

New polymeric thiocyanatoiron(II) complex with *N,N'*-diethylnicotinamide - synthesis, structure, magnetic and spectral properties.

Autorzy

Iveta Ondrejková

S. Galková

Jerzy Mroziński

Julia Kłak

Tadeusz Lis

Zofia Olejnik

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Streszczenie

The iron(II) compound of formula $[\text{Fe}(\text{NCS})_2(\text{dena})_2]_n$ (dena = *N,N'*-diethylnicotinamide) has been prepared by the reaction between iron(III) thiocyanate and dena in ethanol solution. The complex was characterized by elemental analysis, spectral and magnetic measurements. Single-crystal X-ray diffraction methods show that the complex, crystallizing in the triclinic space group, undergoes a phase transition between 220 K and 230 K, connected with the doubling of cell volume. Crystal structures at 230 K (**1a**; HT phase) and 150 K (**1b**; LT phase) are described and a transition mechanism is discussed. In both phases the compound has an extended chain structure, in which the neutral molecule of *N,N'*-diethylnicotinamide acts as a bridging ligand binding through pyridine N atom to one centre and through amide O atom to the neighbouring Fe centre. The Fe^{2+} ion has a slightly distorted *trans*-octahedral environment with FeO_2N_4 chromophore, and all Fe–O and Fe–N bonds in the typical for high-spin iron(II) compounds range. Variable-temperature magnetic susceptibility data in the temperature range 1.8–300 K show that iron(II) is high-spin $S = 2(^5T_{2g})$ and as a result effects due to zero-field splitting are anticipated at low temperatures. The IR spectrum suggested the coordination of *N,N'*-diethylnicotinamide to the central atom of iron(II) as a bridging ligand and NCS group as a monodentate ligand.

Adres publiczny

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