Supporting Information for:

Single-Ion Solvation Free Energies and the Normal Hydrogen Electrode in Methanol, Acetonitrile, and Dimethylsulfoxide

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Standard States

Absolute Solvation Free Energies. In this article all experimental and calculated solvation free energies use a standard state of an ideal gas at a gas-phase concentration of 1 mol/L dissolving as an ideal dilute solution at a liquid-phase concentration of 1 mol/L. The use of a standard state in which the concentration does not change is a natural choice for theoretical work because then the entropy of translation in the gas phase cancels what Ben-Naim calls the entropy of liberation in the liquid-phase solution, and the free energy of solvation is directly related to the solute-solvent coupling.[1]

In computing the vertical legs of the thermochemical cycles illustrated in Schemes 1-7, it is important to ensure that the change in standard-state concentration on going from the gas phase (1 atm) to solution (1 mol/L), is included in the free energy for solutes. When the solution-phase standard-state concentrations are equal, the relationship between solvation free energies tabulated using a standard-state gas-phase pressure of 1 atm and those tabulated using a standard-state gas-phase concentration of 1 mol/L is

$$\Delta G_{\mathrm{S}}^{\circ} = \Delta G_{\mathrm{S}}^{*} + \Delta G^{\circ\rightarrow *} \tag{S1}$$

where

$$\Delta G^{\circ\rightarrow *} = RT \ln\left(\frac{V^{\circ}}{V^{*}}\right) \tag{S2}$$

In the above equation, R is the universal gas constant, T is the temperature, V° is the volume occupied by an ideal gas at a pressure of 1 atm, and V^{*} is the volume occupied by an ideal gas at a concentration of 1 mol/L. The ideal gas law applied to the 1 atm standard state is

$$P^{\circ}V^{\circ} = RT \tag{S3}$$

and this shows that the volume occupied by an ideal gas at 298 K and 1 atm pressure is 24.45 L. Substituting this value into eq S2 gives 1.89 kcal/mol for $\Delta G^{\circ\rightarrow *}$. For an ideal gas at 298 K and 1 bar pressure, eq S3 gives a volume of 24.79 L, and when this value is substituted into eq S2**,** $\Delta G^{\circ\rightarrow *}$ equals 1.90 kcal/mol**.** Because the uncertainties associated with the solution-phase data in this article are larger than 0.01 kcal/mol, we applied the same $\Delta G^{\circ\rightarrow *}$ value (1.9 kcal/mol at 298 K) to solvation free energies tabulated using a gas-phase standard-state concentration of 1 atm and those tabulated using a gas-phase standard-state concentration of 1 bar.

In thermochemical cycle 1, the number of reactants that move from the gas-phase to the solution-phase equals the number of products that move from the gas-phase to the solution-phase. Thus, the standard-state free energy change $\Delta G^{\circ\rightarrow *}$ cancels out in the calculation of $\Delta G_{\mathrm{S}}^{*,\mathrm{con}}(\mathrm{M}^{+})$ (see eq 7). However, this cancellation does not occur in the remaining thermochemical cycles used in this article, so in these cases including the above term is necessary (see eqs 10, 13, 15, 16, and 26).

Conventional Solvation Free Energies. The relationship between the conventional solvation free energy of a monavalent cation and its absolute solvation free energy is

$$\Delta G_{\mathrm{S}}^{*,\mathrm{con}}(\mathrm{M}^{+}) = \Delta G_{\mathrm{S}}^{*}(\mathrm{M}^{+}) - \Delta G_{\mathrm{S}}^{*}(\mathrm{H}^{+}) \qquad \text{(S4)}$$

Substituting eq S1 into the above equation leads to

$$\Delta G_{\mathrm{S}}^{*,\mathrm{con}}(\mathrm{M}^{+}) = \Delta G_{\mathrm{S}}^{\circ,\mathrm{con}}(\mathrm{M}^{+}) \qquad \text{(S5)}$$

Thus, for monovalent cations, conventional solvation free energies tabulated using a standard state gas-phase pressure of 1 atm or 1 bar and a standard-state gas-phase

concentration of 1 mol/L are equal when the standard-state solution-phase concentrations are equal. On the other hand, the relationship between the conventional solvation free energy of a monovalent anion and its absolute solvation free energy is

$$\Delta G_{\mathrm{S}}^{*,\mathrm{con}}(\mathrm{X}^-) = \Delta G_{\mathrm{S}}^{*}(\mathrm{X}^-) + \Delta G_{\mathrm{S}}^{*}(\mathrm{H}^+) \tag{S6}$$

and substituting eq S1 into the above equation leads to

$$\Delta G_{\mathrm{S}}^{*,\mathrm{con}}(\mathrm{X}^-) = \Delta G_{\mathrm{S}}^{\circ,\mathrm{con}}(\mathrm{X}^-) - 2\Delta G^{\circ\rightarrow *} \tag{S7}$$

where at 298 K, $\Delta G^{\circ\rightarrow *}$ equals 1.9 kcal/mol (see above).

Standard Reduction Potentials. For standard reduction potentials, literature values are often tabulated using a standard-state solution-phase concentration of 1 mol solute per 1 kg solvent (molality scale). For water, the difference between standard reduction potentials tabulated on the molality scale and on the molarity scale is very small, whereas for nonaqueous solvents, whose densities deviate significantly from 1 kg L^{-1}, the difference can be larger. The free energy change associated with moving a solute from a standard-state solution-phase concentration of 1 mol solute per 1 kg solvent (molality scale) to a standard-state solution-phase concentration of 1 mol/L (molarity scale) is

$$\Delta G_{\mathrm{molal}\rightarrow\mathrm{molar}}^{*} = -RT\ln\left(\frac{\rho_{\mathrm{liq}}}{\rho^{\mathrm{m}}}\right) \tag{S8}$$

where ρ_{liq} is the density of the solvent in its pure liquid state, and ρ^{m} is 1 kg L^{-1} or, equivalently, 1 g mL^{-1}.

For thermochemical cycle 1, the number of moles of reactants in the solution phase is equal to the number of products in the solution phase. Thus, because the $\Delta G_{\mathrm{molal}\rightarrow\mathrm{molar}}^{*}$ term cancels out, the standard reduction potentials used in this cycle are

equal, regardless of whether they are tabulated on the molality or molarity scale. For thermochemical cycle 2 (silver halide electrode), this cancellation does not occur. The standard reduction potentials used in this cycle can be converted from the molality to the molarity scale through the use of thermochemical cycle 2 and eq S8

$$\text{AgX Electrode}: E_{\text{c}}^{*} = E_{\text{m}}^{*} + \frac{2RT}{F}\ln\left(\frac{\rho_{\text{liq}}}{\rho^{\text{m}}}\right) \tag{S9}$$

where E_{c}^{*} is the standard reduction potential on the molarity scale, E_{m}^{*} is the standard reduction potential on the molality scale, and F is Faraday's constant, which is equal to 23.061 kcal mol^{-1} V^{-1}. In this article, standard reduction potentials at the silver halide electrode in methanol were used to determine conventional solvation free energies. These standard reduction potentials, which are tabulated on the molarity scale, and the resulting conventional solvation free energies, are listed in Table 2. Note that at 298 K, the density of methanol is 0.7914 g mL^{-1} (reference 2) so that $\Delta G_{\text{molal}\rightarrow\text{molar}}^{*}$ equals 0.14 kcal/mol.

Gas-Phase Ion Thermochemistry

Experimental values for the gas-phase free energies of formation of the following monatomic ions have been used in this article to determine conventional solvation free energies: H^{+}, Na^{+}, K^{+}, Rb^{+}, Cs^{+}, Tl^{+}, Ag^{+}, Cl^{-}, Br^{-}, and I^{-}. In this article, all gas-phase free energies of ions are tabulated using the electron convention (EC) and Fermi-Dirac statistics for the thermochemistry of the electron. The following sections provide a detailed description of the different conventions that are commonly used for treating the thermochemistry of the electron, the equations and literature references that were used to

determine the enthalpies, entropies, and free energies of formation of ions listed above, and the equations used to convert entropies computed using a standard-state gas-phase pressure of 1 bar to a standard-state gas-phase pressure of 1 atm.

Thermochemical Conventions for the Electron. The enthalpy of formation of a species is defined as the difference between its enthalpy and the sum of the enthalpies of the species of which it is composed, in their elemental standard states. For cations, the usual approach to determining the enthalpy of formation is to add to the enthalpy of formation of the neutral species the enthalpy change associated with the following reaction

$$M \rightarrow M^+ + e^- \qquad \text{(S10)}$$

For anions, the enthalpy of formation is determined by subtracting from the enthalpy of formation of the neutral species the enthalpy change associated with the following reaction

$$X^- \rightarrow X + e^- \qquad \text{(S11)}$$

The energy changes associated with the chemical reactions above are referred to as the ionization energy and electron affinity, respectively. If these energy differences are measured as threshold energy differences between the lowest electronic, vibrational, and rotational level of the isolated neutral species and the lowest electronic, vibrational, and rotational level of the isolated ionic species, they correspond to 0 K. To convert such enthalpies to enthalpies of reaction at a finite temperature, one must add to the 0 K energy difference the difference between the integrated heat capacities of the products and reactants. In the reactions above, the electron appears as a product, so the special problem arises of how to take into account its enthalpy and heat capacity. Two kinds of

conventions for doing this are the electron convention "EC" and the ion convention "IC".[3]

In the EC, the electron is treated as a standard chemical element, and thus, its standard-state enthalpy of formation is taken to be equal to zero. Assuming the electron to behave as an ideal gas, its integrated heat capacity can then be determined using statistical mechanics. Using conventional Boltzmann statistics yields a value equal to $\frac{5}{2}RT$, or 1.481 kcal/mol at 298 K. The result of following this convention is that the integrated heat capacity of the electron in the standard state is effectively assigned to the ion rather than to itself; this indirect assignment is required in order to satisfy the constraint that the standard-state enthalpy of formation of the electron equal zero at all temperatures. Because the electron is a degenerate Fermi-Dirac gas, a more correct treatment of its heat capacity uses Fermi-Dirac statistics, not Boltzmann statistics. Bartmess[4] has derived values for the heat capacity of the electron using Fermi-Dirac statistics for temperatures up to 1000 K; he reports a value of 0.752 kcal/mol for the integrated heat capacity of the electron at 298 K.

In the second commonly used kind of convention for treating the enthalpy of the electron, the IC, its integrated heat capacity *and* enthalpy of formation are both taken to be zero at all temperatures in the standard state. When this convention is followed, the integrated heat capacity term is eliminated in the expression for the standard-state enthalpy of formation of the ion.

For standard-state enthalpies of formation of ions, the values tabulated following the IC are identical to those one would obtain if one assigned the integrated heat capacity of the electron to itself, rather than to the enthalpy of formation of the accompanying ion,

as is done in the EC. Thus, the relationships between standard-state enthalpies of formation of monovalent ions tabulated following the EC and the IC are

$$\Delta_f H^\circ_T(M^+;EC) = \Delta_f H^\circ_T(M^+;IC) + (H^\circ_T - H^\circ_0)[e^-(g)] \quad (S12)$$

$$\Delta_f H^\circ_T(X^-;EC) = \Delta_f H^\circ_T(X^-;IC) - (H^\circ_T - H^\circ_0)[e^-(g)] \quad (S13)$$

where, as usual, subscript f denotes formation from elements, subscript T or 0 denotes temperature, a superscript $\circ$ denotes standard state, and $(H^\circ_T - H^\circ_0)[e^-(g)]$ is the standard-state integrated heat capacity of the electron at temperature T. Enthalpies of formation tabulated following the EC can be further subdivided into two groups: those determined using an integrated heat capacity of the electron obtained from Boltzmann statistics (EC-B), and those determined using an integrated heat capacity of the electron obtained from Fermi-Dirac statistics (EC-FD).

In this article, enthalpies of formation of ions have been tabulated following the EC-FD convention, although it is important to point out that for *conventional solvation free energies of ions*, there is no intrinsic advantage associated with following any of the three conventions described above; any convention that is followed will lead to identical results for relative values between ions, as long as the same convention is followed *consistently*. However, in chemical reactions where the electron appears as a reactant (e.g., eqs S10 and S11), the enthalpy and the free energy of reaction *does* depend on whether Boltzmann or Fermi-Dirac statistics are used to compute the electron integrated heat capacity and entropy.

Enthalpies of Formation of Ions. The chemical reaction for the formation of H^+ from its elemental standard state is

$$\tfrac{1}{2}H_2(g) \rightarrow H^+(g) + e^-(g) \quad (S14)$$

The standard-state enthalpy change associated with the above chemical reaction can be written as

$$\Delta_f H^\circ_T[H^+(g)] = \Delta_f H^\circ_T[H(g)] + \Delta H^\circ_T(IE) \quad (S15)$$

where $\Delta_f H^\circ_T[H(g)]$ is the standard-state enthalpy change associated with the formation of H from its elemental standard state

$$\tfrac{1}{2}H_2(g) \rightarrow H(g) \quad (S16)$$

and $\Delta H^\circ_T(IE)$ is the standard-state enthalpy change associated with the gas-phase ionization reaction

$$H(g) \rightarrow H^+(g) + e^-(g) \quad (S17)$$

The enthalpy change $\Delta H^\circ_T(IE)$ can be written as

$$\Delta_f H^\circ_T(IE) = IE_0 + (H^\circ_T - H^\circ_0)[H^+(g)] + (H^\circ_T - H^\circ_0)[e^-(g)] - (H^\circ_T - H^\circ_0)[H(g)] \quad (S18)$$

where IE_0 is the gas-phase ionization energy of H at 0 K, and the remaining three terms are the standard-state integrated heat capacities of H^+, the electron, and H, respectively, in the gas phase. Note that the enthalpy of formation of the electron does not appear in eq S15 because in both the IC and the EC it is equal to zero. (The standard-state integrated heat capacity of the electron *does* appear in eq S18, so the final result for the enthalpy of formation of the ion still depends on the convention used for the enthalpy of the electron, as described in the previous section).

For Na^+, K^+, Rb^+, Cs^+, Tl^+, and Ag^+, the chemical reaction for the formation of the ion from its elemental standard state is

$$M(cr) \rightarrow M^+(g) + e^-(g) \quad (S19)$$

where the “cr” stands for “crystalline”, and “g” denotes gas. The standard-state enthalpy change associated with the above chemical reaction can be written as

$$\Delta_f H^\circ_T[M^+(g)] = \Delta H^\circ_T(IE) + \Delta_f H^\circ_T[M(g)] \quad \text{(S20)}$$

where $\Delta_f H^\circ_T[M(g)]$ is the standard-state enthalpy of formation of the neutral species from its elemental standard state

$$M\,(cr) \rightarrow M\,(g) \quad \text{(S21)}$$

and $\Delta H^\circ_T(IE)$ is the standard-state enthalpy change associated with the gas-phase ionization reaction

$$M\,(g) \rightarrow M^+(g) + e^-(g) \quad \text{(S22)}$$

The standard-state enthalpy change $\Delta H^\circ_T(IE)$ can be written as

$$\Delta_f H^\circ_T(IE) = IE_0 + (H^\circ_T - H^\circ_0)[M^+(g)] + (H^\circ_T - H^\circ_0)[e^-(g)] - (H^\circ_T - H^\circ_0)[M(g)] \quad \text{(S23)}$$

where IE_0 is the gas-phase ionization energy of the metal atom at 0 K, and the remaining three terms are the standard-state integrated heat capacities of the metal cation, the electron, and the metal atom in the gas phase, respectively.

For Cl^-, Br^-, and I^-, the chemical reaction for the formation of the ion from its elemental standard state is

$$\tfrac{1}{2}X_2(g/l/cr) + e^-(g) \rightarrow X^-(g) \quad \text{(S24)}$$

where the “g/l/cr” notation has been used to denote $Cl_2(g)$, $Br_2(l)$ and $I_2(cr)$, which are the elemental standard states for Cl, Br, and I. The standard-state enthalpy change associated with the above chemical reaction can be written as

$$\Delta_f H^\circ_T[X^-(g)] = \Delta_f H^\circ_T[X(g)] - \Delta H^\circ_T(EA) \quad \text{(S25)}$$

where $\Delta_f H^\circ_T[X(g)]$ is the standard-state enthalpy of formation of the neutral species from its elemental standard state

$$\tfrac{1}{2}X_2(g/l/cr) \rightarrow X(g) \quad \text{(S26)}$$

and $\Delta H^\circ_T(EA)$ is the standard-state enthalpy change associated with the following chemical reaction

$$X^-(g) \rightarrow X(g) + e^-(g) \quad \text{(S27)}$$

The standard-state enthalpy change $\Delta H^\circ_T(EA)$ can be written as

$$\Delta H^\circ_T(EA) = EA_0 + (H^\circ_T - H^\circ_0)[X(g)] + (H^\circ_T - H^\circ_0)[e^-(g)] - (H^\circ_T - H^\circ_0)[X^-(g)] \quad \text{(S28)}$$

where EA_0 is the gas-phase electron affinity of the halogen atom at 0 K, and the remaining three terms are the integrated heat capacity of the halide anion, the electron, and the halogen atom, respectively, in the gas phase.

For all of the ions listed above, standard-state enthalpies of formation have been tabulated in the NBS tables.[5] Recently, Fawcett reevaluated[6] all of these enthalpies, using improved values for the electron affinities of monatomic anions.[7] In this article, we used the enthalpies of formation reported by Fawcett. These enthalpies, which Fawcett tabulated using the IC, were converted to the EC-FD convention using Bartmess' value for the electron integrated heat capacity (0.752 kcal/mol at 298 K) in eqs S12 and S13. The resulting enthalpies of formation are listed in Table S1. The entropies and free energies in Table S1 are described below.

Entropies and Free Energies of Formation of Ions. The standard-state free energy of formation is related to the enthalpy of formation according to

$$\Delta_f G^\circ_T = \Delta_f H^\circ_T - T\Delta_f S^\circ_T \quad \text{(S29)}$$

where $\Delta_f S^\circ_T$ is the entropy change associated with the formation of the species from its elemental standard state. The chemical reactions for the formation of the ions considered in this work from their elemental standard states are given in eqs S14, S19, and S24. The standard-state entropies of neutral species are listed in the NBS tables.[5] The NBS tables do not list entropies for ions, although for monatomic ions, these can be computed using statistical mechanics. Assuming the ion to behave as an ideal gas, conventional Boltzmann statistics leads to the following expression for the standard-state entropy of a monatomic species[8]

$$S^\circ_T = S^\circ_{T,trans} + S_{T,elec} \tag{S30}$$

where $S^\circ_{T,trans}$ and $S_{T,elec}$ are the translational and electronic contributions to the total entropy (the nuclear spin contribution to the total entropy is taken to be equal to zero). For monatomic species, $S^\circ_{T,trans}$ can be computed using the Sackur-Tetrode equation[8]

$$S^\circ_{trans} = R\ln\left[\left(\frac{2\pi mkT}{h^2}\right)^{3/2}\frac{V^\circ e^{5/2}}{N_A}\right] \tag{S31}$$

where R is the universal gas constant (1.9872 cal mol^{-1} K^{-1}), m is the electron rest mass (9.109 39 × 10^{-31} kg), k is Boltzmann's constant (3.299 86 × 10^{-23} cal K^{-1}), T is the temperature in Kelvin, h is Planck's constant (1.583 67 × 10^{-34} cal s), N_A is Avagadro's number (6.022 14 × 10^{23} mol^{-1}), and V° is the standard-state volume, which can be computed using the ideal gas law

$$P^\circ V^\circ = RT \tag{S32}$$

where P° is the standard-state pressure. In this article, a standard-state gas-phase pressure of 1 atm is used.

The electronic contribution to the entropy, which does not depend on the gas-phase pressure, is given by[8]

$$S_{\text{elec}} = R\ln\sum_{i=0}^{n}(2J_i+1)e^{-\varepsilon_i/kT} \tag{S33}$$

where ε_i is the energy of the ith electronic level and J_i is the associated quantum number for the total angular momentum.

Using eqs S30-S33, along with experimental data[9] for the electronic energy levels of ions, Fawcett[6] computed entropies for all of the ions in Table S1, using a standard-state gas-phase pressure of 1 bar. To convert these entropies to a standard-state gas-phsae pressure of 1 atm, we used the following equation

$$S^\circ_{\text{T,1 atm}} = S^\circ_{\text{T,1 bar}} + R\ln\left(\frac{V^\circ_{\text{1 atm}}}{V^\circ_{\text{1 bar}}}\right) \tag{S34}$$

At 298 K, an ideal gas at 1 atm occupies a volume of 0.0244655 m^3, and at 1 bar a volume of 0.0247897 m^3. Substituting these values into eq S34 gives

$$S^\circ_{\text{298,1 atm}} = S^\circ_{\text{298,1 bar}} - 0.02615\ \text{cal mol}^{-1} \tag{35}$$

For the electron, the value used for the standard-state entropy depends, in addition to the gas-phase pressure, on which convention is followed for its enthalpy. In the IC, the standard-state integrated heat capacity of the electron is taken to equal zero. As a result, the entropy of the electron is not clearly defined, although the usual approach is to assume a value of zero for its entropy when this convention is followed. In the EC the electron is treated as a standard chemical element, so its entropy can be computed in the same way as for monatomic species. Using conventional Boltzmann statistics (eqs S30-S33) leads to a value of 4.988 cal mol^{-1} for the entropy of the electron at 298 K and 1

atm. Of course, as mentioned above, the electron is a degenerate Fermi-Dirac gas, so a more correct treatment of the electron uses Fermi-Dirac statistics. Applying Fermi-Dirac statistics to the electron leads to a value of 5.407 cal mol^{-1} for the entropy at 298 K and 1 atm.[4]

Using the entropies of monatomic ions taken from Fawcett (adjusted for a standard-state gas-phase pressure of 1 atm using eq S35), entropies of neutral species taken from the NBS tables (adjusted for a standard-state gas-phase pressure of 1 atm using eq S35), and the entropy of the electron from Fawcett (5.407 cal mol^{-1} at 298 K and 1 atm), entropies of formation for all of the ions listed in Table S1 were computed following the chemical reactions shown in eqs S14, S19, and S24. These are listed in Table S1. Using the enthalpies and entropies of formation in Table S1, free energies of formation were then computed using eq S29. These free energies of formation, which are the ones used to calculate conventional solvation free energies, are also listed Table S1.

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TABLE S1: Gas-Phase Enthalpies (kcal/mol), Entropies (cal/mol), and Free Energies (kcalmol) of Formation of Monatomic Ions[a]

Ion	$\Delta_f H^\circ_{298}$	$\Delta_f S^\circ_{298,1\ atm}$	$\Delta_f G^\circ_{298,1\ atm}$
H^+	366.4	15.8	361.7
Na^+	144.9	28.5	136.4
K^+	122.2	27.0	114.1
Rb^+	116.4	26.3	108.5
Cs^+	108.7	25.6	101.1
Tl^+	185.1	31.9	175.6
Ag^+	243.4	35.2	232.9
Cl^-	-55.1	4.6	-56.4
Br^-	-51.6	15.5	-56.2
I^-	-45.7	21.2	-52.1

[a]All data are tabulated following the electron convention and Fermi-Dirac statistics for the electron integrated heat capacity and entropy.

TABLE S2: Conventional Solvation Free Energies (kcal/mol) of Unclustered and Clustered Ions in Methanol[a]

	no. of clustering CH_3OH molecules			
ion	0	1	2	3
Cl^-	-335.0[b]	-327.9	-323.9	-322.1
Br^-	-329.3[b]	-323.8	-320.5	-319.2
I^-	-321.7[b]	-318.7	-317.3	-317.1
p-$NO_2C_6H_4O^-$	-318.5	-316.4		
$CH_3CO_2^-$	-337.3	-329.7		
$C_6H_5O^-$	-333.5	-328.3		
$CH_3CH_2CO_2^-$	-336.2	-331.2		
$C_6H_5CO_2^-$	-331.8	-327.5		
p-$FC_6H_4CO_2^-$	-328.0	-324.1		
Na^+	162.4	176.2	187.4	194.4
K^+	180.2	189.8	194.4	197.7
$CH_3NH_3^+$	188.9	197.8		
$(CH_3)_3NH^+$	203.0	208.9	210.5	210.1
NH_4^+	177.9	191.0		
$C_5H_{10}NH_2^+$	200.3	204.9		
pyridineH^+	202.9	208.8		
$C_6H_5NH_3^+$	189.5	196.2		

[a]Conventional solvation free energies are for a temperature of 298 K, and use a standard-state concentration of 1 mol/L in both the gas and aqueous phases. [b]Average value from Tables 2 and 3.

TABLE S3: Conventional Solvation Free Energies (kcal/mol) of Unclustered and Clustered Ions in Acetonitrile[a]

	no. of clustering CH_3CN molecules			
ion	0	1	2	3
Cl^-	-322.6[b]	-316.1	-311.9	-310.0
Br^-	-319.5[b]	-313.8	-310.6	-309.7
I^-	-313.2	-309.5	-307.9	-308.0
$CH_3CO_2^-$	-319.5	-313.1		
NO_3^-	-313.3	-309.0		
$CF_3CO_2^-$	-308.7	-302.7		
$NCCH_2CO_2^-$	-309.6	-305.6		
$C_6H_5CO_2^-$	-316.1	-311.5		
$C_6H_5O^-$	-315.6	-311.5		
Na^+	159.1	179.7	195.2	205.0
K^+	174.7	189.7	200.1	206.9
Rb^+	178.4	190.7	199.2	204.6
Cs^+	187.8	198.5	205.8	210.1
NH_4^+	170.7	188.1	198.7	204.1
$C_6H_5NH_3^+$	183.4	194.8		
$CH_3NH_3^+$	179.8	194.4		
pyridineH^+	193.8	204.7		

[a]Conventional solvation free energies are for a temperature of 298 K, and use a standard-state concentration of 1 mol/L in both the gas and aqueous phases. [b]Average value from Table 3.

TABLE S4: Conventional Solvation Free Energies (kcal/mol) of Unclustered and Clustered Ions in DMSO[a]

	no. of clustering DMSO molecules			
ion	0	1	2	3
F^-	-352.0[b]			
Cl^-	-336.0[c]	-329.3	-326.1	-325.9
Br^-	-333.1[c]	-328.0	-325.9	-326.3
I^-	-328.4	-325.0	-324.5	-326.1
NO_2^-	-329.6	-326.7		
$C_6H_5CO_2^-$	-330.2	-328.2		
$CH_3CO_2^-$	-333.9	-329.5		
$C_6H_5O^-$	-328.4	-326.2		
CH_3O^-	-342.2	-330.6		
$C_2H_5O^-$	-337.9	-329.6		
Na^+	164.4	189.6		
K^+	181.1	201.1	214.2	220.1
pyridineH^+	206.3[b]	218.8[b]		
$C_6H_5NH_3^+$	193.2	206.3		
NH_4^+	179.0	202.3		
$CH_3NH_3^+$	189.9	207.3		

[a]Conventional solvation free energies are for a temperature of 298 K, and use a standard-state concentration of 1 mol/L in both the gas and aqueous phases. [b]This conventional solvation free energy was not used to determine the absolute aqueous solvation free energy of the proton. [c]Average value from Table 3.

TABLE S5: Slopes, Intercepts, and *Y* Values (kcal/mol) for Methanol

n	slope	intercept	Y^a
0	1.0000	0.0	-264.8
1	0.7729	-60.7	-263.8
2	0.5678	-114.1	-262.7
3	0.3923	-159.9	-262.5
average			-263.5

[a] *Y* is the average intersection ordinate of the *n*th straight line with all the others in this table.

TABLE S6: Slopes, Intercepts, and *Y* Values (kcal/mol) for Acetonitrile

n	slope	intercept	Y^a
0	1.0000	0.0	-260.9
1	0.7183	-74.1	-260.6
2	0.3568	-167.1	-259.6
3	0.1387	-223.9	-259.9
average			-260.2

[a] *Y* is the average intersection ordinate of the *n*th straight line with all the others in this table.

TABLE S7: Slopes, Intercepts, and *Y* Values (kcal/mol) for DMSO

n	slope	intercept	Y^a
0	1.0000	0.0	-273.5
1	0.5622	-120.0	-273.5
2	0.2229	-212.7	-273.4
3	-0.0295	-280.7	-272.7
average			-273.3

[a] *Y* is the average intersection ordinate of the *n*th straight line with all the others in this table.

TABLE S8: y_{ij} values (kcal/mol) for Methanol, Acetonitrile, and DMSO

i	*j*	CH_3OH	CH_3CN	DMSO
1	0	-267.3	-263.0	-274.1
2	0	-264.0	-259.8	-273.7
2	1	-261.9	-258.9	-273.6
3	0	-263.1	-260.0	-272.7
3	1	-262.1	-259.7	-272.7
3	2	-262.3	-260.0	-272.8
standard deviation		2.0	1.4	0.6

Cartesian Coordinates of Singly Clustered Ions, Optimized at the B97-1/MG3S Level of Theory.

Name of the unclustered ion is listed first, followed by its molecular formula, the molecular formula of the clustering solvent molecule, and the symmetry point group that the clustered ion belongs to.

Ion: Phenoxide
Formula: C6H5O-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.406479	0.837767	-0.307230
2	6	0	-1.629780	1.476828	-0.152436
3	6	0	-2.797824	0.764397	0.147934
4	6	0	-2.697123	-0.625911	0.288129
5	6	0	-1.483750	-1.283584	0.137917
6	6	0	-0.267055	-0.585155	-0.168071
7	8	0	0.850912	-1.198049	-0.302900
8	1	0	-3.749008	1.272364	0.266579
9	1	0	0.485444	1.409614	-0.547263
10	1	0	-1.678574	2.557885	-0.269097
11	1	0	-3.588466	-1.206159	0.519934
12	1	0	-1.422298	-2.362438	0.249345
13	8	0	3.127384	0.068133	-0.575755
14	6	0	3.471721	0.436924	0.728259
15	1	0	2.242742	-0.407938	-0.528314
16	1	0	2.688148	1.035442	1.219785
17	1	0	4.384673	1.044692	0.694053
18	1	0	3.672703	-0.431742	1.377209

Ion: 4-Nitrophenoxide
Formula: 4-NO2C6H4O-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.599587	-0.556148	-0.372299
2	6	0	0.708287	-0.962088	-0.278649
3	6	0	1.730285	-0.027573	-0.010657
4	6	0	1.400560	1.333543	0.158759
5	6	0	0.095863	1.747647	0.066022
6	6	0	-0.987848	0.827988	-0.203782
7	8	0	-2.187087	1.218530	-0.283256
8	7	0	3.079859	-0.451615	0.086293
9	8	0	3.348131	-1.657167	-0.067286
10	8	0	3.963518	0.392799	0.322923
11	1	0	-1.385821	-1.273328	-0.584100
12	1	0	0.981372	-2.001595	-0.408658
13	1	0	2.199354	2.035362	0.362543
14	1	0	-0.164121	2.792772	0.195432
15	8	0	-4.249827	-0.498341	-0.507673
16	6	0	-4.503713	-0.888199	0.815729
17	1	0	-3.490325	0.135807	-0.490375
18	1	0	-3.622473	-1.335656	1.299946
19	1	0	-5.300095	-1.640011	0.806753
20	1	0	-4.837866	-0.049635	1.446012

Ion: Acetate
Formula: CH3CO2-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.682296	-0.150297	-0.006378
2	6	0	1.133637	0.074954	0.003512
3	8	0	0.751228	1.248897	-0.002527
4	1	0	3.207151	0.800013	-0.010943
5	1	0	2.967940	-0.731955	0.869767
6	1	0	2.955543	-0.732915	-0.885899
7	8	0	0.475388	-0.989347	0.014960
8	8	0	-2.262053	-0.810485	-0.014933
9	1	0	-1.277460	-0.913364	-0.002619
10	6	0	-2.472853	0.588479	0.005628
11	1	0	-1.526306	1.118540	-0.002029
12	1	0	-3.064056	0.903165	-0.862339
13	1	0	-3.037802	0.885172	0.897489

Ion: Propanate
Formula: CH3CH2CO2-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.208456	0.487997	0.028054
2	6	0	0.652365	0.445564	-0.030717
3	8	0	0.122861	-0.701049	0.000959
4	6	0	2.905664	-0.872810	0.046691
5	1	0	2.544911	1.085586	-0.826643
6	1	0	2.475898	1.070150	0.917804
7	8	0	0.082260	1.552963	-0.098725
8	8	0	-2.547972	-1.005962	-0.140664
9	1	0	-1.562230	-0.899737	-0.093447
10	6	0	-3.115433	0.250576	0.140413
11	1	0	-2.378528	1.054560	0.030078
12	1	0	-3.953435	0.440862	-0.546126
13	1	0	-3.518421	0.293184	1.167130
14	1	0	3.996911	-0.765735	0.096127
15	1	0	2.655760	-1.449388	-0.847182
16	1	0	2.575622	-1.465053	0.903053

Ion: Benzoate
Formula: C6H5CO2-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.504712	-1.188689	0.028737
2	6	0	2.892114	-1.323249	0.076697
3	6	0	3.706648	-0.189628	0.068428
4	6	0	3.121585	1.076747	0.011968
5	6	0	1.733830	1.204239	-0.035441
6	6	0	0.909683	0.075182	-0.027550
7	6	0	-0.625722	0.228787	-0.079160
8	8	0	-1.065838	1.393193	-0.124400
9	8	0	-1.270887	-0.855056	-0.068105
10	1	0	0.849919	-2.052360	0.033876
11	1	0	3.340942	-2.311302	0.120275
12	1	0	4.786914	-0.291891	0.105274
13	1	0	3.749715	1.962797	0.004987
14	1	0	1.252683	2.174723	-0.079345
15	8	0	-3.974257	-0.855236	-0.202923
16	6	0	-4.397377	0.398022	0.276344
17	1	0	-2.985597	-0.864360	-0.163722
18	1	0	-5.311311	0.696878	-0.254495
19	1	0	-3.630999	1.166545	0.123218
20	1	0	-4.637248	0.367282	1.353218

Ion: p-Fluorobenzoate
Formula: p-FC6H4CO2-
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072094	-1.143943	0.010510
2	6	0	-2.461882	-1.262878	0.050115
3	6	0	-3.222583	-0.103817	0.038961
4	6	0	-2.649373	1.157793	-0.009955
5	6	0	-1.258033	1.250905	-0.048752
6	6	0	-0.454159	0.108347	-0.038967
7	6	0	1.082801	0.235856	-0.081320
8	8	0	1.540655	1.393261	-0.123326
9	8	0	1.708175	-0.858921	-0.066978
10	1	0	-0.434813	-2.020314	0.017381
11	1	0	-2.953989	-2.228089	0.088724
12	9	0	-4.579353	-0.208104	0.077305
13	1	0	-3.283926	2.036770	-0.017188
14	1	0	-0.760624	2.213125	-0.087388
15	8	0	4.417367	-0.894988	-0.193505
16	6	0	4.855579	0.351626	0.290096
17	1	0	3.429390	-0.891693	-0.157765
18	1	0	5.084404	0.317257	1.369142
19	1	0	4.103406	1.132476	0.129525
20	1	0	5.779216	0.635254	-0.231827

Ion: Ammonium
Formula: NH4+
Solvent: CH3OH
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.231573	-1.436977	0.000000
2	7	0	-1.219769	-1.566256	0.000000
3	1	0	-0.725420	-0.609931	0.000000
4	1	0	-0.958082	-2.097420	0.830431
5	1	0	-0.958082	-2.097420	-0.830431
6	8	0	0.000000	0.777154	0.000000
7	1	0	-0.476551	1.611821	0.000000
8	6	0	1.424561	1.027301	0.000000
9	1	0	1.917803	0.056867	0.000000
10	1	0	1.711461	1.577906	0.896035
11	1	0	1.711461	1.577906	-0.896035

Ion: Methylammonium
Formula: CH3NH3+
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.334402	0.684879	-0.039050
2	6	0	-2.152016	-0.586842	-0.101046
3	1	0	-1.694251	1.319077	0.679413
4	1	0	-1.368602	1.188100	-0.929811
5	1	0	-0.323673	0.457147	0.182975
6	1	0	-3.178133	-0.337287	-0.331221
7	1	0	-2.085042	-1.076109	0.860110
8	1	0	-1.731343	-1.218948	-0.869885
9	8	0	1.190879	-0.130193	0.519659
10	6	0	2.308286	-0.062649	-0.396851
11	1	0	1.538222	-0.024587	1.418506
12	1	0	2.779276	0.913327	-0.362106
13	1	0	1.910305	-0.242145	-1.386664
14	1	0	3.029400	-0.834240	-0.157863

Ion: Trimethylammonium
Formula: (CH3)3NH+
Solvent: CH3OH
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.858649	-0.312824	0.000000
2	1	0	-0.023827	0.239511	0.000000
3	6	0	1.997601	0.663079	0.000000
4	6	0	0.858649	-1.155152	1.240792
5	6	0	0.858649	-1.155152	-1.240792
6	1	0	2.932456	0.116392	0.000000
7	1	0	1.772771	-1.734854	1.275575
8	1	0	1.772771	-1.734854	-1.275575
9	1	0	1.928991	1.280085	-0.886374
10	1	0	1.928991	1.280085	0.886374
11	1	0	0.796335	-0.504995	2.103378
12	1	0	0.001642	-1.815154	1.215782
13	1	0	0.001642	-1.815154	-1.215782
14	1	0	0.796335	-0.504995	-2.103378
15	8	0	-1.493943	1.158207	0.000000
16	1	0	-1.505849	2.126394	0.000000
17	6	0	-2.860921	0.697063	0.000000
18	1	0	-2.825846	-0.384347	0.000000
19	1	0	-3.379639	1.038488	-0.888477
20	1	0	-3.379639	1.038488	0.888477

Ion: Piperidinium
Formula: C5H10NH2+
Solvent: CH3OH
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.117895	-0.092941	0.347143
2	6	0	-2.129852	-1.164884	0.263126
3	6	0	-1.902389	1.350689	0.144143
4	6	0	-2.723892	0.132844	-0.301367
5	6	0	-0.655834	-1.308013	-0.101730
6	6	0	-0.429293	1.193839	-0.218629
7	1	0	0.082902	-0.044611	1.366664
8	1	0	-2.239045	-1.188290	1.353906
9	1	0	-1.997865	1.496053	1.226756
10	1	0	-2.743667	0.082720	-1.395580
11	1	0	-0.514091	-1.376079	-1.182463
12	1	0	-0.282303	1.136305	-1.299036
13	1	0	1.122745	-0.198196	0.082202
14	1	0	-2.661734	-2.038436	-0.119344
15	1	0	-2.272559	2.265139	-0.323841
16	1	0	-3.759027	0.241907	0.025901
17	1	0	-0.189703	-2.176748	0.364584
18	1	0	0.187718	2.005104	0.169446
19	8	0	2.783563	-0.372170	-0.355691
20	1	0	3.084902	-0.961625	-1.051634
21	6	0	3.923008	0.291738	0.223078
22	1	0	3.546478	0.944630	1.009181
23	1	0	4.439948	0.895549	-0.524794
24	1	0	4.611040	-0.432762	0.661862

Ion: Pyridinium
Formula: PyridineH+
Solvent: CH3OH
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.162222	-0.674010	1.178966
2	6	0	0.162222	-2.056085	1.207518
3	6	0	0.162236	-2.754655	0.000000
4	6	0	0.162222	-2.056085	-1.207518
5	6	0	0.162222	-0.674010	-1.178966
6	7	0	0.161952	-0.027777	0.000000
7	1	0	0.162821	-0.055798	2.066755
8	1	0	0.162523	-2.571647	2.158223
9	1	0	0.162460	-3.838019	0.000000
10	1	0	0.162523	-2.571647	-2.158223
11	1	0	0.162821	-0.055798	-2.066755
12	1	0	0.164038	1.017652	0.000000
13	8	0	0.180445	2.686320	0.000000
14	1	0	0.995084	3.195248	0.000000
15	6	0	-0.947702	3.582488	0.000000
16	1	0	-1.843539	2.963862	0.000000
17	1	0	-0.943240	4.207085	-0.894638
18	1	0	-0.943240	4.207085	0.894638

Ion: Anilinium
Formula: C6H5NH3+
Solvent: CH3OH
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.770956	-0.827874	1.217398
2	6	0	-0.770956	-2.221355	1.209043
3	6	0	-0.770586	-2.914473	0.000000
4	6	0	-0.770956	-2.221355	-1.209043
5	6	0	-0.770956	-0.827874	-1.217398
6	6	0	-0.772410	-0.161845	0.000000
7	1	0	-0.773285	-0.283638	2.155909
8	1	0	-0.775716	-2.760234	2.148065
9	1	0	-0.774672	-3.997283	0.000000
10	1	0	-0.775716	-2.760234	-2.148065
11	1	0	-0.773285	-0.283638	-2.155909
12	7	0	-0.738211	1.319646	0.000000
13	1	0	0.261059	1.680221	0.000000
14	1	0	-1.213427	1.693263	0.822052
15	1	0	-1.213427	1.693263	-0.822052
16	8	0	1.823446	2.139566	0.000000
17	1	0	2.529952	1.488537	0.000000
18	6	0	2.386512	3.467164	0.000000
19	1	0	1.552357	4.166744	0.000000
20	1	0	2.988957	3.627315	-0.895113
21	1	0	2.988957	3.627315	0.895113

Ion: NO3-
Formula: NO3-
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016389	1.329605	0.000000
2	6	0	-1.035159	2.785836	0.000000
3	7	0	-1.057649	3.940874	0.000000
4	1	0	0.000000	0.916309	0.000000
5	1	0	-1.526421	0.942065	0.882836
6	1	0	-1.526421	0.942065	-0.882836
7	7	0	0.735220	-1.783179	0.000000
8	8	0	1.315859	-2.888437	0.000000
9	8	0	-0.522977	-1.722461	0.000000
10	8	0	1.409509	-0.713721	0.000000

Ion: Trifluoroacetate
Formula: CF3CO2-
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.684296	-2.849024	0.000000
2	6	0	0.294474	-4.252405	0.000000
3	7	0	-0.008943	-5.367040	0.000000
4	1	0	-0.176804	-2.169194	0.000000
5	1	0	1.283399	-2.618341	0.881767
6	1	0	1.283399	-2.618341	-0.881767
7	6	0	0.069592	0.555240	0.000000
8	6	0	-0.239590	2.109489	0.000000
9	9	0	0.857971	2.892957	0.000000
10	9	0	-0.964325	2.480627	1.084580
11	9	0	-0.964325	2.480627	-1.084580
12	8	0	1.271337	0.251257	0.000000
13	8	0	-0.964325	-0.137826	0.000000

Ion: Cyanoacetate
Formula: NCCH2CO2-
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.887116	-1.760634	0.000000
2	6	0	-3.331671	-1.947022	0.000000
3	7	0	-4.476401	-2.102462	0.000000
4	1	0	-1.592914	-0.703516	0.000000
5	1	0	-1.440949	-2.222976	0.881270
6	1	0	-1.440949	-2.222976	-0.881270
7	6	0	1.029124	0.092052	0.000000
8	6	0	2.427184	0.861036	0.000000
9	6	0	2.384277	2.316635	0.000000
10	1	0	2.983394	0.522348	0.877881
11	1	0	2.983394	0.522348	-0.877881
12	8	0	1.176172	-1.145460	0.000000
13	8	0	0.000000	0.788423	0.000000
14	7	0	2.386097	3.472271	0.000000

Ion: Benzoate
Formula: C6H5CO2-
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.831736	3.137958	0.000000
2	6	0	3.087741	3.875002	0.000000
3	7	0	4.083159	4.462049	0.000000
4	1	0	1.973507	2.047310	0.000000
5	1	0	1.240255	3.387799	0.881587
6	1	0	1.240255	3.387799	-0.881587
7	6	0	0.000000	0.226049	0.000000
8	6	0	-0.841868	-1.071281	0.000000
9	8	0	-0.645249	1.298726	0.000000
10	8	0	1.245626	0.065019	0.000000
11	6	0	-2.375335	-3.428387	0.000000
12	1	0	-2.967624	-4.338333	0.000000
13	6	0	-2.238567	-1.013953	0.000000
14	6	0	-0.223505	-2.325234	0.000000
15	6	0	-3.002419	-2.180903	0.000000
16	6	0	-0.981004	-3.496322	0.000000
17	1	0	-2.698485	-0.032264	0.000000
18	1	0	0.860304	-2.349345	0.000000
19	1	0	-4.086978	-2.121215	0.000000
20	1	0	-0.487031	-4.463614	0.000000

Ion: Acetate
Formula: CH3CO2-
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.977585	1.435916	0.000000
2	6	0	-0.866652	2.886975	0.000000
3	7	0	-0.781192	4.039872	0.000000
4	1	0	0.000000	0.922808	0.000000
5	1	0	-1.520908	1.094473	0.882272
6	1	0	-1.520908	1.094473	-0.882272
7	6	0	0.528290	-1.674192	0.000000
8	6	0	1.261616	-3.045341	0.000000
9	1	0	0.554319	-3.877336	0.000000
10	1	0	1.908582	-3.113719	0.880197
11	1	0	1.908582	-3.113719	-0.880197
12	8	0	-0.724164	-1.698425	0.000000
13	8	0	1.282247	-0.664855	0.000000

Ion: Phenoxide
Formula: C6H5O-
Solvent: CH3CN
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.007075	-1.237963	-0.000014
2	6	0	-3.290355	-0.708491	0.006219
3	6	0	-3.513195	0.675089	0.006464
4	6	0	-2.392192	1.515728	0.000140
5	6	0	-1.100774	1.006082	-0.006182
6	6	0	-0.831135	-0.407753	-0.006608
7	1	0	-1.854273	-2.313835	-0.000105
8	1	0	-4.142285	-1.386444	0.011030
9	1	0	-4.519088	1.081144	0.011332
10	1	0	-2.533939	2.595064	0.000144
11	1	0	-0.245842	1.676951	-0.011135
12	8	0	0.350049	-0.891744	-0.012473
13	6	0	3.291679	-0.868997	0.006705
14	6	0	4.237635	0.235954	0.003323
15	7	0	4.998774	1.104975	0.000772
16	1	0	3.446685	-1.480102	0.898532
17	1	0	2.234899	-0.539268	-0.000457
18	1	0	3.454497	-1.492277	-0.875241

Ion: Anilinium
Formula: C6H5NH3+
Solvent: CH3CN
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.925239	1.078924	0.598496
2	6	0	2.983661	0.253960	0.976077
3	6	0	3.112473	-1.015862	0.418784
4	6	0	2.184875	-1.472133	-0.517103
5	6	0	1.120565	-0.660803	-0.902067
6	6	0	1.016487	0.602271	-0.334252
7	1	0	1.822326	2.070321	1.027434
8	1	0	3.704245	0.608597	1.702087
9	1	0	3.937948	-1.651974	0.712950
10	1	0	2.286385	-2.459616	-0.949353
11	1	0	0.392927	-1.010460	-1.626062
12	7	0	-0.117566	1.463744	-0.737424
13	1	0	-0.074098	2.363040	-0.258020
14	1	0	-1.051545	1.018805	-0.504065
15	1	0	-0.101794	1.654091	-1.740782
16	7	0	-2.559677	0.305533	-0.114143
17	6	0	-3.578632	-0.143384	0.173610
18	6	0	-4.865147	-0.711518	0.537591
19	1	0	-4.985704	-0.683728	1.621941
20	1	0	-5.666930	-0.136057	0.071703
21	1	0	-4.920193	-1.746682	0.196323

Ion: Pyridinium
Formula: PyridineH+
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000455	-1.209337	1.178517
2	6	0	0.000455	-2.591525	1.207375
3	6	0	0.000453	-3.289882	0.000000
4	6	0	0.000455	-2.591525	-1.207375
5	6	0	0.000455	-1.209337	-1.178517
6	7	0	0.000462	-0.564156	0.000000
7	1	0	0.000427	-0.590164	2.065562
8	1	0	0.000443	-3.107433	2.157809
9	1	0	0.000442	-4.373205	0.000000
10	1	0	0.000443	-3.107433	-2.157809
11	1	0	0.000427	-0.590164	-2.065562
12	1	0	0.000402	0.480641	0.000000
13	7	0	0.000160	2.234000	0.000000
14	6	0	-0.000554	3.384249	0.000000
15	6	0	-0.001894	4.837450	0.000000
16	1	0	-1.029301	5.205253	0.000000
17	1	0	0.511705	5.206524	0.889333
18	1	0	0.511705	5.206524	-0.889333

Ion: Ammonium
Formula: NH4+
Solvent: CH3CN
Point Group: C3V

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-2.555079
2	6	0	0.000000	0.000000	-1.103435
3	7	0	0.000000	0.000000	0.046443
4	1	0	0.000000	1.027992	-2.922004
5	1	0	0.890267	-0.513996	-2.922004
6	1	0	-0.890267	-0.513996	-2.922004
7	1	0	0.000000	0.000000	1.690809
8	7	0	0.000000	0.000000	2.765575
9	1	0	0.000000	0.958308	3.114055
10	1	0	-0.829919	-0.479154	3.114055
11	1	0	0.829919	-0.479154	3.114055

Ion: Methylammonium
Formula: CH3NH3+
Solvent: CH3CN
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.054609	3.069208	0.000000
2	6	0	0.465917	1.741409	0.000000
3	7	0	0.000000	0.689759	0.000000
4	1	0	0.264012	3.821665	0.000000
5	1	0	1.673227	3.197307	0.889987
6	1	0	1.673227	3.197307	-0.889987
7	1	0	-0.754751	-0.848876	0.000000
8	7	0	-1.177463	-1.819544	0.000000
9	6	0	-0.105259	-2.866513	0.000000
10	1	0	-1.776426	-1.902382	-0.821274
11	1	0	-1.776426	-1.902382	0.821274
12	1	0	-0.561567	-3.853727	0.000000
13	1	0	0.504669	-2.732520	0.890279
14	1	0	0.504669	-2.732520	-0.890279

Ion: NO2-
Formula: NO2-
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.140472	-0.001376	-0.111999
2	8	0	2.483801	1.065603	-0.011422
3	8	0	2.478600	-1.069383	-0.083071
4	16	0	-1.585639	-0.010470	-0.438627
5	6	0	-0.735573	1.358434	0.383058
6	6	0	-0.721881	-1.332033	0.443797
7	1	0	0.345945	1.264724	0.202392
8	1	0	-1.129811	2.281549	-0.043873
9	1	0	-0.963469	1.312338	1.450803
10	1	0	0.359013	-1.233364	0.260552
11	1	0	-0.955366	-1.241971	1.507528
12	1	0	-1.102717	-2.277815	0.056242
13	8	0	-3.015144	-0.007058	0.020399

Ion: Benzoate
Formula: C6H5CO2-
Solvent: (CH3)2SO
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.014838	2.944633	1.202146
2	6	0	-0.082519	4.337539	1.205782
3	6	0	-0.116453	5.040037	0.000000
4	6	0	-0.082519	4.337539	-1.205782
5	6	0	-0.014838	2.944633	-1.202146
6	6	0	0.019806	2.232132	0.000000
7	1	0	0.012622	2.374332	2.123646
8	1	0	-0.108984	4.878143	2.147382
9	1	0	-0.168916	6.124417	0.000000
10	1	0	-0.108984	4.878143	-2.147382
11	1	0	0.012622	2.374332	-2.123646
12	6	0	0.095372	0.689550	0.000000
13	8	0	0.122438	0.144033	-1.128397
14	8	0	0.122438	0.144033	1.128397
15	1	0	0.273408	-1.959649	-1.278283
16	1	0	0.273408	-1.959649	1.278283
17	6	0	0.408050	-3.049178	-1.349474
18	6	0	0.408050	-3.049178	1.349474
19	16	0	-0.491084	-3.851279	0.000000
20	8	0	-0.113983	-5.304418	0.000000
21	1	0	1.462165	-3.326335	-1.270852
22	1	0	-0.009979	-3.436172	-2.279897
23	1	0	-0.009979	-3.436172	2.279897
24	1	0	1.462165	-3.326335	1.270852

Ion: Acetate
Formula: CH3CO2-
Solvent: (CH3)2SO
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.473048	3.640010	0.000000
2	6	0	0.713625	2.284741	0.000000
3	8	0	-0.536315	2.327439	0.000000
4	1	0	0.782470	4.485683	0.000000
5	1	0	2.121500	3.695711	0.879980
6	1	0	2.121500	3.695711	-0.879980
7	8	0	1.447320	1.257694	0.000000
8	16	0	-0.265500	-2.163488	0.000000
9	6	0	-0.536315	-0.981771	-1.343367
10	6	0	-0.536315	-0.981771	1.343367
11	1	0	-0.375807	-1.516776	-2.280324
12	1	0	0.176559	-0.160816	-1.204376
13	1	0	-1.559431	-0.607402	-1.281421
14	1	0	-0.375807	-1.516776	2.280324
15	1	0	-1.559431	-0.607402	1.281421
16	1	0	0.176559	-0.160816	1.204376
17	8	0	-1.404052	-3.142454	0.000000

Ion: Phenoxide
Formula: C6H5O-
Solvent: (CH3)2SO
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.215573	-2.411980	1.209585
2	6	0	-0.237983	-3.800186	1.199336
3	6	0	-0.249734	-4.524239	0.000000
4	6	0	-0.237983	-3.800186	-1.199336
5	6	0	-0.215573	-2.411980	-1.209585
6	6	0	-0.203174	-1.633760	0.000000
7	1	0	-0.206118	-1.869246	2.151051
8	1	0	-0.246201	-4.335976	2.146833
9	1	0	-0.266711	-5.608801	0.000000
10	1	0	-0.246201	-4.335976	-2.146833
11	1	0	-0.206118	-1.869246	-2.151051
12	8	0	-0.183623	-0.355777	0.000000
13	1	0	-0.198484	1.378045	-1.215240
14	1	0	-0.198484	1.378045	1.215240
15	6	0	-0.215573	2.467709	-1.347330
16	6	0	-0.215573	2.467709	1.347330
17	16	0	0.744812	3.204355	0.000000
18	8	0	0.477731	4.681331	0.000000
19	1	0	-1.233648	2.860924	-1.294818
20	1	0	0.256373	2.774339	-2.281465
21	1	0	0.256373	2.774339	2.281465
22	1	0	-1.233648	2.860924	1.294818

Ion: Methoxide
Formula: CH3O-
Solvent: (CH3)2SO
Point Group: CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.620951	1.239734	0.000000
2	8	0	0.380885	2.726397	0.000000
3	8	0	-0.319106	-2.144426	0.000000
4	6	0	-0.346113	0.508936	1.342691
5	6	0	-0.346113	0.508936	-1.342691
6	1	0	-0.365063	-0.583889	1.163211
7	1	0	-1.349239	0.943177	1.310239
8	1	0	0.146632	0.776109	2.279205
9	1	0	-0.365063	-0.583889	-1.163211
10	1	0	0.146632	0.776109	-2.279205
11	1	0	-1.349239	0.943177	-1.310239
12	6	0	-0.346113	-3.496288	0.000000
13	1	0	-1.377731	-3.944650	0.000000
14	1	0	0.156821	-3.973580	0.885586
15	1	0	0.156821	-3.973580	-0.885586

Ion: Ethoxide
Formula: CH3CH2O-
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.775156	-0.089609	-0.478684
2	8	0	-3.255354	-0.085526	-0.206328
3	8	0	1.655191	0.147060	0.402111
4	6	0	-0.992247	-1.243246	0.674864
5	6	0	-1.061888	1.406945	0.245517
6	1	0	0.094753	-1.046234	0.641514
7	1	0	-1.247680	-2.252159	0.346711
8	1	0	-1.405326	-1.056473	1.669843
9	1	0	0.034408	1.260213	0.269214
10	1	0	-1.475260	1.524316	1.250891
11	1	0	-1.362397	2.246528	-0.383528
12	6	0	2.997969	0.241909	0.471715
13	6	0	3.730799	-0.304587	-0.784017
14	1	0	3.369667	1.296689	0.603932
15	1	0	3.445013	-0.308090	1.346677
16	1	0	4.824718	-0.210109	-0.697631
17	1	0	3.398548	0.242084	-1.673755
18	1	0	3.479541	-1.361415	-0.929672

Ion: Pyridinium
Formula: PyridineH+
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.985402	-1.167230	-0.110659
2	6	0	-3.367915	-1.205426	-0.112948
3	6	0	-4.073743	-0.007811	0.000057
4	6	0	-3.381094	1.197095	0.112547
5	6	0	-1.997860	1.173940	0.109289
6	7	0	-1.343862	0.006645	-0.000896
7	1	0	-1.365578	-2.049965	-0.194564
8	1	0	-3.878105	-2.154852	-0.201787
9	1	0	-5.157023	-0.014057	0.000378
10	1	0	-3.901411	2.140971	0.201704
11	1	0	-1.381337	2.059018	0.192300
12	1	0	-0.280713	0.033450	0.000532
13	8	0	1.241179	0.379334	0.042298
14	16	0	2.511165	-0.443477	-0.071351
15	6	0	3.515063	0.400328	-1.311416
16	6	0	3.484997	-0.023924	1.389590
17	1	0	3.009380	0.280823	-2.268909
18	1	0	3.597987	1.455701	-1.049821
19	1	0	4.495752	-0.076404	-1.349835
20	1	0	2.960006	-0.430646	2.253159
21	1	0	4.466637	-0.491955	1.300643
22	1	0	3.569107	1.060533	1.466942

Ion: Anilinium
Formula: C6H5NH3+
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.082934	0.411855	1.137468
2	6	0	3.102095	1.228693	0.653545
3	6	0	3.722156	0.933303	-0.559605
4	6	0	3.327929	-0.181825	-1.295311
5	6	0	2.310683	-1.008887	-0.821740
6	6	0	1.707588	-0.696090	0.388547
7	1	0	1.597634	0.636993	2.081021
8	1	0	3.412436	2.092096	1.228639
9	1	0	4.516726	1.569715	-0.928629
10	1	0	3.812061	-0.416050	-2.235035
11	1	0	2.004302	-1.881350	-1.389492
12	7	0	0.608680	-1.543574	0.882649
13	1	0	-0.372629	-1.089021	0.704965
14	1	0	0.625126	-2.458010	0.433337
15	1	0	0.689225	-1.700737	1.887340
16	8	0	-1.727410	-0.482745	0.680979
17	16	0	-2.492827	0.132284	-0.484173
18	6	0	-2.879093	1.813801	0.041480
19	6	0	-4.147445	-0.576800	-0.374377
20	1	0	-4.061075	-1.634527	-0.620234
21	1	0	-4.527126	-0.447088	0.639456
22	1	0	-4.787318	-0.079183	-1.104760
23	1	0	-1.938616	2.362488	0.078380
24	1	0	-3.539988	2.265501	-0.700017
25	1	0	-3.348078	1.785315	1.025375

Ion: Ammonium
Formula: NH4+
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.594265	0.000216	-0.436066
2	8	0	-0.641354	0.000819	0.466379
3	1	0	-1.999869	0.003464	0.091815
4	6	0	1.598262	1.370332	0.164154
5	6	0	1.596355	-1.371557	0.164194
6	1	0	2.560170	1.342839	-0.350262
7	1	0	1.722609	1.278640	1.243477
8	1	0	1.072750	2.290739	-0.087657
9	1	0	2.558197	-1.345688	-0.350448
10	1	0	1.069067	-2.291011	-0.087390
11	1	0	1.720962	-1.279742	1.243457
12	7	0	-3.119397	0.000262	-0.033168
13	1	0	-3.383383	-0.168910	-1.001581
14	1	0	-3.524905	-0.731179	0.547972
15	1	0	-3.504931	0.896356	0.258719

Ion: Methylammonium
Formula: CH3NH3+
Solvent: (CH3)2SO
Point Group: C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.214623	-0.029250	-0.466624
2	8	0	-0.167527	-0.021334	0.172994
3	1	0	-1.564820	-0.113350	-0.408352
4	6	0	2.057446	1.410703	0.218167
5	6	0	2.128195	-1.318785	0.402686
6	1	0	3.098420	1.389757	-0.108350
7	1	0	1.983173	1.389340	1.305839
8	1	0	1.564092	2.294544	-0.184590
9	1	0	3.167557	-1.289057	0.071780
10	1	0	1.681918	-2.272984	0.124995
11	1	0	2.049990	-1.154436	1.477747
12	7	0	-2.628374	-0.158845	-0.608238
13	1	0	-2.851042	0.504046	-1.349039
14	1	0	-2.851988	-1.089099	-0.958181
15	6	0	-3.396730	0.146836	0.638904
16	1	0	-4.464692	0.097190	0.437635
17	1	0	-3.121120	1.143717	0.974395
18	1	0	-3.120088	-0.581613	1.397277

END OF SUPPORTING INFORMATION