m42.o05

A complex spin crossover scenario as seen by synchrotron diffraction and Small Angle Neutron Scattering

Dmitry Chernyshov, [a*] Karl Wilhelm Törnroos,[b] Brita Vangdal,[b] Hans-Beat Bürgi,[c] Marc Hostettler[c] and Sergey Grigoriev[d]

[a]Swiss-Norwegian Beam Lines at the ESRF, France, [b]University of Bergen, Norway, [c]University of Berne, Switzerland, and [d]Petersburg Nuclear Physics Institute, Russia. E-mail: dmitry.chernyshov@esrf.fr

Keywords: spin crossover, synchrotron diffraction, SANS

Some octahedral iron(II) complexes assume two spin states - low spin (LS, S=0 singlet $t_{2g}{}^6e_g{}^0$) at low temperature and high spin (HS, S=2, quintet $t_{2g}{}^4e_g{}^2$)) at high temperature. Cooperative interactions between spin-active centres will lead to temperature-dependent correlations between spin states in the crystal structure. In order to elucidate the corresponding correlation length, synchrotron diffraction and small-angle scattering experiments have been done for Fe^{II}(2-pic)$_3$]Cl_2 2-propanol solvate [1]. X-ray diffraction does not reveal any noticeable diffuse scattering. The SANS signal shows no effects other than the dependence of crystal density on temperature. Thus both experiments corroborate the presence of mainly long-range correlations between HS and LS states and support a mean-field scenario of the temperature-induced spin crossover [2, 3].

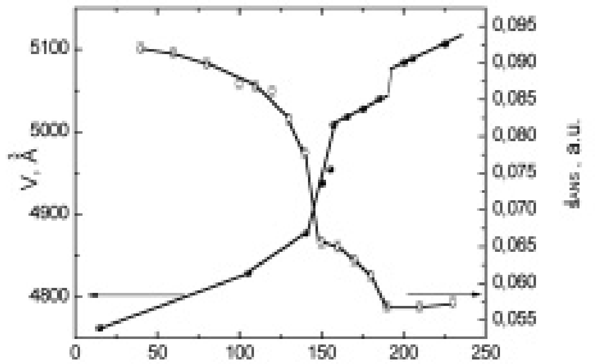

Fig. 1 Intensity of the SANS signal and volume of the unit cell deduced from diffraction experiments, as a function of temperature.

[1] M. Hostettler, K. W. Törnroos, D. Chernyshov, B. Vangdal & H. B. Bürgi, *Angew. Chem. Int. Ed.* 43, 2004, 4589.
[2] K. Boukheddaden, I. Shteto, B. Hôo, and F. Varret, *Phys. Rev.* B62, 2000, 14796.
[3] D. Chernyshov, H.-B. Bürgi, M. Hostettler & K. W. Törnroos, *Phys. Rev.* B70, 2004, 094116.

m43.o01

Structural investigation of light-induced metastable states

Sébastien Pillet

LCM3B, UHP Nancy I, Faculté des sciences, Blvd des aiguillettes, 54506 Vandoeuvre les Nancy, France. E-mail: sebastien.pillet@lcm3b.uhp-nancy.fr

Keywords: metastable structure determination, light induced phenomenon, photo crystallography

Single crystal X-ray diffraction is a particularly well established technique in condensed matter physics that has enabled to draw many structure-properties correlations, especially in molecular solids. Since the pioneering work of P. Coppens in 1967, efficient methods have been developed for the reconstruction of the periodic electron density distribution from high resolution X-ray diffraction data. This technique has been in the past restricted to equilibrium ground state systems; this limit is now overcome and may be extended to non ambient conditions. Indeed, measurements under external perturbation, like electric field [1] or optical excitation [2], are more and more explored owing to the improvements of laboratory and synchrotron diffraction equipment. Many solid state processes can be triggered or initiated through an optical photon absorption process and accordingly, laser light perturbations have been much more developed. These light-induced solid state phenomena range from purely molecular to collective processes like order-disorder or displacive phase transitions. The presentation will cover structural and electron density aspects of light-induced molecular metastable states. Equipment, measurement conditions and sample characteristics will be discussed. Light-induced metastable states of Fe(II) coordination complexes will be described as supporting examples [3].

[1] Hansen *et al.* (2004). *Acta Cryst*. A60, 465.
[2] Coppens *et al.* (2005). *Acta Cryst*. A61, 162.
[3] Legrand *et al.* (2005). *J. Phys. Conf. Series.* 21, 73.