X-ray Absorption Studies of Fe-btr Spin Crossover Complexes

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The aim of this work is to take the advantage of the X-ray absorption spectroscopy to get insight into the evolution of electronic configuration in HS and LS states of the specific absorption atoms at various temperatures and also in the LIESST state. Three Fe spin crossover complexes, (1) Fe(btr)₂(NCS)₂·H₂O^[1] (2) Fe(btr)₃(ClO₄)₂^[2] and a Co doped Fe_xCo_{1-x}(btr)₂(NCS)₂·H₂O^[3] (3) were chosen to be studied. With temperature changing 1 shows an abrupt spin transition with a hysteresis of 25K ($T_{1/2} \downarrow = 119.8$ K and $T_{1/2} \uparrow = 145.1$ K) while 2 was found to behave as a two-step spin crossover complex.

K-edge absorption spectra of 1 and 3 were collected in both RT (HS) and 16K (LS) and also after irradiating by a laser light of 532 nm. The existence of the HS-2 after irradiation in both 1 and 3 is varified by Fe K-edge spectra. However, spin transition only occurs at Fe site not at Co site, though they should be situated on the same site.

Fe L-edge spectra of 2 illustrate a two-step spin transition; one is abrupt and the other one is gradual, which is consistent with the results reported earlier.

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