ADDITIONS AND CORRECTIONS

1997, Volume 101A

Yao-Yuan Chuang and Donald G. Truhlar*: Improved Dual-Level Direct Dynamics Method for Reaction Rate Calculations with Inclusion of Multidimensional Tunneling Effects and Validation for the Reaction of H with *trans*-N_2H_2

Page 3809. In column 1, the description of the requirements for CVT/SCT calculations should read

CVT/SCT	same requirements as CVT/ZCT plus generalized normal mode eigenvectors

In the next section (CVT/LCT), it should be clear that the eigenvectors are required at the generalized transition states, and the additional single-point energies are required along the large-curvature tunneling paths.

Page 3809. In eq 10, ωm should be ω_m.

Page 3812. In Table 4, the dual-level results should be as follows:

6.6	9.0	12	11	5.0
4.0	3.5	4.0	4.3	3.2
3.9	3.7	3.8	4.1	4.3
1.9	1.8	1.7	2.1	2.4
8	9	22	24	21
0	2.19	0.11	0.24	0.14

In footnote *b*, LLL should be LL. In eq 2, MUPD should be MUDL.

Page 3813. In Table 5, line 2, 40 should be 35. In Table 6, lines 5 and 6 should be as follows:

1500	−11	3.5	4.5	3.7	4.5
2000	−11	7.6	8.1	7.2	8.1

Jeffrey S. Pilgrim and Craig A. Taatjes*: Infrared Absorption Probing of the Cl + C_2H_4 Reaction: Direct Measurement of Arrhenius Parameters for Hydrogen Abstraction

Page 4172. Because of arithmetic errors, the determination of the heat of formation of the vinyl radical in the title article[1] suffers from inaccurate temperature corrections. Using tabulated thermochemical data for entropies and heat capacities,[2] an average ΔC_p for the reaction $Cl + C_2H_4 \rightarrow HCl + C_2H_3$ of $+0.19$ cal mol^{-1} K^{-1} is found between 298 and 500 K, and a reaction entropy of $\Delta S_{498} = +8.78$ cal mol^{-1} K^{-1}. The heat of reaction deduced from the equilibrium constant near 498 K is then 7.37 kcal mol^{-1}, which results in a 298 K heat of reaction of 7.33 kcal mol^{-1} and $\Delta H°_{f,298}(C_2H_3) = 70.9 \pm 0.3$ kcal mol^{-1}. The uncertainties reflect the precision associated with the experimental measurements and assume no error in the entropy values. Similarly, correction of the second-law determination from 615 K using the heat capacity values of ref 2 yields an average ΔC_p of -0.15 cal mol^{-1} K^{-1} between 298 and 615 K, giving $\Delta H_{298} = 7.55$ kcal mol^{-1} and $\Delta H°_{f,298}(C_2H_3) = 71.1 \pm 1.3$ kcal mol^{-1}. The results remain in good agreement with determinations from ion cycle measurements[3] and other recent determinations of $\Delta H°_{f,298}(C_2H_3)$,[4,5] and the conclusions of the paper are unaltered. We thank Dr. E. W. Kaiser for calling our attention to this error.

(1) Pilgrim, J. S.; Taatjes, C. A. *J. Phys. Chem. A* **1997**, *101*, 4172.

(2) Gurvich, L. V., Veyts, I. V., Alcock, C. B., Eds. *Thermodynamic Properties of Individual Substances*, 4th ed.; Hemisphere: New York, 1989.

(3) Ervin, K. M.; Gronert, S.; Barlow, S. E.; Gilles, M. K.; Harrison, A. G.; Bierbaum, V. M.; DePuy, C. H.; Lineberger, W. C.; Ellison, G. B. *J. Am. Chem. Soc.* **1990**, *112*, 5750.

(4) Kaiser, E. W.; Wallington, T. J. *J. Phys. Chem.* **1996**, *100*, 4111.

(5) Knyazev, V. D.; Slagle, I. R. *J. Phys. Chem.* **1996**, *100*, 16899.