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Neutron and synchrotron X-ray powder study of copper(II) chloride complex with deuterated 1-ethyltetrazole

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Abstract

The structure of the copper(II) chloride complex with deuterated 1-ethyltetrazole has been investigated in the temperature range of 2-290 K using neutron and synchrotron X-ray powder diffraction. The compound was found to exhibit structural transformation at ca 180 K, without change of space group and main structural motif. At higher temperatures, the complex reveals positional disorder of the ethyl group, whereas no disorder is observed at lower temperatures. Temperature dependence of the lattice parameters, obtained from synchrotron X-ray data, showed main lattice changes at the transformation, explained by structural features of the complex. From the magnetic measurements, the effect of the disorder on paramagnetic behaviour of the compound was found. Detailed structural data of the compound at 2 and 290 K, obtained from neutron powder diffraction data, are reported. © by Oldenbourg Wissenschaftsverlag, München.

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Keywords

Copper(II) complexes, Neutron diffraction, Synchrotron X-ray diffraction, Tetrazoles