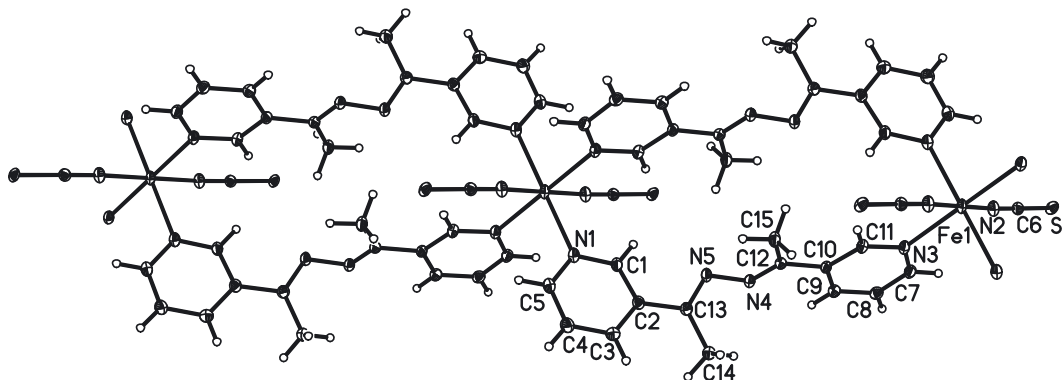


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The crystal structure of one-dimensional coordination polymer bis(thiocyanato)-bis((1*E*,2*E*)-1,2-bis(1-(pyridin-3-yl)ethylidene)-hydrazine $\kappa^2 N:N$)iron(II), (C₃₀H₂₈N₁₀S₂Fe)_n



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Abstract

C₃₀H₂₈N₁₀S₂Fe, monoclinic, *P*2₁/*n* (no. 14), *a* = 9.5643(4) Å, *b* = 16.9693(9) Å, *c* = 9.5997(5) Å, β = 98.531(5)°, *V* = 1540.79(13) Å³, *Z* = 2, *R*_{gt}(*F*) = 0.0457, *wR*_{ref}(*F*²) = 0.1316, *T* = 293 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

The ligand (1*E*,2*E*)-1,2-bis(1-(pyridin-3-yl)ethylidene)-hydrazine (L¹) was synthesized according to the literature method.⁴ The ligand L¹ (47.6 mg, 0.2 mmol) dissolved in

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.20 × 0.14 × 0.08 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.66 mm ^{−1}
Diffractometer, scan mode:	Bruker APEX2, φ and ω scans
θ _{max} , completeness:	25.0°, 100 %
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	5666, 2716, 0.026
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2280
<i>N</i> (<i>param</i>) _{refined} :	198
Programs:	Bruker, ¹ SHELX ^{2,3}

methanol solution (10 mL) was carefully mixed with another methanolic solution (10 mL) containing KSCN (19.4 mg, 0.2 mmol) and anhydrous FeCl₂ (12.7 mg, 0.10 mmol). The resulted solution was stirred for a few minutes and, after filtration, the filtrate was allowed to slowly evaporate in the dark with no disturbance in air at room temperature. Yellow block crystals, obtained after several days were collected and air-dried. Yield: 41.6 mg (64.14 %).

2 Experimental details

Coordinates of hydrogen atoms bonded to the C atoms were refined with constraints or restraints. Their *U*_{iso} values were set to 1.2*U*_{eq} or 1.5*U*_{eq} of the parent atoms.

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3 Comment

Iron(II)-based spin crossover (SCO) complexes, which have been given intense attention due to their easily spin transition behavior between the paramagnetic high-spin (HS) state $t_{2g}^4 e_g^2$ ($S = 2$) and the diamagnetic low-spin (LS) $t_{2g}^6 e_g^0$ ($S = 0$) under the external stimuli (temperature, pressure, light irradiation, guest molecules, and so on),^{5–7} are with various structure types ranging from zero-dimensional clusters to three-dimensional networks. Among of the organic ligands used, due to their moderate coordination ability suitable for tuning the spin state of the central Fe(II) ion, many research have devoted to developing new SCO material with multi-dimensional structure by employing the bispyridine-like compounds as auxiliary ligands. In this paper, we report the structure of a new one-dimensional Fe(II) complex based on a semi-rigid bidentate pyridine-type ligand L^1 , which has been successfully used to prepare the 1D Cd(II), Co(II), Zn(II) and Cu(II) complexes.^{8–11}

As shown in figure, the title neutral Fe(II) complex $[Fe(L^1)_2(NCS)_2]$, which contains two units in the unit cell similar to above mentioned complexes,^{8–11} belongs to loop-like one-dimensional chain structure. The Fe(II) ion in the title complex is involved in octahedral coordination geometry, in which the four equatorial sites were occupied by the four N atoms of L^1 acting as bidentate bridging ligands and two axial positions were coordinated by two N atoms of the thiocyanato ions as terminal ligands. The Fe–N_L1 and Fe–N_{NCS} bond lengths are 2.238(3), 2.253(3) and 2.091(3) Å, respectively, which are basically consistent with the corresponding values found in reported Fe(II) complexes based-on the analogue of L^1 ,^{6,12} demonstrating the slightly distorted octahedral sphere of the central Fe(II) ion and implying also the paramagnetic high spin state nature of the Fe(II) ion. The Fe–NC bond angle is 167.1(3)°, indicating the slight deviation from the linear conformation of these three atoms. Indeed, the angle parameter corresponding to deviations from the ideal octahedron of the 12 cis bond angles is 58.5° at room temperature, markedly larger than the corresponding value in the low spin Fe(II) complex with the metal center being involved in a comparative regular octahedron,¹³ further proving the high spin state of the central Fe(II) ion.

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