

Correction to “Ab Initio Coupled Cluster Determination of the Heats of Formation of C₂H₂F₂, C₂F₂, and C₂F₄”

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The higher order core/valence corrections to the atomization energies listed in Table 3 as “ $\Delta\text{HO}(4)$ est CCSDT(Q)(CV)/cc-pwCVTZ” are incorrect. The correct values are smaller by 0.4–0.5 kcal/mol, which is a significant amount in the present context. In addition, the scaling factor used to scale up the cc-pwCVDZ values should have been 2.30. This error affects the heats of formation listed in Table 4 and in the Abstract. Revised values (kcal/mol) are as follows:

system	$\Delta\text{HO}(4)$	best		
		composite ΣD_0	$\Delta H(0\text{K})$	$\Delta H(298.15\text{K})$
1,1-C ₂ H ₂ F ₂	0.04	562.19 ± 0.64	−82.0 ± 0.6	−83.7 ± 0.6
cis-1,2-C ₂ H ₂ F ₂	0.04	552.51 ± 0.60	−72.3 ± 0.6	−73.9 ± 0.6
trans-1,2-C ₂ H ₂ F ₂	0.04	551.78 ± 0.61	−71.6 ± 0.6	−73.1 ± 0.6
C ₂ F ₄	0.10	573.80 ± 0.79	−160.0 ± 0.8	−160.8 ± 0.8
C ₂ F ₂	0.05	376.21 ± 0.33	0.7 ± 0.3	1.4 ± 0.3

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