Theoretical study of structural, electronic and vibrational properties of a Ni-Salen Complex

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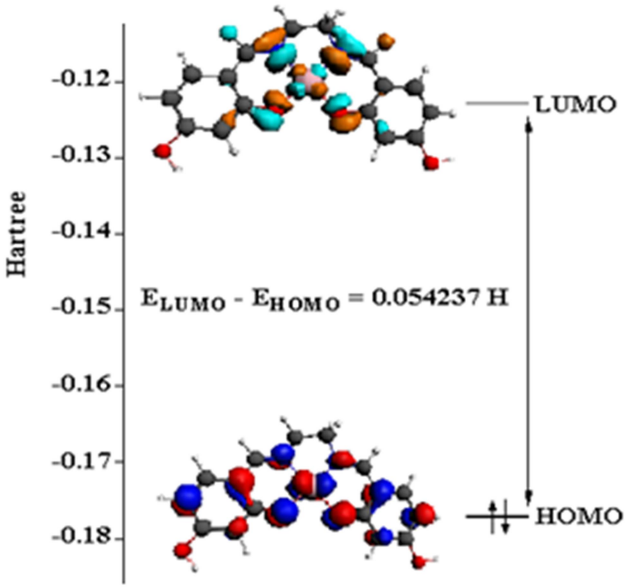

Abstract

Density Functional Theory (DFT) calculations using ADF 2009.01 package was performed for a nickle(II) complex (NiL , H_2L= *N*,*N*'-ethylene bis(4-hydroxysalicylideneimine)) and compared with the results of complex characterization (UV–Vis and FTIR techniques). Electronic spectrum of the Ni(II) complex is dominated by charge transfer and intraligand bands at $\lambda < 436$ nm. DFT calculations showed that the HOMO with -4.824 eV energy is metal-dominated, with the H → L_{+1} (85%) transfer. The magnitude of bond lengths and angles predicted by DFT calculations are comparable to those determined by X-ray crystallography for similar complex which has the same as bonds as mentioned Ni(II) complex.

The good agreement between experimental and theoretical vibration data allowed the assignment of relevant IR bands to molecular vibration modes.

Ultraviolet–visible (UV–Vis) spectrum of the mentioned molecule in the gas phase and ground state was evaluated using DFT with the standard PW91 method and compared with experimental.
Keywords: *Vibration, electronic, DFT, Calculation, PW91, Salen, ADF*