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Addition/Correction

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Correction to "Heats of Formation of MH_xCl_y (M = Si, P, As, Sb) Compounds and Main Group Fluorides from High Level Electronic Structure Calculations"

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The aug-cc-pVQZ value for PbF_4 was incorrectly copied into the spread sheet for the calculation of the total atomization energy, which led to an incorrect calculated heat of formation for PbF_4. The entries in Tables 3 and 4 for PbF_4 were corrected as given below.

Table 3. CCSD(T) Total Atomization Energies and Components for Calculating the Atomization Energies in kcal/mol.[a]

molecule	$\sum D_e$(CBS)[b]	ΔE_{ZPE}[c]	ΔE_{CV}[d]	ΔE_{SR}[e]	ΔE_{SO}[f]	$\sum D_0$ (0 K)[g]
PbF_4 (T_d−$^1A_1$)	335.49	4.43	−	−1.35	−28.95	300.76

[a]The atomic energies were calculated with the R/UCCSD(T) method. [b]Extrapolated by using eq 1 with the aVDZ, aVTZ, and aVQZ basis sets for Si and P compounds and with the awCVDZ, awCVTZ, and awCVQZ basis sets for Ge, As, Sn, Sb, Pb, and Bi compounds. [c]The zero point energies were taken as 0.5 the sum of the appropriate calculated/scaled harmonic frequencies. See text. [d]Core−valence corrections for the Si and P molecules were obtained with the cc-pwCVTZ basis sets at the optimized CCSD(T)/aVTZ geometries. [e]The scalar relativistic correction is based on a CISD(FC)/VTZ MVD calculation and is expressed relative to the CISD result without the MVD correction, i.e., including the existing relativistic effects on Ge, As, Sn, Sb, Pb, and Bi resulting from the use of a relativistic effective core potential. [f]Correction due to the incorrect treatment of the atomic asymptotes as an average of spin multiplets. Values are based on C. Moore's Tables.[44] [g]The theoretical value of $\sum D_0$(0 K) was computed with the CBS-DTQ estimates.

Table 4. Calculated and Experimental CCSD(T) Heats of Formation (kcal/mol)

molecule	theory (0 K)	theory (298 K)	expt (0 K)	expt (298 K)
PbF_4 (T_d)[h]	−180.3 ± 0.3 (−180.2)[v]	−181.1 ± 0.3 (−180.9)[v]		

[h]ΔH_f is based on CBS extrapolation of the awCVDZ, awCVTZ, and awCVQZ energies using eq 1. [v]$\Delta H_{f,0\ K}$(Pb) = 46.76 kcal/mol from ref 1.

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