QUANTUM CHEMICAL CALCULATIONS OF CHEMICAL BOND DEVIATION IN CL2O.

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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 (Fig. 1, Δ). 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 Cl_2O molecule. Hartree-Fock and DFT calculations were performed with Orca 5.0 software [4]. Table 1 summarizes the data obtained: angle Δ appears to be small, about 0.7°. This is a fairly predictable value, keeping in mind the small (relative to water) dipole moment of Cl_2O. The obtained information can be utilized in further research focusing on the interaction of the Cl_2O with various surfaces.

Table 1. Chemical bond deviation angle in Cl_2O

Method	Δ, °
RI BP86 def2-TZVP def2/J	0.6
B3LYP DEF2-SVP	0.7
B3LYP D3BJ def2-TZVP	0.8
B3LYP D4 def2-TZVP	0.8
RHF def2-TZVP	0.8

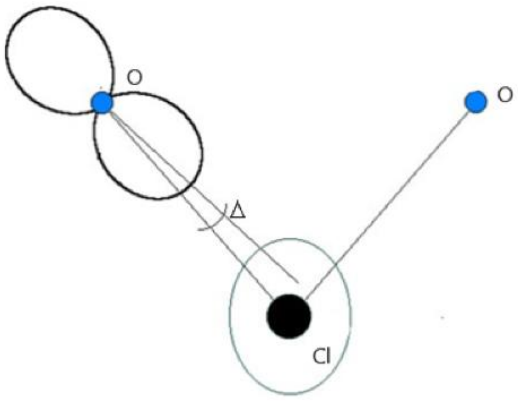

Fig. 1 Chemical bond deviation angle Δ.

References

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