Ab initio Molecular and Solid State Studies of the FeII Spin Cross-over System \([\text{Fe(btz)}_2(\text{NCS})_2]\) (btz = 2.2’-bis-4.5-dihydrothiazine)

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*Ab initio* computations within the density functional theory are reported for the spin cross-over complex \([\text{Fe(btz)}_2(\text{NCS})_2]\) (btz = 2.2’-bis-4.5-dihydrothiazine), where 3\(d^6\) FeII is characterized by high-spin (HS \(t_{2g}^4, e_g^2\)) and low-spin (LS \(t_{2g}^6, e_g^0\)) states. Results of infrared and Raman spectra for the isolated molecule are complemented for the crystalline solid with a full account of the electronic band structure properties: the density of states assessing the crystal field effects and the chemical bonding, assigning a specific role to the Fe–N interactions within the coordination sphere of FeII.

**Key words:** Density Functional Theory, Spin Cross-over (SCO)