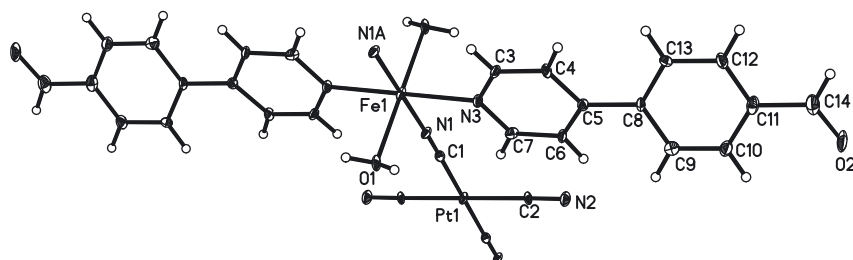


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The crystal structure of *catena*-poly[*diaqua*- μ_2 -*dicyanido*- κ^2 C:*N*-*dicyanido*- κ^1 C-bis(4-(pyridin-4-yl)benzaldehyde- κ^1 N)iron(II)-platinum(II), $C_{28}H_{22}N_6O_4PtFe$



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Abstract

$(C_{28}H_{22}N_6O_4PtFe)_n$, triclinic, $P\bar{1}$ (no. 2), $a = 7.9137(6)$ Å, $b = 8.5766(13)$ Å, $c = 10.970(3)$ Å, $\alpha = 70.266(19)^\circ$, $\beta = 81.258(14)^\circ$, $\gamma = 78.728(11)^\circ$, $V = 684.3(2)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0408$, $wR_{ref}(F^2) = 0.0657$, $T = 293$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

All the chemical reagents were from commercial sources. To a solution of $K_2[Pt(CN)_4]$ (0.10 mmol, 37.7 mg) in water/methanol (4:1, v:v) (10 mL), $FeCl_2$ (0.10 mmol, 12.7 mg) dissolved in methanol and 4-(pyridin-4-yl)benzaldehyde (0.20 mmol, 36.6 mg) were carefully added in sequence. The resulting mixture was stirred for 1 min and filtered at once,

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.14 \times 0.11 \times 0.09$ mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	5.68 mm^{-1}
Diffractometer, scan mode:	Bruker APEX II, φ and ω
θ_{max} , completeness:	25.0° , 99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	4074, 2395, 0.050
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2321
$N(\text{param})_{\text{refined}}$:	184
Programs:	Bruker [1], SHELX [2, 3]

then the filtrate was kept undisturbed at room temperature in the dark for about 1 week. The obtained title yellow block crystals were collected by filtration giving the yield of 46.3 mg (61.1 %).

2 Experimental details

For the H atom of the coordinated water molecule, the coordinates are appointed by the Q peaks with the rational distance from the Fourier map and the U_{iso} value was set to $1.5U_{\text{eq}}$ of the O atom.

3 Comment

The research on coordination polymers (CPs) with switch and memory functions has always been a subject of current interest in the search for new advanced materials with potential applications. Implementation of CPs with electronically labile iron(II) building blocks are able to undergo

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.000000	1.000000	1.000000	0.01442 (12)
Fe1	0.500000	0.500000	1.000000	0.0156 (3)
O1	0.3749 (4)	0.3666 (4)	1.1818 (4)	0.0199 (10)
H1	0.331430	0.293034	1.171651	0.030*
H1A	0.453980	0.332884	1.229547	0.030*
O2	−0.4197 (6)	0.2552 (6)	0.3897 (5)	0.0408 (14)
N1	0.3124 (5)	0.7164 (6)	0.9912 (5)	0.0170 (12)
N2	−0.1901 (6)	0.8664 (6)	0.8318 (5)	0.0234 (13)
N3	0.3387 (5)	0.4127 (5)	0.8931 (5)	0.0154 (12)
C1	0.2018 (7)	0.8239 (7)	0.9923 (6)	0.0145 (13)
C2	−0.1211 (7)	0.9178 (7)	0.8908 (6)	0.0155 (14)
C3	0.3991 (7)	0.2964 (7)	0.8350 (6)	0.0184 (15)
H5	0.510773	0.239522	0.848918	0.022*
C4	0.3092 (7)	0.2543 (7)	0.7564 (6)	0.0185 (14)
H6	0.360874	0.174017	0.716980	0.022*
C5	0.1380 (7)	0.3336 (7)	0.7359 (6)	0.0157 (14)
C6	0.0735 (7)	0.4496 (7)	0.8011 (6)	0.0168 (14)
H8	−0.039914	0.504432	0.792965	0.020*
C7	0.1730 (7)	0.4849 (7)	0.8770 (6)	0.0166 (14)
H9	0.124002	0.562487	0.919498	0.020*
C8	0.0358 (7)	0.3003 (7)	0.6467 (6)	0.0158 (14)
C9	−0.1466 (7)	0.3392 (8)	0.6591 (7)	0.0261 (16)
H15	−0.202337	0.382739	0.724225	0.031*
C10	−0.2416 (8)	0.3129 (7)	0.5753 (7)	0.0247 (16)
H14	−0.361336	0.342311	0.582578	0.030*
C11	−0.1613 (8)	0.2424 (7)	0.4787 (7)	0.0242 (16)
C12	0.0176 (7)	0.2077 (7)	0.4655 (6)	0.0226 (15)
H12	0.073423	0.164987	0.399896	0.027*
C13	0.1146 (7)	0.2360 (7)	0.5492 (6)	0.0175 (14)
H11	0.234644	0.211105	0.539329	0.021*
C14	−0.2631 (9)	0.2194 (8)	0.3877 (7)	0.0332 (18)
H16	−0.204598	0.174367	0.324062	0.040*

cooperative spin crossover (SCO) behavior [4–6]. The use of cyanide as bridging ligands has been proven to be a successful strategy for assembling Fe(II) nodes into a rich diversity of SCO CPs generically known as Hofmann-type compounds [7–10]. In the current work, the reaction of $\text{K}_2[\text{Pt}(\text{CN})_4]$ as precursor with Fe(II) salt as spin center and 4-(pyridin-4-yl)benzaldehyde as mono-dentate terminal ligand was investigated, resulting in unexpectedly an one-dimensional PtFe complex.

As shown in Figure, two trans cyanide groups of $[\text{Pt}(\text{CN})_4]^{2-}$ anion functioning as bidentate ligand that link the Fe(II) cations, forming neutral one-dimensional infinite chains. The coordination sphere of the Pt ion is perfectly square planar. The bond parameters around the central Pt ion are almost equal to each other, indicating that the

coordination or non-coordination of the N atom to the Fe(II) ion has no obvious influence on the geometry of the cyanide precursor. The Fe(II) ion defines a slightly disordered octahedral $[\text{FeN}_4\text{O}_2]$ node with the equatorial positions occupied by four nitrogen atoms from the two cyano groups, which bridge the adjacent Fe(II) centers to define an array of the infinite linear chain. There are two terminal pyridyl ligands, while the axial positions are occupied by two O atoms of the coordinated water molecules. The Fe–N_{cyano}, Fe–N_{pyridyl} and Fe–O bond lengths are 2.233(5), 2.122(4) and 2.137(4) Å, respectively. Under the help of the intermolecular O–H...N ($\text{O}\cdots\text{N} = 2.751(6)$ Å) hydrogen bonds between the O atom of the water molecule and the N atom of the cyanide group and O–H...O ($\text{O}\cdots\text{O} = 2.794(5)$ Å) hydrogen bonds interactions between the O atoms of the water molecule and the formyl group. Thus the 1D chains can be further constructed into 3D supramolecular network structure.

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