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Pentaaqua(isocyanurato)iron(II) isocyanurate dihydrate

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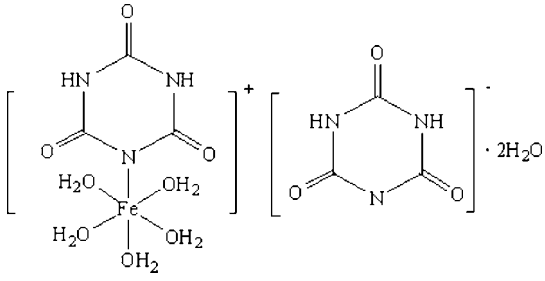
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(N–C) = 0.003 Å; R factor = 0.037; wR factor = 0.113; data-to-parameter ratio = 12.8.

In the title compound, $[Fe(C_3H_2N_3O_3)(H_2O)_5](C_3H_2N_3O_3)\cdot 2H_2O$, the Fe^{II} atom exhibits an $FeNO_5$ octahedral coordination geometry arising from one N-bonded 1,3,5-triazinanyl-2,4,6-trione molecule and five O atoms of water molecules. The uncoordinated 1,3,5-triazinanyl-2,4,6-trione anion and uncoordinated water molecules interact with the cation through O—H···O, O—H···N and N—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For general background, see: Cai *et al.* (2001). For related structures, see: Cai *et al.* (2003). For related literature, see: Cai, *et al.* (2005).



Experimental

Crystal data

$[Fe(C_3H_2N_3O_3)(H_2O)_5](C_3H_2N_3O_3)\cdot 2H_2O$
M_r = 438.11
Monoclinic, $P2_1/n$
a = 14.0563 (2) Å
b = 6.6947 (1) Å
c = 17.2336 (3) Å
β = 97.408 (1)°
V = 1608.19 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 298 (2) K
0.20 × 0.17 × 0.15 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.822, T_{max} = 0.862
14409 measured reflections
3691 independent reflections
3064 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.113
S = 1.07
3691 reflections
289 parameters
25 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O4^{i}	0.839 (10)	1.958 (10)	2.795 (2)	175 (3)
O7—H7A···O2W^{ii}	0.841 (9)	1.905 (11)	2.736 (2)	170 (3)
O8—H8A···O3	0.827 (9)	2.294 (19)	2.904 (2)	131 (2)
O8—H8A···O2^{iii}	0.827 (9)	2.47 (2)	3.147 (2)	140 (2)
O8—H8B···O2W^{iv}	0.829 (10)	1.962 (11)	2.788 (2)	174 (3)
O9—H9B···O1W^{v}	0.833 (10)	1.946 (14)	2.743 (2)	160 (2)
O9—H9A···N5^{iii}	0.843 (10)	2.018 (11)	2.858 (2)	174 (3)
O10—H10A···N5^{i}	0.842 (10)	2.058 (11)	2.895 (2)	172 (2)
O10—H10B···O1W^{vi}	0.841 (9)	1.927 (13)	2.743 (2)	163 (2)
O11—H11A···O5^{vi}	0.835 (10)	2.079 (19)	2.828 (2)	149 (3)
O11—H11B···O2^{vii}	0.835 (10)	1.949 (14)	2.761 (2)	164 (3)
O1W—H1WB···O10^{i}	0.838 (9)	2.179 (17)	2.926 (2)	148 (3)
O1W—H1WB···O9^{i}	0.838 (9)	2.54 (3)	3.075 (3)	123 (3)
O1W—H1WB···O1^{i}	0.838 (9)	2.60 (2)	3.142 (2)	124 (2)
O1W—H1WA···O6^{viii}	0.837 (10)	1.916 (12)	2.736 (2)	166 (3)
O2W—H2WA···O6	0.844 (10)	1.892 (10)	2.734 (2)	176 (3)
O2W—H2WB···O7	0.849 (10)	2.053 (13)	2.859 (2)	158 (3)
N3—H3···O4	0.851 (10)	1.947 (11)	2.790 (2)	170 (3)
N4—H4···O3	0.853 (10)	1.979 (11)	2.829 (2)	174 (3)
N6—H6···O1^{ix}	0.860 (10)	1.979 (11)	2.834 (2)	173 (3)

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, -y+1, -z+1$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, -y, -z+1$; (v) $x-1, y-1, z$; (vi) $x-1, y, z$; (vii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (viii) $-x+1, -y+1, -z+1$; (ix) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2093).

References

Bruker (1998). *SMART* (Version 5.0) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Cai, Y.-P., Chen, C.-L., Zhang, L., Shi, J.-L., Xu, A.-W., Su, C.-Y. & Kang, B.-S. (2003). *Inorg. Chim. Acta*, **342**, 107–113.
Cai, Y.-P., Li, G.-B., Zhan, Q.-G., Sun, F., Zhang, J.-G., Gao, S. & Xu, A.-W. (2005). *J. Solid State Chem.* **178**, 3729–3734.
Cai, Y.-P., Zhang, H.-X., Xu, A.-W., Su, C.-Y., Chen, C.-L., Liu, H.-Q., Zhang, L. & Kang, B.-S. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2429–2434.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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Pentaaqua(isocyanurato)iron(II) isocyanurate dihydrate

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Comment

Recently we reported a series of one-dimensional helical Ag(I) compounds containing 8-hydroxyquinoline coordinating groups (Cai *et al.*, 2001 and 2003). As a part of the structural studies of the compounds involving the oxygen-nitrogen chelating ligand (Cai *et al.*, 2005), here we report the synthesis and structure of the compound, pentaaqua(1,3,5-triazinanyl-2,4,6-trione)iron(II) 1,3,5-triazinanate-2,4,6-trione dihydrate, namely $[Fe(C_3H_2N_3O_3)(H_2O)_5]^+(C_3H_2N_3O_3)^- 2H_2O$ (Scheme 1).

Fig.1 shows that the molecule of $[Fe(C_3H_2N_3O_3)(H_2O)_5]^+(C_3H_2N_3O_3)^- 2H_2O$ consists of one cation $[Fe(C_3H_2N_3O_3)(H_2O)_5]^+$, one anion $(C_3H_2N_3O_3)^-$ and two water molecules. The Fe^{II} atom exhibits a $FeNO_5$ octahedral coordination geometry arising from one N-bonded 1,3,5-triazinanyl-2,4,6-trione molecule and five O atoms of water molecules. The uncoordinated 1,3,5-triazinanyl-2,4,6-trione anion and uncoordinated water molecules interact with the cation through O—H···O, O—H···N and N—H···O hydrogen bonds (Table 1), generating a three-dimensional network.

Experimental

A solution of $FeCl_2$ (200 mg, 1.00 mmol) in CH_3OH (20 ml) was slowly added to a solution of 1,3,5-triazinane-2,4,6-trione (260 mg, 1.95 mmol) in CH_3OH (10 ml). The resultant pale green solution was stirred under N_2 for 2 h at 323 K and then filtered. After addition of diethyl ether (20 ml), the filtrate was cooled to 253 K. Microcrystalline material was collected after 24 h and dried under vacuum (yield: 237 mg, 53%). Green blocks suitable for X-ray diffraction were obtained in 2 d by slow diffusion of diethyl ether into a dilute solution of the title complex in methanol. The assigned structure was substantiated by elemental analysis; calculated for $C_6H_{18}N_6FeO_{13}$: C 16.47, H 4.12, N 19.21%; found: C 16.43, H 4.18, N 19.17%.

Refinement

The structure was solved using direct methods followed by Fourier synthesis. Non-H atoms were refined anisotropically. The water/nitrogen H atoms were located and isotropically refined, with the O—H/N—H and H···H for water molecules distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. All other H atoms were placed in calculated positions (C—H = 0.93 or 0.97 Å), and were included in the refinement using the riding-model approximation. U_{iso} values were set equal to 1.5Ueq(parent atom) for water/nitrogen H atoms and to 1.2Ueq(parent atom) for all other H atoms.

Figures

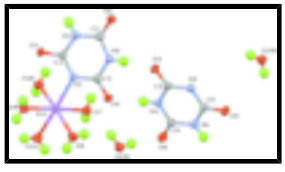


Fig. 1. The structure of title molecule, with its atom-numbering scheme, is shown at the 50% probability level.

Pentaaqua(isocyanurato)iron(II) isocyanurate dihydrate

Crystal data

$[Fe(C_3H_2N_3O_3)(H_2O)_5](C_3H_2N_3O_3)\cdot 2H_2O$	$F_{000} = 904$
$M_r = 438.11$	$D_x = 1.809$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4778 reflections
$a = 14.0563$ (2) Å	$\theta = 2.4$–27.4°
$b = 6.6947$ (1) Å	$\mu = 1.02$ mm^{-1}
$c = 17.2336$ (3) Å	$T = 298$ (2) K
$\beta = 97.408$ (1)°	Block, green
$V = 1608.19$ (4) Å^3	0.20 × 0.17 × 0.15 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3691 independent reflections
Radiation source: fine-focus sealed tube	3064 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 298$(2) K	$\theta_{max} = 27.5^\circ$
φ and ω scans	$\theta_{min} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -18\rightarrow17$
$T_{min} = 0.822$, $T_{max} = 0.862$	$k = -8\rightarrow6$
14409 measured reflections	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.9167P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
3691 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
289 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
25 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based

on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	−0.05822 (2)	0.17964 (5)	0.678490 (17)	0.02687 (13)
O1	−0.01859 (11)	0.1853 (3)	0.87539 (9)	0.0296 (4)
O2	0.30290 (12)	0.2819 (3)	0.93035 (10)	0.0421 (5)
O3	0.17061 (11)	0.1783 (3)	0.68074 (9)	0.0327 (4)
O4	0.41363 (11)	0.1655 (3)	0.75242 (8)	0.0289 (4)
O5	0.60977 (11)	0.2088 (3)	0.56299 (10)	0.0377 (4)
O6	0.28965 (12)	0.2944 (3)	0.50276 (10)	0.0433 (5)
O7	−0.00205 (11)	0.4449 (3)	0.62062 (9)	0.0302 (4)
H7B	0.0276 (17)	0.510 (3)	0.6578 (11)	0.045*
H7A	−0.0367 (17)	0.512 (3)	0.5867 (11)	0.045*
O8	0.00260 (12)	−0.0127 (3)	0.59652 (10)	0.0372 (4)
H8A	0.0619 (7)	−0.014 (4)	0.6028 (18)	0.056*
H8B	−0.0266 (16)	−0.107 (3)	0.5730 (18)	0.056*
O9	−0.13082 (12)	−0.0603 (3)	0.72935 (10)	0.0329 (4)
H9B	−0.1713 (16)	−0.122 (4)	0.6988 (13)	0.049*
H9A	−0.0971 (17)	−0.129 (3)	0.7635 (13)	0.049*
O10	−0.13586 (11)	0.3992 (3)	0.74129 (9)	0.0284 (3)
H10A	−0.0988 (15)	0.472 (3)	0.7713 (13)	0.043*
H10B	−0.1783 (14)	0.459 (3)	0.7112 (13)	0.043*
O11	−0.18778 (12)	0.1871 (3)	0.59092 (10)	0.0404 (5)
H11A	−0.2439 (11)	0.197 (5)	0.6014 (16)	0.061*
H11B	−0.179 (2)	0.201 (5)	0.5442 (8)	0.061*
O1W	0.74356 (12)	0.6644 (3)	0.65640 (9)	0.0329 (4)
H1WB	0.6986 (14)	0.692 (5)	0.6821 (12)	0.049*
H1WA	0.7299 (18)	0.657 (5)	0.6077 (6)	0.049*
O2W	0.09420 (12)	0.3139 (3)	0.49336 (10)	0.0339 (4)
H2WA	0.1543 (8)	0.301 (5)	0.4958 (15)	0.051*
H2WB	0.0736 (17)	0.326 (5)	0.5373 (10)	0.051*
N1	0.06881 (12)	0.1824 (3)	0.77285 (10)	0.0205 (4)
N2	0.14088 (12)	0.2369 (3)	0.90343 (10)	0.0247 (4)
H2	0.1357 (19)	0.244 (4)	0.9520 (7)	0.030*

N3	0.23620 (13)	0.2187 (3)	0.80582 (11)	0.0286 (4)
H3	0.2910 (11)	0.217 (4)	0.7898 (16)	0.034*
N4	0.35144 (13)	0.2299 (3)	0.62800 (10)	0.0246 (4)
H4	0.2955 (10)	0.223 (4)	0.6421 (15)	0.029*
N5	0.51845 (12)	0.1830 (3)	0.66238 (10)	0.0232 (4)
N6	0.45021 (13)	0.2501 (3)	0.53267 (10)	0.0274 (4)
H6	0.4638 (19)	0.262 (4)	0.4856 (8)	0.033*
C1	0.05928 (15)	0.2003 (3)	0.85001 (12)	0.0207 (4)
C2	0.23144 (15)	0.2485 (4)	0.88340 (12)	0.0264 (5)
C3	0.15702 (15)	0.1924 (3)	0.75000 (12)	0.0220 (4)
C4	0.42988 (14)	0.1913 (3)	0.68387 (12)	0.0213 (4)
C5	0.53042 (15)	0.2133 (3)	0.58650 (12)	0.0242 (4)
C6	0.35972 (15)	0.2595 (4)	0.55118 (12)	0.0256 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.02585 (19)	0.0331 (2)	0.02092 (18)	−0.00181 (13)	0.00026 (12)	−0.00010 (12)
O1	0.0202 (7)	0.0491 (10)	0.0200 (7)	−0.0022 (7)	0.0045 (6)	0.0003 (7)
O2	0.0236 (8)	0.0810 (14)	0.0206 (8)	−0.0096 (9)	−0.0013 (6)	−0.0031 (8)
O3	0.0228 (8)	0.0586 (12)	0.0171 (7)	−0.0006 (7)	0.0034 (6)	−0.0039 (7)
O4	0.0259 (8)	0.0444 (10)	0.0171 (7)	0.0045 (7)	0.0052 (6)	0.0065 (6)
O5	0.0188 (8)	0.0717 (13)	0.0231 (8)	0.0025 (8)	0.0048 (6)	0.0027 (8)
O6	0.0200 (8)	0.0872 (16)	0.0216 (8)	0.0053 (8)	−0.0016 (6)	0.0065 (9)
O7	0.0311 (8)	0.0352 (9)	0.0231 (8)	−0.0038 (7)	−0.0002 (6)	0.0045 (7)
O8	0.0258 (8)	0.0480 (11)	0.0378 (9)	−0.0018 (8)	0.0038 (7)	−0.0163 (8)
O9	0.0293 (8)	0.0351 (9)	0.0322 (9)	−0.0057 (7)	−0.0047 (7)	0.0081 (7)
O10	0.0248 (8)	0.0321 (9)	0.0267 (8)	0.0017 (7)	−0.0021 (6)	−0.0028 (7)
O11	0.0227 (8)	0.0769 (14)	0.0206 (8)	0.0017 (9)	−0.0007 (6)	0.0016 (8)
O1W	0.0266 (8)	0.0496 (11)	0.0224 (8)	0.0031 (7)	0.0031 (6)	−0.0009 (7)
O2W	0.0244 (8)	0.0484 (11)	0.0289 (8)	0.0003 (8)	0.0034 (6)	−0.0008 (7)
N1	0.0170 (8)	0.0287 (9)	0.0156 (8)	−0.0003 (7)	0.0019 (6)	−0.0002 (7)
N2	0.0206 (9)	0.0389 (11)	0.0146 (8)	−0.0012 (8)	0.0026 (7)	−0.0025 (8)
N3	0.0160 (8)	0.0514 (13)	0.0187 (9)	−0.0008 (8)	0.0031 (7)	−0.0031 (8)
N4	0.0160 (8)	0.0397 (11)	0.0186 (8)	0.0010 (8)	0.0042 (7)	0.0019 (8)
N5	0.0192 (8)	0.0322 (10)	0.0180 (8)	0.0016 (7)	0.0018 (6)	0.0010 (7)
N6	0.0204 (9)	0.0475 (12)	0.0146 (8)	0.0008 (8)	0.0029 (7)	0.0006 (8)
C1	0.0199 (9)	0.0238 (11)	0.0182 (9)	0.0004 (8)	0.0015 (7)	0.0007 (8)
C2	0.0236 (10)	0.0370 (12)	0.0183 (10)	−0.0012 (9)	0.0012 (8)	0.0009 (9)
C3	0.0207 (10)	0.0275 (11)	0.0175 (9)	0.0004 (8)	0.0010 (7)	−0.0008 (8)
C4	0.0198 (10)	0.0242 (11)	0.0199 (10)	0.0007 (8)	0.0021 (8)	−0.0005 (8)
C5	0.0187 (9)	0.0338 (12)	0.0198 (10)	0.0002 (8)	0.0022 (8)	0.0001 (8)
C6	0.0191 (9)	0.0386 (12)	0.0189 (10)	0.0008 (9)	0.0015 (8)	−0.0010 (9)

Geometric parameters (Å, °)

Fe1—O9	2.1495 (17)	O1W—H1WA	0.837 (10)
Fe1—O8	2.1671 (17)	O2W—H2WA	0.844 (10)
Fe1—O10	2.1973 (16)	O2W—H2WB	0.849 (10)

Fe1—O11	2.2109 (16)	N1—C3	1.350 (3)
Fe1—O7	2.2303 (17)	N1—C1	1.359 (3)
Fe1—N1	2.2549 (16)	N2—C2	1.363 (3)
O1—C1	1.234 (3)	N2—C1	1.397 (3)
O2—C2	1.226 (3)	N2—H2	0.851 (10)
O3—C3	1.237 (3)	N3—C2	1.362 (3)
O4—C4	1.244 (2)	N3—C3	1.385 (3)
O5—C5	1.235 (3)	N3—H3	0.851 (10)
O6—C6	1.228 (3)	N4—C6	1.358 (3)
O7—H7B	0.839 (10)	N4—C4	1.391 (3)
O7—H7A	0.841 (9)	N4—H4	0.853 (10)
O8—H8A	0.827 (9)	N5—C4	1.345 (3)
O8—H8B	0.829 (10)	N5—C5	1.355 (3)
O9—H9B	0.833 (10)	N6—C6	1.352 (3)
O9—H9A	0.843 (10)	N6—C5	1.387 (3)
O10—H10A	0.842 (10)	N6—H6	0.860 (10)
O10—H10B	0.841 (9)	C3—O3	1.237 (3)
O11—H11A	0.835 (10)	C4—O4	1.244 (2)
O11—H11B	0.835 (10)	C6—O6	1.228 (3)
O1W—H1WB	0.838 (9)		
O9—Fe1—O8	93.99 (8)	C1—N1—Fe1	122.52 (14)
O9—Fe1—O10	90.40 (7)	C2—N2—C1	123.87 (18)
O8—Fe1—O10	168.93 (6)	C2—N2—H2	116.6 (18)
O9—Fe1—O11	84.41 (7)	C1—N2—H2	119.4 (18)
O8—Fe1—O11	85.87 (7)	C2—N3—C3	124.30 (19)
O10—Fe1—O11	84.46 (7)	C2—N3—H3	118.8 (19)
O9—Fe1—O7	172.46 (6)	C3—N3—H3	116.9 (19)
O8—Fe1—O7	89.41 (7)	C6—N4—C4	122.80 (19)
O10—Fe1—O7	85.09 (7)	C6—N4—H4	118.9 (18)
O11—Fe1—O7	89.12 (7)	C4—N4—H4	118.0 (18)
O9—Fe1—O7	172.46 (6)	C4—N5—C5	119.60 (18)
O8—Fe1—O7	89.41 (7)	C6—N6—C5	123.98 (18)
O10—Fe1—O7	85.09 (7)	C6—N6—H6	123.2 (19)
O11—Fe1—O7	89.12 (7)	C5—N6—H6	112.8 (19)
O9—Fe1—N1	94.91 (6)	O1—C1—N1	122.93 (19)
O8—Fe1—N1	97.63 (6)	O1—C1—N2	118.11 (19)
O10—Fe1—N1	92.10 (6)	N1—C1—N2	118.96 (18)
O11—Fe1—N1	176.48 (7)	O2—C2—N3	122.3 (2)
O7—Fe1—N1	91.31 (6)	O2—C2—N2	123.7 (2)
O7—Fe1—N1	91.31 (6)	N3—C2—N2	113.95 (18)
Fe1—O7—H7B	103.8 (18)	O3—C3—N1	122.67 (18)
Fe1—O7—H7A	122.0 (19)	O3—C3—N1	122.67 (18)
H7B—O7—H7A	116.2 (14)	O3—C3—N3	118.01 (19)
Fe1—O8—H8A	113.3 (19)	O3—C3—N3	118.01 (19)
Fe1—O8—H8B	124 (2)	N1—C3—N3	119.32 (18)
H8A—O8—H8B	119.0 (15)	O4—C4—N5	123.06 (18)
Fe1—O9—H9B	115.7 (19)	O4—C4—N5	123.06 (18)
Fe1—O9—H9A	116.1 (19)	O4—C4—N4	117.18 (19)
H9B—O9—H9A	116.6 (14)	O4—C4—N4	117.18 (19)

Fe1—O10—H10A	112.6 (18)	N5—C4—N4	119.76 (18)
Fe1—O10—H10B	112.0 (18)	O5—C5—N5	122.86 (19)
H10A—O10—H10B	115.8 (14)	O5—C5—N6	118.40 (19)
Fe1—O11—H11A	125 (2)	N5—C5—N6	118.74 (19)
Fe1—O11—H11B	117 (2)	O6—C6—N6	123.0 (2)
H11A—O11—H11B	117.4 (15)	O6—C6—N6	123.0 (2)
H1WB—O1W—H1WA	116.8 (14)	O6—C6—N4	121.9 (2)
H2WA—O2W—H2WB	114.9 (14)	O6—C6—N4	121.9 (2)
C3—N1—C1	119.42 (17)	N6—C6—N4	115.12 (19)
C3—N1—Fe1	117.50 (13)		
O9—Fe1—N1—C3	134.41 (15)	C1—N1—C3—O3	−179.6 (2)
O8—Fe1—N1—C3	39.71 (16)	Fe1—N1—C3—O3	−8.0 (3)
O10—Fe1—N1—C3	−135.00 (15)	C1—N1—C3—N3	0.6 (3)
O11—Fe1—N1—C3	−146.9 (11)	Fe1—N1—C3—N3	172.28 (16)
O7—Fe1—N1—C3	−49.86 (15)	C2—N3—C3—O3	175.8 (2)
O7—Fe1—N1—C3	−49.86 (15)	C2—N3—C3—O3	175.8 (2)
O9—Fe1—N1—C1	−54.23 (17)	C2—N3—C3—N1	−4.4 (3)
O8—Fe1—N1—C1	−148.93 (16)	C5—N5—C4—O4	−179.8 (2)
O10—Fe1—N1—C1	36.36 (16)	C5—N5—C4—O4	−179.8 (2)
O11—Fe1—N1—C1	24.5 (13)	C5—N5—C4—N4	0.3 (3)
O7—Fe1—N1—C1	121.50 (16)	C6—N4—C4—O4	−179.6 (2)
O7—Fe1—N1—C1	121.50 (16)	C6—N4—C4—O4	−179.6 (2)
C3—N1—C1—O1	−177.2 (2)	C6—N4—C4—N5	0.3 (3)
Fe1—N1—C1—O1	11.6 (3)	C4—N5—C5—O5	179.6 (2)
C3—N1—C1—N2	2.6 (3)	C4—N5—C5—N6	−0.8 (3)
Fe1—N1—C1—N2	−168.57 (15)	C6—N6—C5—O5	−179.7 (2)
C2—N2—C1—O1	177.2 (2)	C6—N6—C5—N5	0.6 (4)
C2—N2—C1—N1	−2.7 (3)	C5—N6—C6—O6	179.2 (2)
C3—N3—C2—O2	−176.0 (2)	C5—N6—C6—O6	179.2 (2)
C3—N3—C2—N2	4.3 (4)	C5—N6—C6—N4	−0.1 (4)
C1—N2—C2—O2	179.5 (2)	C4—N4—C6—O6	−179.7 (2)
C1—N2—C2—N3	−0.7 (3)	C4—N4—C6—O6	−179.7 (2)
C1—N1—C3—O3	−179.6 (2)	C4—N4—C6—N6	−0.4 (3)
Fe1—N1—C3—O3	−8.0 (3)		

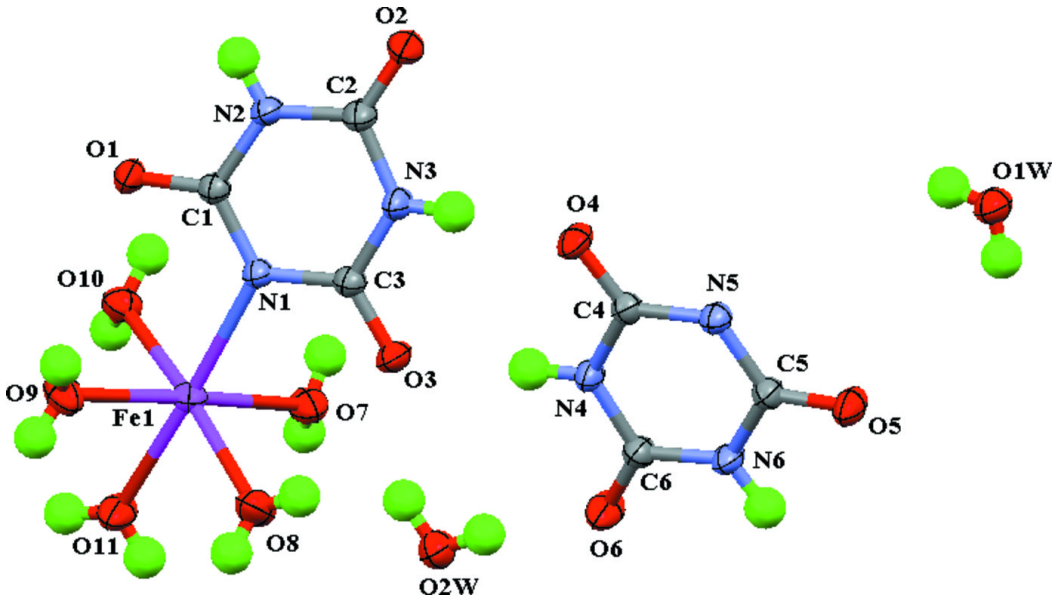
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7B···O4^{i}	0.839 (10)	1.958 (10)	2.795 (2)	175 (3)
O7—H7A···O2W^{ii}	0.841 (9)	1.905 (11)	2.736 (2)	170 (3)
O8—H8A···O3	0.827 (9)	2.294 (19)	2.904 (2)	131 (2)
O8—H8A···O2^{iii}	0.827 (9)	2.47 (2)	3.147 (2)	140 (2)
O8—H8B···O2W^{iv}	0.829 (10)	1.962 (11)	2.788 (2)	174 (3)
O9—H9B···O1W^{v}	0.833 (10)	1.946 (14)	2.743 (2)	160 (2)
O9—H9A···N5^{iii}	0.843 (10)	2.018 (11)	2.858 (2)	174 (3)
O10—H10A···N5^{i}	0.842 (10)	2.058 (11)	2.895 (2)	172 (2)
O10—H10B···O1W^{vi}	0.841 (9)	1.927 (13)	2.743 (2)	163 (2)

O11—H11A···O5^{vi}	0.835 (10)	2.079 (19)	2.828 (2)	149 (3)
O11—H11B···O2^{vii}	0.835 (10)	1.949 (14)	2.761 (2)	164 (3)
O1W—H1WB···O10^{i}	0.838 (9)	2.179 (17)	2.926 (2)	148 (3)
O1W—H1WB···O9^{i}	0.838 (9)	2.54 (3)	3.075 (3)	123 (3)
O1W—H1WB···O1^{i}	0.838 (9)	2.60 (2)	3.142 (2)	124 (2)
O1W—H1WA···O6^{viii}	0.837 (10)	1.916 (12)	2.736 (2)	166 (3)
O2W—H2WA···O6	0.844 (10)	1.892 (10)	2.734 (2)	176 (3)
O2W—H2WB···O7	0.849 (10)	2.053 (13)	2.859 (2)	158 (3)
N3—H3···O4	0.851 (10)	1.947 (11)	2.790 (2)	170 (3)
N4—H4···O3	0.853 (10)	1.979 (11)	2.829 (2)	174 (3)
N6—H6···O1^{ix}	0.860 (10)	1.979 (11)	2.834 (2)	173 (3)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iv) −*x*, −*y*, −*z*+1; (v) *x*−1, *y*−1, *z*; (vi) *x*−1, *y*, *z*; (vii) *x*−1/2, −*y*+1/2, *z*−1/2; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) *x*+1/2, −*y*+1/2, *z*−1/2.

Fig. 1


O2
C2
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O1
N3
C1
O1W
O4
O10
N1
C3
N5
C4
O3
C5
O9
Fe1
O7
N4
O5
N6
C6
O11
O8
O6
O2W