.29	−12.05	−11.59	−11.13	−10.67
225	−13.72	−13.51	−13.28	−13.05	−12.82	−12.36	−11.90	−11.44
250	−14.46	−14.26	−14.04	−13.81	−13.59	−13.13	−12.68	−12.22
300	−15.92	−15.78	−15.57	−15.35	−15.13	−14.69	−14.24	−13.79
350	−17.31	−17.27	−17.11	−16.90	−16.69	−16.26	−15.82	−15.38
400		−18.81	−18.64	−18.45	−18.25	−17.84	−17.41	−16.98
450		−20.30	−20.18	−20.01	−19.83	−19.43	−19.01	−18.59
500			−21.71	−21.57	−21.40	−21.03	−20.63	−20.21
550			−23.22	−23.12	−22.97	−22.63	−22.25	−21.85
600			−24.73	−24.67	−24.55	−24.24	−23.88	−23.49
700				−27.80	−27.70	−27.45	−27.14	−26.78
800					−30.87	−30.67	−30.41	−30.09
900					−34.07	−33.90	−33.68	−33.39
1000						−37.15	−36.98	−36.70

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other *than* H_2O *as a function of* temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Tl^{+3}				
25	51.30	50.86	50.47	50.13	49.82	49.28	48.81	48.39
50	52.49	52.03	51.62	51.26	50.93	50.35	49.83	49.37
75	53.73	53.25	52.83	52.45	52.11	51.49	50.94	50.45
100	55.04	54.53	54.09	53.69	53.33	52.68	52.10	51.59
125	56.40	55.86	55.39	54.97	54.59	53.90	53.30	52.76
150	57.81	57.24	56.73	56.29	55.88	55.16	54.53	53.96
175	59.30	58.67	58.12	57.64	57.21	56.45	55.79	55.19
200	60.85	60.16	59.56	59.04	58.58	57.77	57.07	56.44
225	62.49	61.72	61.06	60.49	59.99	59.12	58.37	57.71
250	64.22	63.34	62.60	61.98	61.43	60.49	59.70	59.00
300	68.04	66.79	65.82	65.08	64.43	63.33	62.42	61.63
350	71.82	70.62	69.15	68.32	67.56	66.28	65.22	64.32
400		72.36	72.48	71.65	70.81	69.34	68.12	67.09
450		69.88	75.59	75.01	74.14	72.49	71.11	69.94
500			78.13	78.36	77.55	75.75	74.19	72.86
550			79.70	81.60	81.03	79.12	77.37	75.88
600			80.15	84.61	84.56	82.63	80.68	79.01
700				89.55	91.72	90.14	87.75	85.68
800					99.07	98.42	95.53	93.00
900					107.01	107.43	103.97	101.02
1000						116.90	112.86	109.67
				Tm^{+}				
25	−159.90	−160.38	−160.81	−161.19	−161.53	−162.14	−162.67	−163.15
50	−158.42	−158.92	−159.36	−159.76	−160.13	−160.78	−161.36	−161.88
75	−156.88	−157.40	−157.87	−158.29	−158.67	−159.36	−159.97	−160.52
100	−155.29	−155.84	−156.33	−156.77	−157.17	−157.89	−158.53	−159.11
125	−153.65	−154.24	−154.75	−155.21	−155.64	−156.39	−157.06	−157.67
150	−151.96	−152.59	−153.14	−153.63	−154.07	−154.86	−155.56	−156.20
175	−150.21	−150.89	−151.48	−152.00	−152.47	−153.31	−154.05	−154.71
200	−148.39	−149.13	−149.77	−150.34	−150.85	−151.73	−152.51	−153.20
225	−146.48	−147.31	−148.02	−148.64	−149.18	−150.13	−150.95	−151.68
250	−144.49	−145.42	−146.22	−146.89	−147.49	−148.51	−149.38	−150.15
300	−140.16	−141.46	−142.50	−143.29	−143.99	−145.17	−146.17	−147.03
350	−135.93	−137.14	−138.67	−139.56	−140.36	−141.74	−142.88	−143.86
400		−135.06	−134.89	−135.76	−136.65	−138.21	−139.52	−140.63
450		−137.66	−131.36	−131.94	−132.86	−134.60	−136.08	−137.34
500			−128.49	−128.17	−129.00	−130.89	−132.56	−133.97
550			−126.70	−124.54	−125.09	−127.08	−128.94	−130.52
600			−126.17	−121.18	−121.15	−123.14	−125.20	−126.97
700				−115.69	−113.23	−114.79	−117.28	−119.46
800					−105.15	−105.67	−108.67	−111.32
900					−96.49	−95.82	−99.39	−102.49
1000						−85.51	−89.69	−93.02
				Valine				
25	−85.30	−84.24	−83.22	−82.23	−81.26	−79.38	−77.55	−75.75
50	−86.44	−85.38	−84.36	−83.37	−82.41	−80.54	−78.73	−76.96
75	−87.72	−86.65	−85.63	−84.65	−83.69	−81.83	−80.03	−78.27
100	−89.12	−88.05	−87.03	−86.05	−85.09	−83.24	−81.44	−79.69
125	−90.65	−89.58	−88.55	−87.57	−86.61	−84.76	−82.97	−81.22
150	−92.28	−91.22	−90.19	−89.20	−88.24	−86.39	−84.60	−82.86
175	−94.03	−92.96	−91.93	−90.94	−89.98	−88.12	−86.33	−84.59
200	−95.87	−94.81	−93.77	−92.77	−91.81	−89.95	−88.16	−86.42
225	−97.82	−96.76	−95.71	−94.71	−93.74	−91.88	−90.08	−88.34
250	−99.86	−98.81	−97.74	−96.73	−95.76	−93.89	−92.09	−90.34
300	−104.25	−103.20	−102.09	−101.05	−100.05	−98.16	−96.35	−94.60
350	−109.28	−108.02	−106.79	−105.70	−104.68	−102.75	−100.92	−99.16
400		−113.47	−111.87	−110.69	−109.62	−107.64	−105.78	−104.00
450		−120.42	−117.37	−116.00	−114.85	−112.80	−110.91	−109.10

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
Valine — Continued								
500		−129.38	−123.38	−121.66	−120.38	−118.23	−116.29	−114.46
550		−137.83	−129.93	−127.65	−126.20	−123.91	−121.91	−120.05
600		−145.66	−136.96	−133.99	−132.30	−129.83	−127.76	−125.86
700		−160.52	−151.60	−147.50	−145.24	−142.34	−140.10	−138.11
800		−175.04	−166.44	−161.74	−159.01	−155.64	−153.22	−151.14
900		−189.59	−181.36	−176.41	−173.35	−169.61	−167.03	−164.89
1000		−204.34	−196.42	−191.38	−188.14	−184.13	−181.45	−179.29
VO^{+2}								
25	−106.70	−107.03	−107.31	−107.55	−107.77	−108.15	−108.46	−108.73
50	−105.89	−106.23	−106.52	−106.78	−107.01	−107.42	−107.77	−108.08
75	−105.06	−105.41	−105.72	−105.99	−106.24	−106.67	−107.04	−107.37
100	−104.22	−104.59	−104.91	−105.19	−105.45	−105.90	−106.30	−106.65
125	−103.36	−103.75	−104.09	−104.39	−104.66	−105.13	−105.55	−105.92
150	−102.48	−102.89	−103.25	−103.57	−103.85	−104.36	−104.79	−105.18
175	−101.57	−102.02	−102.40	−102.74	−103.04	−103.57	−104.03	−104.44
200	−100.62	−101.11	−101.54	−101.90	−102.23	−102.79	−103.27	−103.70
225	−99.64	−100.18	−100.65	−101.05	−101.40	−102.00	−102.51	−102.96
250	−98.61	−99.22	−99.74	−100.18	−100.56	−101.20	−101.75	−102.22
300	−96.35	−97.20	−97.87	−98.39	−98.83	−99.59	−100.21	−100.75
350	−94.16	−94.98	−95.98	−96.55	−97.07	−97.95	−98.67	−99.28
400		−94.16	−94.12	−94.70	−95.27	−96.27	−97.10	−97.80
450		−96.11	−92.45	−92.86	−93.46	−94.58	−95.51	−96.30
500			−91.17	−91.06	−91.62	−92.85	−93.90	−94.79
550			−90.55	−89.37	−89.78	−91.07	−92.26	−93.25
600			−90.69	−87.85	−87.93	−89.24	−90.56	−91.67
700				−85.61	−84.24	−85.34	−86.95	−88.33
800					−80.53	−81.04	−82.97	−84.66
900					−76.54	−76.35	−78.66	−80.63
1000						−71.45	−74.14	−76.27
VO_2^+								
25	−140.30	−140.67	−141.00	−141.28	−141.55	−142.00	−142.40	−142.76
50	−140.08	−140.46	−140.80	−141.10	−141.37	−141.86	−142.29	−142.68
75	−139.91	−140.30	−140.64	−140.96	−141.24	−141.75	−142.20	−142.61
100	−139.79	−140.18	−140.54	−140.86	−141.15	−141.68	−142.14	−142.57
125	−139.70	−140.11	−140.47	−140.80	−141.10	−141.64	−142.12	−142.56
150	−139.65	−140.07	−140.44	−140.78	−141.09	−141.64	−142.14	−142.59
175	−139.62	−140.06	−140.44	−140.79	−141.11	−141.68	−142.19	−142.65
200	−139.62	−140.07	−140.47	−140.84	−141.16	−141.75	−142.27	−142.75
225	−139.63	−140.10	−140.53	−140.90	−141.25	−141.85	−142.39	−142.88
250	−139.66	−140.16	−140.61	−141.00	−141.35	−141.98	−142.54	−143.04
300	−139.72	−140.30	−140.82	−141.25	−141.64	−142.32	−142.91	−143.44
350	−139.89	−140.46	−141.13	−141.60	−142.02	−142.76	−143.39	−143.96
400		−141.29	−141.56	−142.03	−142.48	−143.28	−143.96	−144.57
450		−143.28	−142.13	−142.55	−143.02	−143.88	−144.62	−145.27
500			−142.94	−143.17	−143.64	−144.55	−145.34	−146.04
550			−144.08	−143.90	−144.32	−145.28	−146.13	−146.88
600			−145.58	−144.78	−145.07	−146.06	−146.98	−147.78
700				−147.04	−146.78	−147.71	−148.77	−149.70
800					−148.71	−149.44	−150.67	−151.74
900					−150.76	−151.23	−152.64	−153.84
1000						−153.15	−154.73	−156.00
WO_4^{-2}								
25	−219.15	−218.78	−218.40	−218.02	−217.64	−216.87	−216.09	−215.31
50	−219.35	−218.98	−218.60	−218.23	−217.85	−217.09	−216.33	−215.56
75	−219.48	−219.12	−218.76	−218.39	−218.03	−217.29	−216.54	−215.79
100	−219.55	−219.21	−218.87	−218.52	−218.17	−217.45	−216.73	−216.00

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				WO_4^{-2} — Continued				
125	−219.54	−219.25	−218.93	−218.60	−218.27	−217.59	−216.89	−216.18
150	−219.46	−219.22	−218.94	−218.65	−218.34	−217.69	−217.03	−216.34
175	−219.29	−219.12	−218.90	−218.64	−218.37	−217.77	−217.14	−216.49
200	−219.01	−218.95	−218.80	−218.59	−218.35	−217.82	−217.23	−216.61
225	−218.60	−218.68	−218.62	−218.48	−218.30	−217.84	−217.30	−216.72
250	−218.01	−218.31	−218.38	−218.32	−218.19	−217.82	−217.35	−216.81
300	−216.03	−217.15	−217.63	−217.79	−217.83	−217.68	−217.36	−216.94
350	−211.73	−215.04	−216.47	−216.97	−217.24	−217.39	−217.27	−217.00
400		−212.22	−214.76	−215.80	−216.38	−216.93	−217.07	−216.97
450		−204.36	−212.24	−214.18	−215.22	−216.29	−216.73	−216.85
500			−208.54	−212.00	−213.70	−215.44	−216.25	−216.61
550			−203.40	−209.20	−211.77	−214.35	−215.61	−216.25
600			−197.18	−205.78	−209.43	−213.02	−214.78	−215.75
700				−197.90	−203.67	−209.56	−212.53	−214.21
800					−197.13	−205.17	−209.45	−211.89
900					−190.52	−200.20	−205.69	−208.76
1000						−195.11	−201.53	−204.87
				Xe°				
25	3.22	3.72	4.21	4.68	5.14	6.04	6.92	7.78
50	2.80	3.31	3.81	4.30	4.77	5.69	6.58	7.46
75	2.26	2.79	3.30	3.79	4.27	5.20	6.11	6.99
100	1.63	2.17	2.69	3.18	3.67	4.61	5.52	6.41
125	0.92	1.46	1.99	2.49	2.98	3.93	4.84	5.74
150	0.13	0.68	1.21	1.72	2.21	3.16	4.08	4.98
175	−0.73	−0.18	0.36	0.87	1.37	2.33	3.26	4.16
200	−1.66	−1.10	−0.56	−0.04	0.46	1.43	2.36	3.26
225	−2.65	−2.09	−1.54	−1.02	−0.51	0.46	1.40	2.31
250	−3.71	−3.15	−2.59	−2.05	−1.54	−0.56	0.38	1.30
300	−6.04	−5.45	−4.85	−4.30	−3.77	−2.77	−1.82	−0.89
350	−8.82	−8.05	−7.36	−6.77	−6.22	−5.19	−4.21	−3.28
400		−11.06	−10.11	−9.45	−8.86	−7.79	−6.80	−5.85
450		−15.15	−13.15	−12.35	−11.70	−10.58	−9.56	−8.59
500		−20.67	−16.52	−15.47	−14.73	−13.53	−12.47	−11.49
550		−25.81	−20.28	−18.82	−17.95	−16.65	−15.55	−14.53
600		−30.47	−24.35	−22.39	−21.35	−19.92	−18.77	−17.72
700		−39.15	−32.88	−30.09	−28.64	−26.89	−25.61	−24.51
800		−47.52	−41.47	−38.26	−36.45	−34.37	−32.96	−31.79
900		−55.84	−50.06	−46.66	−44.63	−42.27	−40.74	−39.52
1000		−64.25	−58.70	−55.23	−53.06	−50.51	−48.91	−47.67
				Y^{+3}				
25	−163.80	−164.26	−164.66	−165.02	−165.34	−165.91	−166.41	−166.85
50	−162.27	−162.74	−163.16	−163.54	−163.89	−164.50	−165.04	−165.52
75	−160.68	−161.18	−161.62	−162.01	−162.37	−163.02	−163.59	−164.11
100	−159.04	−159.56	−160.02	−160.44	−160.82	−161.50	−162.10	−162.64
125	−157.35	−157.90	−158.39	−158.83	−159.23	−159.94	−160.57	−161.14
150	−155.60	−156.20	−156.72	−157.18	−157.60	−158.35	−159.01	−159.61
175	−153.79	−154.44	−155.00	−155.50	−155.95	−156.74	−157.43	−158.06
200	−151.91	−152.62	−153.24	−153.78	−154.26	−155.10	−155.83	−156.49
225	−149.96	−150.75	−151.43	−152.02	−152.54	−153.44	−154.21	−154.90
250	−147.90	−148.81	−149.57	−150.21	−150.78	−151.75	−152.57	−153.30
300	−143.46	−144.73	−145.72	−146.49	−147.15	−148.29	−149.24	−150.05
350	−139.08	−140.28	−141.77	−142.63	−143.40	−144.72	−145.81	−146.75
400		−137.98	−137.85	−138.70	−139.55	−141.06	−142.31	−143.38
450		−140.08	−134.16	−134.74	−135.63	−137.31	−138.73	−139.94
500			−131.07	−130.81	−131.63	−133.47	−135.07	−136.43
550			−129.00	−127.00	−127.57	−129.51	−131.31	−132.83
600			−128.10	−123.45	−123.47	−125.43	−127.42	−129.13
700				−117.48	−115.21	−116.78	−119.21	−121.32

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Y^{+3} — Continued				
800					−106.77	−107.38	−110.31	−112.88
900					−97.76	−97.25	−100.75	−103.76
1000						−86.68	−90.77	−94.01
				Yb^{+2}				
25	−128.50	−128.61	−128.69	−128.74	−128.78	−128.81	−128.81	−128.78
50	−128.22	−128.33	−128.42	−128.48	−128.53	−128.58	−128.60	−128.59
75	−127.95	−128.07	−128.16	−128.23	−128.28	−128.35	−128.38	−128.39
100	−127.68	−127.81	−127.91	−127.99	−128.05	−128.13	−128.18	−128.20
125	−127.40	−127.55	−127.66	−127.75	−127.82	−127.92	−127.99	−128.02
150	−127.12	−127.29	−127.42	−127.52	−127.61	−127.72	−127.80	−127.85
175	−126.83	−127.03	−127.18	−127.30	−127.39	−127.54	−127.63	−127.69
200	−126.53	−126.76	−126.93	−127.07	−127.19	−127.35	−127.47	−127.55
225	−126.20	−126.47	−126.68	−126.85	−126.98	−127.18	−127.32	−127.41
250	−125.83	−126.17	−126.43	−126.62	−126.78	−127.01	−127.17	−127.29
300	−124.95	−125.50	−125.89	−126.15	−126.36	−126.68	−126.90	−127.07
350	−123.99	−124.68	−125.34	−125.67	−125.94	−126.36	−126.66	−126.88
400		−124.78	−124.82	−125.18	−125.51	−126.04	−126.43	−126.72
450		−126.37	−124.40	−124.71	−125.09	−125.73	−126.21	−126.57
500			−124.20	−124.26	−124.66	−125.41	−125.99	−126.44
550			−124.35	−123.87	−124.22	−125.07	−125.77	−126.31
600			−124.91	−123.57	−123.77	−124.71	−125.52	−126.16
700				−123.48	−122.90	−123.84	−124.93	−125.79
800					−122.03	−122.73	−124.12	−125.24
900					−121.04	−121.41	−123.13	−124.47
1000						−120.00	−122.04	−123.50
				Yb^{+3}				
25	−153.00	−153.50	−153.94	−154.34	−154.69	−155.33	−155.89	−156.39
50	−151.54	−152.07	−152.53	−152.94	−153.32	−154.00	−154.60	−155.15
75	−150.03	−150.57	−151.06	−151.49	−151.89	−152.60	−153.24	−153.82
100	−148.47	−149.04	−149.54	−149.99	−150.41	−151.16	−151.83	−152.44
125	−146.85	−147.45	−147.98	−148.46	−148.90	−149.68	−150.38	−151.01
150	−145.17	−145.82	−146.38	−146.89	−147.35	−148.17	−148.90	−149.56
175	−143.43	−144.13	−144.74	−145.28	−145.77	−146.64	−147.40	−148.09
200	−141.62	−142.39	−143.05	−143.63	−144.15	−145.07	−145.88	−146.60
225	−139.73	−140.58	−141.31	−141.94	−142.50	−143.48	−144.33	−145.09
250	−137.75	−138.70	−139.52	−140.21	−140.82	−141.87	−142.77	−143.56
300	−133.43	−134.75	−135.81	−136.62	−137.33	−138.55	−139.58	−140.47
350	−129.23	−130.44	−132.00	−132.90	−133.72	−135.13	−136.30	−137.31
400		−128.39	−128.22	−129.11	−130.01	−131.61	−132.95	−134.09
450		−131.06	−124.70	−125.29	−126.22	−128.00	−129.51	−130.80
500			−121.84	−121.52	−122.36	−124.29	−125.98	−127.43
550			−120.08	−117.89	−118.45	−120.47	−122.36	−123.97
600			−119.57	−114.53	−114.50	−116.52	−118.61	−120.41
700				−109.04	−106.56	−108.13	−110.66	−112.87
800					−98.44	−98.97	−101.99	−104.68
900					−89.74	−89.05	−92.66	−95.79
1000						−78.67	−82.87	−86.25
				Zn^{+2}				
25	−35.20	−35.47	−35.70	−35.89	−36.06	−36.34	−36.57	−36.77
50	−34.54	−34.82	−35.06	−35.26	−35.45	−35.76	−36.02	−36.24
75	−33.87	−34.16	−34.41	−34.63	−34.82	−35.16	−35.44	−35.68
100	−33.20	−33.50	−33.76	−33.99	−34.20	−34.55	−34.85	−35.12
125	−32.51	−32.84	−33.11	−33.36	−33.57	−33.95	−34.27	−34.55
150	−31.81	−32.16	−32.46	−32.72	−32.95	−33.35	−33.69	−33.98
175	−31.09	−31.47	−31.79	−32.07	−32.32	−32.75	−33.11	−33.42
200	−30.34	−30.76	−31.12	−31.42	−31.69	−32.15	−32.53	−32.86

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Zn^{+2} — Continued				
225	−29.56	−30.03	−30.43	−30.76	−31.05	−31.55	−31.96	−32.31
250	−28.73	−29.27	−29.72	−30.09	−30.41	−30.95	−31.39	−31.77
300	−26.90	−27.67	−28.27	−28.71	−29.10	−29.73	−30.25	−30.69
350	−25.09	−25.89	−26.80	−27.31	−27.76	−28.51	−29.12	−29.62
400		−25.36	−25.37	−25.89	−26.40	−27.27	−27.98	−28.57
450		−27.21	−24.10	−24.49	−25.03	−26.02	−26.84	−27.51
500			−23.17	−23.13	−23.65	−24.75	−25.68	−26.45
550			−22.81	−21.86	−22.26	−23.45	−24.50	−25.37
600			−23.10	−20.74	−20.87	−22.10	−23.28	−24.27
700				−19.22	−18.12	−19.19	−20.66	−21.91
800					−15.35	−15.95	−17.75	−19.28
900					−12.36	−12.38	−14.54	−16.34
1000						−8.65	−11.18	−13.12
				$Zn(CH_3COO)^+$				
25	−125.66	−125.39	−125.13	−124.86	−124.59	−124.04	−123.50	−122.95
50	−125.98	−125.70	−125.43	−125.15	−124.88	−124.33	−123.78	−123.24
75	−126.44	−126.16	−125.88	−125.60	−125.32	−124.78	−124.23	−123.69
100	−127.01	−126.73	−126.45	−126.18	−125.90	−125.35	−124.81	−124.27
125	−127.69	−127.41	−127.14	−126.86	−126.59	−126.04	−125.50	−124.96
150	−128.46	−128.19	−127.92	−127.65	−127.37	−126.83	−126.30	−125.76
175	−129.32	−129.05	−128.79	−128.52	−128.25	−127.72	−127.18	−126.65
200	−130.24	−129.99	−129.73	−129.47	−129.21	−128.68	−128.15	−127.63
225	−131.23	−131.01	−130.76	−130.50	−130.25	−129.73	−129.21	−128.68
250	−132.28	−132.08	−131.85	−131.60	−131.35	−130.85	−130.33	−129.82
300	−134.49	−134.41	−134.22	−134.00	−133.77	−133.29	−132.79	−132.29
350	−136.84	−136.91	−136.82	−136.63	−136.42	−135.97	−135.51	−135.02
400		−139.86	−139.65	−139.48	−139.29	−138.89	−138.45	−137.99
450		−143.20	−142.68	−142.52	−142.36	−142.00	−141.60	−141.16
500			−145.92	−145.75	−145.62	−145.31	−144.94	−144.53
550			−149.38	−149.16	−149.04	−148.78	−148.46	−148.08
600			−153.06	−152.74	−152.62	−152.41	−152.13	−151.80
700				−160.45	−160.21	−160.08	−159.91	−159.66
800					−168.36	−168.24	−168.19	−168.02
900					−176.99	−176.85	−176.92	−176.83
1000						−185.91	−186.09	−186.03
				$Zn(CH_3COO)_2^0$				
25	−216.45	−215.59	−214.77	−213.98	−213.22	−211.74	−210.32	−208.94
50	−217.20	−216.31	−215.46	−214.65	−213.86	−212.35	−210.90	−209.49
75	−218.25	−217.35	−216.49	−215.66	−214.87	−213.33	−211.86	−210.43
100	−219.57	−218.65	−217.78	−216.95	−216.15	−214.60	−213.11	−211.67
125	−221.12	−220.20	−219.32	−218.48	−217.67	−216.11	−214.62	−213.17
150	−222.87	−221.95	−221.06	−220.22	−219.40	−217.84	−216.34	−214.88
175	−224.81	−223.89	−223.00	−222.15	−221.33	−219.76	−218.26	−216.80
200	−226.93	−226.01	−225.12	−224.27	−223.45	−221.87	−220.36	−218.89
225	−229.20	−228.30	−227.41	−226.55	−225.73	−224.15	−222.63	−221.16
250	−231.62	−230.75	−229.85	−228.99	−228.16	−226.58	−225.06	−223.59
300	−236.88	−236.08	−235.17	−234.31	−233.48	−231.89	−230.36	−228.89
350	−242.65	−241.96	−241.04	−240.17	−239.34	−237.74	−236.21	−234.73
400		−248.37	−247.41	−246.53	−245.69	−244.08	−242.55	−241.06
450		−255.35	−254.25	−253.35	−252.49	−250.88	−249.34	−247.85
500		−262.92	−261.53	−260.59	−259.73	−258.10	−256.55	−255.06
550		−270.81	−269.23	−268.24	−267.35	−265.71	−264.16	−262.66
600		−278.99	−277.32	−276.26	−275.35	−273.69	−272.13	−270.63
700		−296.21	−294.53	−293.35	−292.39	−290.68	−289.10	−287.59
800		−314.57	−312.92	−311.68	−310.67	−308.91	−307.31	−305.79
900		−333.99	−332.37	−331.11	−330.06	−328.27	−326.65	−325.12
1000		−354.39	−352.80	−351.53	−350.46	−348.64	−347.02	−345.48

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$Zn(CH_3COO)_3^-$				
25	−305.74	−304.22	−302.79	−301.42	−300.10	−297.56	−295.14	−292.79
50	−306.63	−305.06	−303.59	−302.18	−300.83	−298.23	−295.74	−293.33
75	−308.02	−306.44	−304.94	−303.52	−302.14	−299.51	−296.99	−294.55
100	−309.83	−308.24	−306.73	−305.30	−303.92	−301.27	−298.74	−296.28
125	−311.99	−310.41	−308.90	−307.47	−306.08	−303.43	−300.89	−298.43
150	−314.46	−312.90	−311.41	−309.98	−308.60	−305.94	−303.40	−300.94
175	−317.21	−315.69	−314.21	−312.79	−311.42	−308.78	−306.24	−303.78
200	−320.21	−318.75	−317.29	−315.89	−314.53	−311.90	−309.37	−306.92
225	−323.42	−322.04	−320.63	−319.25	−317.90	−315.30	−312.78	−310.34
250	−326.80	−325.56	−324.19	−322.84	−321.52	−318.95	−316.45	−314.02
300	−333.88	−333.13	−331.93	−330.68	−329.42	−326.93	−324.49	−322.10
350	−340.61	−341.17	−340.38	−339.28	−338.12	−335.76	−333.40	−331.06
400		−349.47	−349.38	−348.54	−347.52	−345.33	−343.08	−340.81
450		−355.68	−358.72	−358.34	−357.54	−355.58	−353.45	−351.27
500			−368.13	−368.56	−368.09	−366.44	−364.47	−362.39
550			−377.39	−379.12	−379.10	−377.85	−376.08	−374.11
600			−386.65	−389.97	−390.52	−389.76	−388.21	−386.39
700				−412.76	−414.55	−414.93	−413.93	−412.42
800					−440.28	−441.80	−441.39	−440.19
900					−467.90	−470.32	−470.44	−469.51
1000						−500.53	−501.05	−500.22
				$ZnCl^+$				
25	−66.85	−66.86	−66.85	−66.82	−66.78	−66.68	−66.54	−66.39
50	−67.45	−67.46	−67.44	−67.42	−67.38	−67.29	−67.17	−67.03
75	−68.09	−68.10	−68.09	−68.06	−68.03	−67.94	−67.83	−67.70
100	−68.77	−68.78	−68.77	−68.75	−68.72	−68.63	−68.53	−68.41
125	−69.49	−69.50	−69.49	−69.47	−69.44	−69.36	−69.26	−69.14
150	−70.24	−70.25	−70.24	−70.23	−70.20	−70.12	−70.02	−69.91
175	−71.01	−71.03	−71.03	−71.01	−70.99	−70.91	−70.82	−70.71
200	−71.81	−71.83	−71.84	−71.82	−71.80	−71.74	−71.65	−71.54
225	−72.64	−72.66	−72.67	−72.66	−72.65	−72.58	−72.50	−72.40
250	−73.47	−73.52	−73.53	−73.53	−73.51	−73.46	−73.38	−73.29
300	−75.19	−75.27	−75.31	−75.32	−75.32	−75.28	−75.21	−75.13
350	−76.91	−77.08	−77.17	−77.20	−77.21	−77.19	−77.13	−77.06
400		−79.02	−79.10	−79.15	−79.17	−79.17	−79.14	−79.07
450		−80.99	−81.09	−81.16	−81.20	−81.23	−81.21	−81.16
500			−83.13	−83.23	−83.29	−83.35	−83.36	−83.32
550			−85.21	−85.35	−85.44	−85.53	−85.56	−85.55
600			−87.35	−87.52	−87.63	−87.77	−87.82	−87.82
700				−92.04	−92.16	−92.37	−92.49	−92.53
800					−96.88	−97.14	−97.32	−97.42
900					−101.77	−102.06	−102.32	−102.45
1000						−107.15	−107.46	−107.61
				$ZnCl_2^0$				
25	−98.30	−98.01	−97.73	−97.44	−97.16	−96.59	−96.02	−95.45
50	−99.02	−98.72	−98.42	−98.13	−97.84	−97.27	−96.70	−96.13
75	−99.81	−99.51	−99.21	−98.91	−98.62	−98.04	−97.46	−96.89
100	−100.67	−100.36	−100.06	−99.76	−99.46	−98.88	−98.31	−97.74
125	−101.59	−101.28	−100.97	−100.67	−100.37	−99.79	−99.21	−98.64
150	−102.56	−102.24	−101.94	−101.63	−101.34	−100.75	−100.17	−99.60
175	−103.58	−103.26	−102.95	−102.65	−102.35	−101.76	−101.19	−100.62
200	−104.64	−104.33	−104.02	−103.71	−103.41	−102.83	−102.25	−101.68
225	−105.75	−105.44	−105.13	−104.82	−104.52	−103.93	−103.36	−102.79
250	−106.89	−106.59	−106.28	−105.97	−105.67	−105.08	−104.51	−103.94
300	−109.28	−109.01	−108.70	−108.39	−108.09	−107.50	−106.92	−106.35
350	−111.79	−111.57	−111.26	−110.95	−110.65	−110.06	−109.48	−108.91
400		−114.27	−113.95	−113.64	−113.34	−112.75	−112.17	−111.60
450		−117.09	−116.76	−116.45	−116.15	−115.56	−114.98	−114.41

TABLE 1. Calculated apparent standard partial molal Gibbs free energies of formation (in kcal/mol) of aqueous species other than H_2O as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				$ZnCl_2^0$ — Continued				
500		−120.02	−119.69	−119.38	−119.08	−118.48	−117.90	−117.33
550		−123.06	−122.72	−122.41	−122.10	−121.51	−120.93	−120.36
600		−126.20	−125.85	−125.54	−125.23	−124.64	−124.06	−123.49
700		−132.73	−132.39	−132.07	−131.76	−131.16	−130.58	−130.01
800		−139.59	−139.25	−138.93	−138.62	−138.02	−137.44	−136.87
900		−146.75	−146.41	−146.09	−145.78	−145.18	−144.60	−144.02
1000		−154.19	−153.85	−153.52	−153.21	−152.61	−152.03	−151.46
				$ZnCl_3^-$				
25	−129.31	−128.69	−128.09	−127.50	−126.93	−125.81	−124.72	−123.65
50	−129.98	−129.34	−128.72	−128.12	−127.54	−126.40	−125.29	−124.21
75	−130.71	−130.07	−129.45	−128.84	−128.26	−127.11	−126.00	−124.91
100	−131.50	−130.86	−130.24	−129.64	−129.05	−127.91	−126.80	−125.71
125	−132.34	−131.71	−131.10	−130.50	−129.92	−128.78	−127.68	−126.59
150	−133.21	−132.60	−132.00	−131.42	−130.84	−129.72	−128.62	−127.54
175	−134.10	−133.53	−132.95	−132.38	−131.81	−130.70	−129.62	−128.54
200	−135.01	−134.48	−133.93	−133.37	−132.82	−131.74	−130.67	−129.61
225	−135.90	−135.45	−134.93	−134.40	−133.87	−132.82	−131.76	−130.72
250	−136.77	−136.42	−135.96	−135.46	−134.96	−133.93	−132.90	−131.87
300	−138.28	−138.33	−138.04	−137.64	−137.20	−136.27	−135.30	−134.31
350	−138.79	−139.99	−140.11	−139.86	−139.52	−138.71	−137.83	−136.90
400		−141.24	−142.07	−142.08	−141.89	−141.25	−140.47	−139.61
450		−139.80	−143.76	−144.23	−144.26	−143.85	−143.20	−142.44
500			−144.96	−146.25	−146.60	−146.50	−146.01	−145.35
550			−145.49	−148.08	−148.87	−149.18	−148.88	−148.34
600			−145.52	−149.71	−151.07	−151.86	−151.80	−151.39
700				−152.68	−155.30	−157.24	−157.71	−157.61
800					−159.57	−162.64	−163.69	−163.92
900					−164.22	−168.19	−169.78	−170.26
1000						−174.07	−176.05	−176.64
				$ZnCl_4^{-2}$				
25	−161.89	−160.88	−159.92	−158.99	−158.09	−156.35	−154.66	−153.01
50	−162.83	−161.80	−160.82	−159.87	−158.95	−157.17	−155.45	−153.77
75	−163.84	−162.81	−161.82	−160.87	−159.95	−158.16	−156.43	−154.74
100	−164.90	−163.88	−162.90	−161.96	−161.04	−159.26	−157.53	−155.84
125	−166.00	−165.01	−164.05	−163.11	−162.20	−160.44	−158.72	−157.04
150	−167.11	−166.16	−165.23	−164.32	−163.43	−161.69	−159.99	−158.33
175	−168.22	−167.34	−166.45	−165.57	−164.71	−163.00	−161.33	−159.68
200	−169.30	−168.53	−167.70	−166.86	−166.02	−164.36	−162.73	−161.10
225	−170.33	−169.70	−168.95	−168.17	−167.37	−165.77	−164.17	−162.58
250	−171.26	−170.84	−170.20	−169.49	−168.74	−167.22	−165.67	−164.12
300	−172.53	−172.92	−172.65	−172.13	−171.53	−170.20	−168.78	−167.32
350	−171.66	−174.33	−174.92	−174.73	−174.34	−173.27	−172.03	−170.69
400		−174.91	−176.85	−177.19	−177.10	−176.40	−175.37	−174.19
450		−170.05	−178.14	−179.40	−179.76	−179.54	−178.79	−177.79
500			−178.33	−181.23	−182.24	−182.66	−182.25	−181.47
550			−177.12	−182.58	−184.50	−185.73	−185.73	−185.20
600			−174.82	−183.43	−186.50	−188.72	−189.19	−188.95
700				−184.37	−189.87	−194.42	−196.01	−196.41
800					−193.00	−199.82	−202.63	−203.72
900					−196.62	−205.22	−209.14	−210.78
1000						−211.00	−215.74	−217.61

TABLE 2. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of H_2O as a function of temperature and pressure (see text)

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				H_2O				
25	−56.69	−56.47	−56.26	−56.06	−55.86	−55.46	−55.07	−54.70
50	−57.12	−56.91	−56.70	−56.49	−56.28	−55.88	−55.49	−55.11
75	−57.59	−57.38	−57.16	−56.95	−56.74	−56.34	−55.94	−55.56
100	−58.10	−57.88	−57.66	−57.44	−57.23	−56.82	−56.42	−56.03
125	−58.63	−58.41	−58.18	−57.97	−57.75	−57.34	−56.93	−56.54
150	−59.19	−58.96	−58.74	−58.52	−58.30	−57.88	−57.47	−57.06
175	−59.78	−59.55	−59.32	−59.09	−58.87	−58.44	−58.02	−57.62
200	−60.39	−60.16	−59.92	−59.69	−59.46	−59.03	−58.60	−58.19
225	−61.03	−60.79	−60.55	−60.31	−60.08	−59.64	−59.21	−58.79
250	−61.69	−61.45	−61.20	−60.96	−60.72	−60.27	−59.83	−59.40
300	−63.07	−62.83	−62.56	−62.31	−62.06	−61.59	−61.13	−60.69
350	−64.53	−64.30	−64.01	−63.74	−63.47	−62.98	−62.51	−62.05
400		−65.87	−65.54	−65.24	−64.96	−64.44	−63.95	−63.48
450		−67.55	−67.14	−66.81	−66.52	−65.96	−65.45	−64.96
500		−69.36	−68.83	−68.46	−68.13	−67.55	−67.01	−66.50
550		−71.28	−70.59	−70.17	−69.81	−69.19	−68.62	−68.09
600		−73.26	−72.42	−71.94	−71.55	−70.88	−70.28	−69.73
700		−77.37	−76.27	−75.64	−75.17	−74.40	−73.75	−73.15
800		−81.63	−80.31	−79.55	−78.98	−78.10	−77.38	−76.73
900		−86.01	−84.49	−83.60	−82.95	−81.96	−81.16	−80.45
1000		−90.49	−88.79	−87.79	−87.06	−85.95	−85.07	−84.31
1100		−95.07	−93.20	−92.10	−91.29	−90.06	−89.10	−88.28
1200		−99.74	−97.71	−96.50	−95.62	−94.28	−93.25	−92.37
1300		−104.49	−102.30	−100.99	−100.04	−98.60	−97.49	−96.55
1400		−109.31	−106.97	−105.57	−104.55	−103.02	−101.83	−100.83
1500		−114.21	−111.72	−110.23	−109.14	−107.51	−106.25	−105.20
1600		−119.18	−116.54	−114.95	−113.80	−112.08	−110.75	−109.64
1700		−124.21	−121.42	−119.75	−118.53	−116.72	−115.33	−114.17
1800		−129.31	−126.37	−124.61	−123.33	−121.43	−119.97	−118.76
1900		−134.46	−131.38	−129.54	−128.19	−126.20	−124.68	−123.42
2000		−139.67	−136.45	−134.52	−133.11	−131.04	−129.46	−128.14

T, °C	7.5	10.0	12.5	15.0	20.0	25.0	30.0
25	−53.78						
50	−54.18	−53.29	−52.43				
75	−54.62	−53.72	−52.84	−51.99			
100	−55.08	−54.17	−53.29	−52.43	−50.77		
125	−55.58	−54.66	−53.77	−52.90	−51.23	−49.61	
150	−56.09	−55.16	−54.27	−53.39	−51.71	−50.09	−48.52
175	−56.64	−55.70	−54.79	−53.91	−52.21	−50.58	−49.01
200	−57.20	−56.25	−55.33	−54.45	−52.74	−51.10	−49.51
225	−57.78	−56.82	−55.90	−55.00	−53.28	−51.63	−50.04
250	−58.39	−57.42	−56.48	−55.58	−53.85	−52.19	−50.59
300	−59.65	−58.66	−57.71	−56.79	−55.03	−53.36	−51.74
350	−60.98	−59.96	−59.00	−58.06	−56.28	−54.59	−52.96
400	−62.37	−61.33	−60.35	−59.40	−57.59	−55.88	−54.24
450	−63.82	−62.76	−61.75	−60.79	−58.96	−57.22	−55.57
500	−65.33	−64.24	−63.21	−62.23	−60.37	−58.62	−56.95
550	−66.88	−65.77	−64.72	−63.72	−61.84	−60.07	−58.38
600	−68.48	−67.34	−66.27	−65.25	−63.34	−61.55	−59.85
700	−71.81	−70.61	−69.50	−68.45	−66.48	−64.65	−62.92
800	−75.30	−74.04	−72.87	−71.78	−69.76	−67.89	−66.13
900	−78.93	−77.60	−76.39	−75.26	−73.18	−71.26	−69.46
1000	−82.69	−81.29	−80.02	−78.85	−76.71	−74.75	−72.92
1100	−86.56	−85.09	−83.77	−82.56	−80.35	−78.34	−76.48
1200	−90.54	−89.00	−87.63	−86.37	−84.09	−82.04	−80.14
1300	−94.62	−93.01	−91.58	−90.28	−87.93	−85.83	−83.90
1400	−98.79	−97.11	−95.62	−94.27	−91.86	−89.71	−87.74
1500	−103.05	−101.29	−99.75	−98.36	−95.87	−93.67	−91.66
1600	−107.39	−105.56	−103.96	−102.52	−99.97	−97.70	−95.65
1700	−111.81	−109.90	−108.25	−106.77	−104.13	−101.82	−99.72
1800	−116.30	−114.32	−112.61	−111.08	−108.37	−106.00	−103.86

TABLE 2. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of H_2O as a function of temperature and pressure (see text) — Continued

t, °C	7.5	10.0	12.5	15.0	20.0	25.0	30.0
				H_2O			
1900	−120.86	−118.80	−117.04	−115.46	−112.68	−110.25	−108.06
2000	−125.48	−123.35	−121.53	−119.91	−117.05	−114.56	−112.33

t, °C	40.0	50.0	75.0	100.0	125.0	150.0	200.0
25							
50							
75							
100							
125							
150							
175							
200							
225	−47.00						
250	−47.54	−44.63					
300	−48.67	−45.75					
350	−49.86	−46.93	−40.08				
400	−51.12	−48.17	−41.31	−34.97	−29.01		
450	−52.43	−49.46	−42.59	−36.25	−30.30	−24.66	−14.09
500	−53.79	−50.81	−43.91	−37.58	−31.64	−26.01	−15.50
550	−55.19	−52.20	−45.29	−38.95	−33.02	−27.40	−16.94
600	−56.64	−53.64	−46.71	−40.36	−34.43	−28.83	−18.41
700	−59.67	−56.63	−49.66	−43.31	−37.38	−31.79	−21.41
800	−62.83	−59.77	−52.76	−46.40	−40.47	−34.88	−24.51
900	−66.13	−63.03	−56.00	−49.61	−43.68	−38.10	−27.72
1000	−69.54	−66.42	−59.34	−52.95	−47.01	−41.42	−31.03
1100	−73.06	−69.91	−62.80	−56.40	−50.45	−44.85	−34.43
1200	−76.67	−73.50	−66.36	−59.94	−53.99	−48.38	−37.94
1300	−80.38	−77.18	−70.01	−63.58	−57.62	−52.01	−41.53
1400	−84.17	−80.94	−73.74	−67.30	−61.34	−55.71	−45.20
1500	−88.04	−84.78	−77.55	−71.10	−65.13	−59.50	−48.96
1600	−91.98	−88.69	−81.43	−74.98	−69.00	−63.37	−52.80
1700	−95.99	−92.67	−85.39	−78.92	−72.95	−67.30	−56.70
1800	−100.07	−96.72	−89.41	−82.94	−76.95	−71.30	−60.68
1900	−104.22	−100.83	−93.49	−87.01	−81.03	−75.37	−64.72
2000	−108.42	−105.00	−97.62	−91.14	−85.15	−79.49	−68.82

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol)of 22 minerals as a function of temperature and pressure (see text)

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Albite				
25	−888.94	−887.74	−886.54	−885.34	−884.14	−881.75	−879.35	−876.96
50	−890.22	−889.03	−887.83	−886.63	−885.43	−883.04	−880.64	−878.24
75	−891.61	−890.42	−889.22	−888.02	−886.82	−884.43	−882.03	−879.63
100	−893.10	−891.90	−890.70	−889.51	−888.31	−885.91	−883.52	−881.12
125	−894.67	−893.48	−892.28	−891.09	−889.89	−887.49	−885.10	−882.70
150	−896.34	−895.15	−893.95	−892.76	−891.56	−889.16	−886.77	−884.37
175	−898.09	−896.91	−895.71	−894.51	−893.32	−890.92	−888.52	−886.13
200	−899.91	−898.75	−897.56	−896.36	−895.16	−892.76	−890.37	−887.97
225	−901.81	−900.68	−899.48	−898.28	−897.08	−894.69	−892.29	−889.89
250	−903.78	−902.68	−901.48	−900.28	−899.09	−896.69	−894.29	−891.90
300	−907.91	−906.92	−905.72	−904.52	−903.33	−900.93	−898.53	−896.14
350	−912.26	−911.46	−910.26	−909.06	−907.87	−905.47	−903.07	−900.68
400		−916.28	−915.09	−913.89	−912.69	−910.29	−907.90	−905.50
450		−921.38	−920.18	−918.98	−917.79	−915.39	−912.99	−910.60
500		−926.74	−925.54	−924.34	−923.14	−920.75	−918.35	−915.95
550		−932.34	−931.14	−929.94	−928.74	−926.35	−923.95	−921.56
600		−938.18	−936.98	−935.78	−934.58	−932.18	−929.79	−927.39
700		−950.51	−949.32	−948.12	−946.92	−944.52	−942.13	−939.73
800		−963.68	−962.48	−961.28	−960.08	−957.68	−955.29	−952.89
900		−977.60	−976.40	−975.20	−974.00	−971.61	−969.21	−966.81
1000		−992.22	−991.02	−989.82	−988.62	−986.23	−983.83	−981.44
				Albite, Low				
25	−888.94	−887.74	−886.54	−885.35	−884.15	−881.76	−879.37	−876.98
50	−890.22	−889.03	−887.83	−886.64	−885.44	−883.05	−880.66	−878.27
75	−891.61	−890.42	−889.22	−888.03	−886.83	−884.44	−882.05	−879.65
100	−893.10	−891.90	−890.71	−889.51	−888.32	−885.92	−883.53	−881.14
125	−894.67	−893.48	−892.29	−891.09	−889.90	−887.50	−885.11	−882.72
150	−896.34	−895.15	−893.96	−892.76	−891.57	−889.18	−886.78	−884.39
175	−898.09	−896.91	−895.72	−894.52	−893.33	−890.93	−888.54	−886.15
200	−899.91	−898.76	−897.56	−896.36	−895.17	−892.78	−890.38	−887.99
225	−901.81	−900.68	−899.48	−898.29	−897.09	−894.70	−892.31	−889.92
250	−903.78	−902.68	−901.49	−900.29	−899.09	−896.70	−894.31	−891.92
300	−907.90	−906.91	−905.72	−904.52	−903.32	−900.93	−898.54	−896.15
350	−912.23	−911.43	−910.23	−909.03	−907.84	−905.45	−903.05	−900.66
400		−916.21	−915.01	−913.81	−912.62	−910.23	−907.84	−905.44
450		−921.24	−920.04	−918.85	−917.65	−915.26	−912.87	−910.48
500		−926.51	−925.31	−924.12	−922.92	−920.53	−918.14	−915.75
550		−932.01	−930.81	−929.62	−928.42	−926.03	−923.64	−921.24
600		−937.72	−936.52	−935.33	−934.13	−931.74	−929.35	−926.96
700		−949.75	−948.56	−947.36	−946.17	−943.77	−941.38	−938.99
800		−962.55	−961.35	−960.15	−958.96	−956.57	−954.17	−951.78
900		−976.04	−974.84	−973.65	−972.45	−970.06	−967.67	−965.28
1000		−990.19	−988.99	−987.80	−986.60	−984.21	−981.82	−979.43
				Albite, High				
25	−887.14	−885.94	−884.74	−883.54	−882.34	−879.94	−877.54	−875.14
50	−888.50	−887.30	−886.10	−884.90	−883.70	−881.29	−878.89	−876.49
75	−889.95	−888.75	−887.55	−886.35	−885.15	−882.75	−880.35	−877.95
100	−891.51	−890.31	−889.11	−887.91	−886.71	−884.31	−881.91	−879.51
125	−893.15	−891.96	−890.76	−889.56	−888.36	−885.96	−883.56	−881.16
150	−894.89	−893.70	−892.50	−891.30	−890.10	−887.70	−885.30	−882.90
175	−896.71	−895.53	−894.33	−893.13	−891.93	−889.53	−887.13	−884.73
200	−898.60	−897.44	−896.24	−895.04	−893.84	−891.44	−889.04	−886.64
225	−900.57	−899.43	−898.23	−897.03	−895.83	−893.43	−891.03	−888.63
250	−902.61	−901.51	−900.31	−899.11	−897.91	−895.51	−893.10	−890.70
300	−906.87	−905.88	−904.68	−903.48	−902.27	−899.87	−897.47	−895.07
350	−911.33	−910.53	−909.33	−908.13	−906.93	−904.53	−902.13	−899.73
400		−915.45	−914.25	−913.05	−911.85	−909.45	−907.05	−904.65
450		−920.64	−919.44	−918.24	−917.04	−914.64	−912.24	−909.84
500		−926.07	−924.87	−923.67	−922.47	−920.07	−917.67	−915.27

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Albite, High — Continued				
550		−931.74	−930.54	−929.34	−928.14	−925.74	−923.34	−920.94
600		−937.63	−936.43	−935.23	−934.03	−931.63	−929.23	−926.83
700		−950.04	−948.84	−947.64	−946.44	−944.04	−941.64	−939.24
800		−963.23	−962.03	−960.83	−959.63	−957.23	−954.83	−952.43
900		−977.15	−975.95	−974.75	−973.55	−971.15	−968.75	−966.35
1000		−991.75	−990.55	−989.35	−988.15	−985.75	−983.35	−980.95
				Analcime				
25	−740.73	−739.57	−738.41	−737.25	−736.08	−733.76	−731.44	−729.12
50	−742.18	−741.02	−739.86	−738.70	−737.54	−735.22	−732.90	−730.57
75	−743.73	−742.57	−741.41	−740.25	−739.09	−736.77	−734.45	−732.13
100	−745.38	−744.23	−743.07	−741.90	−740.74	−738.42	−736.10	−733.78
125	−747.13	−745.97	−744.81	−743.65	−742.49	−740.17	−737.85	−735.53
150	−748.96	−747.81	−746.65	−745.49	−744.33	−742.01	−739.69	−737.36
175	−750.87	−749.73	−748.57	−747.41	−746.25	−743.93	−741.61	−739.29
200	−752.86	−751.74	−750.58	−749.42	−748.26	−745.94	−743.62	−741.30
225	−754.93	−753.83	−752.67	−751.51	−750.35	−748.03	−745.70	−743.38
250	−757.06	−755.99	−754.83	−753.67	−752.51	−750.19	−747.87	−745.55
300	−761.51	−760.55	−759.39	−758.23	−757.07	−754.74	−752.42	−750.10
350	−766.16	−765.38	−764.22	−763.06	−761.90	−759.58	−757.26	−754.94
400		−770.48	−769.32	−768.16	−767.00	−764.68	−762.36	−760.04
450		−775.84	−774.68	−773.52	−772.36	−770.04	−767.71	−765.39
500		−781.43	−780.27	−779.11	−777.95	−775.63	−773.31	−770.99
550		−787.25	−786.09	−784.93	−783.77	−781.45	−779.13	−776.81
600		−793.29	−792.13	−790.97	−789.81	−787.49	−785.17	−782.85
700		−806.00	−804.84	−803.68	−802.52	−800.20	−797.87	−795.55
800		−819.48	−818.32	−817.16	−816.00	−813.68	−811.36	−809.04
900		−833.70	−832.54	−831.38	−830.22	−827.90	−825.58	−823.26
1000		−848.62	−847.46	−846.30	−845.14	−842.81	−840.49	−838.17
				Andalusite				
25	−583.51	−582.90	−582.28	−581.67	−581.05	−579.82	−578.59	−577.36
50	−584.10	−583.48	−582.87	−582.25	−581.64	−580.40	−579.17	−577.94
75	−584.75	−584.13	−583.51	−582.90	−582.28	−581.05	−579.82	−578.59
100	−585.45	−584.84	−584.22	−583.60	−582.99	−581.76	−580.53	−579.29
125	−586.21	−585.60	−584.99	−584.37	−583.75	−582.52	−581.29	−580.06
150	−587.03	−586.42	−585.81	−585.19	−584.57	−583.34	−582.11	−580.88
175	−587.90	−587.30	−586.68	−586.07	−585.45	−584.22	−582.99	−581.76
200	−588.82	−588.23	−587.61	−586.99	−586.38	−585.15	−583.92	−582.68
225	−589.79	−589.21	−588.59	−587.97	−587.36	−586.13	−584.89	−583.66
250	−590.80	−590.23	−589.62	−589.00	−588.39	−587.16	−585.92	−584.69
300	−592.95	−592.44	−591.82	−591.20	−590.59	−589.36	−588.12	−586.89
350	−595.23	−594.82	−594.20	−593.58	−592.97	−591.74	−590.50	−589.27
400		−597.36	−596.75	−596.13	−595.52	−594.29	−593.05	−591.82
450		−600.07	−599.46	−598.84	−598.23	−596.99	−595.76	−594.53
500		−602.93	−602.32	−601.70	−601.08	−599.85	−598.62	−597.39
550		−605.93	−605.32	−604.70	−604.08	−602.85	−601.62	−600.39
600		−609.07	−608.45	−607.84	−607.22	−605.99	−604.76	−603.53
700		−615.72	−615.11	−614.49	−613.88	−612.65	−611.41	−610.18
800		−622.86	−622.24	−621.62	−621.01	−619.78	−618.54	−617.31
900		−630.42	−629.81	−629.19	−628.58	−627.35	−626.11	−624.88
1000		−638.40	−637.79	−637.17	−636.55	−635.32	−634.09	−632.86
				Boehmite				
25	−219.60	−219.37	−219.13	−218.90	−218.67	−218.20	−217.73	−217.26
50	−219.84	−219.60	−219.37	−219.13	−218.90	−218.43	−217.97	−217.50
75	−220.10	−219.86	−219.63	−219.40	−219.16	−218.70	−218.23	−217.76
100	−220.39	−220.15	−219.92	−219.69	−219.45	−218.99	−218.52	−218.05
125	−220.70	−220.47	−220.23	−220.00	−219.77	−219.30	−218.83	−218.37

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

T, C°	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Bochmite — Continued				
150	−221.04	−220.81	−220.57	−220.34	−220.11	−219.64	−219.17	−218.70
175	−221.40	−221.17	−220.94	−220.70	−220.47	−220.00	−219.53	−219.07
200	−221.78	−221.56	−221.32	−221.09	−220.86	−220.39	−219.92	−219.45
225	−222.19	−221.97	−221.73	−221.50	−221.26	−220.80	−220.33	−219.86
250	−222.61	−222.40	−222.16	−221.93	−221.70	−221.23	−220.76	−220.30
300	−223.52	−223.33	−223.09	−222.86	−222.63	−222.16	−221.69	−221.22
350	−224.49	−224.34	−224.10	−223.87	−223.64	−223.17	−222.70	−222.24
400		−225.43	−225.19	−224.96	−224.73	−224.26	−223.79	−223.33
450		−226.60	−226.36	−226.13	−225.90	−225.43	−224.96	−224.49
500		−227.84	−227.60	−227.37	−227.14	−226.67	−226.20	−225.74
550		−229.15	−228.92	−228.68	−228.45	−227.98	−227.51	−227.05
600		−230.53	−230.30	−230.06	−229.83	−229.36	−228.90	−228.43
700		−233.49	−233.26	−233.02	−232.79	−232.32	−231.86	−231.39
800		−236.70	−236.47	−236.24	−236.00	−235.54	−235.07	−234.60
900		−240.16	−239.93	−239.69	−239.46	−238.99	−238.53	−238.06
1000		−243.85	−243.61	−243.38	−243.15	−242.68	−242.21	−241.75
				Corundum				
25	−378.17	−377.86	−377.56	−377.25	−376.95	−376.33	−375.72	−375.11
50	−378.49	−378.19	−377.88	−377.58	−377.27	−376.66	−376.05	−375.44
75	−378.86	−378.55	−378.24	−377.94	−377.63	−377.02	−376.41	−375.80
100	−379.26	−378.95	−378.65	−378.34	−378.03	−377.42	−376.81	−376.20
125	−379.69	−379.39	−379.08	−378.78	−378.47	−377.86	−377.25	−376.64
150	−380.17	−379.86	−379.56	−379.25	−378.95	−378.34	−377.72	−377.11
175	−380.67	−380.37	−380.07	−379.76	−379.46	−378.84	−378.23	−377.62
200	−381.21	−380.92	−380.61	−380.30	−380.00	−379.39	−378.78	−378.16
225	−381.78	−381.49	−381.19	−380.88	−380.57	−379.96	−379.35	−378.74
250	−382.38	−382.10	−381.79	−381.49	−381.18	−380.57	−379.96	−379.35
300	−383.66	−383.40	−383.10	−382.79	−382.49	−381.88	−381.27	−380.65
350	−385.03	−384.83	−384.52	−384.22	−383.91	−383.30	−382.69	−382.08
400		−386.36	−386.05	−385.75	−385.44	−384.83	−384.22	−383.61
450		−387.99	−387.69	−387.38	−387.08	−386.47	−385.85	−385.24
500		−389.73	−389.42	−389.12	−388.81	−388.20	−387.59	−386.98
550		−391.55	−391.25	−390.94	−390.64	−390.02	−389.41	−388.80
600		−393.46	−393.16	−392.85	−392.55	−391.94	−391.33	−390.71
700		−397.54	−397.23	−396.93	−396.62	−396.01	−395.40	−394.79
800		−401.92	−401.61	−401.30	−401.00	−400.39	−399.78	−399.16
900		−406.57	−406.27	−405.96	−405.66	−405.05	−404.43	−403.82
1000		−411.49	−411.19	−410.88	−410.57	−409.96	−409.35	−408.74
				Diaspore				
25	−220.15	−219.94	−219.73	−219.51	−219.30	−218.88	−218.45	−218.03
50	−220.37	−220.16	−219.95	−219.74	−219.53	−219.10	−218.68	−218.25
75	−220.63	−220.41	−220.20	−219.99	−219.78	−219.35	−218.93	−218.50
100	−220.90	−220.69	−220.48	−220.27	−220.05	−219.63	−219.21	−218.78
125	−221.20	−220.99	−220.78	−220.57	−220.36	−219.93	−219.51	−219.08
150	−221.53	−221.32	−221.11	−220.90	−220.68	−220.26	−219.83	−219.41
175	−221.88	−221.67	−221.46	−221.25	−221.03	−220.61	−220.18	−219.76
200	−222.25	−222.04	−221.83	−221.62	−221.41	−220.98	−220.56	−220.13
225	−222.64	−222.44	−222.23	−222.02	−221.80	−221.38	−220.96	−220.53
250	−223.06	−222.86	−222.65	−222.44	−222.22	−221.80	−221.37	−220.95
300	−223.94	−223.76	−223.55	−223.34	−223.12	−222.70	−222.28	−221.85
350	−224.89	−224.75	−224.53	−224.32	−224.11	−223.68	−223.26	−222.84
400		−225.81	−225.60	−225.38	−225.17	−224.75	−224.32	−223.90
450		−226.95	−226.74	−226.52	−226.31	−225.89	−225.46	−225.04
500		−228.16	−227.95	−227.74	−227.52	−227.10	−226.67	−226.25
550		−229.44	−229.23	−229.02	−228.81	−228.38	−227.96	−227.53
600		−230.79	−230.58	−230.37	−230.16	−229.73	−229.31	−228.88
700		−233.70	−233.48	−233.27	−233.06	−232.64	−232.21	−231.79
800		−236.85	−236.64	−236.43	−236.22	−235.79	−235.37	−234.94

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Diaspore — Continued				
900		−240.25	−240.04	−239.83	−239.61	−239.19	−238.76	−238.34
1000		−243.88	−243.67	−243.46	−243.25	−242.82	−242.40	−241.97
				Gibbsite				
25	−276.03	−275.64	−275.26	−274.88	−274.50	−273.73	−272.97	−272.21
50	−276.46	−276.08	−275.69	−275.31	−274.93	−274.17	−273.40	−272.64
75	−276.93	−276.55	−276.17	−275.79	−275.41	−274.64	−273.88	−273.12
100	−277.46	−277.07	−276.69	−276.31	−275.93	−275.17	−274.40	−273.64
125	−278.02	−277.64	−277.26	−276.88	−276.49	−275.73	−274.97	−274.20
150	−278.63	−278.25	−277.87	−277.49	−277.10	−276.34	−275.58	−274.81
175	−279.27	−278.90	−278.52	−278.14	−277.75	−276.99	−276.23	−275.46
200	−279.96	−279.59	−279.21	−278.83	−278.45	−277.68	−276.92	−276.16
225	−280.69	−280.33	−279.94	−279.56	−279.18	−278.42	−277.65	−276.89
250	−281.45	−281.10	−280.72	−280.34	−279.95	−279.19	−278.43	−277.66
300	−283.08	−282.77	−282.38	−282.00	−281.62	−280.86	−280.09	−279.33
350	−284.84	−284.59	−284.21	−283.82	−283.44	−282.68	−281.92	−281.15
400		−286.56	−286.18	−285.80	−285.42	−284.65	−283.89	−283.12
450		−288.68	−288.30	−287.92	−287.54	−286.77	−286.01	−285.25
500		−290.95	−290.57	−290.18	−289.80	−289.04	−288.27	−287.51
550		−293.36	−292.97	−292.59	−292.21	−291.45	−290.68	−289.92
600		−295.90	−295.52	−295.14	−294.76	−294.00	−293.23	−292.47
700		−301.41	−301.03	−300.65	−300.27	−299.50	−298.74	−297.98
800		−307.46	−307.08	−306.70	−306.32	−305.55	−304.79	−304.02
900		−314.04	−313.65	−313.27	−312.89	−312.13	−311.36	−310.60
1000		−321.13	−320.74	−320.36	−319.98	−319.22	−318.45	−317.69
				Jadeite				
25	−682.07	−681.35	−680.63	−679.91	−679.19	−677.74	−676.30	−674.85
50	−682.91	−682.19	−681.47	−680.74	−680.02	−678.58	−677.14	−675.69
75	−683.82	−683.10	−682.38	−681.66	−680.94	−679.49	−678.05	−676.61
100	−684.82	−684.09	−683.37	−682.65	−681.93	−680.49	−679.04	−677.60
125	−685.88	−685.16	−684.44	−683.72	−682.99	−681.55	−680.11	−678.66
150	−687.01	−686.30	−685.57	−684.85	−684.13	−682.69	−681.24	−679.80
175	−688.21	−687.50	−686.78	−686.06	−685.34	−683.89	−682.45	−681.00
200	−689.47	−688.77	−688.05	−687.33	−686.61	−685.16	−683.72	−682.27
225	−690.79	−690.11	−689.38	−688.66	−687.94	−686.50	−685.05	−683.61
250	−692.17	−691.50	−690.78	−690.06	−689.34	−687.89	−686.45	−685.01
300	−695.07	−694.47	−693.75	−693.03	−692.30	−690.86	−689.42	−687.97
350	−698.14	−697.66	−696.94	−696.22	−695.50	−694.05	−692.61	−691.16
400		−701.06	−700.34	−699.62	−698.90	−697.45	−696.01	−694.57
450		−704.66	−703.94	−703.22	−702.50	−701.05	−699.61	−698.16
500		−708.45	−707.73	−707.00	−706.28	−704.84	−703.39	−701.95
550		−712.41	−711.69	−710.97	−710.25	−708.80	−707.36	−705.91
600		−716.54	−715.82	−715.10	−714.38	−712.94	−711.49	−710.05
700		−725.29	−724.57	−723.85	−723.13	−721.68	−720.24	−718.80
800		−734.64	−733.91	−733.19	−732.47	−731.03	−729.58	−728.14
900		−744.53	−743.81	−743.09	−742.37	−740.92	−739.48	−738.04
1000		−754.95	−754.23	−753.50	−752.78	−751.34	−749.90	−748.45
				K-Feldspar				
25	−897.07	−895.77	−894.47	−893.16	−891.86	−889.26	−886.66	−884.06
50	−898.39	−897.09	−895.79	−894.49	−893.19	−890.59	−887.98	−885.38
75	−899.81	−898.51	−897.21	−895.91	−894.61	−892.01	−889.40	−886.80
100	−901.33	−900.03	−898.73	−897.43	−896.12	−893.52	−890.92	−888.32
125	−902.93	−901.64	−900.34	−899.04	−897.74	−895.13	−892.53	−889.93
150	−904.63	−903.34	−902.04	−900.74	−899.44	−896.84	−894.24	−891.63
175	−906.42	−905.14	−903.84	−902.54	−901.24	−898.63	−896.03	−893.43
200	−908.28	−907.02	−905.72	−904.42	−903.12	−900.52	−897.92	−895.31
225	−910.23	−908.99	−907.69	−906.39	−905.09	−902.49	−899.89	−897.28

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, C°	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				K-Feldspar — Continued				
250	−912.25	−911.05	−909.75	−908.45	−907.15	−904.54	−901.94	−899.34
300	−916.48	−915.40	−914.10	−912.80	−911.49	−908.89	−906.29	−903.69
350	−920.92	−920.05	−918.75	−917.45	−916.15	−913.55	−910.94	−908.34
400		−924.99	−923.69	−922.39	−921.09	−918.49	−915.89	−913.28
450		−930.21	−928.91	−927.61	−926.30	−923.70	−921.10	−918.50
500		−935.68	−934.38	−933.07	−931.77	−929.17	−926.57	−923.97
550		−941.39	−940.09	−938.79	−937.48	−934.88	−932.28	−929.68
600		−947.33	−946.03	−944.73	−943.43	−940.82	−938.22	−935.62
700		−959.86	−958.56	−957.26	−955.96	−953.35	−950.75	−948.15
800		−973.19	−971.89	−970.59	−969.28	−966.68	−964.08	−961.48
900		−987.25	−985.95	−984.65	−983.35	−980.74	−978.14	−975.54
1000		−1001.99	−1000.69	−999.39	−998.09	−995.49	−992.88	−990.28
				Kalsilite				
25	−482.98	−482.27	−481.55	−480.83	−480.12	−478.69	−477.26	−475.82
50	−483.81	−483.09	−482.38	−481.66	−480.94	−479.51	−478.08	−476.65
75	−484.69	−483.98	−483.26	−482.54	−481.83	−480.40	−478.97	−477.53
100	−485.63	−484.92	−484.20	−483.48	−482.77	−481.34	−479.90	−478.47
125	−486.62	−485.91	−485.19	−484.48	−483.76	−482.33	−480.90	−479.47
150	−487.66	−486.95	−486.24	−485.52	−484.81	−483.37	−481.94	−480.51
175	−488.75	−488.05	−487.33	−486.62	−485.90	−484.47	−483.04	−481.61
200	−489.89	−489.19	−488.48	−487.76	−487.04	−485.61	−484.18	−482.75
225	−491.06	−490.38	−489.67	−488.95	−488.23	−486.80	−485.37	−483.94
250	−492.28	−491.62	−490.90	−490.19	−489.47	−488.04	−486.61	−485.18
300	−494.81	−494.22	−493.50	−492.79	−492.07	−490.64	−489.21	−487.78
350	−497.46	−496.98	−496.27	−495.55	−494.83	−493.40	−491.97	−490.54
400		−499.90	−499.19	−498.47	−497.75	−496.32	−494.89	−493.46
450		−502.97	−502.26	−501.54	−500.82	−499.39	−497.96	−496.53
500		−506.18	−505.47	−504.75	−504.03	−502.60	−501.17	−499.74
550		−509.53	−508.82	−508.10	−507.38	−505.95	−504.52	−503.09
600		−513.02	−512.30	−511.59	−510.87	−509.44	−508.01	−506.58
700		−520.35	−519.63	−518.91	−518.20	−516.77	−515.34	−513.90
800		−528.11	−527.40	−526.68	−525.97	−524.53	−523.10	−521.67
900		−536.28	−535.56	−534.85	−534.13	−532.70	−531.27	−529.84
1000		−544.80	−544.09	−543.37	−542.66	−541.22	−539.79	−538.36
				Kaolinite				
25	−908.50	−907.31	−906.12	−904.93	−903.74	−901.37	−898.99	−896.61
50	−909.76	−908.57	−907.39	−906.20	−905.01	−902.63	−900.25	−897.87
75	−911.15	−909.96	−908.77	−907.58	−906.39	−904.01	−901.63	−899.25
100	−912.64	−911.46	−910.27	−909.08	−907.89	−905.51	−903.13	−900.75
125	−914.26	−913.07	−911.88	−910.69	−909.50	−907.12	−904.75	−902.37
150	−915.97	−914.80	−913.61	−912.42	−911.23	−908.85	−906.47	−904.09
175	−917.80	−916.63	−915.44	−914.25	−913.06	−910.68	−908.30	−905.92
200	−919.72	−918.56	−917.37	−916.18	−915.00	−912.62	−910.24	−907.86
225	−921.73	−920.60	−919.41	−918.22	−917.03	−914.65	−912.27	−909.90
250	−923.83	−922.74	−921.55	−920.36	−919.17	−916.79	−914.41	−912.03
300	−928.28	−927.29	−926.10	−924.91	−923.72	−921.34	−918.96	−916.59
350	−933.00	−932.21	−931.02	−929.83	−928.64	−926.26	−923.88	−921.50
400		−937.47	−936.28	−935.09	−933.90	−931.53	−929.15	−926.77
450		−943.07	−941.88	−940.69	−939.50	−937.12	−934.74	−932.36
500		−948.98	−947.79	−946.60	−945.41	−943.04	−940.66	−938.28
550		−955.20	−954.01	−952.82	−951.64	−949.26	−946.88	−944.50
600		−961.72	−960.53	−959.34	−958.15	−955.77	−953.39	−951.02
700		−975.61	−974.42	−973.23	−972.04	−969.66	−967.28	−964.90
800		−990.58	−989.39	−988.20	−987.01	−984.63	−982.25	−979.87
900		−1006.57	−1005.39	−1004.20	−1003.01	−1000.63	−998.25	−995.87
1000		−1023.56	−1022.37	−1021.18	−1019.99	−1017.61	−1015.23	−1012.85

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

	Pressure, kbar							
T, °C	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Kyanite				
25	−583.88	−583.36	−582.83	−582.30	−581.78	−580.72	−579.67	−578.61
50	−584.41	−583.89	−583.36	−582.83	−582.31	−581.25	−580.20	−579.14
75	−585.00	−584.48	−583.95	−583.42	−582.90	−581.84	−580.79	−579.73
100	−585.65	−585.13	−584.60	−584.07	−583.55	−582.49	−581.44	−580.39
125	−586.36	−585.84	−585.31	−584.78	−584.25	−583.20	−582.15	−581.09
150	−587.12	−586.60	−586.07	−585.55	−585.02	−583.97	−582.91	−581.86
175	−587.94	−587.42	−586.89	−586.37	−585.84	−584.79	−583.73	−582.68
200	−588.80	−588.29	−587.77	−587.24	−586.71	−585.66	−584.60	−583.55
225	−589.72	−589.22	−588.69	−588.16	−587.64	−586.58	−585.53	−584.47
250	−590.67	−590.19	−589.66	−589.14	−588.61	−587.56	−586.50	−585.45
300	−592.72	−592.28	−591.75	−591.23	−590.70	−589.65	−588.59	−587.54
350	−594.90	−594.55	−594.02	−593.50	−592.97	−591.92	−590.86	−589.81
400		−596.99	−596.46	−595.94	−595.41	−594.36	−593.30	−592.25
450		−599.59	−599.06	−598.54	−598.01	−596.96	−595.90	−594.85
500		−602.34	−601.82	−601.29	−600.76	−599.71	−598.66	−597.60
550		−605.24	−604.71	−604.19	−603.66	−602.61	−601.55	−600.50
600		−608.27	−607.75	−607.22	−606.69	−605.64	−604.59	−603.53
700		−614.73	−614.20	−613.67	−613.15	−612.09	−611.04	−609.98
800		−621.66	−621.13	−620.61	−620.08	−619.03	−617.97	−616.92
900		−629.04	−628.51	−627.98	−627.46	−626.40	−625.35	−624.30
1000		−636.83	−636.30	−635.78	−635.25	−634.19	−633.14	−632.09
				Microcline, Maximum				
25	−897.07	−895.77	−894.47	−893.17	−891.87	−889.27	−886.67	−884.07
50	−898.40	−897.10	−895.80	−894.50	−893.20	−890.60	−888.00	−885.40
75	−899.82	−898.53	−897.23	−895.93	−894.63	−892.03	−889.43	−886.83
100	−901.35	−900.05	−898.75	−897.45	−896.15	−893.55	−890.95	−888.36
125	−902.97	−901.67	−900.37	−899.07	−897.77	−895.17	−892.58	−889.98
150	−904.67	−903.38	−902.08	−900.78	−899.49	−896.89	−894.29	−891.69
175	−906.46	−905.18	−903.88	−902.59	−901.29	−898.69	−896.09	−893.49
200	−908.33	−907.07	−905.77	−904.47	−903.17	−900.57	−897.97	−895.37
225	−910.27	−909.04	−907.74	−906.44	−905.14	−902.54	−899.94	−897.34
250	−912.28	−911.08	−909.79	−908.49	−907.19	−904.59	−901.99	−899.39
300	−916.48	−915.41	−914.11	−912.81	−911.51	−908.91	−906.31	−903.71
350	−920.89	−920.02	−918.72	−917.42	−916.12	−913.52	−910.92	−908.32
400		−924.90	−923.60	−922.30	−921.00	−918.40	−915.80	−913.20
450		−930.04	−928.74	−927.44	−926.14	−923.54	−920.94	−918.34
500		−935.42	−934.12	−932.82	−931.52	−928.92	−926.32	−923.72
550		−941.03	−939.73	−938.43	−937.13	−934.53	−931.93	−929.33
600		−946.85	−945.55	−944.25	−942.95	−940.35	−937.76	−935.16
700		−959.12	−957.82	−956.53	−955.23	−952.63	−950.03	−947.43
800		−972.16	−970.86	−969.56	−968.26	−965.67	−963.07	−960.47
900		−985.91	−984.61	−983.31	−982.01	−979.41	−976.82	−974.22
1000		−1000.33	−999.03	−997.73	−996.43	−993.83	−991.23	−988.63
				Muscovite				
25	−1340.32	−1338.64	−1336.96	−1335.28	−1333.59	−1330.23	−1326.86	−1323.50
50	−1342.12	−1340.44	−1338.76	−1337.08	−1335.39	−1332.03	−1328.66	−1325.30
75	−1344.08	−1342.40	−1340.72	−1339.04	−1337.35	−1333.99	−1330.62	−1327.26
100	−1346.19	−1344.52	−1342.83	−1341.15	−1339.47	−1336.10	−1332.73	−1329.37
125	−1348.45	−1346.78	−1345.09	−1343.41	−1341.73	−1338.36	−1335.00	−1331.63
150	−1350.85	−1349.18	−1347.50	−1345.82	−1344.14	−1340.77	−1337.40	−1334.04
175	−1353.38	−1351.73	−1350.05	−1348.36	−1346.68	−1343.32	−1339.95	−1336.58
200	−1356.04	−1354.41	−1352.73	−1351.05	−1349.36	−1346.00	−1342.63	−1339.27
225	−1358.82	−1357.23	−1355.54	−1353.86	−1352.18	−1348.81	−1345.45	−1342.08
250	−1361.72	−1360.17	−1358.48	−1356.80	−1355.12	−1351.75	−1348.39	−1345.02
300	−1367.81	−1366.42	−1364.74	−1363.05	−1361.37	−1358.01	−1354.64	−1351.27
350	−1374.27	−1373.14	−1371.46	−1369.77	−1368.09	−1364.73	−1361.36	−1357.99
400		−1380.30	−1378.62	−1376.94	−1375.26	−1371.89	−1368.52	−1365.16
450		−1387.89	−1386.20	−1384.52	−1382.84	−1379.47	−1376.11	−1372.74

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

		Pressure, kbar						
T, °C	*Sat.*	*0.5*	*1.0*	*1.5*	2.0	3.0	4.0	5.0
				Muscovite — Continued				
500		−1395.87	−1394.18	−1392.50	−1390.82	−1387.45	−1384.09	−1380.72
550		−1404.22	−1402.54	−1400.86	−1399.17	−1395.81	−1392.44	−1389.08
600		−1412.94	−1411.25	−1409.57	−1407.89	−1404.52	−1401.16	−1397.79
700		−1431.37	−1429.69	−1428.01	−1426.32	−1422.96	−1419.59	−1416.23
800		−1451.06	−1449.38	−1447.69	−1446.01	−1442.65	−1439.28	−1435.92
900		−1471.90	−1470.22	−1468.54	−1466.85	−1463.49	−1460.12	−1456.76
1000		−1493.81	−1492.13	−1490.45	−1488.77	−1485.40	−1482.03	−1478.67
				Nepheline				
25	−475.50	−474.85	−474.20	−473.56	−472.91	−471.62	−470.32	−469.03
50	−476.27	−475.63	−474.98	−474.33	−473.68	−472.39	−471.09	−469.80
75	−477.11	−476.46	−475.81	−475.16	−474.52	−473.22	−471.93	−470.63
100	−478.00	−477.35	−476.70	−476.06	−475.41	−474.11	−472.82	−471.53
125	−478.94	−478.30	−477.65	−477.00	−476.36	−475.06	−473.77	−472.47
150	−479.94	−479.30	−478.65	−478.00	−477.36	−476.06	−474.77	−473.47
175	−480.98	−480.35	−479.70	−479.05	−478.41	−477.11	−475.82	−474.52
200	−482.07	−481.45	−480.80	−480.15	−479.51	−478.21	−476.92	−475.62
225	−483.21	−482.59	−481.95	−481.30	−480.65	−479.36	−478.06	−476.77
250	−484.38	−483.79	−483.14	−482.49	−481.85	−480.55	−479.26	−477.96
300	−486.84	−486.30	−485.65	−485.01	−484.36	−483.06	−481.77	−480.48
350	−489.41	−488.98	−488.33	−487.68	−487.04	−485.74	−484.45	−483.15
400		−491.81	−491.16	−490.51	−489.87	−488.57	−487.28	−485.98
450		−494.78	−494.14	−493.49	−492.84	−491.55	−490.25	−488.96
500		−497.89	−497.25	−496.60	−495.95	−494.66	−493.36	−492.07
550		−501.13	−500.48	−499.84	−499.19	−497.89	−496.60	−495.30
600		−504.49	−503.84	−503.20	−502.55	−501.25	−499.96	−498.66
700		−511.55	−510.91	−510.26	−509.61	−508.32	−507.02	−505.73
800		−519.04	−518.40	−517.75	−517.10	−515.81	−514.51	−513.22
900		−526.93	−526.28	−525.63	−524.98	−523.69	−522.39	−521.10
1000		−535.17	−534.53	−533.88	−533.23	−531.94	−530.64	−529.35
				Paragonite				
25	−1331.65	−1330.07	−1328.49	−1326.90	−1325.32	−1322.15	−1318.98	−1315.81
50	−1333.39	−1331.81	−1330.22	−1328.64	−1327.05	−1323.89	−1320.72	−1317.55
75	−1335.28	−1333.70	−1332.11	−1330.53	−1328.95	−1325.78	−1322.61	−1319.44
100	−1337.32	−1335.74	−1334.16	−1332.57	−1330.99	−1327.82	−1324.66	−1321.49
125	−1339.51	−1337.94	−1336.35	−1334.77	−1333.18	−1330.02	−1326.85	−1323.68
150	−1341.84	−1340.27	−1338.69	−1337.10	−1335.52	−1332.35	−1329.18	−1326.02
175	−1344.30	−1342.74	−1341.16	−1339.57	−1337.99	−1334.82	−1331.66	−1328.49
200	−1346.88	−1345.35	−1343.76	−1342.18	−1340.60	−1337.43	−1334.26	−1331.09
225	−1349.58	−1348.08	−1346.50	−1344.91	−1343.33	−1340.16	−1336.99	−1333.83
250	−1352.40	−1350.94	−1349.36	−1347.77	−1346.19	−1343.02	−1339.85	−1336.69
300	−1358.33	−1357.02	−1355.44	−1353.85	−1352.27	−1349.10	−1345.93	−1342.77
350	−1364.62	−1363.56	−1361.97	−1360.39	−1358.81	−1355.64	−1352.47	−1349.30
400		−1370.53	−1368.94	−1367.36	−1365.78	−1362.61	−1359.44	−1356.27
450		−1377.91	−1376.33	−1374.74	−1373.16	−1369.99	−1366.82	−1363.66
500		−1385.68	−1384.10	−1382.52	−1380.93	−1377.77	−1374.60	−1371.43
550		−1393.83	−1392.25	−1390.67	−1389.08	−1385.92	−1382.75	−1379.58
600		−1402.35	−1400.76	−1399.18	−1397.60	−1394.43	−1391.26	−1388.09
700		−1420.40	−1418.82	−1417.23	−1415.65	−1412.48	−1409.32	−1406.15
800		−1439.76	−1438.18	−1436.59	−1435.01	−1431.84	−1428.67	−1425.50
900		−1460.34	−1458.75	−1457.17	−1455.59	−1452.42	−1449.25	−1446.08
1000		−1482.07	−1480.49	−1478.91	−1477.32	−1474.16	−1470.99	−1467.82
				Pyrophyllite				
25	−1259.02	−1257.50	−1255.97	−1254.44	−1252.91	−1249.86	−1246.80	−1243.75
50	−1260.53	−1259.00	−1257.47	−1255.94	−1254.42	−1251.36	−1248.31	−1245.25
75	−1262.17	−1260.65	−1259.12	−1257.59	−1256.06	−1253.01	−1249.95	−1246.90
100	−1263.96	−1262.43	−1260.90	−1259.38	−1257.85	−1254.79	−1251.74	−1248.68

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Pyrophyllite — Continued				
125	−1265.87	−1264.35	−1262.82	−1261.30	−1259.77	−1256.71	−1253.66	−1250.60
150	−1267.92	−1266.40	−1264.88	−1263.35	−1261.82	−1258.77	−1255.71	−1252.66
175	−1270.08	−1268.58	−1267.06	−1265.53	−1264.00	−1260.95	−1257.89	−1254.84
200	−1272.36	−1270.89	−1269.36	−1267.83	−1266.30	−1263.25	−1260.19	−1257.14
225	−1274.76	−1273.31	−1271.78	−1270.25	−1268.72	−1265.67	−1262.61	−1259.56
250	−1277.25	−1275.84	−1274.31	−1272.79	−1271.26	−1268.20	−1265.15	−1262.09
300	−1282.51	−1281.25	−1279.72	−1278.19	−1276.67	−1273.61	−1270.56	−1267.50
350	−1288.10	−1287.08	−1285.55	−1284.02	−1282.50	−1279.44	−1276.39	−1273.33
400		−1293.31	−1291.79	−1290.26	−1288.73	−1285.68	−1282.62	−1279.57
450		−1299.93	−1298.41	−1296.88	−1295.35	−1292.30	−1289.24	−1286.19
500		−1306.92	−1305.39	−1303.87	−1302.34	−1299.28	−1296.23	−1293.17
550		−1314.26	−1312.73	−1311.21	−1309.68	−1306.62	−1303.57	−1300.51
600		−1321.94	−1320.42	−1318.89	−1317.36	−1314.31	−1311.25	−1308.20
700		−1338.28	−1336.75	−1335.23	−1333.70	−1330.64	−1327.59	−1324.53
800		−1355.85	−1354.32	−1352.80	−1351.27	−1348.21	−1345.16	−1342.10
900		−1374.59	−1373.06	−1371.53	−1370.01	−1366.95	−1363.90	−1360.84
1000		−1394.44	−1392.91	−1391.38	−1389.85	−1386.80	−1383.74	−1380.69
				Quartz				
25	−204.65	−204.38	−204.10	−203.83	−203.56	−203.03	−202.49	−201.95
50	−204.90	−204.63	−204.36	−204.09	−203.82	−203.28	−202.74	−202.20
75	−205.18	−204.91	−204.64	−204.37	−204.10	−203.56	−203.02	−202.48
100	−205.49	−205.21	−204.94	−204.67	−204.40	−203.86	−203.32	−202.78
125	−205.81	−205.54	−205.26	−204.99	−204.72	−204.18	−203.64	−203.10
150	−206.15	−205.88	−205.60	−205.33	−205.06	−204.52	−203.97	−203.43
175	−206.51	−206.24	−205.96	−205.69	−205.42	−204.88	−204.33	−203.79
200	−206.88	−206.62	−206.34	−206.07	−205.80	−205.25	−204.71	−204.17
225	−207.28	−207.02	−206.74	−206.47	−206.20	−205.65	−205.11	−204.56
250	−207.68	−207.43	−207.16	−206.88	−206.61	−206.06	−205.52	−204.98
300	−208.54	−208.32	−208.04	−207.77	−207.49	−206.94	−206.40	−205.85
350	−209.45	−209.27	−208.99	−208.71	−208.44	−207.89	−207.34	−206.79
400		−210.28	−210.00	−209.73	−209.45	−208.90	−208.35	−207.80
450		−211.35	−211.07	−210.80	−210.52	−209.97	−209.42	−208.87
500		−212.48	−212.20	−211.93	−211.65	−211.09	−210.54	−209.99
550		−213.67	−213.39	−213.11	−212.83	−212.28	−211.72	−211.17
600		−214.91	−214.62	−214.35	−214.07	−213.51	−212.95	−212.40
700		−217.56	−217.27	−216.99	−216.71	−216.14	−215.57	−215.01
800		−220.37	−220.09	−219.81	−219.52	−218.96	−218.39	−217.82
900		−223.34	−223.06	−222.78	−222.49	−221.93	−221.36	−220.79
1000		−226.46	−226.17	−225.89	−225.61	−225.04	−224.47	−223.91
				Sanidine, High				
25	−895.43	−894.13	−892.83	−891.52	−890.22	−887.62	−885.01	−882.40
50	−896.85	−895.54	−894.24	−892.94	−891.63	−889.03	−886.42	−883.82
75	−898.36	−897.06	−895.75	−894.45	−893.15	−890.54	−887.94	−885.33
100	−899.97	−898.67	−897.36	−896.06	−894.76	−892.15	−889.55	−886.94
125	−901.67	−900.37	−899.07	−897.77	−896.46	−893.86	−891.25	−888.65
150	−903.46	−902.17	−900.87	−899.56	−898.26	−895.66	−893.05	−890.45
175	−905.33	−904.06	−902.75	−901.45	−900.15	−897.54	−894.94	−892.33
200	−907.29	−906.03	−904.72	−903.42	−902.12	−899.51	−896.91	−894.30
225	−909.31	−908.08	−906.78	−905.47	−904.17	−901.56	−898.96	−896.35
250	−911.41	−910.21	−908.91	−907.61	−906.30	−903.70	−901.09	−898.49
300	−915.78	−914.70	−913.40	−912.10	−910.80	−908.19	−905.58	−902.98
350	−920.36	−919.48	−918.18	−916.88	−915.58	−912.97	−910.37	−907.76
400		−924.54	−923.23	−921.93	−920.63	−918.02	−915.42	−912.81
450		−929.84	−928.54	−927.24	−925.94	−923.33	−920.72	−918.12
500		−935.39	−934.09	−932.79	−931.48	−928.88	−926.27	−923.67
550		−941.17	−939.87	−938.57	−937.26	−934.66	−932.05	−929.45
600		−947.17	−945.87	−944.56	−943.26	−940.65	−938.05	−935.44
700		−959.78	−958.48	−957.17	−955.87	−953.27	−950.66	−948.06

TABLE 3. Calculated apparent standard molal Gibbs free energies of formation (in kcal/mol) of 22 minerals as a function of temperature and pressure (see text) — Continued

T, °C	Pressure, kbar							
	Sat.	0.5	1.0	1.5	2.0	3.0	4.0	5.0
				Sanidine, High — Continued				
800		−973.16	−971.86	−970.55	−969.25	−966.65	−964.04	−961.43
900		−987.25	−985.95	−984.64	−983.34	−980.73	−978.13	−975.52
1000		−1002.00	−1000.70	−999.40	−998.09	−995.49	−992.88	−990.28
				Sillimanite				
25	−583.02	−582.42	−581.83	−581.23	−580.63	−579.44	−578.25	−577.05
50	−583.63	−583.03	−582.43	−581.84	−581.24	−580.05	−578.86	−577.66
75	−584.30	−583.70	−583.10	−582.51	−581.91	−580.72	−579.53	−578.33
100	−585.02	−584.43	−583.83	−583.24	−582.64	−581.45	−580.25	−579.06
125	−585.81	−585.21	−584.62	−584.02	−583.42	−582.23	−581.04	−579.85
150	−586.65	−586.06	−585.46	−584.86	−584.27	−583.07	−581.88	−580.69
175	−587.54	−586.95	−586.35	−585.76	−585.16	−583.97	−582.78	−581.58
200	−588.48	−587.90	−587.30	−586.71	−586.11	−584.92	−583.72	−582.53
225	−589.46	−588.90	−588.30	−587.71	−587.11	−585.92	−584.72	−583.53
250	−590.49	−589.95	−589.35	−588.75	−588.16	−586.96	−585.77	−584.58
300	−592.68	−592.18	−591.59	−590.99	−590.39	−589.20	−588.01	−586.81
350	−594.99	−594.59	−594.00	−593.40	−592.81	−591.61	−590.42	−589.23
400		−597.18	−596.58	−595.98	−595.39	−594.19	−593.00	−591.81
450		−599.91	−599.32	−598.72	−598.12	−596.93	−595.74	−594.55
500		−602.80	−602.20	−601.61	−601.01	−599.82	−598.63	−597.43
550		−605.83	−605.23	−604.64	−604.04	−602.85	−601.66	−600.46
600		−608.99	−608.40	−607.80	−607.21	−606.01	−604.82	−603.63
700		−615.70	−615.11	−614.51	−613.91	−612.72	−611.53	−610.34
800		−622.88	−622.29	−621.69	−621.10	−619.90	−618.71	−617.52
900		−630.50	−629.91	−629.31	−628.71	−627.52	−626.33	−625.14
1000		−638.53	−637.93	−637.34	−636.74	−635.55	−634.36	−633.16

TABLE 4. Calculated apparent standard molal Gibbs free energies (in kcal/mol) of 18 gases as a function of temperature (see text)

	Gases								
T, °C	Ar	CH_4	C_2H_4	CO	CO_2	H_2	H_2O	H_2S	He
25	0.00	−12.12	16.28	−32.78	−94.25	0.00	−54.53	−8.02	0.00
50	−0.93	−13.24	14.96	−33.97	−95.54	−0.79	−55.65	−9.26	−0.76
75	−1.87	−14.38	13.63	−35.17	−96.84	−1.59	−56.80	−10.51	−1.53
100	−2.82	−15.54	12.29	−36.39	−98.17	−2.40	−58.11	−11.78	−2.30
125	−3.78	−16.71	10.94	−37.61	−99.50	−3.23	−59.29	−13.07	−3.09
150	−4.74	−17.90	9.58	−38.85	−100.86	−4.06	−60.48	−14.36	−3.88
175	−5.71	−19.10	8.20	−40.10	−102.23	−4.91	−61.68	−15.67	−4.68
200	−6.69	−20.32	6.82	−41.36	−103.61	−5.77	−62.90	−17.00	−5.49
225	−7.68	−21.55	5.43	−42.63	−105.01	−6.63	−64.12	−18.33	−6.31
250	−8.67	−22.79	4.02	−43.90	−106.42	−7.50	−65.36	−19.68	−7.13
300	−10.67	−25.33	1.19	−46.48	−109.28	−9.28	−67.87	−22.40	−8.79
350	−12.70	−27.91	−1.68	−49.09	−112.19	−11.08	−70.41	−25.17	−10.47
400	−14.74	−30.55	−4.58	−51.73	−115.15	−12.91	−72.99	−27.97	−12.17
450	−16.80	−33.23	−7.50	−54.40	−118.15	−14.77	−75.60	−30.81	−13.89
500	−18.88	−35.96	−10.46	−57.09	−121.18	−16.65	−78.25	−33.69	−15.62
550	−20.97	−38.74	−13.44	−59.81	−124.26	−18.56	−80.92	−36.59	−17.37
600	−23.08	−41.57	−16.45	−62.55	−127.38	−20.48	−83.62	−39.53	−19.14
700	−27.35	−47.35	−22.53	−68.10	−133.71	−24.40	−89.10	−45.49	−22.72
800	−31.66	−53.30	−28.70	−73.73	−140.16	−28.39	−94.69	−51.57	−26.35
900	−36.02	−59.42	−34.94	−79.43	−146.74	−32.45	−100.37	−57.74	−30.02
1000	−40.42	−65.71	−41.26	−85.20	−153.42	−36.57	−106.13	−64.01	−33.74

T, °C	Kr	N_2	NH_3	Ne	O_2	Rn	S_2	SO_2	Xe
25	0.00	0.00	−3.93	0.00	0.00	0.00	18.95	−71.75	0.00
50	−0.99	−1.15	−5.09	−0.88	−1.23	−1.06	17.58	−73.24	−1.02
75	−1.98	−2.32	−6.27	−1.77	−2.48	−2.13	16.19	−74.75	−2.05
100	−2.98	−3.50	−7.46	−2.67	−3.74	−3.20	14.79	−76.28	−3.08
125	−4.00	−4.69	−8.66	−3.57	−5.01	−4.29	13.38	−77.83	−4.13
150	−5.02	−5.89	−9.89	−4.49	−6.29	−5.38	11.95	−79.40	−5.18
175	−6.04	−7.10	−11.12	−5.41	−7.59	−6.48	10.51	−80.98	−6.25
200	−7.08	−8.32	−12.37	−6.34	−8.89	−7.59	9.06	−82.57	−7.31
225	−8.12	−9.55	−13.63	−7.27	−10.21	−8.70	7.60	−84.18	−8.39
250	−9.17	−10.79	−14.91	−8.21	−11.53	−9.82	6.12	−85.81	−9.47
300	−11.28	−13.30	−17.49	−10.11	−14.20	−12.08	3.15	−89.10	−11.65
350	−13.41	−15.84	−20.12	−12.03	−16.91	−14.36	0.13	−92.44	−13.85
400	−15.57	−18.41	−22.79	−13.98	−19.65	−16.66	−2.92	−95.82	−16.07
450	−17.74	−21.00	−25.51	−15.94	−22.42	−18.97	−6.00	−99.26	−18.31
500	−19.93	−23.62	−28.26	−17.91	−25.21	−21.31	−9.11	−102.73	−20.56
550	−22.13	−26.27	−31.05	−19.91	−28.03	−23.66	−12.24	−106.24	−22.84
600	−24.35	−28.94	−33.88	−21.91	−30.87	−26.02	−15.41	−109.79	−25.12
700	−28.84	−34.34	−39.64	−25.97	−36.63	−30.80	−21.81	−117.00	−29.74
800	−33.37	−39.82	−45.53	−30.08	−42.46	−35.62	−28.31	−124.33	−34.41
900	−37.95	−45.37	−51.55	−34.24	−48.38	−40.49	−34.88	−131.79	−39.12
1000	−42.57	−50.99	−57.69	−38.44	−54.36	−45.40	−41.54	−139.36	−43.88

TABLE 5. Chemical formulas of the 97 aqueous organic species considered in the present study

Organic species	Formula	Organic species	Formula
1-Butanamime	$C_4H_9NH_2$	Formaldehyde	HCHO
1-Butanol	C_4H_9OH	Formate	$HCOO^-$
1-Butene	C_4H_8	Formic Acid	HCOOH
1-Butyne	C_4H_6	Glutamic Acid	$C_5H_9NO_4$
1-Heptanamine	$C_7H_{15}NH_2$	Glutamine	$C_5H_{10}N_2O_3$
1-Heptanol	$C_7H_{15}OH$	Glycine	$C_2H_5NO_2$
1-Heptene	C_7H_{14}	Heptanoate	$C_6H_{13}COO^-$
1-Heptyne	C_7H_{12}	Heptanoic Acid	$C_6H_{13}COOH$
1-Hexanamine	$C_6H_{13}NH_2$	Hexanoate	$C_5H_{11}COO^-$
1-Hexanol	$C_6H_{13}OH$	Hexanoic Acid	$C_5H_{11}COOH$
1-Hexene	C_6H_{12}	Isoleucine	$C_6H_{13}NO_2$
1-Hexyne	C_6H_{10}	Leucine	$C_6H_{13}NO_2$
1-Octanamine	$C_8H_{17}NH_2$	Methanamine	CH_3NH_2
1-Octanol	$C_8H_{17}OH$	Methane	CH_4
1-Octene	C_8H_{16}	Methanol	CH_3OH
1-Octyne	C_8H_{14}	Methionine	$C_5H_{11}NO_2S$
1-Pentanamine	$C_5H_{11}NH_2$	Monochloroacetate	CH_2ClCOO^-
1-Pentanol	$C_5H_{11}OH$	Monochloroacetic Acid	$CH_2ClCOOH$
1-Pentene	C_5H_{10}	Monochloroacetyl Chloride	$CH_2ClCOCl$
1-Pentyne	C_5H_8	N-Butane	C_4H_{10}
1-Propanamine	$C_3H_7NH_2$	N-Butylbenzene	$C_6H_5C_4H_9$
1-Propanol	C_3H_7OH	N-Heptane	C_7H_{16}
1-Propene	C_3H_6	N-Heptylbenzene	$C_6H_5C_7H_{15}$
1-Propyne	C_3H_4	N-Hexane	C_6H_{14}
2-Butanone	C_4H_8O	N-Hexylbenzene	$C_6H_5C_6H_{13}$
2-Heptanone	$C_7H_{14}O$	N-Octane	C_8H_{18}
2-Hexanone	$C_6H_{12}O$	N-Octylbenzene	$C_6H_5C_8H_{17}$
2-Octanone	$C_8H_{16}O$	N-Pentane	C_5H_{12}
2-Pentanone	$C_5H_{10}O$	N-Pentylbenzene	$C_6H_5C_5H_{11}$
A-Aminobutyric Acid	$C_4H_9NO_2$	N-Propylbenzene	$C_6H_5C_3H_7$
Acetate	CH_3COO^-	Octanoate	$C_7H_{15}COO^-$
Acetic Acid	CH_3COOH	Octanoic Acid	$C_7H_{15}COOH$
Acetyl Chloride	CH_3COCl	Pentanoate	$C_4H_9COO^-$
Acetone	C_3H_6O	Pentanoic Acid	C_4H_9COOH
Alanine	$C_3H_7NO_2$	Phenol	C_6H_5OH
Asparagine	$C_4H_8N_2O_3$	Phenylalanine	$C_9H_{11}NO_2$
Aspartic Acid	$C_4H_7NO_4$	Propane	C_3H_8
Benzene	C_6H_6	Propanoate	$C_2H_5COO^-$
Butanoate	$C_3H_7COO^-$	Propanoic Acid	C_2H_5COOH
Butanoic Acid	C_3H_7COOH	Serine	$C_3H_7NO_3$
Dichloroacetate	$CHCl_2COO^-$	Threonine	$C_4H_9NO_3$
Dichloroacetic Acid	$CHCl_2COOH$	Toluene	$C_6H_5CH_3$
Dichloroacetyl Chloride	$CHCl_2COCl$	Trichloroacetate	CCl_3COO^-
Ethanamine	$C_2H_5NH_2$	Trichloroacetic Acid	CCl_3COOH
Ethane	C_2H_6	Trichloroacetyl Chloride	CCl_3COCl
Ethanol	C_2H_5OH	Tryptophan	$C_{11}H_{12}N_2O_2$
Ethylbenzene	$C_6H_5C_2H_5$	Tyrosine	$C_9H_{11}NO_3$
Ethylene	C_2H_4	Valine	$C_5H_{11}NO_2$
Ethyne	C_2H_2		

TABLE 6. Index of the aqueous species considered in the present study and their references

Species	Reference	Page	Species	Reference	Page
1-Butanamide	SH2	1408	BO_2^-	SH1	1433
1-Butanol	SH2	1408	Ba^{+2}	SH1	1433
1-Butene	SH2	1408	$BaCO_3^\circ$	SSH	1433
1-Butyne	SH2	1409	$BaCl^+$	SSH	1434
1-Heptanamine	SH2	1409	BaF^+	SSH	1434
1-Heptanol	SH2	1409	Be^{+2}	SH1	1434
1-Heptene	SH2	1410	BeO_2^{-2}	SH1	1435
1-Heptyne	SH2	1410	Br^-	SH1	1435
1-Hexanamine	SH2	1411	Br_3^-	SH1	1436
1-Hexanol	SH2	1411	BrO^-	SH1	1436
1-Hexene	SH2	1411	BrO_3^-	SH1	1436
1-Hexyne	SH2	1412	BrO_4^-	SH1	1437
1-Octanamine	SH2	1412	CN^-	SH1	1437
1-Octanol	SH2	1413	CO°	SM	1438
1-Octene	SH2	1413	CO_2°	SHS	1438
1-Octyne	SH2	1413	CO_3^{-2}	SH1	1438
1-Pentanamine	SH2	1414	Ca^{+2}	SH1	1439
1-Pentanol	SH2	1414	$Ca(CH_3COO)^+$	SK	1439
1-Pentene	SH2	1414	$Ca(CH_3COO)_2^\circ$	SK	1440
1-Pentyne	SH2	1415	$CaCO_3^\circ$	SSH	1440
1-Propanamine	SH2	1415	$CaCl^+$	SSH	1440
1-Propanol	SH2	1416	$CaCl_2^\circ$	SSH	1441
1-Propene	SH2	1416	$CaHCO_3^+$	SSH	1441
1-Propyne	SH2	1416	CaF^+	SSH	1441
2-Butanone	SH2	1417	$CaSO_4^\circ$	SSH	1442
2-Heptanone	SH2	1417	Cd^{+2}	SH1	1442
2-Hexanone	SH2	1418	Ce^{+3}	SH1	1443
2-Octanone	SH2	1418	Cl^-	SH1	1443
2-Pentanone	SH2	1418	ClO^-	SH1	1443
A-Aminobutyric Acid	SH2	1419	ClO_2^-	SH1	1444
Acetate	SH2	1419	ClO_3^-	SH1	1444
Acetic Acid	SH2	1419	ClO_4^-	SH1	1445
Acetone	SH2	1420	Co^{+2}	SH1	1445
Acetyl Chloride	H1	1420	Co^{+3}	SH1	1445
Alanine	SH2	1421	CrO_4^{-2}	SH1	1446
Asparagine	SH2	1421	$Cr_2O_7^{-2}$	SH1	1446
Aspartic Acid	SH2	1421	Cs^+	SH1	1446
Ag^+	SH1	1422	$CsBr^\circ$	SSH	1447
Ag^{+2}	SH1	1422	$CsCl^\circ$	SSH	1447
$Ag(CH_3COO)^\circ$	SK	1423	CsI°	SSH	1448
$Ag(CH_3COO)_2^-$	SK	1423	Cu^+	SH1	1448
$Ag(CO_3)^-$	SSH	1423	Cu^{+2}	SH1	1448
$Ag(CO_3)_2^{-3}$	SSH	1424	$Cu(CH_3COO)^\circ$	SK	1449
$AgCl^\circ$	SSH	1424	$Cu(CH_3COO)_2^-$	SK	1449
$AgCl_2^-$	SSH	1424	$Cu(CH_3COO)^+$	SK	1450
$AgCl_3^{-2}$	SSH	1425	$Cu(CH_3COO)_2^\circ$	SK	1450
$AgCl_4^{-3}$	SSH	1425	$Cu(CH_3COO)_3^-$	SK	1450
$AgNO_3^\circ$	SSH	1426	Dichloroacetate	H1	1451
Al^{+3}	PH1	1426	Dichloroacetic Acid	H1	1451
$Al(CH_3COO)^{+2}$	*	1426	Dichloroacetyl Chloride	H1	1451
$Al(CH_3COO)_2^+$	*	1427	Dy^{+3}	SH1	1452
$AlHO_2^\circ$	PH1	1427	Ethanamine	SH2	1452
$Al(OH)^{+2}$	PH1	1428	Ethane	SH2	1453
$Al(OH)_2^+$	PH1	1428	Ethanol	SH2	1453
AlO_2^-	PH1	1428	Ethylbenzene	SH2	1453
Ar°	SHS	1429	Ethylene	SH2	1454
Au^+	SH1	1429	Ethyne	SH2	1454
Au^{+3}	SH1	1429	Er^{+3}	SH1	1455
$Au(CH_3COO)^\circ$	SK	1430	Eu^{+2}	SH1	1455
$Au(CH_3COO)_2^-$	SK	1430	Eu^{+3}	SH1	1455
Benzene	SH2	1431	Formaldehyde	ScS	1456
Butanoate	SH2	1431	Formate	SH2	1456
Butanoic Acid	SH2	1431	Formic Acid	SH2	1456
BF_4^-	SH1	1432	F^-	SH1	1457
$B(OH)_3^\circ$	SHS	1432	Fe^{+2}	SH1	1457

TABLE 6. Index of the aqueous species considered in the present study and their references — Continued

Species	Reference	Page	Species	Reference	Page
Fe^{+3}	SH1	1458	KOH°	PH3	1483
$Fe(CH_3COO)^{+}$	SK	1458	HSO_4^{-}	SSH	1483
$Fe(CH_3COO)_2^{\circ}$	SK	1458	Kr°	SHS	1483
$FeCl^{+}$	SSH	1459	Leucine	SH2	1484
$FeCl_2^{\circ}$	SSH	1459	La^{+3}	SH1	1484
Glutamic Acid	SH2	1460	Li^{+}	SH1	1485
Glutamine	SH2	1460	$Li(CH_3COO)^{\circ}$	SK	1485
Glycine	SH2	1460	$Li(CH_3COO)_2^{-}$	SK	1485
Ga^{+3}	SH1	1461	$LiCl^{\circ}$	SSH	1486
Gd^{+3}	SH1	1461	Lu^{+3}	SH1	1486
Heptanoate	SH2	1461	Methanamine	SH2	1486
Heptanoic Acid	SH2	1462	Methane	SH2	1487
Hexanoate	SH2	1462	Methanol	SH2	1487
Hexanoic Acid	SH2	1463	Methionine	SH2	1488
H^{+}	SH1	1463	Monochloroacetate	H1	1488
H_2°	SHS	1463	Monochloroacetic Acid	H1	1488
$HAsO_4^{-2}$	SH1	1464	Monochloroacetyl Chloride	H1	1489
$H_2AsO_3^{-}$	SH1	1464	Mg^{+2}	SH1	1489
$H_2AsO_4^{-}$	SH1	1465	$Mg(CH_3COO)^{+}$	SK	1490
HBr°	PH2	1465	$Mg(CH_3COO)_2^{\circ}$	SK	1490
HCN°	SM	1465	$MgCO_3^{\circ}$	SSH	1490
HCO_3^{-}	SH1	1466	$MgCl^{+}$	SSH	1491
HCl°	PH2	1466	MgF^{+}	SSH	1491
$HCrO_4^{-}$	SH1	1466	$MgHCO_3^{+}$	SSH	1491
HF°	SHS	1467	Mn^{+2}	SH1	1492
HF_2^{-}	SH1	1467	$MnCl^{+}$	SSH	1492
HO_2^{-}	SH1	1468	MnO_4^{-}	SH1	1493
HPO_4^{-2}	SH1	1468	MnO_4^{-2}	SSH	1493
$H_2PO_4^{-}$	SH1	1468	$MnSO_4^{\circ}$	SSH	1493
$H_2P_2O_7^{-2}$	SH1	1469	MoO_4^{-2}	SH1	1494
$H_3PO_4^{\circ}$	SHS	1469	N-Butane	SH2	1494
$H_3P_2O_7^{-}$	SH1	1470	N-Butylbenzene	SH2	1495
HS^{-}	SH1	1470	N-Heptane	SH2	1495
HSO_3^{-}	SH1	1470	N-Heptylbenzene	SH2	1495
HSO_4^{-}	SH1	1471	N-Hexane	SH2	1496
HSO_5^{-}	SH1	1471	N-Hexylbenzene	SH2	1496
H_2S°	SHS	1471	N-Octane	SH2	1496
HSe^{-}	SH1	1472	N-Octylbenzene	SH2	1497
$HSeO_3^{-}$	SH1	1472	N-Pentane	SH2	1497
$HSeO_4^{-}$	SH1	1473	N-Pentylbenzene	SH2	1498
$HSiO_3^{-}$	SSH	1473	N-Propylbenzene	SH2	1498
HVO_4^{-2}	SH1	1473	N_2°	SHS	1498
$H_2VO_4^{-}$	SH1	1474	NH_3°	SHS	1499
He°	SHS	1474	NH_4^{+}	SH1	1499
Hg^{+2}	SH1	1475	NO_2^{-}	SH1	1500
Hg_2^{+2}	SH1	1475	NO_3^{-}	SH1	1500
$Hg(CH_3COO)^{+}$	SK	1475	Na^{+}	SH1	1500
$Hg(CH_3COO)_2^{\circ}$	SK	1476	$NaAlO_2^{\circ}$	PH1	1501
$Hg(CH_3COO)_3^{-}$	SK	1476	$NaBr^{\circ}$	SSH	1501
Ho^{+3}	SH1	1476	$Na(CH_3COO)^{\circ}$	SK	1501
Isoleucine	SH2	1477	$Na(CH_3COO)_2^{-}$	SK	1502
I^{-}	SH1	1477	$NaCl^{\circ}$	SSH	1502
I_3^{-}	SH1	1478	NaF°	SSH	1503
IO^{-}	SH1	1478	$NaHSiO_3^{\circ}$	SSH	1503
IO_3^{-}	SH1	1478	NaI°	SSH	1503
IO_4^{-}	SH1	1479	$NaOH^{\circ}$	PH1	1504
In^{+3}	SH1	1479	Nd^{+3}	SH1	1504
K^{+}	SH1	1480	Ne°	SHS	1505
$KAlO_2^{\circ}$	PH3	1480	Ni^{+2}	SH1	1505
KBr°	SSH	1480	$Ni(CH_3COO)^{+}$	SK	1505
$K(CH_3COO)^{\circ}$	SK	1481	$Ni(CH_3COO)_2^{\circ}$	SK	1506
$K(CH_3COO)_2^{-}$	SK	1481	$Ni(CH_3COO)_3^{-}$	SK	1506
KCl°	PH2	1481	$NiCl^{+}$	SSH	1506
$KHSO_4^{\circ}$	SSH	1482	Octanoate	SH2	1507
KI°	SSH	1482	Octanoic Acid	SH2	1507

TABLE 6. Index of the aqueous species considered in the present study and their references — Continued

Species	Reference	Page
O_2°	SHS	1508
OH^-	SH1	1508
Pentanoate	SH2	1508
Pentanoic Acid	SH2	1509
Phenol	SH2	1509
Phenylalanine	SH2	1510
Propane	SH2	1510
Propanoate	SH2	1510
Propanoic Acid	SH2	1511
PO_4^{-3}	SH1	1511
Pb^{+2}	SH1	1511
$Pb(CH_3COO)^+$	SK	1512
$Pb(CH_3COO)_2^\circ$	SK	1512
$PbCl^+$	SSH	1513
$PbCl_2^\circ$	SSH	1513
$PbCl_3^-$	SSH	1513
$PbCl_4^{-2}$	SSH	1514
Pd^{+2}	SH1	1514
$PdCl^+$	SaS	1515
$PdCl_2^\circ$	SaS	1515
$PdCl_3^-$	SaS	1515
$PdCl_4^{-2}$	SaS	1516
$PdOH^+$	SaS	1516
PdO°	SaS	1516
Pr^{+3}	SH1	1517
Ra^{+2}	SH1	1517
Rb+	SH1	1518
$RbBr^\circ$	SSH	1518
$RbCl^\circ$	SSH	1518
RbF°	SSH	1519
RbI°	SSH	1519
ReO_4^-	SH1	1520
Rn°	SHS	1520
Serine	SH2	1520
S_2^{-2}	SH1	1521
SO_2°	SHS	1521
SO_3^{-2}	SH1	1521
SO_4^{-2}	SH1	1522
$S_2O_3^{-2}$	SH1	1522
$S_2O_4^{-2}$	SH1	1523
$S_2O_5^{-2}$	SH1	1523
$S_2O_6^{-2}$	SH1	1523
$S_2O_8^{-2}$	SH1	1524
S_3^{-2}	SH1	1524
$S_3O_6^{-2}$	SH1	1525
S_4^{-2}	SH1	1525
$S_4O_6^{-2}$	SH1	1525
S_5^{-2}	SH1	1526
$S_5O_6^{-2}$	SH1	1526
Sc^{+3}	SH1	1526
SeO_3^{-2}	SH1	1527
SeO_4^{-2}	SH1	1527
SiF_6^{-2}	SH1	1528
SiO_2°	SHS	1528
Sm^{+2}	SH1	1528
Sm^{+3}	SH1	1529
Sn^{+2}	SH1	1529
Sr^{+2}	SH1	1530
$SrCO_3^\circ$	SSH	1530
$SrCl^+$	SSH	1530
SrF^+	SSH	1531
Threonine	SH2	1531
Trichloroacetate	H1	1531
Trichloroacetic Acid	H1	1532
Trichloroacetyl Chloride	H1	1532
Toluene	SH2	1533
Tryptophan	SH2	1533
Tyrosine	SH2	1533
Tb^{+3}	SH1	1534
Tl^+	SH1	1534
Tl^{+3}	SH1	1535
Tm^{+3}	SH1	1535
Valine	SH2	1535
VO^{+2}	SH1	1536
VO_2^+	SH1	1536
WO_4^{-2}	SH1	1536
Xe°	SHS	1537
Y^{+3}	SH1	1537
Yb^{+2}	SH1	1538
Yb^{+3}	SH1	1538
Zn^{+2}	SH1	1538
$Zn(CH_3COO)^+$	SK	1539
$Zn(CH_3COO)_2^\circ$	SK	1539
$Zn(CH_3COO)_3^-$	SK	1540
$ZnCl^+$	SSH	1540
$ZnCl_2^\circ$	SSH	1540
$ZnCl_3^-$	SSH	1541
$ZnCl_4^{-2}$	SSH	1541

References:

H1: Helgeson (1992a)
PH1: Pokrovskii and Helgeson (1995a)
PH2: Pokrovskii and Helgeson (1995b)
PH3: Pokrovskii and Helgeson (1995c)
SH1: Shock and Helgeson (1988)
SH2: Shock and Helgeson (1990)
SaS: Sassani and Shock (1990)
ScS: Schulte and Shock (1993)
SHS: Shock *et al.* (1989)
SK: Shock and Koretsky (1993)
SM: Shock and McKinnon (1993)
SSH: Sverjensky *et al.* (1995)

*: Computed using equation of state parameters generated from the procedure outlined by Shock and Koretsky (1993) together with values of ΔG, ΔS and ΔV consistent with the thermodynamic properties of aqueous Al^{+3} reported by Pokrovskii and Helgeson (1995a). The resulting equation of state parameters are:

Parameter	$Al(CH_3COO)^{+2}$	$Al(CH_3COO)_2^+$
$\overline{\Delta G}_f^\circ$ (cal/mol)	−208564	−299359
$\overline{S}^\circ_{P_r,T_r}$ (cal/mol/K)	−32.77	8.52
$a_1\times10$ (cal/mol/bar)	2.1643	8.5167
$a_2\times10^{-2}$ (cal/mol)	−2.4961	13.0156
a_3 (cal K/mol/bar)	6.7288	0.6302
$a_4\times10^{-4}$ (cal K/mol)	−2.6757	−3.317
c_1 (cal/mol/K)	63.2437	109.3239
$c_2\times10^{-4}$ (cal K/mol)	11.8151	31.4722
$\omega\times10^{-5}$ (cal/mol)	1.5579	0.4210

TABLE 7. Index of minerals considered in the present study and their chemical formulas

Mineral	Formula	Page
Albite	$NaAlSi_3O_8$	1544
Albite, Low	$NaAlSi_3O_8$	1544
Albite, High	$NaAlSi_3O_8$	1544
Analcime	$NaAlSi_2O_6 \cdot H_2O$	1545
Andalusite	Al_2SiO_5	1545
Boehmite	AlO(OH)	1545
Corundum	Al_2O_3	1546
Diaspore	AlO(OH)	1546
Gibbsite	$Al(OH)_3$	1547
Jadeite	$NaAl(SiO_3)_2$	1547
K-Feldspar	$KAlSi_3O_8$	1547
Kalsilite	$KAlSiO_4$	1548
Kaolinite	$Al_2Si_2O_5(OH)_4$	1548
Kyanite	Al_2SiO_5	1549
Microcline, Maximum	$KAlSi_3O_8$	1549
Muscovite	$KAl_2(AlSi_3)O_{10}(OH)_2$	1549
Nepheline	$NaAlSiO_4$	1550
Paragonite	$NaAl_2(AlSi_3)O_{10}(OH)_2$	1550
Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$	1550
Quartz	SiO_2	1551
Sanidine, High	$KAlSi_3O_8$	1551
Sillimanite	Al_2SiO_5	1552

7. Acknowledgments

The research described above was supported by the National Science Foundation (NSF grants EAR 74–14280, EAR 77–14492, EAR 81–15859, EAR 83–19401, EAR 84–15235, EAR 86–06052, and EAR 91–17393), the Department of Energy (DOE Grant DE–FG03–85ER–13419) and the committee on Research at the University of California, Berkeley. We are indebted to Barbara L. Ransom, William M. Murphy, Jacques Schott, Christophe Monnin, and Jan Amend for helpful discussions, encouragement, and assistance during the course of this study. The impetus for the present communication stems from a conversation one of us (HCH) had long ago (1981) with George Skippen, Terry Gordon, and Edgar Froese in Ottawa, all of whom urged generation for field geologists of a written compilation of values for aqueous species, minerals and gases at high temperatures and pressures. We regret that it has taken nearly 15 years to produce such a compilation.

8. References

Anderson, G. M. and C. W. Berman, The solubility of quartz in supercritical water, Am. J. Sci. **263,** 494 (1965).

Apps, J. A., J. M. Neil, and C. H. Jun, Thermochemical properties of gibbsite, bayerite, boehmite, diaspore, and of the aluminate ion between 0 and 350 °C, Division of Waste Management., Office of Nuclear Material Safety and Safeguards. US NRC NUREG/CR-5271-LBL 21482 (1989).

Barany. R. and K. K. Kelley, Heats and free energies of formation of gibbsite, kaolinite, halloysite and dickite, U.S. Bur. Mines Report **5825,** 13p (1961).

Benson, S. W., Thermochemical Kinetics, New York, John Wiley & Sons, p. 223 (1968).

Benson, B. B., and D, Krause, Jr., Empirical laws for dilute solutions of polar gases," J. Chem. Phys. **64,** 655 (1976).

Bourcier, W. L., K. Knauss, and K. J. Jackson, Aluminum hydrolysis constants to 250 °C from bohemite solubilite measurements, Geochim. Cosmochim. Acta **57,** 747 (1993).

Castet, S., J.-L. Dandurand, J. Schott, and R. Gout, Boehmite solubility and aqueous aluminum speciation in hydrothermal solutions (90–350 °C): Experimental study and modeling, Geochim. Cosmochim. Acta **57,** 4869 (1993).

Claussen, W. F. and M. F. Polglase, Solubilities and structures in aqueous aliphatic hydrocarbon solutions, J. Am. Chem. Soc. **74,** 4817 (1952).

Crovetto, R., R. Fernandez-Prini, and M. L. Japas, Solubilities of inert gases and methane in H_2O and D_2O in the temperature range 300 to 600 K, J. Chem. Phys. **76,** 1077 (1982).

Devidal, J.-L. Solubilite et cinetique de dissolution/precipitation de la kaolinite en millieu hydrothermal: approche experimental et modelisation. Ph. D. Thesis, Université Paul Sabatier, Toulouse, France (1994).

Drummond, S. E., Boiling and mixing of hydrothermal fluids: Effects on mineral deposition. Ph. D. Thesis, Pennsylvania State University, p. 400 (1981).

Ellis, A. J. and R. M. Golding, The solubility of carbon dioxide above 100 °C in water and in sodium chloride solutions, Am. J. Sci. **261,** 47 (1963).

Fortier, J.-L., P.-A. Leduc, and J. E. Desnoyers, Thermodynamic properties of alkali halides. II. Enthalpies of dilution and heat capacities in water at 25 °C J. Soln. Chem. **3,** 323 (1974).

Frantz, J. D. and W. M. Marshall, Electrical conductances and ionization constants of calcium chloride and magnesium chloride in aqueous solutions at temperatures to 600 °C and pressures to 4000 bars, Am. J. Sci.. **282,** 1666 (1984).

Haar, L., J. S. Gallagher, and G. S. Kell, NBS/NRC Steam Tables. Hemisphere Publishing Corporation, p. 320 (1984).

Harned H. S. and R. Davis Jr., The ionization constant of carbonic acid in water and the solubility of carbon dioxide in water and aqueous salt solutions from 0 to 50°, J. Am. Chem. Soc. **65,** 2030 (1943).

Heinrich C. A. and T. M. Seward, A spectrographic study of aqueous iron (II) chloride complexing from 25 to 200 °C, Geochim. Cosmochim. Acta **54,** 2207 (1990).

Helgeson, H. C., Errata: Thermodynamics of minerals, reactions, and aqueous solutions at high pressures and temperatures, Am. J. Sci. **282,** 1143 (1982).

Helgeson, H. C., Errata II: Thermodynamics of minerals, reactions, and aqueous solutions at high pressures and temperatures, Am. J. Sci. **285,** 845 (1985).

Helgeson, H. C., Calculation of the thermodynamic properties and relative stabilities of aqueous acetic and chloroacetic acids, acetate and chloroacetates, and acetyl and chloroacetyl chlorides at high and low temperatures and pressures, Applied Geochem. **7,** 291 (1992a).

Helgeson, H. C., Effects of complex formation in flowing fluids on the hydrothermal solubilities of minerals as a function of fluid pressure in the critical and supercritical regions of the system H_2O, Geochim. Cosmochim. Acta **56,** 3191 (1992b).

Helgeson, H. C. and D. H. Kirkham, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: I. Summary of the thermodynamic/electrostatic properties of the solvent, Am. J. Sci. **274,** 1089 (1974a).

Helgeson, H. C. and D. H. Kirkham, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: II. Debye-Hückel parameters for activity coefficients and relative partial molal properties, Am. J. Sci. **274,** 1199 (1974b).

Helgeson, H. C. and D. H. Kirkham, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: III. Equation of state for aqueous species at infinite dilution, Am. J. Sci. **276,** 97 (1976).

Helgeson, H. C., J. M. Delaney, H. W. Nesbitt, and D. K. Bird, Summary and critique of the thermodynamic properties of rock forming minerals, Am. J. Sci. **278A,** 1 (1978).

Helgeson, H. C., D. H. Kirkham, and G. C. Flowers, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: IV. Calculation of activity coefficients, osmotic coefficients and apparent molal and relative partial molal properties to 600 °C and 5 kbar, Am. J. Sci. **281,** 1249 (1981).

Helgeson, H. C., E. H. Oelkers, E. L. Shock, and D. A. Sverjensky, Calculation of the thermodynamic and transport properties of aqueous species at supercritical temperatures and pressures, Soc. Fran. Chimie Proceed. Inter. Con. Supercritical Fluids **1,** 279 (1988a).

Helgeson, H. C., E. L. Shock, D. A. Sverjensky, and E. H. Oelkers, Calculation of equilibrium constants for reactions among minerals, gases and aqueous species in geothermal systems, Rendiconti della Societa Italiana di Mineralogia e Petrologia, **43,** 1159 (1988b).

Hemley, J.J., J.W Montoya, J. W. Marinenko, and R.W. Luce, Equilibria in the system Al_2O_3—SiO_2—H_2O and some general implications for alteration/mineralization processes, Economic Geology, **75,** 210–228 (1980).

Hill, P. G., A unified fundamental equation for the thermodynamic properties of H_2O, J. Phys. Chem. Ref. Data **19,** 1233 (1990).

Hwang, W.L. Stability and kinetics of kaolinite to boehmite conversion under hydrothermal conditions, Chemical Geology **105,** 197–214 (1993).

Ikkatai, T. and N. Okada, Viscosity, specific gravity and equilibrium concentrations of sodium aluminate solutions in Gerhard, G and P.T. Stroup eds. Extractive Metalurge of Aluminum, Interscience Publishers, New York, p. 159–173 (1962).

Jackson, K. J. and H. C. Helgeson, Chemical and thermodynamic constraints on the hydrothermal transport and deposition of tin: II Interpretation of phase relations in the Southeast Asian tin belt, Econ. Geol. **80,** 1365 (1985).

Johnson, J. W. and D. Norton, Critical phenomena in hydrothermal systems: State, thermodynamic, electrostatic, and transport properties of H_2O in the critical region, Am. J. Sci. **291,** 541 (1991).

Johnson, J. W., E. H. Oelkers, and H. C. Helgeson, CRT92: A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bars and 0° to 1000 °C, Computers and Geosciences, **18,** 889 (1992).

Jonte, J. H. and D. S. Martin, The solubility of silver chloride and the formation of complexes in chloride solution, J. Amer. Chem. Soc. **74,** 2052 (1952).

Kelley, K. K., Contributions to the data on theoretical metallurgy. XIII. High temperature heat content, heat capacity and entropy data for elements and inorganic compounds, U.S. Bur. Mines Bull. **548,** 232 (1960).

Kennedy, G.C., A portion of the system silica-water, Econ. Geol., **45,** 629 (1950).

Kittrick, J. A., Free energy of formation of kaolinite from solubility measurements, Am. Mineralogist **52,** 1457–1466 (1966).

Klots, C. E., and B. B. Benson, Solubilities of nitrogen, oxygen and argon in distilled water, J. Marine Res. **21,** 48 (1963).

Kuyunko, N. S., S. D. Malinin and I. L. Khodakovski, An experimental study of aluminum ion hydrolysis at 150, 200, and 250 °C, Geochem. Internat. **20,** 76 (1983).

Lei, Y. W., H. K. Mao, and R. J. Hemley, Thermal expansivity, bulk modulus, and melting curve of H_2O-ice VII to 20 Gpa, J. Chem. Phys. **99,** 5369 (1993).

May, H.W., D.G. Kinniburgh, P.A. Helmke, and M.L. Jackson, Aqueous dissolution, solubilities and thermodynamic stabilities of common aluminosilicate clay minerals: kaolinite and smectites, Geochim. Cosmochim. Acta **50,** 1667–1677 (1986).

Millero, F. J., The partial molal volume of electrolytes in aqueous solution, in Horne, R. A., ed., Water and aqueous solutions: New York, John Wiley & Sons, Inc, 519 (1972).

Mironov, V. E., Radiochemical data on the solubility of sliver chloride, Radiochimica **4,** 707 (1962).

Morey, G. W., R. O. Fournier, and J. J. Rowe, The solubility of quartz in water in the temperature interval from 25° to 300 °C, Geochim. Cosmochim. Acta **26,** 1029 (1962).

Morrison, T. J. and F. Billett, The salting out of non-electrolytes. Part II. The effect of variation of the non-electrolyte, J. Chem. Soc. **1952,** 3819 (1952).

Morrison, T. J. and N. B. Johnstone, Solubilities of the inert gases in water, J. Chem. Soc., **1954,** 3819 (1954).

Nagy, K., A.E. Blum, and A.C. Lasaga, Dissolution and precipitation kinetics of kaolinite at 80°C and pH 3: The dependance on solution saturation state, Am. J. Sci. **291,** 649–686 (1991).

Oelkers, E. H., and H. C. Helgeson, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Dissociation constants for supercritical alkali metal halides at temperatures from 400° to 800 °C and pressures from 500 to 4000 bars, J. Phys. Chem. **92,** 1631 (1988).

Oelkers, E. H., and H. C. Helgeson, Triple ion anions and polynuclear complexing in supercritical electrolyte solutions, Geochim. Cosmochim. Acta **54,** 727 (1990).

Oelkers, E. H. and H. C. Helgeson, Calculation of the activity coefficients and degrees of formation of neutral ion pairs in supercritical electrolyte solutions," Geochim. Cosmochim. Acta **55,** 1235. (1991).

Oelkers, E. H. and H. C. Helgeson, Calculation of dissociation constants and relative stabilities of polyatomic clusters of 1:1 electrolytes in hydrothermal solutions at supercritical pressures and temperatures, Geochim. Cosmochim. Acta **57,** 2673 (1993a).

Oelkers, E. H. and H. C. Helgeson, Multiple ion association in supercritical aqueous solutions of single electrolytes, Science **261,** 888 (1993b).

Quist, A. S. and W. L. Marshall, Electrical conductances of aqueous sodium chloride solutions from 0 to 800 °C and at pressures to 4000 bars, J. Phys. Chem. **72,** 648 (1968).

Palmer, D. A. and S. E. Drummond, Potentiometric determination of the molal formation constants of ferrous acetate complexes in aqueous solutions to high temperatures, J. Phys. Chem. **92,** 6795 (1988).

Pokrovskii, V. A. and H. C. Helgeson, Thermodynamic properties of aqueous species and the solubilities of minerals at high pressures and temperatures: The system Al_2O_3—H_2O—NaCl, Submitted to Am. J. Sci. (1995a).

Pokrovskii, V. A. and H. C. Helgeson, Thermodynamic properties of aqueous species and the solubilities of minerals at high pressures and temperatures: A thermodynamic interpretation of mineral equilibria in the system K_2O—Na_2O—Al_2O_3—SiO_2—H_2O—HCl at temperatures to 700 °C and pressures to 5 kbar, Submitted to Geochim. Cosmochim. Acta. (1995b).

Pokrovskii, V. A. and H. C. Helgeson, Thermodynamic properties of aqueous species and the solubilities of minerals at high pressures and temperatures: The system Al_2O_3-H_2O-KOH, submitted to Chem. Geol. (1995c).

Potter, R. W. and M. A. Clynne, The solubility of the noble gases He, Ar, Kr, and Xe in water up to the critical point, J. Soln. Chem. **7,** 837 (1978).

Price, L. C., Aqueous solubility of methane at elevated pressures and temperatures," Am. Assoc. Petrol. Geol. Bull. 63, 1527 (1979).

Russell, A. H., J. D. Edwards, and C. S. Taylor, Solubility of hydrated aluminunas in NaOH solutions, J. Metals **203,** 1123 (1955).

Sassani, D. C. and E. L. Shock, Speciation and solubility of palladium in aqueous magmatic-hydrothermal solutions: Geology, **18,** 925 (1990).

Sassani D. C. and E. L. Shock, Estimation of standard partial molal entropies of aqueous ions at 25 °C and 1 bar, Geochim. Cosmochim. Acta **56,** 3895 (1992).

Schulte, M. D. and E. L. Shock, Aldhydes in hydrothermal solution: Standard molal properties and relative stabilities at high temperatures and pressures, Geochim. Cosmochim. Acta **57,** 3835 (1993).

Seward, T. M., The stability of chloride complexes of silver in hydrothermal solutions up to 350 °C, Geochim. Cosmochim. Acta **40,** 1329 (1976).

Seward, T. M., The formation of lead (II) chloride complexes to 300 °C: A spectrophotometric study, Geochim. Cosmochim. Acta **48,** 121 (1984).

Shock, E. L., The stability of peptides in high temperature aqueous solutions, Geochim. Cosmochim. Acta **56,** 3481 (1992).

Shock, E. L., Hydrothermal dehydration of aqueous organic compounds: Geochim. Cosmochim. Acta **57,** 3341 (1993).

Shock, E. L., Organic acids in hydrothermal solutions: Standard molal thermodynamic properties of carboxylic acids, and estimates of dissociation constants at high temperatures and pressures, Am. J. Sci. **295,** 496 (1995).

Shock. E. L. and H. C. Helgeson, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Correlation algorithms for ionic species and equation of state predictions to 5 kbar and 1000 °C, Geochim. Cosmochim. Acta **52,** 2009 (1988).

Shock. E. L. and H. C. Helgeson, Corrections to: Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Correlation algorithms for ionic species and equation of state predictions to 5 kbar and 1000 °C, Geochim. Cosmochim. Acta **53,** 215 (1989).

Shock, E. L. and H. C. Helgeson, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Standard partial molal properties of organic aqueous species, Geochim. Cosmochim. Acta **54,** 915 (1990).

Shock, E. L. and C. M. Koretsky, Metal-organic complexes in geochemical processes: Calculation of standard partial molal thermodynamic properties of aqueous acetate complexes at high pressures and temperatures, Geochim. Cosmochim. Acta **57,** 4899 (1993).

Shock, E. L. and W. B. McKinnon, Hydrothermal processing of cometary volatiles - Application to Triton, Icarus **106,** 464 (1993).

Shock, E. L., H. C. Helgeson, and D. A. Sverjensky, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Standard partial molal properties of inorganic neutral species, Geochim. Cosmochim. Acta **53,** 2157 (1989).

Shock, E. L., E. H. Oelkers, J. W. Johnson, D. A. Sverjensky, and H. C. Helgeson, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Effective electrostatic radii, dissociation constants and the standard molal properties to 1000 °C and 5 kbar. J. Chem. Soc. Farad. Trans. **88,** 803 (1992).

Sverjensky, D. A., Calculation of the thermodynamic properties of aqueous species and the solubilities of minerals in supercritical electrolyte solutions, Reviews in Mineralogy, **17,** 177 (1987).

Sverjensky, D. A., E. L. Shock, and H. C. Helgeson, Prediction of the thermodynamic properties of aqueous metal complexes to 1000 °C and 5 kbar, (in preparation) (1995).

Tanger, H. C. and H. C. Helgeson, Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Revised equation of state for the standard partial molal properties of ions and electrolytes, Am. J. Sci. **288,** 19 (1988).

Verdes, G., Solubilité des hydroxydes d'aluminium entre 20 et 300 °C. Propriétés thermodynamiques des principales espèces naturalles du systèmes Al_2O_3—H_2O. Thèse de l'Université Paul-Sabatier, Toulouse.

Verdes, G., R. Gout, and Castet, S. Thermodynamic properties of the aluminate ion and of bayerite, boehmite, diaspore and gibbsite, Eur. J. Min. **4,** 767 (1992).

Wagman, D. D., W. H. Evans, V. B. Parker, R. H. Schumm, I. Hallow, S. S. 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, p. 392 (1982).

Weill, D. F. and W. S. Fyfe, The solubility of quartz in H_2O in the range 1000 to 4000 bars and 400° to 500 °C, Geochim. Cosmochim. Acta **28,** 1243 (1964).

Wesolowski, D.J., Aluminum speciation and equilibria in aqueous solution: I. The solubility of gibbsite in the system Na—K—Cl—OH—$Al(OH)_4$ from 1 to 100 °C, Geochim. Cosmochim. Acta **56,** 1065–1091 (1992).

Wiebe, R and V. L. Gaddy, The solubility of helium in water at 0, 50, 75, and 100° from 25 to 1000 atmospheres, J. Am. Chem. Soc. **56,** 76 (1935).

Yatsimirskii, K. B. and T. I. Fedorova, The stability of acetate complexes of bivalent chromium, Zhurnal. Neoragnicheskoi Khimii **1,** 2310 (1956).

Zawisza, A. and B. Malesinska, Solubility of carbon dioxide in liquid water and of water in gaseous carbon dioxide in the range 0.2–5MPa. and at temperatures up to 473 K, J. Chem. Eng. Data **26,** 388 (1981).