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QUANTUM CHEMICAL CALCULATIONS OF CHEMICAL BOND DEVIATION IN CLO2

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In many small molecules the direction of the chemical bond, defined as the direction of the greatest change in the molecule's energy, appears not to coincide with the segment connecting the nuclei in a molecule. This phenomenon, first described in [1], is referred to as chemical bond deviation and has been thoroughly examined using classical 3N matrix method, e.g. [2], and ab initio methods, e,g. [3].The present paper describes the quantum chemical calculations applied to determine the chemical bond deviation in ClO2 molecule. Hartree-Fock and DFT calculations were performed with Orca 5.0 software [4]. The chemical bond deviation angle Δ appears to be small, about 0.7 degrees. This is a fairly predictable value, keeping in mind the small (relative to water) dipole moment of ClO2. The obtained information can be utilized in further research focusing on the interaction of the ClO2 with various surfaces.

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