10.1071/CH14188_AC

Australian Journal of Chemistry 2014, 67(11), 1563-1573

Supplementary Material

Thermal Spin Crossover Behaviour of Two-dimensional Hofmann-type Coordination Polymers Incorporating Photoactive Ligands

Florence Ragon,[A] Korcan Yaksi,[A] Natasha F. Sciortino,[A] Guillaume Chastanet,[B] Jean-François Létard,[B] Deanna M. D'Alessandro,[A] Cameron J. Kepert[A] and Suzanne M. Neville[AC]

[A]School of Chemistry, The University of Sydney, NSW 2006, Australia.

[B]CNRS, Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

[C]Corresponding author: suzanne.neville@sydney.edu.au

Contents:

S1. Thermogravimetric analysis

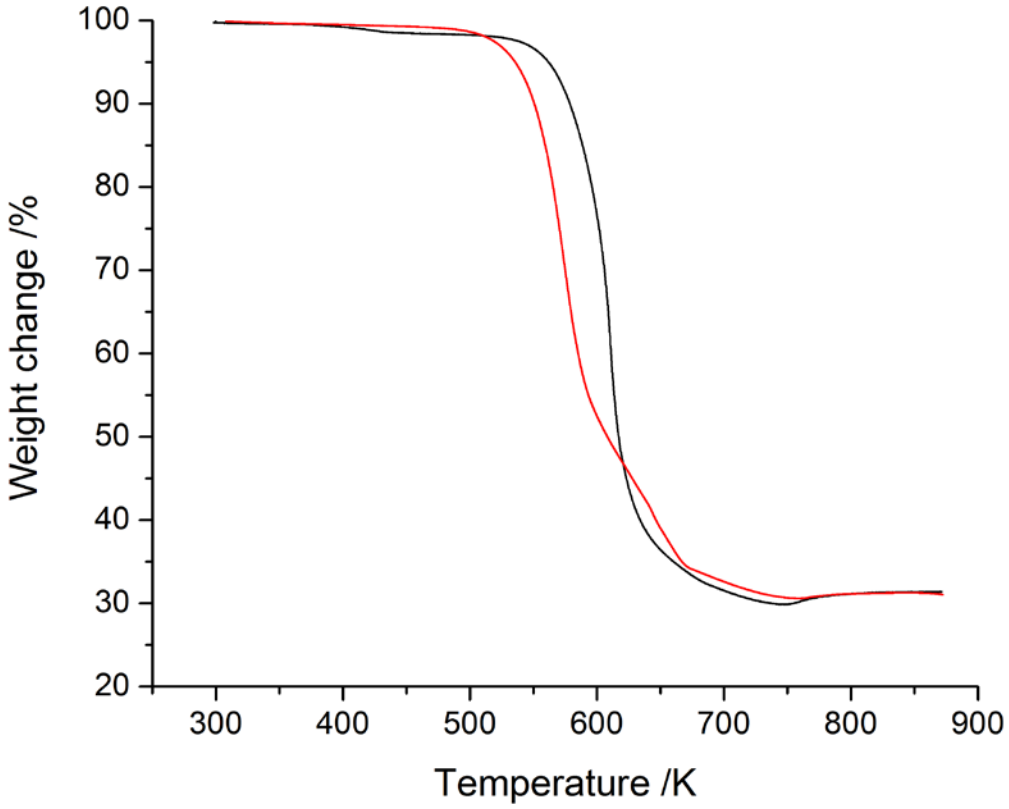


Figure S1: Thermogravimetry curves of compounds **A** (red) and **B** (black).

S2. Synchrotron-Based Powder X-ray Diffraction

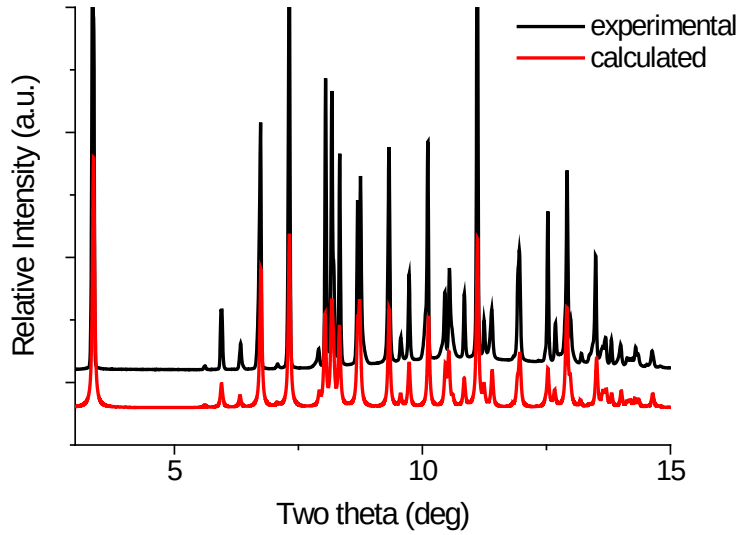


Figure S2: Comparison powder X-ray diffraction data of **A** (200 K, black) and the simulated pattern generated from single crystal X-ray data (220 K, red).

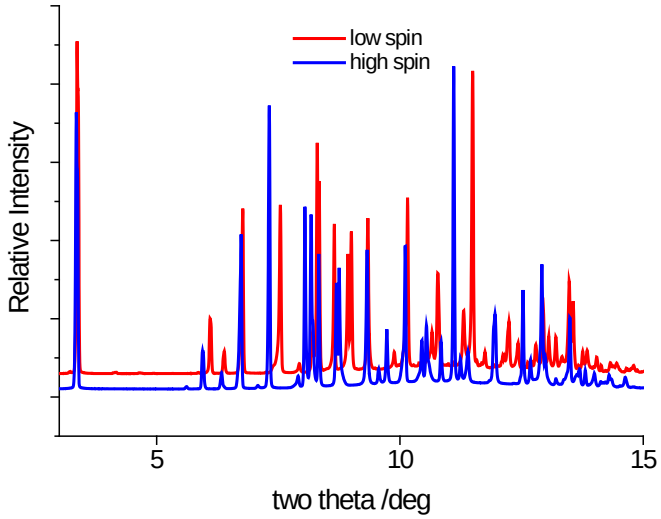


Figure S3: Comparison powder X-ray diffraction data of **A** in the HS (blue) and LS (red) states.

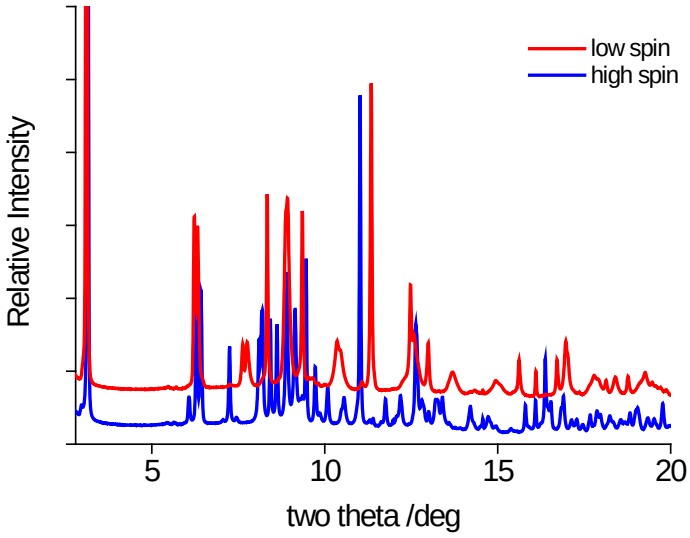
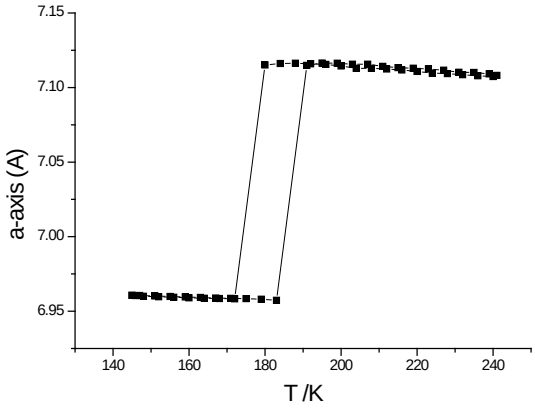
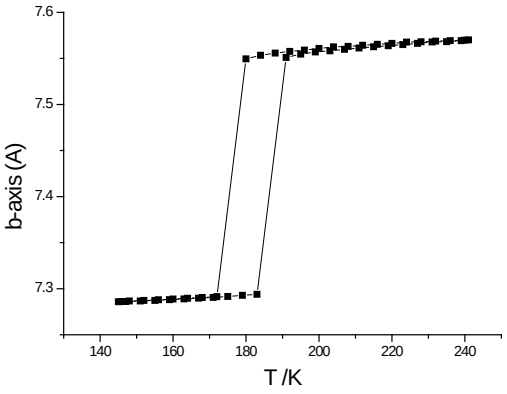


Figure S4: Powder X-ray diffraction data of **B** in the HS (280 K, blue) and LS (220 K, red) states highlighting the significant change in peak position and intensity.





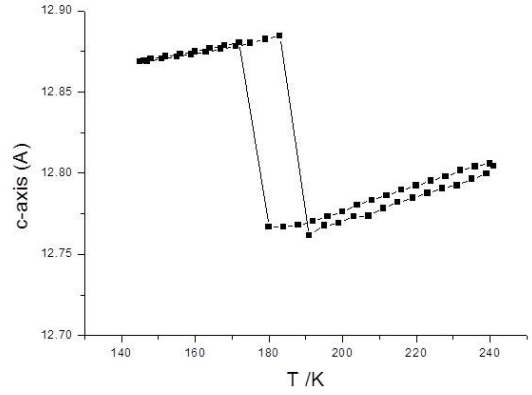


Figure S5: Powder X-ray diffraction unit cell versus temperature data for **A** from Le Bail fitting.

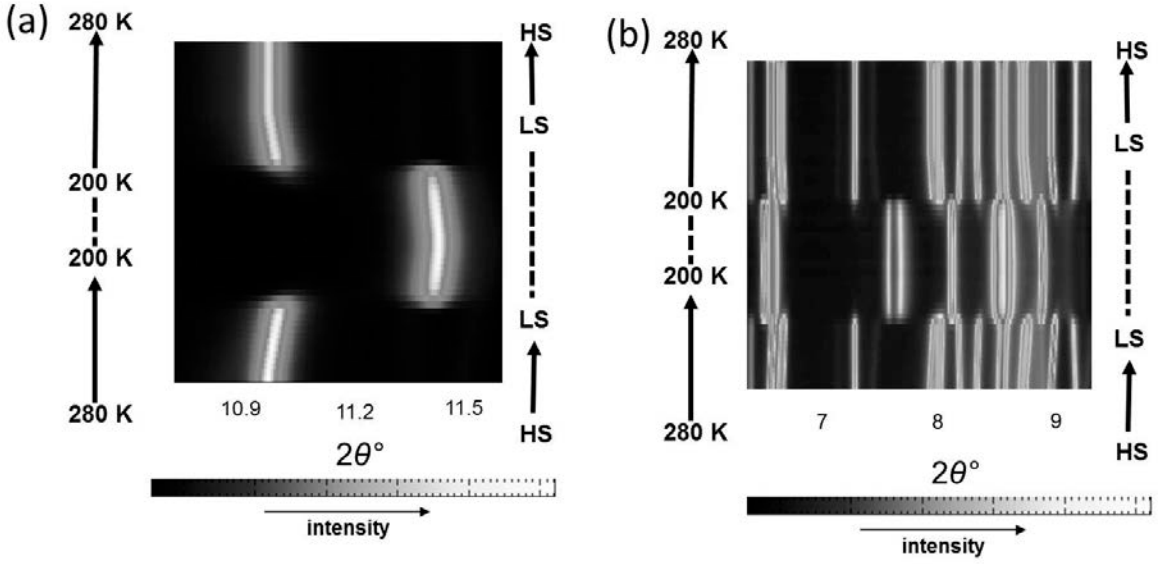


Figure S6: Variable temperature synchrotron powder X-ray diffraction data of **B**. (a) Single peak evolution over the range 10.8-11.6 °, highlighting the abrupt shift in Bragg reflection (0 -1 2) with temperature. (b) Peak evolution over the range 6-10 °, highlighting the shift in Bragg reflections in both directions.

S3. Single crystal X-ray diffraction

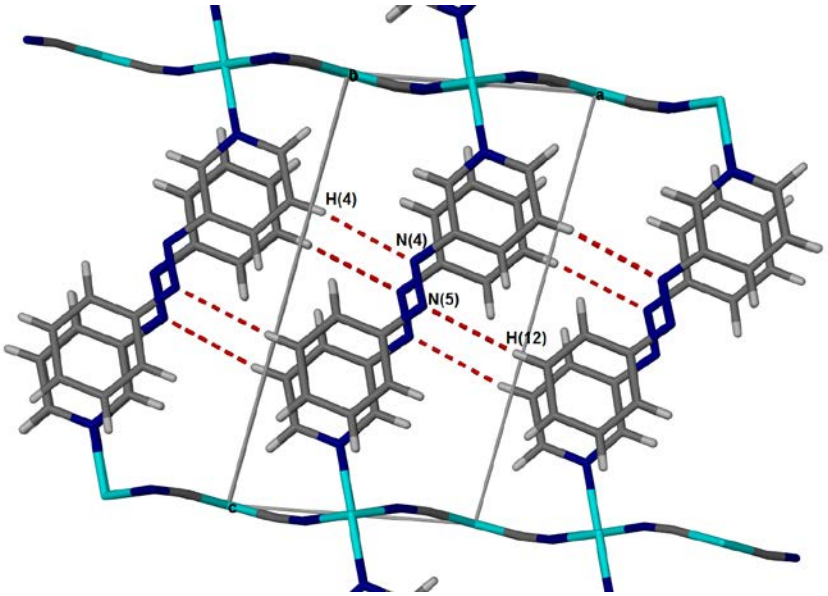


Figure S7: Structural representation of the weak hydrogen-bonding interactions between adjacent ligands in **A** (150 K, see Table 2).

S4. Temperature Dependent Magnetic Susceptibility Measurements

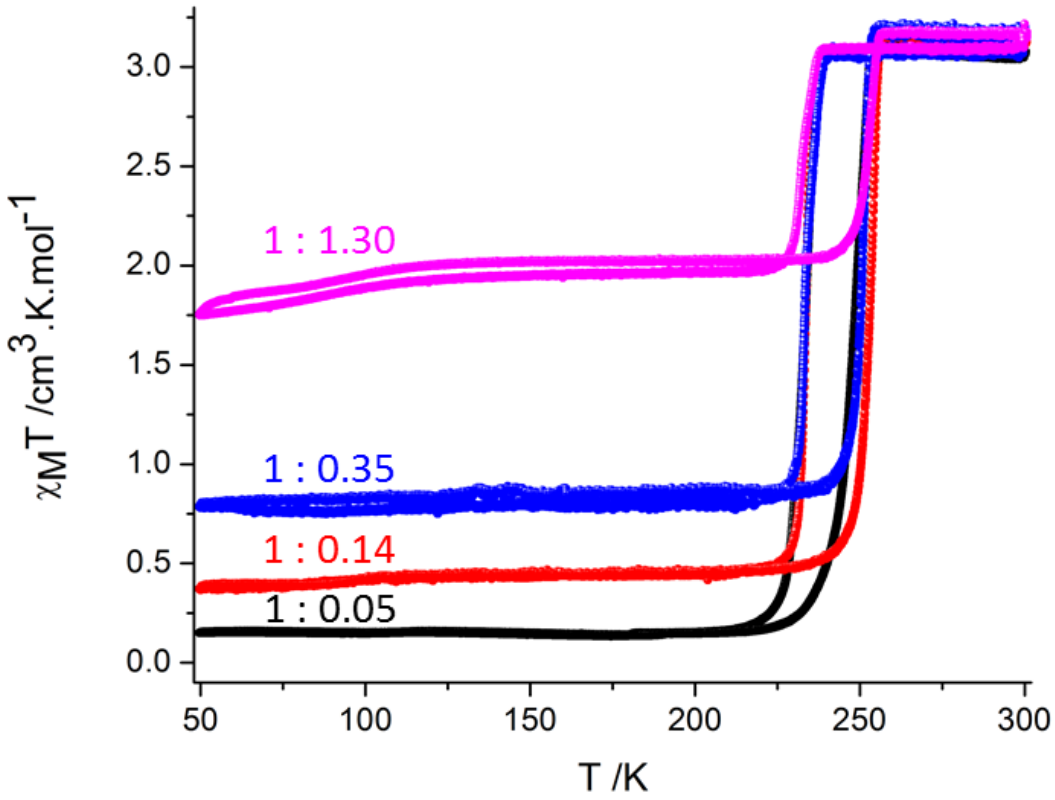


Figure S8: $\chi_M T$ *versus* temperature for SCO of **B** with different degrees of completeness of the HS to LS transition. Assuming a value around 0 $cm^3.K.mol^{-1}$ for a complete LS transition, the ratio of **B : B·(4-PAP)** have been calculated and is indicated on the curve.