"KS-HEAT" part II: case studies on molecules of special interest

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HEAT [1], or High-Accuracy Extrapolated *ab. initio* Thermochemistry, is one of several composite methods (see also Wn [2], FPA [3], and FPD [4]) used to predict molecular enthalpies of formation. As an extension of HEAT, "KS-HEAT" has been designed to approach the "semi-spectroscopic" accuracy range of 20 cm^{-1}, as opposed to the standard 1 kJ mol^{-1} accuracy. In a recently published work [5], KS-HEAT was reported to reproduce ATcT (TN v. 1.124 [6]) 0K enthalpies of formation of HF, CO, N_2, and H_2O to within 13 cm^{-1}.

In part II, we report KS-HEAT's performance on a few problems of historical interest. The ammonia inversion barrier, methylene singlet-triplet state energy gap, water dimerization energy, and bifluoride bond energy are investigated. Additionally, progress on using KS-HEAT to predict enthalpies of formation for a series of carbon and hydrogen containing molecules, which include CH, CH_2, CH_4, acetylene, and vinylidene, is given.

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