

## Accepted Manuscript

Theoretical Study of Bromine Halocarbons: Accurate Enthalpies of Formation

Kameron Jorgensen, Melissa Cadena

PII: S2210-271X(18)30249-4

DOI: <https://doi.org/10.1016/j.comptc.2018.08.016>

Reference: COMPTC 12331

To appear in: *Computational & Theoretical Chemistry*

Received Date: 14 July 2018

Revised Date: 22 August 2018

Accepted Date: 23 August 2018



Please cite this article as: K. Jorgensen, M. Cadena, Theoretical Study of Bromine Halocarbons: Accurate Enthalpies of Formation, *Computational & Theoretical Chemistry* (2018), doi: <https://doi.org/10.1016/j.comptc.2018.08.016>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

**Theoretical Study of Bromine Halocarbons: Accurate Enthalpies of Formation**

Kameron Jorgensen\* and Melissa Cadena

Department of Biology and Chemistry, Texas A&M International University, Laredo, Texas, 78041,  
United States

**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

\*Corresponding author: Email: Kameron.jorgensen@tamiu.edu. Mail: Department of Biology and Chemistry, Texas A&M International University, 5201 University Boulevard, Laredo, Texas, 78041

Download English Version:

<https://daneshyari.com/en/article/10135434>

Download Persian Version:

<https://daneshyari.com/article/10135434>

[Daneshyari.com](https://daneshyari.com)