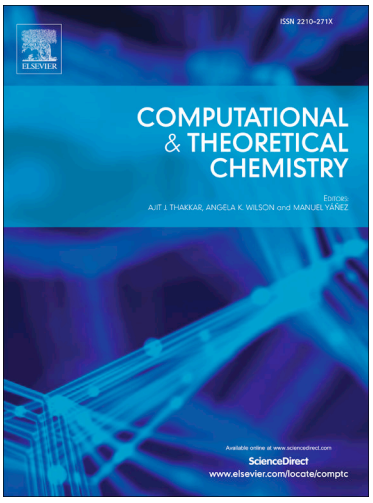

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Theoretical Study of Bromine Halocarbons: Accurate Enthalpies of Formation

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Abstract

The gas phase enthalpies of formation of sixty-five C_1 and C_2 bromine compounds have been calculated using G3, G4, the correlation consistent Composite Approach (ccCA) and CCSD(T)/CBS. Several compounds investigated have importance in atmospheric chemistry due to their global warming potentials. Compounds investigated include chlorine and fluorine containing bromine compounds, and bromine hydrocarbons. Computational methods have been compared to experimental and theoretical values when available. All methods investigated calculate enthalpies of formation that are in agreement with available ATcT, each with a greater than 0.999 R^2 value and mean absolute deviations (MADs) of 1.2 kcal/mol, 0.6 kcal/mol, 0.7 kcal/mol, and 0.6 kcal/mol for G3, G4, ccCA, and CCSD(T), respectively. The importance of molecular spin-orbit corrections is noted. The molecular spin-orbit correction for tetrabromomethane increased the enthalpy of formation by 2.7 kcal/mol to an enthalpy of formation of 27.5 kcal/mol when using CCSD(T)/CBS.

Keywords: Bromine, Halocarbons, Enthalpy of Formation, Composite Methods, Atmospheric Chemistry

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