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An Ab Initio Molecular Orbital Theory and Density Functional Theory Study of Fluorous 1,3-Dion Compounds

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Abstract : Quantum mechanical calculations of energies, geometries, and vibrational wavenumbers of fluorous 1,3-dion compounds are carried out using density functional theory (DFT/B3LYP) method with LANL2DZ basis sets. The calculated HOMO and LUMO energies show that charge transfer occurs in the molecules. The thermodynamic functions of fluorous 1,3-dion compounds have been performed at B3LYP/LANL2DZ basis sets. The theoretical spectrograms for F NMR spectra of fluorous 1,3-dion compounds have also been constructed. The F NMR nuclear shieldings of fluoride ligands in fluorous 1,3-dion compounds have been studied quantum chemical.

Keywords : density function theory, natural bond orbital, HOMO, LOMO, fluorous
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