INTERMOLECULAR INTERACTIONS BETWEEN THE SUPEROXIDE RADICAL AND HYDROGEN FLUORIDE

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This work concerns theoretical characterization of the nature of intermolecular interaction between the superoxide radical and hydrogen fluoride. The long-range intermolecular potential energy surface of the superoxide-HF complex was examined using the CCSD(T)/aug-cc-pVXZ, X=1, 2, 3, 4, and 5, level of theory. Our preliminary results show a minimum energy structure that corresponds to a non-linear planar geometry of Cs symmetry. In this structure, the hydrogen atom of the HF moiety is bonded to one of the oxygen atoms of the superoxide radical via a very strong hydrogen bond that is comparable to ionic bond (D_e = 41.4 kcal/mol). Such an ionic hydrogen bond causes elongation of the H-F bond length in the complex by about 0.1 angstroms. These results as well as those of vibrational frequency calculations will be presented.