

# Poster Presentations

**[MS31-P06] Crystallographic studies of spin crossover in  $[\text{Fe}(\text{abpt})_2(\text{NCS})_2]$  polymorphs**  
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$[\text{Fe}(\text{abpt})_2(\text{NCS})_2]$  (*abpt* = 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole) is a spin crossover compound with four structurally different polymorphs (**A-D**). [1-5] Three of these (**A**, **C** and **D**) undergo temperature induced spin crossover of the iron centre from high spin to low spin upon cooling and also display light induced excited spin-state trapping (LIESST) at low temperature. Magnetic data, room temperature crystal structures [1-5] and crystallographic studies of the thermal and light induced spin transitions in **C** and **D** have been published previously. [3-5] Herein we report structural studies of polymorph **A**; in particular the gradual thermal spin transition with  $T_{1/2} \sim 180$  K, the pressure induced and low temperature light induced spin transitions and also relaxation of the LIESST structure at 30 K. Full characterization of the thermal, pressure and light induced transformations in this interesting polymorphic system will help us to understand the predominant factors, both steric and electronic, favouring the spin transition.

N. Moliner, M. C. Muñoz, S. Létard, J.-F. Létard, X. Solans, R. Burriel, M. Castro, O. Kahn and J. A. Real, *Inorg. Chim. Acta*, 1999, **291**, 279-288.

[2] A. B. Gaspar, M. Carmen Muñoz, N. Moliner, V. Ksenofontov, G. Levchenko, P. Gülich and Antonio Real, *Monatsh. Chem.*, 2003, **134**, 285-294. [3] C.-F. Sheu, S.-M. Chen, S.-C. Wang, G.-H. Lee, Y.-H. Liu and Y. Wang, *Chem. Commun.*, 2009, 7512-7514. [4] C.-H. Shih, C.-F. Sheu, K. Kato, K. Sugimoto, J. Kim, Y. Wang and M. Takata, *Dalton Trans.*, 2010, **39**, 9794-9800.

[5] C.-F. Sheu, C.-H. Shih, K. Sugimoto, B.-M. Cheng, M. Takata and Y. Wang, *Chem. Commun.*, 2012, **48**, 5715-5717.

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