ADDITIONS AND CORRECTIONS

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S. Sekušak, H. Güsten, and A. Sabljić* : An *ab Initio* Study on Reactivity of Fluoroethane with Hydroxyl Radical: Application of G2 Theory

Page 6218. An inadequate correction was used for thermal energy adjustment of barrier heights (ΔE_0(298 K)) in Table 8. The correct table is given below.

TABLE 8

reaction	ΔE_0(298 K)	ΔH_f(298 K)
(R1)	1.95	−18.36
(R2a)	3.26	
(R2b)	4.34	−14.87
expt[a]	1.49−2.44	−23.00[b]

[a] References 7 and 8. [b] Estimated value for reaction R1.

Page 6221. An inadequate correction was used for thermal energy adjustment of barrier heights (ΔE_0(298 K)) in Table 14. The correct table is given below.

TABLE 14

	PUMP4/6-311+G(2d,p)//UMP2/6-31G(d,p)		PUMP2/6-311+G(2d,p)//UMP2/6-31G(d,p)		expt	
reacting system	ΔE_0(298 K)	ΔH_f(298 K)	ΔE_0(298 K)	ΔH_f(298 K)	E_a(298 K)	ΔH_r(298 K)
$[CH_3CHF\cdot\cdot H\cdot\cdot OH]$	3.11	−16.35	2.75	−20.22	1.49−2.44[a]	−23.0[b]
$[CH_2FCH_2\cdot\cdot H\cdot\cdot OH$ (rot1)]	5.14	−13.13	4.38	−16.93		
$[CH_2FCH_2\cdot\cdot H\cdot\cdot OH$ (rot2)]	3.85	−13.13	2.94	−16.93		
$[CH_3CHCl\cdot\cdot H\cdot\cdot OH]$		−17.85	2.06	−21.44	0.75−2.04[c]	
$[CH_2ClCH_2\cdot\cdot H\cdot\cdot OH$ (rot1)]		−14.42	3.52	−18.25		
$[CH_2ClCH_2\cdot\cdot H\cdot\cdot OH$ (rot2)]		−14.42	2.57	−18.25		
$[CH_3CH_2\cdot\cdot H\cdot\cdot OH]$	3.62	−14.93	3.02	−18.76	2.11−2.28[d]	−18.96[e]

[a] References 7 and 8. [b] Estimated value. [c] Reference 37. [d] Reference 3b. [e] Reference 9.

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M. F. Mesleh, J. M. Hunter, A. A. Shvartsburg, G. C. Schatz,* and M. F. Jarrold*: Structural Information from Ion Mobility Measurements: Effects of the Long-Range Potential

Page 16082. By fitting the temperature dependence of the mobility of C_{60}^+ fullerene in helium by an additive pairwise Lennard-Jones potential for C−He interactions plus an ion induced dipole term, we obtained Lennard-Jones parameters of $\epsilon = 1.34$ meV and $\sigma = 3.068$ Å. Here ϵ is the well depth and σ is the distance where the potential becomes positive. When comparing this potential with the Lennard-Jones potential between C and He atoms introduced by Amos et al.,[1] and adopted in studies of helium incorporation into fullerene cages,[2−5] we erroneously stated that the latter has $\sigma = 3.33$ Å. In fact, the parameters for that potential are $\epsilon = 1.61$ meV or 1.63 meV and $\sigma = 2.97$ Å. Mobilities calculated with the parameters $\epsilon = 1.62$ meV and $\sigma = 3.33$ Å deviate from our measured mobilities, over an 80−400 K temperature range, by 15−20%. However, mobilities calculated with $\epsilon = 1.62$ meV and $\sigma = 2.97$ Å differ from the experimental values by only a few percent.

References and Notes

(1) Amos, A.; Palmer, T. F.; Walters, A.; Burrows, B. L. *Chem. Phys. Lett.* **1990,** ***172,*** **503.**

(2) Pang, L.; Brisse, F. J. *J. Chem. Phys.* **1993**, *97*, 8562.

(3) Son, M. S.; Sung, Y. K. *Chem. Phys. Lett.* **1995**, *245*, 113.

(4) DiCamillo, B. A.; Hettich, R. L.; Guiochon, G.; Compton, R. N.; Saunders, M.; Jimenez-Vasquez, H. A.; Khong, A.; Cross, R. J. *J. Phys. Chem.* **1996**, *100*, 9197.

(5) Jimenez-Vazquez, H. A.; Cross, R. J. *J. Chem. Phys.* **1996**, *104*, 5589.