ADDITIONS AND CORRECTIONS

2000, Volume 104A

LeAnn B. Tichenor, John L. Graham, Takahiro Yamada, Philip H. Taylor,* Jingping Peng, Xiaohua Hu, and Paul Marshall: : Kinetic and Modeling Studies of the Reaction of Hydroxyl Radicals with Tetrachloroethylene.

Page 1700. Two errors were made in the creation of Table 2, "Input QRRK Parameters". The B parameters in reactions −1 through 6 were mistakenly divided by Avogadro's number. Another error was made in the parameters "*n*" and "*C*" for reaction −1. The corrected parameters used in the calculation are shown below. The errors in Table 2 do not change the results of the calculation shown in Figure 8 or the conclusion of the study.

TABLE 2: Input QRRK Parameters[a]

	reaction	*B* (s^{-1} or cm^3/(molecule s))	*n*	*C* (kcal/mol)
1	$C_2Cl_4 + OH \Rightarrow C\bullet Cl_2CCl_2OH$	9.90E−21	2.69	−0.7
−1	$C\bullet Cl_2CCl_2OH \Rightarrow C_2Cl_4 + OH$	1.15E+5	2.69	37.5
2	$C\bullet Cl_2CCl_2OH \Rightarrow CCl_3C\bullet ClOH$	1.09E+12	0.26	14.4
−2	$CCl_3C\bullet ClOH \Rightarrow C\bullet Cl_2CCl_2OH$	5.74E+10	0.71	9.80
3	$CCl_3C\bullet ClOH \Rightarrow CCl_3CClO + H$	5.75E+9	1.58	33.0
4	$CCl_3C\bullet ClOH \Rightarrow CCl_2CClOH + Cl$	1.69E+13	0.00	18.8
5	$C\bullet Cl_2CCl_2OH \Rightarrow CCl_2CClOH + Cl$	1.69E+13	0.00	23.5
6	$C\bullet Cl_2CCl_2OH \Rightarrow CCl_2HCClO + Cl$	1.75E+9	0.89	42.7

[a] Grouped geometric mean frequencies of the adduct with effective degeneracies: 337.2 cm^{-1} (8.580), 401.1 cm^{-1} (3.871), 1285.2 cm^{-1} (4.550) Lennard-Jones Parameters: C_2Cl_4OH adduct: $\sigma = 6.056$ Å, $\epsilon/k = 564.3$ K He bath gas: $\sigma = 2.576$ Å, $\epsilon/k = 470.0$ K.

10.1021/jp003764+
Published on Web 12/5/2000

1996, Volume 100

Bhupinder Madan and Kim Sharp*: : Heat Capacity Changes Accompanying Hydrophobic and Ionic Solvation: A Monte-Carlo and Random Network Model Study

Page 7713. In this work[1] we described the application of the Random Network (RN) model of Henn and Kauzmann[2] to the calculation of hydration heat capacities of solutes. An equation of state for the heat capacity in this model may be derived from the temperature derivative of either the enthalpy or entropy

$$C_p = \frac{\partial H}{\partial T} = T\frac{\partial S}{\partial T} \tag{1}$$

We presented an expression for the heat capacity derived from Henn and Kauzmann's expression for enthalpy (C_p^H). An expression for the heat capacity may also be derived from their equation of state for entropy as

$$C_p^S = \frac{0.2783kT}{(\theta^2 + {\theta_o}^2)} + \frac{(1.648 - 0.5538d) \times 10^{-3}kT}{({s_o}^2 + s^2)} - k\sum_{i=1}^{6} \frac{h\nu_i}{2kT}\left(\frac{h}{2k}\frac{\partial \nu_i}{\partial T} - \frac{h\nu_i}{2kT}\right)\bigg/\sinh^2\left(\frac{h\nu_i}{2kT}\right) \tag{2}$$

where

$$\nu_i = \nu_i^o/\exp(3.777 \times 10^{-4}\theta^2 + 1.015(d - 2.75)) \tag{3}$$

$$\frac{\partial \nu_i}{\partial T} = -3.86 \times 10^{-4}\nu_i \tag{4}$$

The three terms in eq 2 describe contributions from hydrogen bond (H-bond) bending, stretching, and vibrations, respectively, *k* is the Boltzmann constant, *T* is temperature, and *h* is the Planck constant. The H-bond structural parameters *d* (mean H-bond length), *s* (standard deviation in H-bond length), and θ (root mean square H-bond angle) are obtained from explicit water simulations. Henn and Kauzmann's values for the reference point standard deviation and rms angle, s_o and θ_o, are 0.09 Å and 2.93°, respectively, and for the six reference point water vibrational frequencies, ν_i^o, are 555, 660, 840, 60, 230, 315 cm^{-1}.[2] The numerical constants in the first two terms of eq 2 and in eq 4 account for the temperature dependence of *d*, *s*, and θ as determined in ref 1. The expression for heat capacity contributions from H-bond stretching, bending, and vibration derived from the entropy, C_p^S, is somewhat simpler than that obtained from the enthalpy, C_p^H. Hence we used C_p^S rather than C_p^H to extract numerical values of hydration heat capacities of solutes from the simulation data. It subsequently came to our attention that because *S* and *H* are derived independently in the random network model, rather than from a single expression for the partition function or ΔG, the numerical values of C_p^S and C_p^H may differ significantly. To reproduce the published values of hydration C_p from our simulation results, the reader must have the expression for C_p^S, which we provide here.

References

(1) Madan, B.; Sharp, K. A. *J. Phys. Chem.* **1996**, *100*, 7713−21.
(2) Henn, A. R.; Kauzmann, W. *J. Phys. Chem.* **1989**, *93*, 3770−3783.

10.1021/jp003954k
Published on Web 12/02/2000