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# Triethylammonium bis{2-[(2-oxido-5-nitrobenzylidene)amino]benzoato}-ferrate(III) monohydrate

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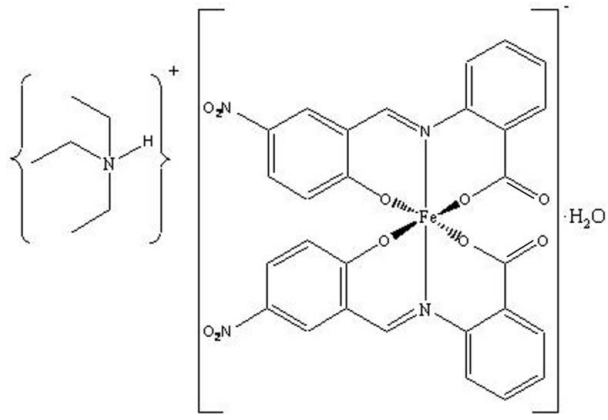
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.011 Å; disorder in solvent or counterion; $R$ factor = 0.081; $wR$ factor = 0.242; data-to-parameter ratio = 13.8.

In the title compound, $[NH(C_2H_5)_3][Fe(C_{14}H_8N_2O_5)_2]\cdot H_2O$, the iron(III) ion is hexacoordinated by four O atoms in the basal plane [Fe—O distances in the range 1.904 (4)–1.909 (4) Å] and two N atoms in the axial plane [Fe—N = 1.981 (4) and 1.985 (4) Å] of two tridentate fully deprotonated 2-{[(2-oxido-5-nitrophenyl)methylene]amino}benzoato ($H_2L$) ligands, forming a tetragonally elongated octahedral geometry. The triethylammonium cations and complex anions are linked by N—H···O hydrogen bonds into chains parallel to [100]. Disordered water molecules (occupancy ratio 0.6:0.4) occupy the voids in the crystal structure.

## Related literature

For the stuctures of related compexes, including those with phenyl-salicyliden-imine (PSI) ligands similar to $H_2L$, see: Rotondo *et al.* (2009); Patel (2009); Patel *et al.* (2008); Laye & Sanudo (2009); Lu *et al.* (2006); Rosair *et al.* (2002). For bond-valence sums, see: Brown & Altermatt (1985).



## Experimental

### Crystal data

$(C_6H_{16}N)[Fe(C_{14}H_8N_2O_5)_2]\cdot H_2O$
$M_r$ = 742.50
Monoclinic, $P2_1/c$
$a$ = 10.2688 (3) Å
$b$ = 14.7128 (4) Å
$c$ = 25.0800 (7) Å
$\beta$ = 97.230 (2)°
$V$ = 3759.03 (18) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.46 mm$^{-1}$
$T$ = 296 K
0.35 × 0.05 × 0.04 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.855, $T_{max}$ = 0.982
20469 measured reflections
6432 independent reflections
5305 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.242
$S$ = 1.13
6432 reflections
466 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.61 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5$A$···O7 | 0.91 | 2.00 | 2.865 (13) | 159 |

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZK2002).

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# supporting information

*Acta Cryst.* (2011). E**67**, m593–m594 [doi:10.1107/S1600536811011196]

## Triethylammonium bis{2-[(2-oxido-5-nitrobenzylidene)amino]-benzoato}ferrate(III) monohydrate

**Eduard N. Chygorin, Svetlana R. Petrusenko, Volodymyr N. Kokozay, Yuri O. Smal and Volodymyr V. Bon**

### S1. Comment

There is growing interest in transition metal complexes with phenyl-salicyliden-imines (PSI) ligands due to their important applications and pharmacological activities (Rotondo *et al.*, 2009, Patel, 2009, Patel *et al.*, 2008, Laye & Sanudo, 2009). Here we represent a new complex with nitro-substituted PSI ligand, 2-(((2-hydroxy-5-nitrophenyl)-methylene)amino)benzoic acid ($H_2L$), wich was obtained as by-product during the invistigation of the system Co – $FeCl_2{\cdot}4H_2O$ – $MnCl_2{\cdot}4H_2O$ – $H_2L$ – $Et_3N$ – DMF.

The synthesis of $\{NH(C_2H_5)_3\}[Fe(C_{14}H_8NO_5)_2]{\cdot}H_2O$, **I**, is carried out in air that leads to stabilization of iron(III) ion. The formation of the complex can be understood if one considers the following reaction scheme: $FeCl_2{\cdot}4H_2O + 2H_2L + 3Et_3N + 0.25O_2 \rightarrow (NHEt_3)[Fe^{III}L_2] + 2Et_3N{\cdot}HCl + 9H_2O$

The crystal structure of **I** consists of triethylammonium cations and complex anions (Fig. 1) linked together by "strong" N—H···O hydrogen bonds (Fig. 2). The Fe centre is hexacoordinated in an axially elongated octahedral fashion ($FeO_4N_2$-chromophore) with oxidation state Fe(III), as it can be seen from close examination of the structured parameters and bond-valence sum calculations (Brown & Altermatt, 1985). Angular deviations from octahedral geometry are not significant, less than 5° for *cis*- and *trans*-angles.

In the crystal packing of **I** there are channels along the *a* axis (Fig. 3), accounting in total 610.7 Å$^3$ per unit cell, *i.e.* some 16.2% of the total volume. The voids were examined using *PLATON* (Spek, 2009). The channels are occupied by disordered water molecules.

### S2. Experimental

2-aminobenzoic acid (0.51 g, 3.75 mmol), 5-Nitrosalicylaldehyde (0.63 g, 3.75 mmol), and triethylamine (0.53 ml, 3.75 mmol) were dissolved in DMF (25 ml) in this order, forming a yellow solution and magnetically stirred at 50 – 60°C (10 min). Then, cobalt powder (0.08 g, 1.25 mmol), $FeCl_2{\cdot}4H_2O$ (0.25 g, 1.25 mmol) and $MnCl_2{\cdot}4H_2O$ (0.26 g, 1.25 mmol) were successfully added to the hot yellow solution with stirring about 2 h. Red crystals suitable for X-ray analysis were isolated by adding of *i*PrOH from the dark red solution after 1 day. Yield: 0.34 g, 0.32% (per Fe). Elemental analysis for $C_{34}H_{34}Fe_1N_5O_{11}$ (Mr=744.52). Calcd: C, 54.85; N, 9.41; H, 4.6; Fe, 7.5. Found: C, 54.5; N, 9.6; H, 4.6; Fe, 7.2. The compound is sparingly soluble in DMSO and DMF, and it is stable in air. The infrared spectrum of solid recorded using KBr disk shows an adsorption at 3440 cm$^{-1}$, which attributed to $\nu$(OH) of $H_2O$ solvation molecules. The presence in IR spectrum of a band at 1680 cm$^{-1}$ attributable to the $\nu(C{=}N)_{imine}$ stretching frequency together with the absence of the band due to the $\nu$(C=O) of the carbonyl indicates the formation of the Schiff base (Fig. 4).

### S3. Refinement

Structure solution by direct methods in the space group $P2_1/c$, followed by refinement, based on $F^2$, of atomic coordinates and anisotropic displacement parameters, was performed using the programs *SHELX97* (Sheldrick, 2008) successively. H atoms bonded to C atoms were found in successive difference Fourier maps and refined using a riding model, with C–H = 0.93 Å and with $U_{iso}$(H)=1.2$U_{eq}$(C). O11 appeared to be highly disordered and was split in two positions with 0.4 and 0.6 occurrence. The H-atoms bonded to disordered oxygen O11 cannot be located from difference map. On this ground, both positions of O11 are refined without H atoms.

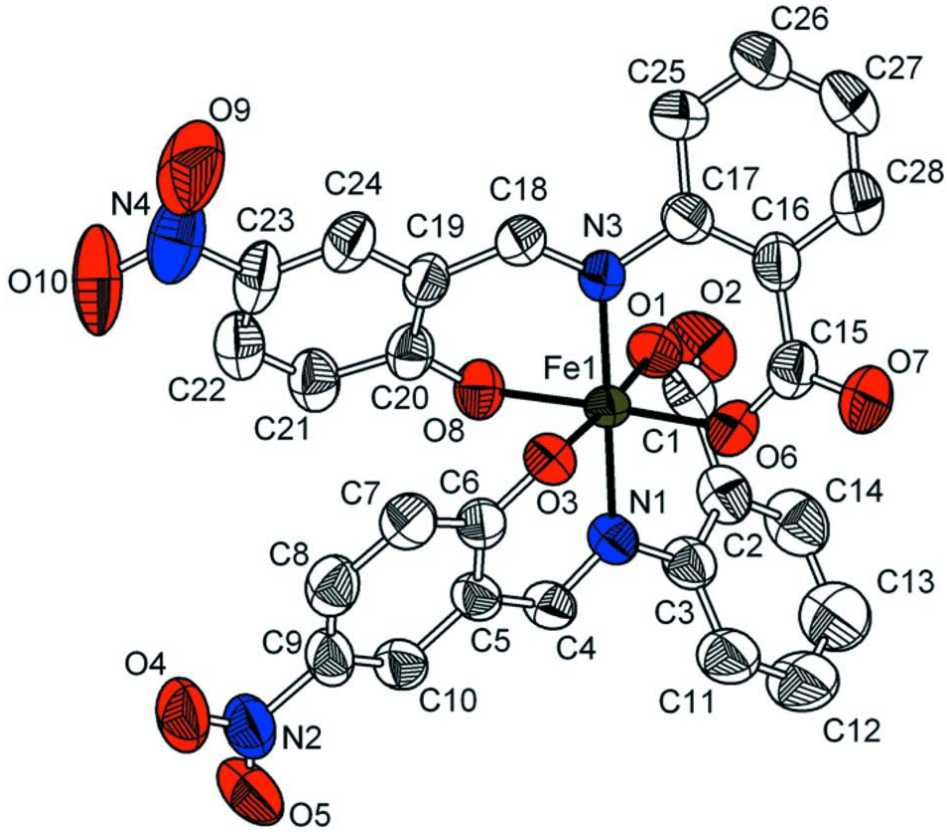


**Figure 1**

The structure of $[Fe(C_{14}H_8NO_5)_2]^-$ with atom labels and 50% probability displacement elipsoides. The H atoms have been omitted.

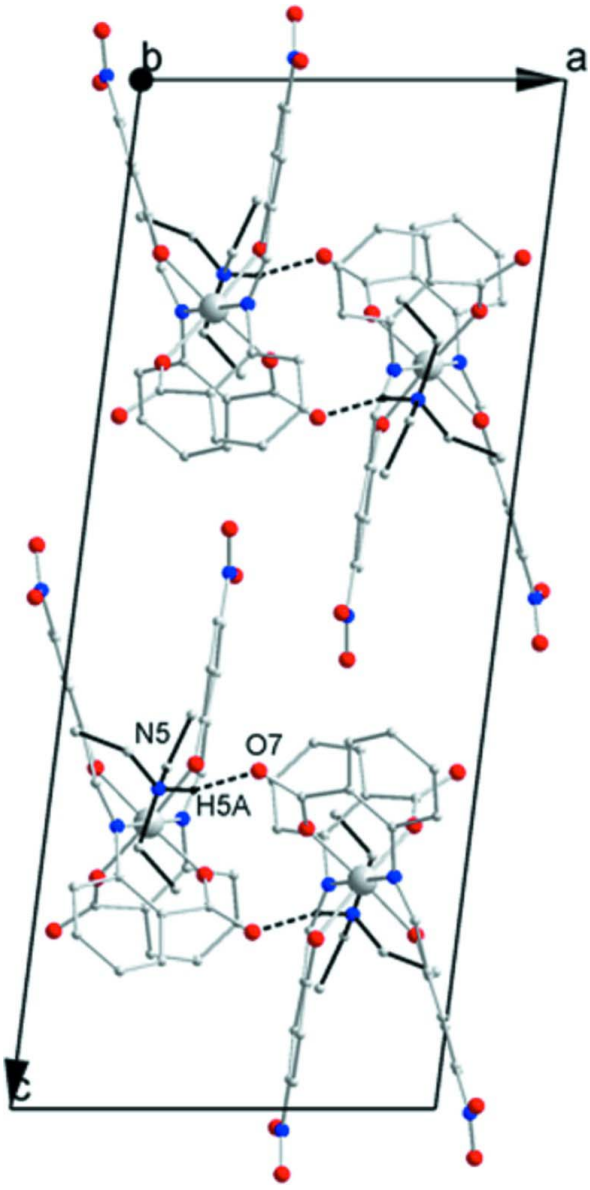


**Figure 2**

The packing of complex **I**, viewed down the *b* axis, showing N–H···O hydrogen bonds linking in pairs of the complex cations and anions. H atoms not involved in hydrogen bonding have been omitted.

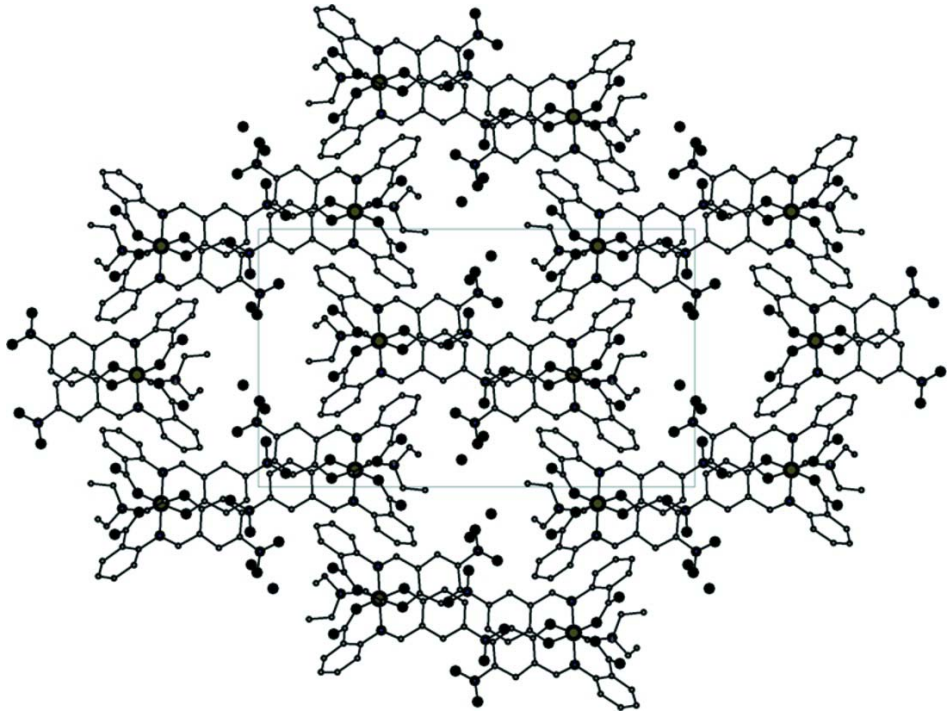

**Figure 3**

The packing of complex **I**, viewed down the *a* axis, demonstrating the voids occupied by water molecules.

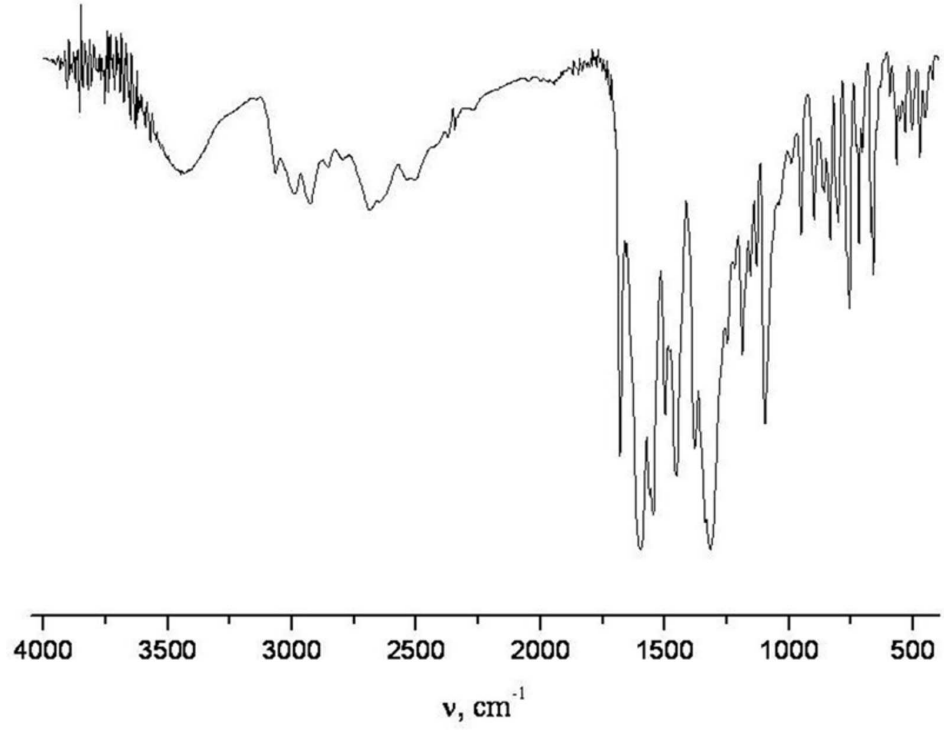


**Figure 4**

The IR spectrum of complex **I** ($cm^{-1}$): 3440, 3065, 2989, 2928, 2861, 2793, 1678, 1592, 1550, 1508, 1457, 1371,1321, 1184, 1107, 955, 895, 862, 836, 801, 750, 715.

**Triethylammonium bis{2-[(2-oxido-5-nitrobenzylidene)amino]benzoato}ferrate(III) monohydrate**

*Crystal data*

$(C_6H_{16}N)[Fe(C_{14}H_8N_2O_5)_2]\cdot H_2O$
$M_r = 742.50$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.2688$ (3) Å
$b = 14.7128$ (4) Å
$c = 25.0800$ (7) Å
$\beta = 97.230$ (2)°
$V = 3759.03$ (18) Å$^3$
$Z = 4$
$F(000) = 1540$
$D_x = 1.312$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5575 reflections
$\theta = 5.8$–$25.0°$
$\mu = 0.46$ mm$^{-1}$
$T = 296$ K
Prism, red
0.35 × 0.05 × 0.04 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.855$, $T_{max} = 0.982$
20469 measured reflections
6432 independent reflections
5305 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.1°$, $\theta_{min} = 5.8°$
$h = -12\rightarrow12$
$k = -17\rightarrow17$
$l = -29\rightarrow28$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.081$
$wR(F^2) = 0.242$
$S = 1.13$
6432 reflections
466 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2 + 8.9019P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å$^{-3}$
$\Delta\rho_{min} = -0.61$ e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Fe1 | 0.76042 (6) | 0.43361 (4) | 0.27782 (3) | 0.0393 (3) | |
| N1 | 0.6821 (4) | 0.5564 (3) | 0.28195 (17) | 0.0488 (10) | |
| N2 | 0.6448 (5) | 0.5933 (6) | 0.5208 (2) | 0.0771 (16) | |
| N3 | 0.8339 (4) | 0.3095 (3) | 0.27462 (17) | 0.0495 (10) | |

| | | | | | |
|---|---|---|---|---|---|
| N4 | 1.0827 (7) | 0.2486 (7) | 0.5039 (3) | 0.103 (2) | |
| N5 | 0.2528 (12) | 0.4148 (8) | 0.1890 (4) | 0.139 (3) | |
| H5A | 0.3355 | 0.3918 | 0.1905 | 0.167* | |
| O1 | 0.8649 (4) | 0.4740 (3) | 0.22465 (16) | 0.0605 (10) | |
| O2 | 0.9514 (5) | 0.5716 (3) | 0.1731 (2) | 0.0854 (14) | |
| O3 | 0.6678 (3) | 0.3946 (2) | 0.33491 (14) | 0.0506 (8) | |
| O4 | 0.6579 (5) | 0.5525 (5) | 0.5635 (2) | 0.0986 (18) | |
| O5 | 0.6314 (6) | 0.6749 (5) | 0.5180 (2) | 0.1001 (18) | |
| O6 | 0.6131 (4) | 0.4005 (3) | 0.22741 (16) | 0.0605 (10) | |
| O7 | 0.4835 (4) | 0.3151 (4) | 0.1717 (2) | 0.0804 (13) | |
| O8 | 0.9015 (4) | 0.4666 (3) | 0.33112 (15) | 0.0556 (9) | |
| O9 | 1.0951 (9) | 0.1671 (6) | 0.4971 (3) | 0.137 (3) | |
| O10 | 1.1067 (8) | 0.2867 (5) | 0.5476 (2) | 0.132 (3) | |
| O11A | 0.741 (3) | 0.1967 (14) | 0.4845 (9) | 0.160 (4) | 0.40 |
| O11B | 0.6751 (18) | 0.1050 (10) | 0.5340 (6) | 0.160 (4) | 0.60 |
| C1 | 0.8614 (6) | 0.5491 (4) | 0.1981 (2) | 0.0588 (14) | |
| C2 | 0.7424 (6) | 0.6079 (4) | 0.1954 (2) | 0.0593 (14) | |
| C3 | 0.6571 (6) | 0.6104 (4) | 0.2343 (2) | 0.0556 (13) | |
| C4 | 0.6518 (5) | 0.5896 (4) | 0.3267 (2) | 0.0509 (12) | |
| H4A | 0.6265 | 0.6503 | 0.3269 | 0.061* | |
| C5 | 0.6544 (5) | 0.5397 (4) | 0.3761 (2) | 0.0487 (11) | |
| C6 | 0.6607 (5) | 0.4436 (4) | 0.3777 (2) | 0.0482 (11) | |
| C7 | 0.6597 (5) | 0.3994 (5) | 0.4274 (2) | 0.0597 (14) | |
| H7A | 0.6607 | 0.3362 | 0.4289 | 0.072* | |
| C8 | 0.6571 (6) | 0.4482 (5) | 0.4737 (2) | 0.0673 (16) | |
| H8A | 0.6607 | 0.4185 | 0.5066 | 0.081* | |
| C9 | 0.6491 (5) | 0.5417 (5) | 0.4714 (2) | 0.0625 (15) | |
| C10 | 0.6460 (5) | 0.5879 (4) | 0.4237 (2) | 0.0581 (14) | |
| H10A | 0.6384 | 0.6509 | 0.4230 | 0.070* | |
| C11 | 0.5449 (8) | 0.6639 (4) | 0.2276 (3) | 0.0780 (19) | |
| H11A | 0.4867 | 0.6636 | 0.2532 | 0.094* | |
| C12 | 0.5208 (10) | 0.7188 (5) | 0.1812 (3) | 0.096 (3) | |
| H12A | 0.4460 | 0.7551 | 0.1763 | 0.115* | |
| C13 | 0.6048 (10) | 0.7192 (5) | 0.1442 (4) | 0.099 (3) | |
| H13A | 0.5885 | 0.7563 | 0.1140 | 0.118* | |
| C14 | 0.7160 (8) | 0.6643 (5) | 0.1507 (3) | 0.0787 (19) | |
| H14A | 0.7735 | 0.6652 | 0.1249 | 0.094* | |
| C15 | 0.5931 (5) | 0.3311 (4) | 0.1968 (2) | 0.0573 (13) | |
| C16 | 0.7025 (6) | 0.2670 (4) | 0.1898 (2) | 0.0597 (14) | |
| C17 | 0.8148 (6) | 0.2571 (4) | 0.2260 (2) | 0.0554 (13) | |
| C18 | 0.8964 (5) | 0.2712 (4) | 0.3170 (2) | 0.0531 (12) | |
| H18A | 0.9137 | 0.2093 | 0.3152 | 0.064* | |
| C19 | 0.9408 (5) | 0.3170 (4) | 0.3664 (2) | 0.0533 (13) | |
| C20 | 0.9450 (5) | 0.4139 (4) | 0.3703 (2) | 0.0510 (12) | |
| C21 | 0.9988 (6) | 0.4511 (5) | 0.4194 (2) | 0.0635 (15) | |
| H21A | 1.0056 | 0.5140 | 0.4226 | 0.076* | |
| C22 | 1.0412 (6) | 0.3991 (5) | 0.4623 (3) | 0.0700 (17) | |
| H22A | 1.0744 | 0.4259 | 0.4948 | 0.084* | |

| | | | | |
|---|---|---|---|---|
| C23 | 1.0348 (6) | 0.3054 (6) | 0.4577 (2) | 0.0738 (18) |
| C24 | 0.9887 (6) | 0.2630 (5) | 0.4103 (2) | 0.0641 (15) |
| H24A | 0.9892 | 0.2000 | 0.4075 | 0.077* |
| C25 | 0.9163 (7) | 0.1966 (5) | 0.2154 (3) | 0.0730 (18) |
| H25A | 0.9941 | 0.1926 | 0.2386 | 0.088* |
| C26 | 0.8961 (10) | 0.1443 (6) | 0.1697 (3) | 0.104 (3) |
| H26A | 0.9595 | 0.1022 | 0.1628 | 0.125* |
| C27 | 0.7844 (10) | 0.1530 (6) | 0.1342 (3) | 0.107 (3) |
| H27A | 0.7737 | 0.1179 | 0.1031 | 0.129* |
| C28 | 0.6886 (8) | 0.2124 (5) | 0.1438 (3) | 0.086 (2) |
| H28A | 0.6128 | 0.2168 | 0.1194 | 0.104* |
| C29 | 0.2660 (14) | 0.5053 (12) | 0.1683 (9) | 0.165 (6) |
| H29A | 0.1813 | 0.5351 | 0.1667 | 0.198* |
| H29B | 0.3266 | 0.5386 | 0.1939 | 0.198* |
| C30 | 0.309 (3) | 0.5136 (18) | 0.1172 (11) | 0.274 (13) |
| H30A | 0.2453 | 0.5464 | 0.0935 | 0.411* |
| H30B | 0.3211 | 0.4542 | 0.1027 | 0.411* |
| H30C | 0.3914 | 0.5458 | 0.1207 | 0.411* |
| C31 | 0.1695 (12) | 0.3468 (13) | 0.1528 (6) | 0.172 (7) |
| H31A | 0.2154 | 0.3332 | 0.1222 | 0.206* |
| H31B | 0.1642 | 0.2907 | 0.1728 | 0.206* |
| C32 | 0.0405 (15) | 0.3743 (10) | 0.1332 (6) | 0.161 (5) |
| H32A | 0.0069 | 0.3363 | 0.1035 | 0.241* |
| H32B | 0.0415 | 0.4364 | 0.1216 | 0.241* |
| H32C | −0.0145 | 0.3688 | 0.1613 | 0.241* |
| C33 | 0.2234 (16) | 0.4065 (15) | 0.2459 (7) | 0.192 (7) |
| H33A | 0.1400 | 0.4359 | 0.2488 | 0.230* |
| H33B | 0.2136 | 0.3426 | 0.2541 | 0.230* |
| C34 | 0.323 (2) | 0.4457 (12) | 0.2862 (7) | 0.204 (8) |
| H34A | 0.3114 | 0.4224 | 0.3211 | 0.306* |
| H34B | 0.3136 | 0.5107 | 0.2862 | 0.306* |
| H34C | 0.4086 | 0.4299 | 0.2778 | 0.306* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0418 (4) | 0.0346 (4) | 0.0414 (4) | 0.0049 (3) | 0.0053 (3) | −0.0007 (3) |
| N1 | 0.058 (2) | 0.044 (2) | 0.045 (2) | −0.0014 (19) | 0.0095 (19) | −0.0020 (18) |
| N2 | 0.061 (3) | 0.117 (5) | 0.053 (3) | −0.003 (3) | 0.008 (2) | −0.019 (3) |
| N3 | 0.053 (2) | 0.051 (2) | 0.043 (2) | 0.0046 (19) | −0.0002 (18) | −0.0003 (18) |
| N4 | 0.104 (5) | 0.128 (6) | 0.070 (5) | −0.019 (5) | −0.013 (4) | 0.038 (4) |
| N5 | 0.156 (9) | 0.152 (9) | 0.113 (7) | −0.003 (7) | 0.033 (6) | −0.005 (6) |
| O1 | 0.056 (2) | 0.073 (3) | 0.054 (2) | 0.0044 (19) | 0.0148 (17) | −0.001 (2) |
| O2 | 0.084 (3) | 0.093 (3) | 0.086 (3) | −0.025 (3) | 0.038 (3) | −0.003 (3) |
| O3 | 0.054 (2) | 0.0494 (19) | 0.049 (2) | −0.0039 (16) | 0.0104 (15) | −0.0029 (16) |
| O4 | 0.084 (3) | 0.165 (6) | 0.047 (3) | 0.004 (3) | 0.009 (2) | −0.011 (3) |
| O5 | 0.124 (5) | 0.112 (5) | 0.068 (3) | 0.006 (4) | 0.026 (3) | −0.032 (3) |
| O6 | 0.055 (2) | 0.067 (2) | 0.058 (2) | 0.0076 (18) | −0.0025 (17) | 0.0048 (19) |

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|---|---|---|---|---|---|---|
| O7 | 0.059 (2) | 0.099 (3) | 0.077 (3) | −0.004 (2) | −0.014 (2) | −0.010 (3) |
| O8 | 0.057 (2) | 0.055 (2) | 0.053 (2) | −0.0113 (17) | 0.0005 (17) | 0.0015 (17) |
| O9 | 0.182 (7) | 0.120 (6) | 0.098 (5) | 0.012 (5) | −0.034 (5) | 0.046 (4) |
| O10 | 0.166 (6) | 0.170 (6) | 0.049 (3) | −0.052 (5) | −0.028 (3) | 0.030 (3) |
| O11A | 0.213 (13) | 0.127 (8) | 0.131 (9) | 0.005 (8) | −0.009 (8) | −0.001 (7) |
| O11B | 0.213 (13) | 0.127 (8) | 0.131 (9) | 0.005 (8) | −0.009 (8) | −0.001 (7) |
| C1 | 0.064 (3) | 0.065 (3) | 0.050 (3) | −0.015 (3) | 0.014 (3) | −0.010 (3) |
| C2 | 0.075 (4) | 0.052 (3) | 0.051 (3) | −0.007 (3) | 0.010 (3) | 0.001 (2) |
| C3 | 0.074 (4) | 0.043 (3) | 0.051 (3) | 0.004 (3) | 0.009 (3) | 0.000 (2) |
| C4 | 0.058 (3) | 0.044 (3) | 0.052 (3) | 0.003 (2) | 0.011 (2) | −0.005 (2) |
| C5 | 0.046 (3) | 0.056 (3) | 0.046 (3) | 0.001 (2) | 0.012 (2) | −0.006 (2) |
| C6 | 0.041 (2) | 0.058 (3) | 0.047 (3) | −0.002 (2) | 0.008 (2) | −0.001 (2) |
| C7 | 0.056 (3) | 0.070 (3) | 0.055 (3) | 0.002 (3) | 0.015 (2) | 0.010 (3) |
| C8 | 0.059 (3) | 0.093 (5) | 0.050 (3) | 0.004 (3) | 0.010 (3) | 0.010 (3) |
| C9 | 0.050 (3) | 0.096 (5) | 0.043 (3) | 0.000 (3) | 0.009 (2) | −0.010 (3) |
| C10 | 0.048 (3) | 0.069 (3) | 0.058 (3) | 0.003 (3) | 0.010 (2) | −0.011 (3) |
| C11 | 0.106 (5) | 0.064 (4) | 0.064 (4) | 0.027 (4) | 0.014 (4) | 0.007 (3) |
| C12 | 0.135 (7) | 0.074 (5) | 0.081 (5) | 0.042 (5) | 0.020 (5) | 0.021 (4) |
| C13 | 0.146 (8) | 0.071 (5) | 0.079 (5) | 0.023 (5) | 0.018 (5) | 0.024 (4) |
| C14 | 0.109 (5) | 0.069 (4) | 0.061 (4) | −0.002 (4) | 0.023 (4) | 0.008 (3) |
| C15 | 0.054 (3) | 0.069 (4) | 0.048 (3) | −0.001 (3) | 0.003 (2) | 0.007 (3) |
| C16 | 0.071 (3) | 0.061 (3) | 0.045 (3) | 0.001 (3) | −0.004 (3) | −0.001 (2) |
| C17 | 0.066 (3) | 0.052 (3) | 0.048 (3) | 0.008 (3) | 0.007 (2) | −0.002 (2) |
| C18 | 0.058 (3) | 0.049 (3) | 0.051 (3) | 0.008 (2) | 0.001 (2) | 0.001 (2) |
| C19 | 0.044 (3) | 0.068 (3) | 0.046 (3) | 0.003 (2) | −0.002 (2) | 0.002 (2) |
| C20 | 0.043 (3) | 0.061 (3) | 0.048 (3) | −0.007 (2) | 0.001 (2) | 0.002 (2) |
| C21 | 0.056 (3) | 0.080 (4) | 0.054 (3) | −0.011 (3) | 0.003 (3) | −0.004 (3) |
| C22 | 0.065 (4) | 0.092 (5) | 0.052 (3) | −0.014 (3) | 0.000 (3) | −0.004 (3) |
| C23 | 0.062 (4) | 0.107 (5) | 0.048 (3) | −0.008 (4) | −0.009 (3) | 0.018 (3) |
| C24 | 0.057 (3) | 0.076 (4) | 0.058 (4) | 0.006 (3) | −0.001 (3) | 0.015 (3) |
| C25 | 0.082 (4) | 0.075 (4) | 0.061 (4) | 0.030 (3) | 0.006 (3) | −0.007 (3) |
| C26 | 0.141 (7) | 0.093 (5) | 0.073 (5) | 0.051 (5) | −0.009 (5) | −0.026 (4) |
| C27 | 0.138 (7) | 0.108 (6) | 0.071 (5) | 0.030 (6) | −0.007 (5) | −0.039 (5) |
| C28 | 0.097 (5) | 0.091 (5) | 0.065 (4) | 0.013 (4) | −0.015 (4) | −0.019 (4) |
| C29 | 0.124 (9) | 0.159 (13) | 0.211 (19) | 0.009 (9) | 0.013 (10) | 0.006 (12) |
| C30 | 0.38 (4) | 0.26 (3) | 0.19 (2) | −0.02 (2) | 0.07 (2) | 0.070 (18) |
| C31 | 0.092 (7) | 0.285 (19) | 0.132 (10) | −0.001 (10) | −0.013 (7) | −0.075 (11) |
| C32 | 0.165 (13) | 0.163 (12) | 0.159 (12) | −0.012 (10) | 0.041 (10) | −0.060 (10) |
| C33 | 0.151 (12) | 0.29 (2) | 0.133 (12) | 0.040 (13) | 0.010 (9) | −0.069 (13) |
| C34 | 0.26 (2) | 0.205 (16) | 0.126 (11) | 0.014 (14) | −0.043 (13) | −0.039 (11) |

*Geometric parameters (Å, º)*

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| Fe1—O3 | 1.904 (4) | C12—H12A | 0.9300 |
| Fe1—O8 | 1.906 (4) | C13—C14 | 1.391 (11) |
| Fe1—O1 | 1.908 (4) | C13—H13A | 0.9300 |
| Fe1—O6 | 1.909 (4) | C14—H14A | 0.9300 |
| Fe1—N3 | 1.981 (4) | C15—C16 | 1.493 (8) |

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| Fe1—N1 | 1.985 (4) | C16—C17 | 1.382 (8) |
| N1—C4 | 1.299 (7) | C16—C28 | 1.399 (9) |
| N1—C3 | 1.431 (7) | C17—C25 | 1.420 (8) |
| N2—O5 | 1.209 (8) | C18—C19 | 1.432 (8) |
| N2—O4 | 1.219 (8) | C18—H18A | 0.9300 |
| N2—C9 | 1.460 (8) | C19—C24 | 1.396 (8) |
| N3—C18 | 1.300 (7) | C19—C20 | 1.429 (8) |
| N3—C17 | 1.436 (7) | C20—C21 | 1.397 (8) |
| N4—O9 | 1.220 (10) | C21—C22 | 1.348 (9) |
| N4—O10 | 1.230 (10) | C21—H21A | 0.9300 |
| N4—C23 | 1.462 (9) | C22—C23 | 1.385 (10) |
| N5—C29 | 1.443 (18) | C22—H22A | 0.9300 |
| N5—C33 | 1.50 (2) | C23—C24 | 1.373 (9) |
| N5—C31 | 1.537 (16) | C24—H24A | 0.9300 |
| N5—H5A | 0.9100 | C25—C26 | 1.375 (10) |
| O1—C1 | 1.289 (7) | C25—H25A | 0.9300 |
| O2—C1 | 1.225 (7) | C26—C27 | 1.367 (12) |
| O3—C6 | 1.301 (6) | C26—H26A | 0.9300 |
| O6—C15 | 1.280 (7) | C27—C28 | 1.359 (11) |
| O7—C15 | 1.241 (7) | C27—H27A | 0.9300 |
| O8—C20 | 1.288 (6) | C28—H28A | 0.9300 |
| C1—C2 | 1.492 (9) | C29—C30 | 1.41 (3) |
| C2—C3 | 1.392 (8) | C29—H29A | 0.9700 |
| C2—C14 | 1.394 (9) | C29—H29B | 0.9700 |
| C3—C11 | 1.387 (9) | C30—H30A | 0.9600 |
| C4—C5 | 1.436 (8) | C30—H30B | 0.9600 |
| C4—H4A | 0.9300 | C30—H30C | 0.9600 |
| C5—C10 | 1.400 (8) | C31—C32 | 1.413 (17) |
| C5—C6 | 1.417 (7) | C31—H31A | 0.9700 |
| C6—C7 | 1.409 (8) | C31—H31B | 0.9700 |
| C7—C8 | 1.368 (9) | C32—H32A | 0.9600 |
| C7—H7A | 0.9300 | C32—H32B | 0.9600 |
| C8—C9 | 1.379 (10) | C32—H32C | 0.9600 |
| C8—H8A | 0.9300 | C33—C34 | 1.46 (2) |
| C9—C10 | 1.373 (9) | C33—H33A | 0.9700 |
| C10—H10A | 0.9300 | C33—H33B | 0.9700 |
| C11—C12 | 1.412 (10) | C34—H34A | 0.9600 |
| C11—H11A | 0.9300 | C34—H34B | 0.9600 |
| C12—C13 | 1.346 (12) | C34—H34C | 0.9600 |

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| O3—Fe1—O8 | 87.53 (16) | O7—C15—O6 | 121.5 (6) |
| O3—Fe1—O1 | 175.55 (16) | O7—C15—C16 | 118.0 (6) |
| O8—Fe1—O1 | 88.07 (17) | O6—C15—C16 | 120.6 (5) |
| O3—Fe1—O6 | 89.54 (16) | C17—C16—C28 | 118.1 (6) |
| O8—Fe1—O6 | 176.91 (17) | C17—C16—C15 | 124.6 (5) |
| O1—Fe1—O6 | 94.87 (18) | C28—C16—C15 | 117.3 (5) |
| O3—Fe1—N3 | 88.95 (17) | C16—C17—C25 | 121.0 (5) |
| O8—Fe1—N3 | 90.20 (17) | C16—C17—N3 | 120.9 (5) |

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| O1—Fe1—N3 | 90.46 (18) | C25—C17—N3 | 118.1 (5) |
| O6—Fe1—N3 | 90.70 (17) | N3—C18—C19 | 125.1 (5) |
| O3—Fe1—N1 | 89.48 (17) | N3—C18—H18A | 117.5 |
| O8—Fe1—N1 | 90.51 (17) | C19—C18—H18A | 117.5 |
| O1—Fe1—N1 | 91.17 (18) | C24—C19—C20 | 120.6 (5) |
| O6—Fe1—N1 | 88.50 (18) | C24—C19—C18 | 117.1 (5) |
| N3—Fe1—N1 | 178.24 (18) | C20—C19—C18 | 122.1 (5) |
| C4—N1—C3 | 118.4 (4) | O8—C20—C21 | 119.8 (5) |
| C4—N1—Fe1 | 122.0 (4) | O8—C20—C19 | 123.0 (5) |
| C3—N1—Fe1 | 119.6 (3) | C21—C20—C19 | 117.2 (5) |
| O5—N2—O4 | 122.6 (6) | C22—C21—C20 | 122.2 (6) |
| O5—N2—C9 | 118.8 (6) | C22—C21—H21A | 118.9 |
| O4—N2—C9 | 118.5 (7) | C20—C21—H21A | 118.9 |
| C18—N3—C17 | 117.6 (4) | C21—C22—C23 | 119.4 (6) |
| C18—N3—Fe1 | 121.1 (4) | C21—C22—H22A | 120.3 |
| C17—N3—Fe1 | 121.2 (3) | C23—C22—H22A | 120.3 |
| O9—N4—O10 | 124.1 (7) | C24—C23—C22 | 122.2 (6) |
| O9—N4—C23 | 118.8 (8) | C24—C23—N4 | 118.1 (7) |
| O10—N4—C23 | 117.1 (9) | C22—C23—N4 | 119.6 (7) |
| C29—N5—C33 | 117.3 (14) | C23—C24—C19 | 118.2 (6) |
| C29—N5—C31 | 117.2 (13) | C23—C24—H24A | 120.9 |
| C33—N5—C31 | 110.2 (12) | C19—C24—H24A | 120.9 |
| C29—N5—H5A | 103.2 | C26—C25—C17 | 118.0 (6) |
| C33—N5—H5A | 103.2 | C26—C25—H25A | 121.0 |
| C31—N5—H5A | 103.2 | C17—C25—H25A | 121.0 |
| C1—O1—Fe1 | 130.3 (4) | C27—C26—C25 | 121.1 (7) |
| C6—O3—Fe1 | 122.5 (3) | C27—C26—H26A | 119.4 |
| C15—O6—Fe1 | 130.9 (4) | C25—C26—H26A | 119.4 |
| C20—O8—Fe1 | 122.8 (3) | C28—C27—C26 | 120.8 (7) |
| O2—C1—O1 | 121.5 (6) | C28—C27—H27A | 119.6 |
| O2—C1—C2 | 119.1 (6) | C26—C27—H27A | 119.6 |
| O1—C1—C2 | 119.3 (5) | C27—C28—C16 | 120.9 (7) |
| C3—C2—C14 | 118.2 (6) | C27—C28—H28A | 119.5 |
| C3—C2—C1 | 124.7 (5) | C16—C28—H28A | 119.5 |
| C14—C2—C1 | 117.2 (6) | C30—C29—N5 | 117.5 (17) |
| C11—C3—C2 | 121.0 (5) | C30—C29—H29A | 107.9 |
| C11—C3—N1 | 118.4 (5) | N5—C29—H29A | 107.9 |
| C2—C3—N1 | 120.5 (5) | C30—C29—H29B | 107.9 |
| N1—C4—C5 | 124.9 (5) | N5—C29—H29B | 107.9 |
| N1—C4—H4A | 117.5 | H29A—C29—H29B | 107.2 |
| C5—C4—H4A | 117.5 | C29—C30—H30A | 109.5 |
| C10—C5—C6 | 119.3 (5) | C29—C30—H30B | 109.5 |
| C10—C5—C4 | 118.6 (5) | H30A—C30—H30B | 109.5 |
| C6—C5—C4 | 122.0 (5) | C29—C30—H30C | 109.5 |
| O3—C6—C7 | 118.8 (5) | H30A—C30—H30C | 109.5 |
| O3—C6—C5 | 122.5 (5) | H30B—C30—H30C | 109.5 |
| C7—C6—C5 | 118.7 (5) | C32—C31—N5 | 116.5 (13) |
| C8—C7—C6 | 120.8 (6) | C32—C31—H31A | 108.2 |

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| C8—C7—H7A | 119.6 | N5—C31—H31A | 108.2 |
| C6—C7—H7A | 119.6 | C32—C31—H31B | 108.2 |
| C7—C8—C9 | 119.6 (6) | N5—C31—H31B | 108.2 |
| C7—C8—H8A | 120.2 | H31A—C31—H31B | 107.3 |
| C9—C8—H8A | 120.2 | C31—C32—H32A | 109.5 |
| C10—C9—C8 | 121.8 (6) | C31—C32—H32B | 109.5 |
| C10—C9—N2 | 118.9 (6) | H32A—C32—H32B | 109.5 |
| C8—C9—N2 | 119.3 (6) | C31—C32—H32C | 109.5 |
| C9—C10—C5 | 119.6 (6) | H32A—C32—H32C | 109.5 |
| C9—C10—H10A | 120.2 | H32B—C32—H32C | 109.5 |
| C5—C10—H10A | 120.2 | C34—C33—N5 | 114.7 (16) |
| C3—C11—C12 | 118.8 (7) | C34—C33—H33A | 108.6 |
| C3—C11—H11A | 120.6 | N5—C33—H33A | 108.6 |
| C12—C11—H11A | 120.6 | C34—C33—H33B | 108.6 |
| C13—C12—C11 | 120.6 (7) | N5—C33—H33B | 108.6 |
| C13—C12—H12A | 119.7 | H33A—C33—H33B | 107.6 |
| C11—C12—H12A | 119.7 | C33—C34—H34A | 109.5 |
| C12—C13—C14 | 120.3 (7) | C33—C34—H34B | 109.5 |
| C12—C13—H13A | 119.9 | H34A—C34—H34B | 109.5 |
| C14—C13—H13A | 119.9 | C33—C34—H34C | 109.5 |
| C13—C14—C2 | 121.0 (7) | H34A—C34—H34C | 109.5 |
| C13—C14—H14A | 119.5 | H34B—C34—H34C | 109.5 |
| C2—C14—H14A | 119.5 | | |

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| O3—Fe1—N1—C4 | 30.7 (4) | C7—C8—C9—C10 | −1.2 (9) |
| O8—Fe1—N1—C4 | −56.8 (4) | C7—C8—C9—N2 | 179.2 (5) |
| O1—Fe1—N1—C4 | −144.9 (4) | O5—N2—C9—C10 | 4.0 (9) |
| O6—Fe1—N1—C4 | 120.2 (4) | O4—N2—C9—C10 | −174.4 (6) |
| N3—Fe1—N1—C4 | 57 (6) | O5—N2—C9—C8 | −176.5 (6) |
| O3—Fe1—N1—C3 | −149.0 (4) | O4—N2—C9—C8 | 5.2 (8) |
| O8—Fe1—N1—C3 | 123.5 (4) | C8—C9—C10—C5 | −1.6 (8) |
| O1—Fe1—N1—C3 | 35.4 (4) | N2—C9—C10—C5 | 177.9 (5) |
| O6—Fe1—N1—C3 | −59.4 (4) | C6—C5—C10—C9 | 2.5 (8) |
| N3—Fe1—N1—C3 | −123 (6) | C4—C5—C10—C9 | −179.6 (5) |
| O3—Fe1—N3—C18 | −54.7 (4) | C2—C3—C11—C12 | −2.4 (10) |
| O8—Fe1—N3—C18 | 32.8 (4) | N1—C3—C11—C12 | 178.8 (6) |
| O1—Fe1—N3—C18 | 120.9 (4) | C3—C11—C12—C13 | 0.2 (13) |
| O6—Fe1—N3—C18 | −144.2 (4) | C11—C12—C13—C14 | 0.9 (14) |
| N1—Fe1—N3—C18 | −81 (6) | C12—C13—C14—C2 | 0.2 (13) |
| O3—Fe1—N3—C17 | 122.5 (4) | C3—C2—C14—C13 | −2.3 (10) |
| O8—Fe1—N3—C17 | −150.0 (4) | C1—C2—C14—C13 | 178.0 (7) |
| O1—Fe1—N3—C17 | −61.9 (4) | Fe1—O6—C15—O7 | 170.2 (4) |
| O6—Fe1—N3—C17 | 32.9 (4) | Fe1—O6—C15—C16 | −10.4 (8) |
| N1—Fe1—N3—C17 | 96 (6) | O7—C15—C16—C17 | −158.3 (6) |
| O3—Fe1—O1—C1 | −108 (2) | O6—C15—C16—C17 | 22.3 (9) |
| O8—Fe1—O1—C1 | −100.2 (5) | O7—C15—C16—C28 | 20.7 (9) |
| O6—Fe1—O1—C1 | 78.8 (5) | O6—C15—C16—C28 | −158.7 (6) |
| N3—Fe1—O1—C1 | 169.6 (5) | C28—C16—C17—C25 | 3.2 (10) |

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| N1—Fe1—O1—C1 | −9.8 (5) | C15—C16—C17—C25 | −177.9 (6) |
| O8—Fe1—O3—C6 | 46.6 (4) | C28—C16—C17—N3 | −178.6 (6) |
| O1—Fe1—O3—C6 | 54 (2) | C15—C16—C17—N3 | 0.4 (9) |
| O6—Fe1—O3—C6 | −132.5 (4) | C18—N3—C17—C16 | 146.0 (6) |
| N3—Fe1—O3—C6 | 136.8 (4) | Fe1—N3—C17—C16 | −31.3 (7) |
| N1—Fe1—O3—C6 | −44.0 (4) | C18—N3—C17—C25 | −35.7 (8) |
| O3—Fe1—O6—C15 | −102.1 (5) | Fe1—N3—C17—C25 | 147.0 (5) |
| O8—Fe1—O6—C15 | −120 (3) | C17—N3—C18—C19 | 170.4 (5) |
| O1—Fe1—O6—C15 | 77.3 (5) | Fe1—N3—C18—C19 | −12.3 (8) |
| N3—Fe1—O6—C15 | −13.2 (5) | N3—C18—C19—C24 | 170.6 (6) |
| N1—Fe1—O6—C15 | 168.4 (5) | N3—C18—C19—C20 | −13.5 (9) |
| O3—Fe1—O8—C20 | 46.8 (4) | Fe1—O8—C20—C21 | −149.8 (4) |
| O1—Fe1—O8—C20 | −132.6 (4) | Fe1—O8—C20—C19 | 30.0 (7) |
| O6—Fe1—O8—C20 | 65 (3) | C24—C19—C20—O8 | −179.6 (5) |
| N3—Fe1—O8—C20 | −42.1 (4) | C18—C19—C20—O8 | 4.6 (8) |
| N1—Fe1—O8—C20 | 136.3 (4) | C24—C19—C20—C21 | 0.2 (8) |
| Fe1—O1—C1—O2 | 165.6 (4) | C18—C19—C20—C21 | −175.5 (5) |
| Fe1—O1—C1—C2 | −17.5 (8) | O8—C20—C21—C22 | 177.5 (6) |
| O2—C1—C2—C3 | −155.9 (6) | C19—C20—C21—C22 | −2.4 (9) |
| O1—C1—C2—C3 | 27.0 (8) | C20—C21—C22—C23 | 1.7 (10) |
| O2—C1—C2—C14 | 23.7 (8) | C21—C22—C23—C24 | 1.1 (11) |
| O1—C1—C2—C14 | −153.3 (6) | C21—C22—C23—N4 | 179.0 (6) |
| C14—C2—C3—C11 | 3.4 (9) | O9—N4—C23—C24 | 9.0 (12) |
| C1—C2—C3—C11 | −176.9 (6) | O10—N4—C23—C24 | −170.3 (7) |
| C14—C2—C3—N1 | −177.8 (5) | O9—N4—C23—C22 | −169.0 (8) |
| C1—C2—C3—N1 | 1.9 (8) | O10—N4—C23—C22 | 11.7 (11) |
| C4—N1—C3—C11 | −36.8 (8) | C22—C23—C24—C19 | −3.2 (10) |
| Fe1—N1—C3—C11 | 142.9 (5) | N4—C23—C24—C19 | 178.9 (6) |
| C4—N1—C3—C2 | 144.4 (5) | C20—C19—C24—C23 | 2.5 (9) |
| Fe1—N1—C3—C2 | −35.9 (7) | C18—C19—C24—C23 | 178.4 (6) |
| C3—N1—C4—C5 | 171.3 (5) | C16—C17—C25—C26 | −3.8 (11) |
| Fe1—N1—C4—C5 | −8.4 (7) | N3—C17—C25—C26 | 177.9 (7) |
| N1—C4—C5—C10 | 166.9 (5) | C17—C25—C26—C27 | 3.0 (14) |
| N1—C4—C5—C6 | −15.2 (8) | C25—C26—C27—C28 | −1.5 (17) |
| Fe1—O3—C6—C7 | −145.1 (4) | C26—C27—C28—C16 | 0.8 (15) |
| Fe1—O3—C6—C5 | 34.6 (6) | C17—C16—C28—C27 | −1.6 (12) |
| C10—C5—C6—O3 | 179.6 (5) | C15—C16—C28—C27 | 179.3 (8) |
| C4—C5—C6—O3 | 1.8 (8) | C33—N5—C29—C30 | 172.4 (18) |
| C10—C5—C6—C7 | −0.6 (7) | C31—N5—C29—C30 | −53 (2) |
| C4—C5—C6—C7 | −178.5 (5) | C29—N5—C31—C32 | −53.9 (18) |
| O3—C6—C7—C8 | 177.6 (5) | C33—N5—C31—C32 | 83.7 (17) |
| C5—C6—C7—C8 | −2.2 (8) | C29—N5—C33—C34 | −60.7 (19) |
| C6—C7—C8—C9 | 3.1 (9) | C31—N5—C33—C34 | 161.8 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5*A*···O7 | 0.91 | 2.00 | 2.865 (13) | 159 |