

ADDITIONS AND CORRECTIONS

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W. Sean McGivern, Agnes Derecskei-Kovacs, Simon W. North,* and Joseph S. Francisco*: Computationally Efficient Methodology To Calculate C–H and C–X (X = F, Cl, and Br) Bond Dissociation Energies in Haloalkanes.

Page 436. The corrections of the experimental bond dissociation enthalpies to 0 K to give the values provided in Tables 3, 5, 8, and 9 have been incorrectly and inconsistently applied. In the tables and the corresponding text, we have compared our calculated 0 K bond dissociation energies to these values. To provide a correct comparison of our calculated results to experiment, we have included thermal corrections to our calculated values, which are shown in Table 1 below. The experimental values given in Table 1 represent bond dissociation enthalpies at 298 K. The calculated 0 K bond dissociation energies and conclusions of the paper remain unchanged. The apparent agreement between the thermally corrected results using our methodology and experiment, however, is much better than previously advertised, differing by less than 2 kcal/mol for the entire set of molecules examined.

TABLE 1: Corrected MP2/cc-pVtz C–X (X = H, F, Cl, and Br) Bond Dissociation Enthalpies at 0 K ($D_0^{0\text{ K}}$) and 298 K ($D_0^{298\text{ K}}$)

reaction	raw MP2/cc-pVtz energy	total correction factor	zero-point correction	$D_0^{0\text{ K}}$	$D_0^{298\text{ K}}$	expt ^a
CH ₃ F → CH ₃ + F	117.6	−3.3	−6.3	108.0	109.7	109.8 ^b
CH ₃ Cl → CH ₃ + Cl	88.6	−1.8	−5.4	81.4	83.0	83.8 ^b
CH ₃ Br → CH ₃ + Br	79.1	−4.5	−4.9	69.7	71.2	70.9 ± 0.3 ^c
CH ₂ F ₂ → CH ₂ F + F	127.7	−3.3	−5.1	119.3	120.7	119.4 ^{b,d}
CH ₂ Cl → CH ₂ Cl + Cl	84.7	−1.8	−4.4	78.5	80.0	80.9 ± 1 ^e
CH ₂ Br → CH ₂ Br + Br	75.2	−4.5	−3.7	67.0	68.2	69.8 ± 2 ^e
CHF ₃ → CHF ₂ + F	135.0	−3.3	−3.9	127.8	129.1	127.6 ^{b,d}
CHCl ₃ → CHCl ₂ + Cl	80.1	−1.8	−2.7	75.6	76.6	78.4 ^{b,d}
CHBr ₃ → CHBr ₂ + Br	70.4	−4.5	−2.1	63.8	64.6	66 ± 4 ^f
CH ₄ → CH ₃ + H	110.6	+1.9	−9.7	102.8	104.4	105.1 ^b
CH ₃ F → CH ₂ F + H	106.5	+2.4	−9.2	99.7	101.2	101.3 ± 1 ^b
CH ₃ Cl → CH ₂ Cl + H	105.9	+1.4	−9.6	97.7	99.4	99.5 ± 0.6 ^g
CH ₃ Br → CH ₂ Br + H	107.1	+1.3	−9.5	98.9	100.6	101.6 ± 1 ^e
CH ₂ F ₂ → CHF ₂ + H	106.4	+2.4	−8.8	100.0	101.5	102.3 ^{b,d}
CH ₂ Cl ₂ → CHCl ₂ + H	101.1	+1.4	−8.7	93.8	95.3	95.6 ± 0.6 ^g
CH ₂ Br ₂ → CHBr ₂ + H	103.5	+1.3	−8.5	96.3	97.8	99.7 ± 1.8 ^e
CHF ₃ → CF ₃ + H	111.2	+2.4	−8.5	105.1	106.6	106.7 ± 0.7 ^e
CHCl ₃ → CCl ₃ + H	100.0	+1.4	−8.2	93.2	94.7	95.8 ± 1 ^e
CHBr ₃ → CBr ₃ + H	99.9	+1.3	−8.0	93.2	94.6	96 ± 1.6 ^e

^a Reaction enthalpies at 298 K. ^b Chase, M. W. *NIST-JANAF Thermochemical Tables*, 4th ed. *J. Phys. Chem. Ref. Data Monogr.* **9** **1998**, 1–1951.

^c Pickard, J. M.; Rodgers, A. S. *Int. J. Chem. Kinet.* **1983**, *15*, 569. ^d Zhang, Z.; Pollard, R. *Thermochim. Acta* **1995**, *257*, 21. ^e Tschuikow-Roux, E.; Paddison, S. *Int. J. Chem. Kinet.* **1992**, *24*, 639. ^f Miller, W. J.; Palmer, H. B. *J. Chem. Phys.* **1964**, *40*, 3701. ^g Seetula, J. A. *J. Chem. Soc., Faraday Trans.* **1996**, *92*, 3069.

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