

# DFT study of conformers of Haloacetic Acid using Energy Decomposition Analysis

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## ABSTRACT

We employed density functional theory (DFT) calculations to investigate the conformational properties of haloacetic acids (HAAs,  $XCH_2COOH$ ,  $X=F, Cl, Br, \text{ and } I$ ), acetic acid derivatives with a hydrogen atom substituted by a halogen atom. The conformers were generated by varying the dihedral angle ( $\angle X-C-C=O$ ,  $X= F, Cl, Br, \text{ and } I$ ), and the effects of different halogen substituents (fluorine to iodine) on molecular structure and relative energies were analyzed. The optimal DFT functional ( $\omega B97XD$ ) was determined by comparing coupled-cluster singles and doubles with perturbative triples (CCSD(T)) results. Potential energy surfaces (PESs) were then calculated with  $\omega B97XD$  as a function of the HAA dihedral angle. Significant differences in calculated PESs were observed between halogen substituents (see Fig. 1). Energy decomposition analysis (EDA) of HAAs was used to elucidate the origins of these PES variations.

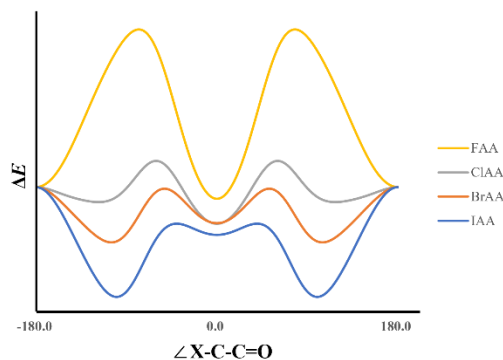


Figure1: Potential energy surfaces with respect to dihedral angle ( $\angle X-C-C=O$ ,  $X=F, Cl, Br, \text{ and } I$ ) of haloacetic acids.