MS29-2-3 Rare low-spin to high-spin transition by cooling a desolvated [2x2] Fe(II) metallogrid revealed by crystallographic studies
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Abstract
Spin crossover (SCO) complexes are prototypes of materials with bi- or multi-stability in the solid state. The structural evolution during their spin transition is a key feature to establish the foundations of how to utilize this type of material. Here, we used single crystal X-ray crystallography to study the molecular reorganisation during the thermal SCO of a solvated and a desolvated [2 × 2] tetranuclear metallogrid of the form $[FeII_4LMe_4](BF_4)_4$ ($[LMe]^-$ = 4-methyl-3,5-bis{6-(2,2′-bipyridyl)}pyrazolate), here called **FE4**. A multi-temperature crystallographic investigation exhibits the influence of the solvent effect in the number of spin transitions that occur in the solid sample, observed by the expansion of the average Fe-N bond length of one crystallographic-symmetry independent metal atoms where the SCO take place. While the solvated crystals show a single gradual phase transition from a 3HS-1LS to a 2HS-2LS configuration in the 400K to 250K range, the desolvated crystals show two SCO: a gradual 3HS-1LS to 2HS-2LS transition in the 400K to 140K range and the reverse transition from 2HS-2LS to 3HS-1LS by further cooling to 80K. The present work highlights the importance of the solvent effect in SCO complexes and open new questions about the control of the bi-/multi-stability in SCO solids.

References
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