TABLE I: Dissociative Bond Enthalpies
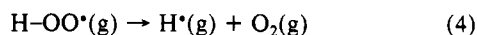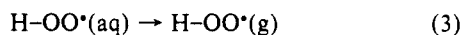
bond	$\Delta H°_{DBE}$/kcal mol^{-1}			
	Sawyer calcd[a]	Sawyer lit.[a]	JANAF calcd[b]	this work
H–OH	119	119	119.9	
H–O•	106	102	102.3	
H–O$^-$	116		110.8	
H–OOH	90	88	82.5	
H–OO$^-$	80	59	(68.9)[c]	69.1
H–OO•	59	47	51.6	51.8

[a] Reference 1. [b] Reference 2. [c] The heat of formation of HO$_2^-$ is taken from ref 4 but corrected for the newer value for the heat of formation of the hydroperoxo radical given in ref 2.
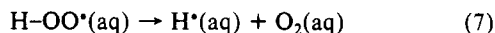
these assumptions is defensible if the claimed objective is "accurate values".

Table I lists values obtained by Sawyer and comparison literature values cited by him. Four of the comparison values date from 1965 to 1979 and one from 1983. At the outset it therefore seemed appropriate to calculate the several bond dissociation enthalpies from a more recent compendium of thermodynamic data.[2] These appear in column four of the table. The last column of the table contains two values we calculate according to the prescription given below. Sawyer's approach gives bond energies in these two instances that are 12 and 21 kcal/mol greater than the "long-accepted values". By implication, he believes that the latter are incorrect by the stated amounts.

We now examine the case of H–OO•, for which Sawyer's value and the "accepted" value differ by 12 kcal/mol. The thermochemical cycle that will yield $\Delta H°_{DBE}$ is

$$H-OO•(aq) \rightarrow H-OO•(g) \quad (3)$$

$$H-OO•(g) \rightarrow H•(g) + O_2(g) \quad (4)$$

$$H•(g) \rightarrow H•(aq) \quad (5)$$

$$O_2(g) \rightarrow O_2(aq) \quad (6)$$

the sum of which is

$$H-OO•(aq) \rightarrow H•(aq) + O_2(aq) \quad (7)$$

Reaction 4 is the desired gas-phase bond-dissociation reaction. Note that $-\Delta G°_{BF} = \Delta G°_7$ and $\Delta S°_4 = \Delta S°_{DBE}$. This cycle yields

$$\Delta H°_{DBE} = -\Delta G°_{BF} + T\Delta S°_{DBE} - \Delta G°_3 - \Delta G°_5 - \Delta G°_6 \quad (8)$$

The first two terms in eq 8 are in Sawyer's formula, eq 1, but not the last three.

Data taken from ref 2 yield $\Delta S°_4 = 21.7$ cal/K, and hence $T\Delta S°_{DBE} = 6.5$ kcal/mol, not the constant value of 7.8 kcal/mol used by Sawyer. Sawyer's cited value for the HO$_2$/H$_2$O$_2$ reduction potential of 1.44 V when combined with the standard Gibbs energy of formation for aqueous H$_2$O$_2$ of 32.0 kcal/mol[3] leads to a standard Gibbs energy of formation for HO$_2$(aq) of +1.2 kcal/mol. The corresponding quantity for HO$_2$(g) = 3.44 kcal/mol[2] and hence $\Delta G°_3 = 2.2$ kcal/mol. A similar calculation gives $\Delta G°_5 = -0.2$ kcal/mol while $\Delta G°_6 = \Delta G°_f$ for O$_2$(aq) = 3.9 kcal/mol.[3] Sawyer's tabulated redox potentials yield $\Delta G°_7 = 51.2$ kcal/mol. When all these values are substituted into eq 8, we find $\Delta H°_{DBE} = 51.8$ kcal/mol, in excellent agreement with the JANAF value given in column four of the table.

The bond dissociation enthalpy for H–OO$^-$ may be calculated readily from $\Delta H°_{DBE}$ for H–OO• by adding the electron affinity (EA) of HO$_2$, 27.4 kcal/mol,[4] and subtracting EA for O$_2$, 10.1 kcal/mol.[5] This yields 69.1 kcal/mol for $\Delta H°_{DBE}$ of HO$_2^-$, again

in good agreement with the result calculated essentially from gas-phase enthalpy of formation data. It is not, of course, surprising that accurate redox potentials used in an appropriate thermochemical cycle can lead to accurate thermodynamic results. Sawyer, however, has handled them improperly. Any agreement between his results and "accepted" ones is fortuitous.

(5) Celotta, R. J.; Bennett, R. A.; Hall, J. L.; Seigel, M. W.; Levine, J. *Phys. Rev.* **1972**, *A6*, 631.

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Comments on "Reevaluation of the Bond-Dissociation Energies (ΔH_{DBE}) for H–OH, H–OOH, H–OO$^-$, H–O•, H–OO$^-$, and H–OO•"[†]

Sir: In a recent letter by Sawyer,[1] it was suggested that new values of the bond dissociation energies (BDE), defined for bond-breaking processes in the gas phase at 298 K, for a number of hydrogen- and oxygen-containing species could be determined from half-cell potentials. Discrepancies with "accepted" values for HO$_2$ and HO$_2^-$ were noted. We wish to point out that the bond dissociation energies for H–OO and H–OO$^-$ that were derived by Sawyer are in serious disagreement with those established in the past decade by gas-phase chemical kinetics and photoelectron spectroscopy. These bond energies have been simply and accurately deduced from experimental measurements of the heats of formation of HO$_2$ and HO$_2^-$ and of the electron affinity of HO$_2$. These results were not cited by Sawyer. Moreover, computations utilizing half-cell potentials for the derivation of bond dissociation energies must account for substantial solvation effects. When properly calculated, these BDEs are, in fact, in accord with established values.

Kinetic Determinations

We take serious exception to Sawyer's statement that the bond energies of polyatomic molecules extracted from kinetic data are usually subject to considerable error. On the contrary, kinetic measurements provide a basis for accurate data on many species including highly reactive radicals[2] and ions.[3] The observation of a large rate coefficient for a gas-phase reaction at room temperature indicates that the reaction is not greatly endothermic, i.e., $\Delta H_r \leq 2$ kcal mol^{-1}. The measurement of both the forward and reverse rate coefficients of a reaction defines the equilibrium constant and hence the free energy change for the reaction:

$$K = k_f/k_r = \exp[-\Delta G°/RT] \quad (1)$$

When the entropies of all species are known and the heats of formation of all but one of the reactants or products is well-established, the heat of formation of the remaining species may be deduced.

Heat of Formation of HO$_2$. Several reactions involving the HO$_2$ radical have been studied to gain information on the thermochemistry of this important species.[4] The gas-phase rate coefficients for reactions 2 and 3 have been measured as a function

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

(3) Wagman, D. D.; Evans, W. H.; Parker, V. B.; Schumm, R. H.; Halow, I.; Bailey, S. M.; Churney, K. L.; Nuttall, R. L. *J. Phys. Chem. Ref. Data* **1982**, *11*, Suppl. 1.

(4) Bierbaum, V. M.; Schmitt, R. J.; DePuy, C. H.; Mead, R. D.; Schulz, P. A.; Linebarger, W. C. *J. Am. Chem. Soc.* **1981**, *103*, 6262.

[†] The first H–OO$^-$ in the original title should have read H–O$^-$.
(1) Sawyer, D. T. *J. Phys. Chem.* **1989**, *93*, 7977.
(2) McMillen, D. F.; Golden, D. M. *Ann. Rev. Phys. Chem.* **1982**, *33*, 493.
(3) Lias, S. G.; Bartmess, J. E.; Liebman, J. F.; Holmes, J. L.; Levin, R. D.; Mallard, W. G. *J. Phys. Chem. Ref. Data* **1988**, *17*, Suppl. No. 1.
(4) The thermochemical history of HO$_2$ up to 1982 is reviewed by: Shum, L. G. S.; Benson, S. W. *J. Phys. Chem.* **1983**, *87*, 3479.

of temperature to determine $\Delta H^\circ_{f,298}(HO_2)$. (All thermochemical quantities discussed herein are at a nominal temperature of 298 K. Temperature values will be omitted from thermochemical symbols.) The forward rate coefficients at room temperature for both reactions 2 and 3 have been measured by several workers[5,6]

$$HO_2 + NO \rightarrow OH + NO_2 \qquad (2)$$

$$HO_2 + Cl \rightarrow OH + ClO \qquad (3)$$
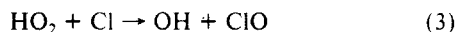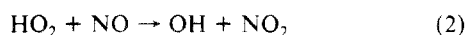
and found to be relatively large ($\sim 8 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $\sim 9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, respectively), indicating that neither reaction is significantly endothermic. This fact contradicts the thermochemical data derived by Sawyer; his BDE(H–OO) implies $\Delta H^\circ_f(HO_2) = -6.9$ kcal mol^{-1}, which makes reactions 2 and 3 endothermic by 2.6 and 11.4 kcal mol^{-1}, respectively. Further, the direct measurements of the reverse rate coefficients for reactions 2 and 3 provide two independent determinations for $\Delta H^\circ_f(HO_2)$ (2.5 ± 0.6[7] and 3.0 ± 0.4[8] kcal mol^{-1}) which are in good agreement. The latter value is recommended as discussed in ref 8. This $\Delta H^\circ_f(HO_2)$ defines the BDE(H–OO):

$$HO_2 \rightarrow H + O_2 \qquad BDE = 49.1 \text{ kcal mol}^{-1} \qquad (4)$$
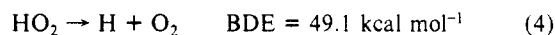
This value is 9.9 kcal mol^{-1} below that reported by Sawyer.

Heat of Formation of HO_2^-. The photoelectron spectroscopy of HO_2^- has been studied by Ellison and co-workers,[9] and the electron affinity of the hydroperoxyl radical has been determined:

$$e + HO_2 \rightarrow HO_2^- \qquad EA = 1.078 \pm 0.017 \text{ eV} \qquad (5)$$
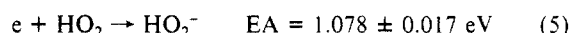
This value, combined with the heat of formation of HO_2 and the integrated heat capacity of the electron,[10] yields the heat of formation of the hydroperoxide ion, $\Delta H^\circ_f(HO_2^-) = -23.3 \pm 0.6$ kcal mol^{-1}. This value directly determines BDE(H–O$_2^-$):

$$HO_2^- \rightarrow H + O_2^- \qquad BDE = 63.8 \text{ kcal mol}^{-1} \qquad (6)$$

This value is 16.2 kcal mol^{-1} lower than that recommended by Sawyer. These disagreements are significant since the total error in the measured heat of formation and bond dissociation energies are estimated to be less than 1 kcal mol^{-1}.

Moreover, gas-phase ion chemistry[12] provides a totally independent check on the $\Delta H^\circ_f(HO_2^-)$ that was derived from the combined results of chemical kinetics and photoelectron spectroscopy. The $\Delta H^\circ_f(HO_2^-)$ was determined by using the flowing afterglow technique by measuring the forward and reverse reaction rate coefficients for two proton-transfer reactions, (7) and (8).

$$CF_3^- + H_2O_2 \leftrightarrow HO_2^- + HCF_3 \qquad (7)$$

$$F^- + H_2O_2 \leftrightarrow HO_2^- + HF \qquad (8)$$
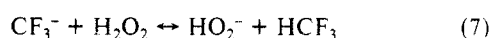
The resulting value,[13] $\Delta H^\circ_f(HO_2^-) = -23.7 \pm 1.5$ kcal mol^{-1}, while less precise, corroborates the thermochemistry given above. The

(5) Howard, C. J.; Evenson, K. M. *Geophys. Res. Lett.* **1977**, *4*, 437. Leu, M.-T. *J. Chem. Phys.* **1979**, *70*, 1662. Glaschick-Schimpf, I.; Leiss, A.; Monkhouse, P. B.; Schurath, U.; Becker, K. H.; Fink, E. H. *Chem. Phys. Lett.* **1979**, *67*, 318. Hack, W.; Preuss, A. W.; Temps, F.; Wagner, H. G.; Hoyermann, K. *Int. J. Chem. Kinet.* **1980**, *12*, 851. Thrush, B. A.; Wilkinson, J. P. T. *Chem. Phys. Lett.* **1981**, *81*, 1.
(6) Lee, Y.-P.; Howard, C. J. *J. Chem. Phys.* **1982**, *77*, 756. Cattell, F. C.; Cox, R. A. *J. Chem. Soc., Faraday Trans. 2* **1986**, *82*, 1413.
(7) Howard, C. J. *J. Am. Chem. Soc.* **1980**, *102*, 6937.
(8) Hills, A. J.; Howard, C. J. *J. Chem. Phys.* **1984**, *81*, 4458; Other studies of the OH + ClO reaction are in good agreement: Leu, M.-T.; Lin, C.-L. *Geophys. Res. Lett.* **1979**, *6*, 425. Ravishankara, A. R.; Eisele, F. L.; Wine, P. H. *J. Chem. Phys.* **1983**, *78*, 1140. Burrows, J. P.; Wallington, T. J.; Wayne, R. P. *J. Chem. Soc., Faraday Trans. 2* **1984**, *80*, 957. Poulet, G.; Laverdet, G.; LeBras, G. *J. Phys. Chem.* **1986**, *90*, 159.
(9) Oakes, J. M.; Harding, L. B.; Ellison, G. B. *J. Chem. Phys.* **1985**, *83*, 5400.
(10) The heat capacity of the electron must be accounted for following the convention of ref 11.
(11) Chase, M. W., Jr.; Davies, C. A.; Downey, J. R., Jr.; Frurip, D. J.; McDonald, R. A.; Syverud, A. N. *JANAF Thermochemical Tables*, 3rd ed.; *J. Phys. Chem. Ref. Data* **1985**, *14*, Suppl. No. 1.
(12) Bierbaum, V. M.; Schmitt, R. J.; DePuy, C. H.; Mead, R. D.; Schulz, P. A.; Lineberger, W. C. *J. Am. Chem. Soc.* **1981**, *103*, 6262.

TABLE I: Comparison of BDE Values at 298 K

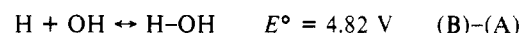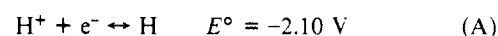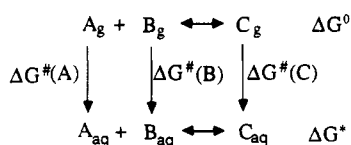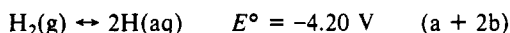| bond	BDE, kcal mol^{-1}	
	Sawyer	recommended[a]
(1) H–OH $\leftrightarrow$ H + OH	119	119
(2) H–O $\leftrightarrow$ H + O	106	102
(3) H–O$^-$ $\leftrightarrow$ H + O$^-$	116	111
(4) H–OOH $\leftrightarrow$ H + OOH	90	87.7[b]
(5) H–OO$^-$ $\leftrightarrow$ H + OO$^-$	80	63.8[b]
(6) H–OO $\leftrightarrow$ H + OO	59	49.1[b]

[a] Based on data in ref 11. [b] Incorporates data discussed in text.

excellent agreement among these independent approaches strongly confirms the validity of the bond dissociation energies that are derived.

The BDE values suggested by Sawyer as well as our recommended values are listed in Table I. If one accepts Sawyer's value for BDE(H–OO), the $\Delta H^\circ_f(HO_2)$ must be revised to -6.9 kcal mol^{-1}, because the error cannot be in the heats of formation of H or O$_2$. If we also accept Sawyer's value of 90 kcal mol^{-1} for BDE(H–OOH), we must also revise the $\Delta H^\circ_f(H_2O_2)$ to -45 kcal mol^{-1} from the accepted value of -32.6 kcal mol^{-1}. An error of this magnitude is extremely unlikely. Is there an explanation for these discrepancies?

Explanation

BDE(H–OH). Sawyer uses the example of the BDE in water to illustrate how he computes the values that he favors. He argues that the following algebraic treatment of the appropriate half-cell potentials leads, through the Nernst equation, to the value of ΔG for the reaction of interest:

$$H^+ + e^- \leftrightarrow H \qquad E^\circ = -2.10 \text{ V} \qquad (A)$$

$$OH + H^+ + e^- \leftrightarrow H–OH \qquad E^\circ = 2.72 \text{ V} \qquad (B)$$

$$H + OH \leftrightarrow H–OH \qquad E^\circ = 4.82 \text{ V} \qquad (B)–(A)$$

Converting to kcal mol^{-1}, $\Delta G = -4.82 \times 23.1 = -111.3$ kcal mol^{-1}.

Sawyer assumes ΔS to be -26 eu. (The gas-phase value is[11] $\Delta S^\circ = -26.2$ eu.) Thus he says that $\Delta G = \Delta H - T\Delta S$ and $\Delta H = -111.3 - (300 \times 0.026) = -111.3 - 7.8 = -119.1$ kcal mol^{-1}, which is, of course, the correct numerical value of the BDE in water.

He then goes on to correct all values of ΔG by the same $T\Delta S$ value, 7.8 kcal mol^{-1}.

The problem is that the value of ΔG obtained from the Nernst equation refers to *aqueous species at standard states of unit molality.* These values cannot be combined simply with the gas-phase entropy change, which in addition to being for different species (i.e., nonaqueous) refers to standard states of 1 atm! The fact that Sawyer's example calculation leads to the correct value for water indicates that ΔG^*, where the asterisk refers to the unit molality standard state, and ΔG°, where the superscript refers to the standard state of 1 atm, must be numerically equal in this particular case.

For each species in the chemical equation we can define the free energy of solvation, $\Delta G^\#$, a quantity directly related to Henry's law coefficients. The thermodynamic symbol reminds us that the standard states of gaseous and aqueous species are not the same. The requirement that ΔG^* be numerically equivalent to ΔG° implicit in Sawyer's analysis can be restated as

$$\Delta G^* - \Delta G^\circ \equiv \Delta[\Delta G^\#] = 0$$

This can be seen diagramatically in Scheme I.

(13) The threshold photodetachment studies of HO$_2^-$ in ref 12 are superseded by the photoelectron studies of ref 9. The flowing afterglow studies of ref 12 which yield the $\Delta H^\circ_f(HO_2^-)$ and the gas-phase acidity of hydrogen peroxide are valid. The value of $\Delta H^\circ_f(HO_2^-)$ reported here is slightly modified due to revised thermochemical data for the species in eq 7 and 8.

SCHEME I

$$A_g + B_g \leftrightarrow C_g \qquad \Delta G^0$$

$$\Delta G^\#(A) \Big\downarrow \quad \Big\downarrow \Delta G^\#(B) \quad \Big\downarrow \Delta G^\#(C)$$

$$A_{aq} + B_{aq} \leftrightarrow C_{aq} \qquad \Delta G^*$$

If we examine the individual species involved in the bond dissociation of water we find

$$H_2(g) \leftrightarrow 2H^+(aq) + 2e^-(aq) \qquad E^\circ = 0.0 \text{ V} \qquad (a)$$

$$H^+(aq) + e^-(aq) \leftrightarrow H(aq) \qquad E^\circ = -2.10 \text{ V} \qquad (b)$$

$$H_2(g) \leftrightarrow 2H(aq) \qquad E^\circ = -4.20 \text{ V} \qquad (a + 2b)$$

$$2\Delta G_f^*(H)(aq) - \Delta G_f^\circ(H_2)(g) = 97.0 \text{ kcal mol}^{-1}$$

We know very well[11] that

$$H_2(g) \leftrightarrow 2H(g) \qquad \Delta G^\circ = 97.1 \text{ kcal mol}^{-1}$$

and thus

$$H(g) \leftrightarrow H(aq) \qquad \Delta G^\# \approx 0 \text{ kcal mol}^{-1}$$

Also it is well documented that[14]

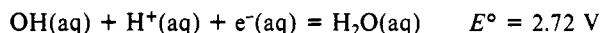$$H_2O(g) \leftrightarrow H_2O(aq) \qquad \Delta G^\# = -2.0 \text{ kcal mol}^{-1}$$

and since[11]

$$\Delta G_f^\circ(H_2O)(g) = -54.6 \text{ kcal mol}^{-1}$$

we see that

$$\Delta G_f^*(H_2O)(aq) = -56.6 \text{ kcal mol}^{-1}$$

Now, we can compute the value of $\Delta G^\#$ for OH:

$$OH(aq) + H^+(aq) + e^-(aq) = H_2O(aq) \qquad E^\circ = 2.72 \text{ V}$$

$$\Delta G^* = -62.8 \text{ kcal mol}^{-1}$$

$$\Delta G_f^*(H_2O)(aq) - \Delta G_f^*(OH)(aq) - \Delta G_f^*(H^+)(aq) -$$
$$\Delta G_f^*(e^-)(aq) = -62.8 \text{ kcal mol}^{-1}$$

The values for the aqueous proton and electron are both zero by convention; therefore, $\Delta G_f^*(OH(aq)) = -56.6 + 62.8 = 6.2$ kcal mol^{-1}, which taken together with the value in the gas phase, $\Delta G_f^\circ(OH(g)) = 8.2$ kcal mol^{-1}, yields

$$OH(g) \leftrightarrow OH(aq) \qquad \Delta G^\# = -2.0 \text{ kcal mol}^{-1}$$

So finally, for bond formation

$$\Delta G^*(BF) = \Delta G_f^*(H_2O)(aq) - \Delta G_f^*(H)(aq) -$$
$$\Delta G_f^*(OH)(aq) = [\Delta G_f^\circ(H_2O)(g) - 2.0] - [\Delta G_f^\circ(H)(g) -$$
$$0] - [\Delta G_f^\circ(OH)(g) - 2.0] = \Delta G^\circ(BF)!$$

Thus in this case $\Delta(\Delta G^\#) \approx 0$, and the procedure used by Sawyer works *accidentally* for water.

BDE(H–OOH). Sawyer's result for reaction 4 is $\Delta G^*(4) = 81.8$ kcal mol^{-1}. The gas-phase value is very well-known to be $\Delta G^\circ(4) = 79.9$ kcal mol^{-1}. The heat of formation of HO$_2$ has a value of 3.0 ± 0.4 kcal mol^{-1} as discussed above. Since all the other necessary thermodynamic values are available,[11] we can use the electrochemical data to calculate the free energy of solvation for HO$_2$.

We have already shown that the aquation free energy for H atoms is essentially zero. Also, $\Delta G^\#(H_2O_2) = -6.8$ kcal mol^{-1}.[14] The combination of all these numbers yields $\Delta G^\#(HO_2) = -4.9$ kcal mol^{-1}, viz.

$$\Delta G^\#(HO_2) = \Delta G^*(4) - \Delta G^\circ(4) - \Delta G^\#(H) + \Delta G^\#(H_2O_2) =$$
$$81.8 - 79.9 - 0 - 6.8 = -4.9 \text{ kcal mol}^{-1}$$

BDE(H–OO). For reaction 6 Sawyer lists $\Delta G^*(6) = 51.3$ kcal mol^{-1}. From the value deduced above for $\Delta G^\#(HO_2) = -4.9$ kcal mol^{-1} and from Wagman et al.[14] as well as Henry's law measurements[15] (corrected for standard state differences by $RT \ln [H_2O]$), we have $\Delta G^\#(O_2) = +3.9$ kcal mol^{-1}. The free energy change for the gas-phase process is

$$\Delta G^\circ(6) = \Delta G^*(6) - \Delta G^\#(H) - \Delta G^\#(O_2) + \Delta G^\#(HO_2)$$

$$\Delta G^\circ(6) = \Delta G^*(6) - 0 - 3.9 + (-4.9) = 51.3 - 8.8 =$$
$$42.5 \text{ kcal mol}^{-1}$$

which agrees with the known[11] value of 42.5 kcal mol^{-1}.

BDE(H–O⁻). From $\Delta G^*(3) = 108.6$ kcal mol^{-1} listed by Sawyer, a value of $\Delta G^\#(O^-) = +0.8$ kcal mol^{-1} can be deduced, since the value of $\Delta G^\#(OH^-) = -4.3$ kcal mol^{-1} is known.[14] The gas-phase values are very well established.[11]

BDE(H–OO⁻). The value of $\Delta G^*(5) = 72.3$ kcal mol^{-1} compares with the gas-phase value of $\Delta G^\circ(5) = 56.7$ kcal mol^{-1} (using the value for $\Delta H_f^\circ(HO_2^-) = -23.3 \pm 0.6$ discussed above and[16] $S^\circ(HO_2^-) = 53 \pm 1$ eu). A value of $\Delta G_f^*(O_2^-) = 4.6$ kcal mol^{-1} can be computed since we know that the value of $\Delta G_f^*(H) = 48.5$ kcal mol^{-1} and $\Delta G_f^*(HO_2^-) = -19.2$ kcal mol^{-1}.[14] (This last quantity was computed from the values for the enthalpy of formation and the entropy of HO$_2^-$ listed in ref 14, rather than their value of the free energy, which does not correspond correctly to these former quantities.) If all these data are correct, this would mean that $\Delta G^\#(O_2^-) = 14.8$ kcal mol^{-1} since $\Delta G_f^\circ(O_2^-) = -10.2$ kcal mol^{-1}.

Conclusion

The gas-phase values of the bond dissociation energies discussed by Sawyer have been accurately determined experimentally. The half-cell potentials cited by Sawyer are in good agreement with this well-known gas-phase thermochemistry, when solvation effects are properly taken into account.

(14) Wagman, D. D.; Evans, W. H.; Parker, V. B.; Schumm, R. H.; Halow, I.; Bailey, S. M.; Churney, K. L.; Nuttall, R. L. The NBS tables of chemical thermodynamic properties. Selected values for inorganic and C1 and C2 organic substances in SI units. *J. Phys. Chem. Ref. Data* **1982**, *11*, Suppl. No. 2.

(15) Wilhelm, E.; Battino, R.; Wilcock, R. J. *Chem. Rev.* **1977**, *77*, 219.

(16) Benson, S. W.; Nangia, P. S. *J. Am. Chem. Soc.* **1980**, *102*, 2843.

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