s12.m34.o5 Stacking disorder in the hexagonal form of tris(bicyclo[2.1.1]hexeno)benzene

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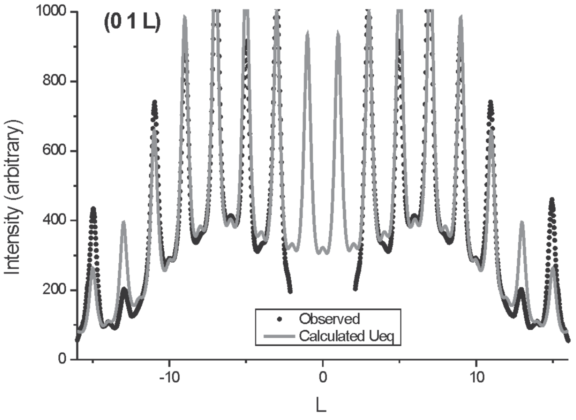
Keywords: Tris(bicyclo[2.1.1]hexeno)benzene; Diffuse scattering; Stacking-faults

X-ray diffractograms of the hexagonal polymorph of the title compound are dominated by diffuse scattering due to heavily faulted layer stacking. Strong diffuse scattering is observed along lattice rows parallel to **c*** with indices $-h + k \neq 3n$ (figure) [1]. The stacking disorder originates from molecules of $\bar{6}m2$ molecular symmetry forming layers with p $\bar{6}m2$ layer symmetry, higher than the symmetry of any stack of consecutive layers. There are three different ways to stack a third layer on top of a pair of consecutive layers. The energy differences between these three different stacking sequences are minute because they depend on next nearest neighbor interactions only [2]. The choice of stacking mode during crystal growth is therefore nearly random. This is the origin of the stacking faults and the corresponding diffuse scattering. The disorder has been analyzed quantitatively with an explicit analytical model based on Markov chains. It provides a closed formula for the intensity along **c*** as the product of a layer form factor with an interference function depending on three stacking probabilities [3]. The probabilities affect the intensities only around integer l, adjusting them reproduces the observed profile of diffuse intensity quite well. However there is an additional modulation that is not reproduced by this model and is tentatively assigned to an imperfect layer form factor.



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s13.m35.o1 Interplay between spin conversion and structural phase transformation: unusual spin crossover in an iron(II) complex

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Keywords: Spin Crossover; Molecular Crystals; Phase Transition

Iron(II) tris(2-picolylamine) dichloride 2-propanol solvate, a new compound showing spin crossover, has been investigated by X-ray diffraction and SQUID techniques. The spin transition scenario of this compound comprises a stable intermediate phase (IP) bracketed between two first-order transitions. Single crystal diffraction data collected at 10 temperatures between 100 and 250 K show that the asymmetric unit of the IP is twice as large as those of the high spin (HS) and low spin (LS) phases (fig., bottom), and that in the IP the iron complexes and the solvent molecules are partially ordered (fig., middle). The IP-phase is located in the HS part of the magnetization curve (fig., top) contrary to what has been found for the ethanol solvate where it occurs at a HS fraction of ~0.5 [1]. The low temperature part of the IP shows an unusual triangular hysteresis loop. The origin of this unusual shape and a possible mechanism of the spin transition scenario will be discussed.

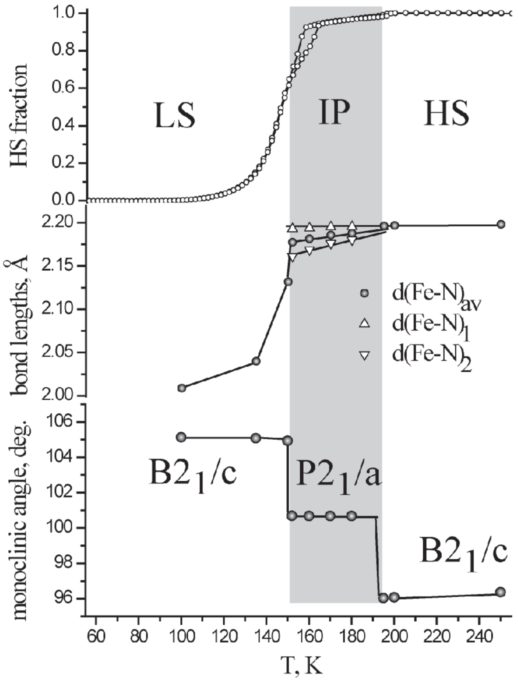

Figure. *Magnetization, structural and symmetry properties of iron(II) tris(2-picolylamine) dichloride 2-propanol solvate.*

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