

# ADDITIONS AND CORRECTIONS

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**A. F. Lago and Tomas Baer\***: A Photoelectron Photoion Coincidence Study of the Vinyl Bromide and Tribromoethane Ion Dissociation Dynamics: Heats of Formation of  $C_2H_3^+$ ,  $C_2H_3Br$ ,  $C_2H_3Br^+$ ,  $C_2H_3Br_2^+$ , and  $C_2H_3Br_3$

Page 3036. It has recently come to our attention that an onset energy ( $12.301 \pm 0.035$  eV) for the sequential loss of Br atoms from 1,1,2-tribromoethane ions,  $C_2H_3Br_3^+ \rightarrow C_2H_3Br^+ + 2Br$ , did not agree with a calculated onset.<sup>1</sup> Upon further investigation, we have come to the conclusion that our mass assignment for the product (vinyl bromide) ion was incorrect. The reaction in our photoionization mass spectrometer, in fact, was  $C_2H_3Br_3^+ \rightarrow C_2H_2Br^+ + Br + HBr$ . Because we had used the vinyl bromide ion as an anchor for establishing the thermochemistry of the 1,1,2-tribromoethane molecule, the reported heat of formation of this molecule ( $53.5 \pm 4.3$  kJ/mol) is incorrect. Without significant additional work, we cannot derive a heat of formation of  $C_2H_3Br_3$  or its ion. A further consequence is that the heat of formation of the Br loss product,  $C_2H_3Br_2^+$ , is also incorrect. The results and discussion concerning the vinyl bromide molecule and ion and the vinyl radical and ion are correct.

## References and Notes

- (1) Wang, L. *J. Phys. Chem. A* **2008**, *112*, 4951.

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**Michael E. Harding,\* Jürgen Gauss, Klaus Pflüger, and Hans-Joachim Werner**: High-Accuracy Extrapolated Ab Initio Thermochemistry of Vinyl Chloride

Page 13623. The temperature corrections calculated on the basis of the harmonic approximation and thus also the standard heats of formation  $\Delta_f H^{0, \text{harmonic}}$  of the nonlinear molecules at 298.15 K have to be corrected by  $+1/2 RT$ . For this reason  $\Delta E_1^{\text{harmonic}}(298.15 \text{ K})$  and  $\Delta_f H^{\text{harmonic}}(298.15 \text{ K})$  of reaction R2 in Table 5 have to be revised to  $-6.92$  and  $-114.10$  kJ/mol, respectively. Additionally two rows in Table 3 were switched. The correct values are given in Table 1 of this erratum. Furthermore, typographical errors occurred in Table 2. The calculated total atomization energy of acetylene is 1626.15 kJ/mol, and the heading of the last column has to be changed to ATcT-total.

**TABLE 1: Calculated Standard Enthalpies of Formation at Standard Conditions (in kJ/mol) in Comparison with Experimental Values**

	Cl <sub>2</sub>	acetylene	ethylene	vinyl chloride
$\Delta_f H^{0, \text{harmonic}}(298.15 \text{ K})$	0.51	228.42	52.42	22.15
$\Delta_f H^{0, \text{anharmonic}}(298.15 \text{ K})$	0.52	228.32	52.45	22.20

The reported corrections leave the conclusions in our paper unchanged. In fact, excellent agreement is now noted between the temperature corrections obtained by the harmonic and anharmonic models.

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