A Novel Spin Transition Curve in [tris(2-picolylamine)Fe^(II)]Cl₂ Allyl Solvate

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The title compound exhibits a temperature dependent spin crossover with an intermediate plateau in the spin transition curve (STC) around 111K at an unusual high-spin concentration of about 30%. This is well below the plateau with a 50% concentration observed for the isomorphous ethanol solvate [1].

We report here single crystal diffraction data collected at 200, 132, 111 and 94K. The systematic absences are consistent with $B2_1/c$ space group symmetry at 200 and 132K. At 111K, *i.e.* in the range of the plateau, a superstructure is observed. The consequential reflections violate the original *B*-centering and lead to $P2_1/c$ space group symmetry with a doubled unit cell volume. At 94K the original $B2_1/c$ symmetry is recovered, thus indicating a reentrant sequence of phase transformations [2].

This observation shows that, as in the cases of the ethanol and 2propanol solvates [1,3], a plateau in the STC reflects the appearance of a new ordered structure. The plateau region is likely a result of the coupling of the spin conversion with the concurrent conformational ordering of the crystal architecture.

[1] Chernyshov D., Hostettler M., Törnroos K. W., Bürgi H.-B., *Angew. Chem. Int. Ed.* 2003, **42**, 3825. [2] Chernyshov D., Bürgi H.-B., Hostettler M., Törnroos K. W., *Phys. Rev.* B, 2004, **70**, 094116. [3] *in preparation.* **Keywords: spin crossover, phase transition, order-disorder**