Contribution ID: **187** Type: **Poster**

Nuclear Inelastic Scattering and Density Functional Theory Studies of Spin Crossover Compound ligand [Fe(1,2,4-triazole)2(1,2,4-triazolato)](BF4)2

Tuesday 18 September 2018 17:15 (15 minutes)

Since it has been synthesized [1], the Fe(trzH)2(trz) complex is one the most investigated spin crossover systems [2]. It contains the 1D polymeric chains and reveals the spin transition with the hysteresis of 40 K. In order to understand its vibrational properties we performed Nuclear Inelastic Scattering (NIS) experiments at the temperatures corresponding to its high-spin and low-spin states [3]. The DFT calculations for linear oligonuclear (n=7,9) models of the compound yielded the normal vibrations and electronic energies for high-spin and low-spin isomers of three different models, differing in the distribution of anionic trz- ligands and BF4- anions. On the basis of the obtained energies the structure exhibiting the centrosymmetric Fe(trzH)4(trz-)2 coordination core for each but the terminal irons is proposed. The the distribution of the BF4- anions in the structure is close to that obtained on the basis of X-ray powder diffraction studies by Grossjean et al [4]. The NIS spectra of the parent complex diluted in the matrix of the corresponding Zn(II) complex show the change of the spectral pattern of the low-spin centres. That is shown, on the basis of the DFT calculations, to be the result of the change of the structure of the neighbours.

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Session Classification: Poster session 2

Track Classification: P8 Functional materials and materials science