Ab initio Molecular and Solid State Studies of the Fe^{II} Spin Cross-over System $[Fe(btz)_2(NCS)_2]$ (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 $[Fe(btz)_2(NCS)_2]$ (btz = 2.2′-bis-4.5-dihydrothiazine), where $3d^6$ Fe^{II} 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 Fe^{II}.

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