



Crystal structure of poly[[diaquatetra- μ_2 -cyanido-platinum(II)iron(II)] methanol 4/3-solvate]: a three-dimensional Hofmann clathrate analogue

Volodymyr M. Hiiuk,^{a,b,c} Vasyl Mykhailovych,^d Sergiu Shova,^e Irina A. Golenya^a and Il'ya A. Gural'skiy^{a,b,*}

Received 14 October 2021

Accepted 17 January 2022

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: coordination compounds; iron(II); clathrate; platinum; cyanido ligand; crystal structure.

CCDC reference: 2142647

Supporting information: this article has supporting information at journals.iucr.org/e

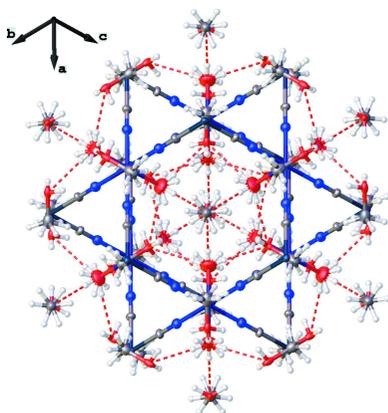
^aDepartment of Chemistry, Taras Shevchenko National University of Kyiv, 64 Volodymyrska St, 01601 Kyiv, Ukraine, ^bUkrOrgSyntez Ltd, 67 Chervonotkatska St, 02094 Kyiv, Ukraine, ^cFaculty of Natural Sciences, National University of Kyiv-Mohyla Academy, 2 Skovorody St, 04070 Kyiv, Ukraine, ^dFaculty of Electrical Engineering and Computer Science & Research Center, MANSiD, Stefan cel Mare University, 13 Universitatii St., 720229 Suceava, Romania, and ^eDepartment of Inorganic Polymers, "Petru Poni", Institute of Macromolecular Chemistry, Romanian Academy of Science, Aleea Grigore Ghica Voda 41-A, Iasi 700487, Romania. *Correspondence e-mail: igolenya@ua.fm

In the title polymeric coordination compound, $\{[\text{FePt}(\text{CN})_4(\text{H}_2\text{O})_2] \cdot 1.33\text{CH}_3\text{OH}\}_n$, the Fe^{II} cation (site symmetry $4/m\bar{m}.m$) is coordinated by the N atoms of four cyanide anions (CN^-) and the O atoms of two water molecules, forming a nearly regular $[\text{FeN}_4\text{O}_2]$ octahedron. According the Fe—N and Fe—O bond lengths, the Fe^{II} atom is in the high-spin state. The cyanide anions act in a bridging manner to connect the Fe^{II} and Pt^{II} atoms. The $[\text{Pt}(\text{CN})_4]^{2-}$ moieties (Pt with site symmetry $4/m\bar{m}.m$) have a perfect square-planar shape. The latter anion is located perpendicular to the FeN_4 plane, thus ensuring the creation of a three-dimensional framework. The crystal structure features methanol solvent molecules of which 4/3 were located per Fe^{II} cation. These solvent molecules are located in hexagonal pores; they interact with coordinating water molecules through weak hydrogen bonds. Other guest molecules could not be modelled in a satisfactory way and their contribution to the scattering was removed by a mask procedure.

1. Chemical context

Cyanide-based complexes form a large group of coordination compounds, which can offer numerous structures and functionalities. As a result of the ability of the cyanide anion to act in a bridging way, this group often links two different metal cations, enabling the formation of one-, two- or three-dimensional frameworks. The beginning of the investigation of cyanide-based complexes dates back to the 18th century when Prussian blue was discovered (Dacarro *et al.*, 2018). Since then, hundreds of cyanide-based complexes have been obtained and proven to be efficient as molecular magnets, in separation, condensation, storage, catalysis, polymer synthesis, switching, *etc* (Zakaria & Chikyow, 2017).

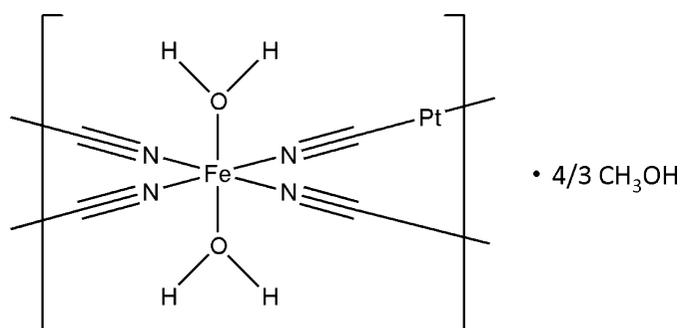
Among all cyanide-based complexes, Hofmann clathrate analogues attract considerable attention. This is a group of polymeric coordination complexes with general formula $[M(L)_x\{M'(\text{CN})_y\}_z \cdot n(\text{guest/solvent})]$ where M has an octahedral coordination environment with two L ligands in axial positions and four N atoms of bridging cyanide groups in equatorial positions, which link M and M' metals into infinite layers (Powell & Rayner, 1949; Hofmann & Küspert, 1897). If the L ligand is bridging as well (*e.g.* pyrazine), the creation of a



OPEN ACCESS

three-dimensional framework is observed (Niel *et al.*, 2001). In addition, the chemical composition of Hofmann clathrates can easily be modified by variation of the guest/solvent molecules.

One of the attractive properties of Hofmann clathrate analogues is the ability of some complexes of this class to undergo spin crossover under the influence of external stimuli (Carmen Muñoz & Real, 2011; Kucheriv *et al.*, 2021). The change of spin state can be observed in complexes of general formula $[\text{Fe}(L)_x\{\text{M}'(\text{CN})_y\}_z]$ where L = azine or azole ligand, $\text{M}' = \text{Cu}, \text{Ag}, \text{Au}$ for $y = 2, z = 2$, and $\text{M}' = \text{Ni}, \text{Pt}, \text{Pd}$ for $y = 4, z = 1$ (Shylin *et al.*, 2020; Kuzevanova *et al.*, 2021).



In this paper we report a $[\text{FePt}(\text{CN})_4(\text{H}_2\text{O})_2] \cdot 4/3\text{CH}_3\text{OH}$,_{*n*} coordination polymer with a non-classical Hofmann-type framework.

2. Structural commentary

The Fe^{II} cation (site symmetry $4/m\bar{m}.m$; Wyckoff position 3*c*) exists in an $[\text{FeN}_4\text{O}_2]$ coordination environment (Fig. 1), which is formed by the N atoms of four cyanide anions in equatorial positions [$\text{Fe1}-\text{N1} = 2.155(18) \text{ \AA}$] and the O atoms of two water molecules in axial positions [$\text{Fe1}-\text{O1} = 2.15(2) \text{ \AA}$]. The similar lengths of the Fe–O and Fe–N bonds provide an almost ideal octahedral environment. The $\text{Fe}^{\text{II}}-\text{O}$ and $\text{Fe}^{\text{II}}-\text{N}$ bond lengths indicate that, at the temperature of the

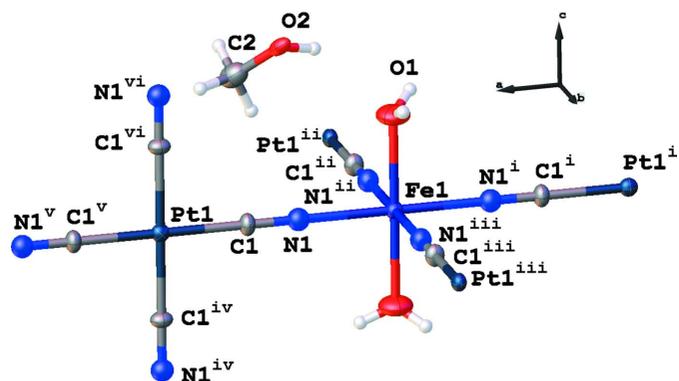


Figure 1

A fragment of the crystal structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1-x, 1-y, +z$; (ii) $y, 1-x, +z$; (iii) $1-y, x, z$; (iv) $1-z, y, -1+x$; (v) $2-x, 1-y, z$; (vi) $1+z, y, 1-x$; (vii) $x, 1-y, -z$].

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1A}\cdots\text{O2}$	0.82	2.20	3.020 (18)	175

diffraction study, Fe^{II} is in the high-spin state. The cyanide anions connect the Fe^{II} and Pt^{II} atoms, whereby the latter (site symmetry $4/m\bar{m}.m$; Wyckoff position 3*d*) has a perfect square-planar environment with a $\text{Pt1}-\text{C1}$ bond length of $1.953(17) \text{ \AA}$. Contrary to classical Hofmann clathrate arrangements (Kucheriv *et al.*, 2021), the tetracyanidoplatinate(II) anions in the title compound are located perpendicular to the FeN_4 plane, which ensures the creation of a three-dimensional framework (Fig. 2). As a result of the cubic symmetry of the crystal structure, no deviation from linearity is observed for the Fe–N–C–Pt fragments.

The title compound incorporates $4/3$ methanol solvent molecules per $[\text{FePt}(\text{CN})_4(\text{H}_2\text{O})_2]$ unit, which are located in hexagonal pores (Fig. 3) and interact with the coordinating water molecules through $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1). The framework features some additional highly disordered guest molecules, which could not be modelled satisfactorily. Their contribution to the scattering was removed with a mask procedure implemented in *OLEX2* (Dolomanov *et al.*, 2009). These disordered guest molecules reside in two types of void with total volumes of 138.3 and 20.3 \AA^3 corresponding to 36.4 and 2.6 electrons, respectively.

In comparison, two similar coordination compounds, *viz.* $[\text{Fe}(\text{H}_2\text{O})_2[\text{Pt}(\text{CN})_4] \cdot 2\text{acetone}$ (Kuzevanova *et al.*, 2019) and $[\text{Fe}(\text{H}_2\text{O})_2[\text{Ni}(\text{CN})_4] \cdot 2\text{dioxane}$ (Yuge *et al.*, 1997), form infinite $[\text{FeM}^{\text{II}}(\text{CN})_4]_\infty$ layers. The size of the available voids between the cyanidometallate layers in these two compounds allows the acetone or dioxane molecules to rotate freely, thus leading to a high disorder of the solvent. Both of these compounds, as well as the title compound, represent specta-

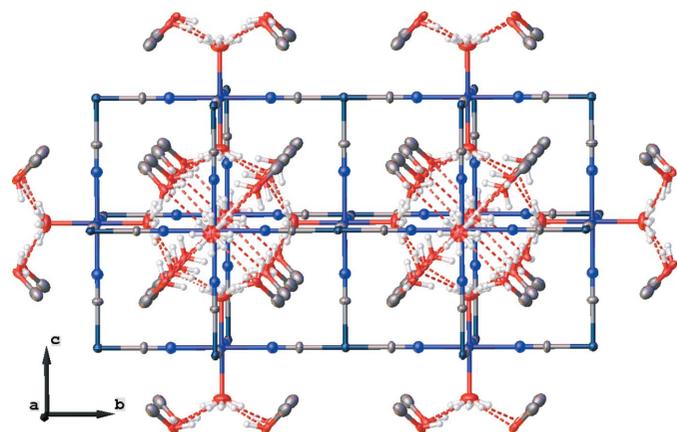


Figure 2

View of the crystal structure of the title compound along the a axis showing the three-dimensional coordination framework. Hydrogen bonds are shown as red dashed lines. Hydrogen atoms of the methyl group of the methanol solvent molecules are omitted for clarity.

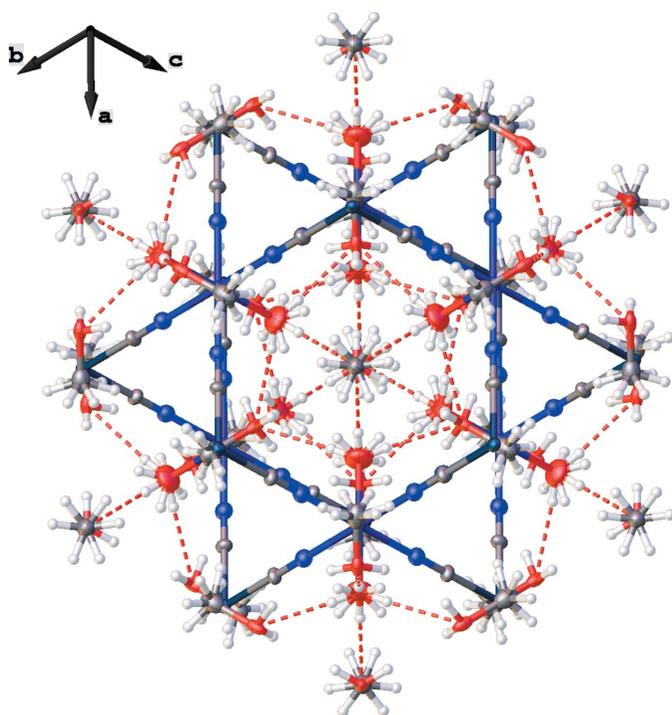


Figure 3
View of the crystal structure of the title compound showing the methanol solvent molecules, which are located in hexagonal pores. Hydrogen bonds are shown as red dashed lines.

cular examples of how variation of the guest/solvent molecule can significantly influence the crystal structure of the coordination framework. Whereas small molecules of methanol can fit inside the hexagonal pores of a three-dimensional framework, bulkier acetone or dioxane molecules cannot be placed there, thus inducing the creation of layers.

3. Database survey

A survey of the Cambridge Structural Database (Version 5.40; Groom *et al.*, 2016) revealed 106 framework structures containing Fe–N–C–Pt fragments. Among them there are three structures with an [FeN₅O] coordination environment [AMIJEN (Kucheriv *et al.*, 2016), ZOHBEG and ZOHBIK (Wong *et al.*, 2019)], three structures with an [FeN₄O₂] coordination environment [CEMJAI (Piñero-López *et al.*, 2017), HOCRAU (Zhang *et al.*, 2014) and OKITAF (Haraguchi *et al.*, 2016)] and three structures that have two different Fe^{II} cations forming [FeN₄O₂] and [FeN₆] octahedra [AMIJOX (Kucheriv *et al.*, 2016) and VOKLIS, VOKLIS01 (Sciortino *et al.*, 2014)].

4. Synthesis and crystallization

Crystals of the title compound were grown by slow diffusion between three layers in a 3 ml tube. The first layer was a solution of K₂[Pt(CN)₄] (0.02 mmol) in water (0.5 ml), the second was a mixture of water/methanol (1:1, 1.5 ml) and the third layer was a solution of Fe(OTs)₂·6H₂O (0.02 mmol)

Table 2
Experimental details.

Crystal data	
Chemical formula	[FePt(CN) ₄ (H ₂ O) ₂] ₂ ·1.33CH ₄ O
<i>M_r</i>	433.77
Crystal system, space group	Cubic, <i>Pm</i> $\bar{3}$ <i>m</i>
Temperature (K)	293
<i>a</i> (Å)	10.5089 (3)
<i>V</i> (Å ³)	1160.56 (10)
<i>Z</i>	3
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	9.96
Crystal size (mm)	0.04 × 0.04 × 0.04
Data collection	
Diffractometer	Xcalibur, Eos
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2021)
<i>T</i> _{min} , <i>T</i> _{max}	0.930, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	2210, 336, 273
<i>R</i> _{int}	0.091
(sin θ/λ) _{max} (Å ⁻¹)	0.688
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.055, 0.133, 1.07
No. of reflections	336
No. of parameters	23
No. of restraints	13
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	2.15, −1.36

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

(OTs = *p*-toluenesulfonate) in methanol (0.5 ml). After two weeks, colourless crystals grew in the middle layer; these were collected and maintained under the mother solution until measured.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms of water molecules and the methanol OH group were placed at calculated positions and refined as riding on the bonded O atom. The occupancy of methanol atoms was refined and found to be equal to approximately 0.5 and later restrained to half-occupancy. As a result of symmetry restrictions, H atoms of the water molecule are disordered over four positions and were constrained to have an occupancy of 1/4. The three H atoms of the methyl group are disordered over two sets of sites, and were refined as for an idealized methyl group and were allowed to rotate about the O–C bond. The H atom of the OH group is disordered over three sites. Its occupancy was restrained to coincide with half-occupancy of the complete molecule.

Funding information

Funding for this research was provided by: Ministry of Education and Science of Ukraine (grant No. 19BF037-01M); H2020 Marie Skłodowska-Curie Actions (grant No. 734322). VMH thanks the Yuchymenko Family Endowment Fund for financial support.

References

- Carmen Muñoz, M. & Real, J. A. (2011). *Coord. Chem. Rev.* **255**, 2068–2093.
- Dacarro, G., Taglietti, A. & Pallavicini, P. (2018). *Molecules*, **23**, 1414.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Haraguchi, T., Otsubo, K., Sakata, O., Kawaguchi, S., Fujiwara, A. & Kitagawa, H. (2016). *Chem. Commun.* **52**, 6017–6020.
- Hofmann, K. A. & Küspert, F. (1897). *Z. Anorg. Chem.* **15**, 204–207.
- Kucheriv, O. I., Fritsky, I. O. & Gural'skiy, I. A. (2021). *Inorg. Chim. Acta*, **521**, 120303.
- Kucheriv, O. I., Shylin, S. I., Ksenofontov, V., Dechert, S., Haukka, M., Fritsky, I. O. & Gural'skiy, I. A. (2016). *Inorg. Chem.* **55**, 4906–4914.
- Kuzevanova, I. S., Kucheriv, O. I., Hiiuk, V. M., Naumova, D. D., Shova, S., Shylin, S. I., Kotsyubynsky, V. O., Rotaru, A., Fritsky, I. O. & Gural'skiy, I. A. (2021). *Dalton Trans.* **50**, 9250–9258.
- Kuzevanova, I. S., Naumova, D. D., Terebilenko, K. V., Shova, S. & Gural'skiy, I. A. (2019). *Acta Cryst.* **E75**, 1536–1539.
- Niel, V., Martinez-Agudo, J. M., Carmen Muñoz, M., Gaspar, A. B. & Real, J. A. (2001). *Inorg. Chem.* **40**, 3838–3839.
- Piñeiro-López, L., Valverde-Muñoz, F. J., Serebyuk, M. & Znovnyak, K. (2017). *IUCrData*, **2**, x171413.
- Powell, H. M. & Rayner, J. H. (1949). *Nature*, **163**, 566–567.
- Rigaku OD (2021). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sciortino, N. F., Neville, S. M., Létard, J.-F., Moubaraki, B., Murray, K. S. & Kepert, C. J. (2014). *Inorg. Chem.* **53**, 7886–7893.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Shylin, S. I., Kucheriv, O. I., Shova, S., Ksenofontov, V., Tremel, W. & Gural'skiy, I. A. (2020). *Inorg. Chem.* **59**, 6541–6549.
- Wong, B. J. C., Xu, D., Bao, S.-S., Zheng, L.-M. & Lei, J. (2019). *Appl. Mater. Interfaces*, **11**, 12986–12992.
- Yuge, H., Kim, C., Iwamoto, T. & Kitazawa, T. (1997). *Inorg. Chim. Acta*, **257**, 217–224.
- Zakaria, M. B. & Chikyow, T. (2017). *Coord. Chem. Rev.* **352**, 328–345.
- Zhang, M., Li, B.-B., Sun, J., Kong, X.-P., Gu, P.-P., Chen, Y.-Y. & Yuan, A.-H. (2014). *Z. Anorg. Allg. Chem.* **640**, 1007–1011.

supporting information

Acta Cryst. (2022). E78, 216-219 [https://doi.org/10.1107/S2056989022000573]

Crystal structure of poly[[diaquatetra- μ_2 -cyanido-platinum(II)iron(II)] methanol 4/3-solvate]: a three-dimensional Hofmann clathrate analogue

Volodymyr M. Hiiuk, Vasyl Mykhailovych, Sergiu Shova, Irina A. Golenya and Il'ya A. Gural'skiy

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Poly[[diaquatetra- μ_2 -cyanido-platinum(II)iron(II)] methanol 1.33-solvate]

Crystal data

[FePt(CN)₄(H₂O)₂]:1.33CH₄O

$M_r = 433.77$

Cubic, *Pm* $\bar{3}$ *m*

$a = 10.5089$ (3) Å

$V = 1160.56$ (10) Å³

$Z = 3$

$F(000) = 600$

$D_x = 1.862$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 449 reflections

$\theta = 1.9$ – 21.7°

$\mu = 9.96$ mm⁻¹

$T = 293$ K

Cube, clear intense colourless

$0.04 \times 0.04 \times 0.04$ mm

Data collection

Xcalibur, Eos
diffractometer

Radiation source: fine-focus sealed X-ray tube,
Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.1593 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2021)

$T_{\min} = 0.930$, $T_{\max} = 1.000$

2210 measured reflections

336 independent reflections

273 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.091$

$\theta_{\max} = 29.3^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -9 \rightarrow 8$

$k = -14 \rightarrow 14$

$l = -5 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.133$

$S = 1.07$

336 reflections

23 parameters

13 restraints

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 2.15$ e Å⁻³

$\Delta\rho_{\min} = -1.36$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pt1	1.000000	0.500000	0.000000	0.0374 (5)	
Fe1	0.500000	0.500000	0.000000	0.0395 (12)	
N1	0.7051 (17)	0.500000	0.000000	0.059 (4)	
C1	0.8141 (17)	0.500000	0.000000	0.047 (4)	
O1	0.500000	0.500000	0.2049 (19)	0.112 (9)	
H1A	0.549690	0.450310	0.238738	0.168*	0.25
H1B	0.423680	0.500000	0.233848	0.168*	0.25
O2	0.6888 (17)	0.3112 (17)	0.3112 (17)	0.049 (7)	0.5
H2	0.610990	0.294000	0.294000	0.073*	0.1667
C2	0.7666 (19)	0.2334 (19)	0.2334 (19)	0.088 (14)	0.5
H2A	0.728153	0.224628	0.151003	0.132*	0.0833
H2B	0.775372	0.151003	0.271847	0.132*	0.0833
H2C	0.848997	0.271847	0.224628	0.132*	0.0833

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.0420 (6)	0.0282 (7)	0.0420 (6)	0.000	0.000	0.000
Fe1	0.0399 (16)	0.0399 (16)	0.039 (2)	0.000	0.000	0.000
N1	0.060 (11)	0.054 (10)	0.064 (11)	0.000	0.000	0.000
C1	0.032 (9)	0.046 (10)	0.063 (12)	0.000	0.000	0.000
O1	0.144 (15)	0.144 (15)	0.047 (14)	0.000	0.000	0.000
O2	0.049 (7)	0.049 (7)	0.049 (7)	-0.019 (7)	-0.019 (7)	0.019 (7)
C2	0.088 (14)	0.088 (14)	0.088 (14)	-0.021 (11)	-0.021 (11)	0.021 (11)

Geometric parameters (\AA , $^\circ$)

Pt1—C1 ⁱ	1.953 (17)	O1—H1A	0.8198
Pt1—C1 ⁱⁱ	1.953 (17)	O1—H1A ^{ix}	0.8198
Pt1—C1 ⁱⁱⁱ	1.953 (17)	O1—H1B ^{ix}	0.8579
Pt1—C1	1.953 (17)	O1—H1B ^x	0.8579
Fe1—N1	2.155 (18)	O1—H1B ^{viii}	0.8579
Fe1—N1 ^{iv}	2.155 (18)	O1—H1B	0.8579
Fe1—N1 ^v	2.155 (18)	O2—H2	0.8565
Fe1—N1 ^{vi}	2.155 (18)	O2—H2 ^{xi}	0.8565
Fe1—O1 ^v	2.15 (2)	O2—H2 ^{xii}	0.8565
Fe1—O1	2.15 (2)	O2—C2	1.42 (2)
N1—C1	1.15 (2)	C2—H2A	0.9600
O1—H1A ^{vii}	0.8198	C2—H2B	0.9600

O1—H1A ^{viii}	0.8198	C2—H2C	0.9600
C1 ⁱ —Pt1—C1 ⁱⁱⁱ	180.0	H1A—O1—H1A ^{ix}	79.1
C1 ⁱⁱⁱ —Pt1—C1	90.0	H1A ^{viii} —O1—H1B ^x	116.2
C1 ⁱ —Pt1—C1	90.0	H1A—O1—H1B ^x	41.4
C1 ⁱ —Pt1—C1 ⁱⁱ	90.0	H1A ^{vii} —O1—H1B ^{viii}	116.2
C1 ⁱⁱⁱ —Pt1—C1 ⁱⁱ	90.0	H1A ^{vii} —O1—H1B ^{ix}	41.4
C1 ⁱⁱ —Pt1—C1	180.0	H1A—O1—H1B	116.2
N1—Fe1—N1 ^v	180.0	H1A ^{vii} —O1—H1B ^x	41.4
N1 ^{vi} —Fe1—N1 ^{iv}	180.0	H1A—O1—H1B ^{ix}	116.2
N1 ^v —Fe1—N1 ^{iv}	90.0	H1A—O1—H1B ^{viii}	41.4
N1—Fe1—N1 ^{vi}	90.0	H1A ^{ix} —O1—H1B ^x	116.2
N1 ^v —Fe1—N1 ^{vi}	90.0	H1A ^{ix} —O1—H1B ^{viii}	41.4
N1—Fe1—N1 ^{iv}	90.0	H1A ^{viii} —O1—H1B ^{viii}	116.2
O1 ^v —Fe1—N1 ^{vi}	90.0	H1A ^{viii} —O1—H1B ^{ix}	41.4
O1 ^v —Fe1—N1 ^{iv}	90.0	H1A ^{ix} —O1—H1B ^{ix}	116.2
O1—Fe1—N1 ^v	90.0	H1B—O1—H1A ^{vii}	116.2
O1—Fe1—N1 ^{vi}	90.0	H1B—O1—H1A ^{ix}	41.4
O1—Fe1—N1 ^{iv}	90.0	H1B—O1—H1A ^{viii}	41.4
O1 ^v —Fe1—N1	90.0	H1B ^{ix} —O1—H1B ^{viii}	138.4
O1—Fe1—N1	90.0	H1B ^{viii} —O1—H1B ^x	82.8
O1 ^v —Fe1—N1 ^v	90.0	H1B—O1—H1B ^{viii}	82.8
O1 ^v —Fe1—O1	180.0	H1B—O1—H1B ^{ix}	82.8
C1—N1—Fe1	180.0	H1B—O1—H1B ^x	138.4
N1—C1—Pt1	180.0	H1B ^{ix} —O1—H1B ^x	82.8
Fe1—O1—H1A ^{viii}	115.740 (1)	H2 ^{xi} —O2—H2 ^{xii}	111.0
Fe1—O1—H1A ^{ix}	115.740 (1)	H2—O2—H2 ^{xii}	111.0
Fe1—O1—H1A	115.7	H2—O2—H2 ^{xi}	111.0
Fe1—O1—H1A ^{vii}	115.740 (2)	C2—O2—H2	107.9
Fe1—O1—H1B	110.8	C2—O2—H2 ^{xii}	107.857 (3)
Fe1—O1—H1B ^{ix}	110.8	C2—O2—H2 ^{xi}	107.857 (8)
Fe1—O1—H1B ^x	110.799 (2)	O2—C2—H2A	109.5
Fe1—O1—H1B ^{viii}	110.8	O2—C2—H2B	109.5
H1A ^{ix} —O1—H1A ^{viii}	79.1	O2—C2—H2C	109.5
H1A—O1—H1A ^{viii}	128.5	H2A—C2—H2B	109.5
H1A—O1—H1A ^{vii}	79.1	H2A—C2—H2C	109.5
H1A ^{ix} —O1—H1A ^{vii}	128.5	H2B—C2—H2C	109.5
H1A ^{viii} —O1—H1A ^{vii}	79.1		

Symmetry codes: (i) $-z+1, -y+1, x-1$; (ii) $-x+2, -y+1, -z$; (iii) $z+1, y, -x+1$; (iv) $-y+1, -x+1, z$; (v) $-x+1, -y+1, -z$; (vi) $y, x, -z$; (vii) $-y+1, x, z$; (viii) y, x, z ; (ix) $y, -x+1, z$; (x) $-x+1, -y+1, z$; (xi) $-z+1, -x+1, y$; (xii) $-y+1, z, -x+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O2	0.82	2.20	3.020 (18)	175