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Tris[2-(benzyliminomethyl)phenolato-κ^2N,O]iron(III)

Hai-Bin Gong,* Lei Wang and Wei-Tao Zhao

Xuzhou Central Hospital, Xuzhou 221009, People's Republic of China
Correspondence e-mail: adler_20008@yahoo.com.cn

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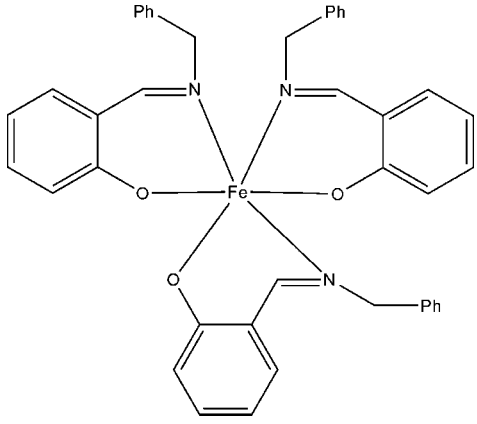
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.058; wR factor = 0.152; data-to-parameter ratio = 15.0.

In the title compound, $[Fe(C_{14}H_{12}NO)_3]$, the Fe^{III} atom has a slightly distorted octahedral geometry and is coordinated by three Schiff base ligands, *viz.* 2-(benzyliminomethyl)-phenolate. The crystal structure is stabilized by intramolecular C—H···O and C—H···N hydrogen bonds.

Related literature

For related literature, see: Liu *et al.* (2004); You & Zhu (2004); You *et al.* (2004, 2005); Zhu, Xia *et al.* (2003); Zhu, Zeng *et al.* (2003).



Experimental

Crystal data

$[Fe(C_{14}H_{12}NO)_3]$
M_r = 686.59
Triclinic, $P\overline{1}$
a = 9.3470 (8) Å
b = 10.9248 (13) Å
c = 16.7702 (19) Å
α = 95.42 (3)°
β = 96.47 (3)°
γ = 93.88 (3)°
V = 1688.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.828, T_{max} = 0.908
7053 measured reflections
6624 independent reflections
4330 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
S = 1.04
6624 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O3	0.97	2.34	2.830 (2)	111
C22—H22B···O1	0.97	2.52	2.978 (2)	109
C22—H22B···N3	0.97	2.59	3.018 (2)	107
C36—H36B···O1	0.97	2.29	2.938 (2)	123

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BX2126).

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supporting information

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S1. Comment

Due to its interesting physical and biological properties, many iron complexes with amines or imines have been structurally studied (Liu *et al.*, 2004; You & Zhu, 2004; You *et al.*,2004, 2005; Zhu, Xia *et al.*, 2003; Zhu, Zeng *et al.*, 2003). We report here the title structure of (I). Compound (I) is an electronically neutral mononuclear iron (III) compound (Fig. 1). In the complex the central iron(III) atom is six coordinated by three nitrogen atoms and three oxygen atoms from three Schiff base ligands. In the crystal structure, (I) is stabilized by intramolecular C—H···O and C—H···N hydrogen bonds.

S2. Experimental

Benzylamine and salicylaldehyde were available commercially and were used without further purification. Benzylamine (0.3 mmol, 32.0 mg) and salicylaldehyde (0.3 mmol, 36.7 mg) were dissolved in acetonitrile solution (20 ml). The mixture was stirred for 1 h to obtain a clear red solution of HL (0.3 mmol), where HL is 2-(benzyliminomethyl)phenol.To the solution of HL was added a solution of

$Fe(ClO_4)_2\times6\times H_2O$ (0.1 mmol, 38.9 mg) in acetonitrile (10 ml), with stirring. After keeping the resulting solution in air for 2 days, yielding large purple crystals. The crystals were isolated, washed three times with acetonitrile and methanol (yield 79%).

S3. Refinement

C-bound H atoms were included in the riding model approximation with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

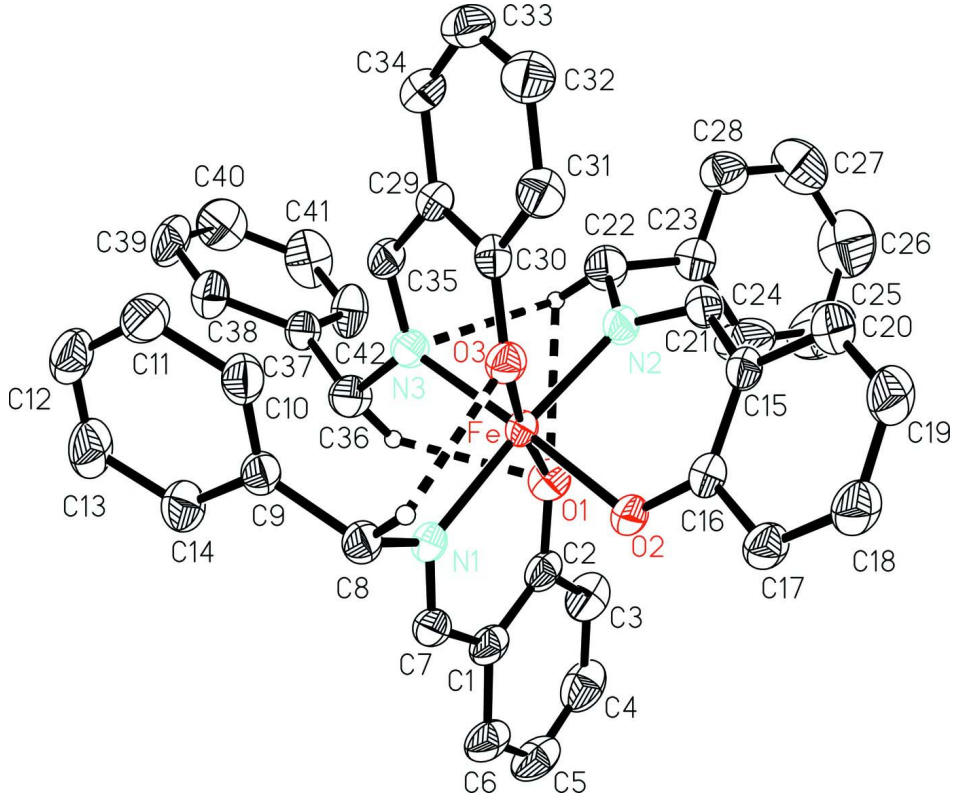

Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms unrelated to the hydrogen bonds have been omitted for clarity, showing hydrogen bond interactions as dashed lines.

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Crystal data

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$M_r = 686.59$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.3470\ (8)$ Å
$b = 10.9248\ (13)$ Å
$c = 16.7702\ (19)$ Å
$\alpha = 95.42\ (3)°$
$\beta = 96.47\ (3)°$
$\gamma = 93.88\ (3)°$
$V = 1688.6\ (3)$ Å^3
$Z = 2$
$F(000) = 718$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2702 reflections
$\theta = 2.7–27.9°$
$\mu = 0.49$ mm^{-1}
$T = 293$ K
Prism, purple
0.40 × 0.30 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.828$, $T_{max} = 0.908$
7053 measured reflections
6624 independent reflections
4330 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.2°$
$h = 0\rightarrow11$
$k = -13\rightarrow13$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.152$
$S = 1.04$
6624 reflections
442 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
$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 0.6392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe	0.82215 (5)	0.23502 (4)	0.78274 (3)	0.03716 (16)
O1	1.0232 (3)	0.2737 (2)	0.78948 (16)	0.0554 (7)
O2	0.7939 (3)	0.4060 (2)	0.79542 (15)	0.0497 (6)
O3	0.6202 (3)	0.2022 (2)	0.76423 (15)	0.0458 (6)
N1	0.8205 (3)	0.2453 (2)	0.89852 (18)	0.0440 (7)
N2	0.8234 (3)	0.2396 (3)	0.66785 (18)	0.0461 (7)
N3	0.8477 (3)	0.0590 (3)	0.77627 (18)	0.0449 (7)
C1	1.0614 (4)	0.3518 (3)	0.9288 (3)	0.0515 (10)
C2	1.1043 (4)	0.3354 (3)	0.8506 (3)	0.0511 (10)
C3	1.2425 (5)	0.3852 (4)	0.8396 (3)	0.0690 (13)
H3	1.2742	0.3734	0.7891	0.083*
C4	1.3309 (5)	0.4502 (4)	0.9013 (4)	0.0800 (15)
H4	1.4216	0.4821	0.8921	0.096*
C5	1.2884 (5)	0.4696 (4)	0.9774 (4)	0.0767 (15)
H5	1.3490	0.5158	1.0188	0.092*
C6	1.1556 (5)	0.4201 (4)	0.9913 (3)	0.0646 (12)
H6	1.1274	0.4318	1.0427	0.077*
C7	0.9239 (4)	0.3019 (3)	0.9480 (2)	0.0492 (9)
H7	0.9087	0.3118	1.0020	0.059*
C8	0.6871 (4)	0.2082 (3)	0.9334 (2)	0.0498 (9)
H8A	0.6051	0.2382	0.9025	0.060*
H8B	0.6934	0.2474	0.9882	0.060*
C9	0.6603 (4)	0.0696 (3)	0.9346 (2)	0.0491 (9)
C10	0.5434 (5)	0.0044 (4)	0.8898 (3)	0.0606 (11)
H10	0.4807	0.0448	0.8560	0.073*

C11	0.5173 (6)	−0.1225 (4)	0.8942 (3)	0.0735 (13)
H11	0.4382	−0.1663	0.8633	0.088*
C12	0.6085 (6)	−0.1811 (4)	0.9442 (3)	0.0737 (14)
H12	0.5919	−0.2654	0.9470	0.088*
C13	0.7231 (6)	−0.1176 (4)	0.9900 (3)	0.0779 (15)
H13	0.7840	−0.1581	1.0246	0.093*
C14	0.7501 (5)	0.0081 (4)	0.9854 (3)	0.0657 (12)
H14	0.8292	0.0512	1.0169	0.079*
C15	0.6688 (4)	0.4070 (3)	0.6628 (2)	0.0469 (9)
C16	0.7035 (4)	0.4535 (3)	0.7443 (2)	0.0462 (9)
C17	0.6398 (4)	0.5617 (3)	0.7711 (3)	0.0554 (10)
H17	0.6631	0.5964	0.8242	0.066*
C18	0.5452 (5)	0.6154 (4)	0.7204 (3)	0.0678 (12)
H18	0.5058	0.6869	0.7394	0.081*
C19	0.5059 (5)	0.5666 (4)	0.6413 (3)	0.0706 (13)
H19	0.4377	0.6023	0.6080	0.085*
C20	0.5700 (5)	0.4642 (4)	0.6128 (3)	0.0627 (11)
H20	0.5470	0.4325	0.5591	0.075*
C21	0.7481 (4)	0.3114 (3)	0.6284 (2)	0.0519 (10)
H21	0.7441	0.3011	0.5725	0.062*
C22	0.9185 (5)	0.1603 (4)	0.6228 (3)	0.0639 (12)
H22A	0.8593	0.0906	0.5933	0.077*
H22B	0.9875	0.1282	0.6616	0.077*
C23	1.0000 (4)	0.2252 (4)	0.5645 (3)	0.0560 (10)
C24	1.0837 (6)	0.3340 (5)	0.5903 (4)	0.1012 (19)
H24	1.0897	0.3679	0.6437	0.121*
C25	1.1584 (8)	0.3918 (7)	0.5359 (6)	0.142 (3)
H25	1.2131	0.4659	0.5527	0.171*
C26	1.1532 (8)	0.3413 (8)	0.4574 (5)	0.126 (3)
H26	1.2052	0.3801	0.4215	0.151*
C27	1.0715 (7)	0.2346 (7)	0.4328 (3)	0.1002 (19)
H27	1.0670	0.1998	0.3797	0.120*
C28	0.9951 (5)	0.1775 (4)	0.4861 (3)	0.0682 (12)
H28	0.9387	0.1045	0.4683	0.082*
C29	0.6256 (4)	0.0056 (3)	0.6874 (2)	0.0460 (9)
C30	0.5625 (4)	0.1171 (3)	0.7069 (2)	0.0452 (9)
C31	0.4290 (4)	0.1352 (4)	0.6627 (3)	0.0578 (11)
H31	0.3837	0.2067	0.6745	0.069*
C32	0.3658 (5)	0.0481 (4)	0.6025 (3)	0.0719 (13)
H32	0.2786	0.0624	0.5737	0.086*
C33	0.4289 (5)	−0.0614 (4)	0.5834 (3)	0.0701 (13)
H33	0.3855	−0.1192	0.5420	0.084*
C34	0.5557 (5)	−0.0814 (4)	0.6269 (3)	0.0607 (11)
H34	0.5969	−0.1553	0.6159	0.073*
C35	0.7575 (4)	−0.0208 (3)	0.7334 (2)	0.0494 (9)
H35	0.7788	−0.1029	0.7317	0.059*
C36	0.9731 (5)	0.0181 (4)	0.8270 (3)	0.0612 (11)
H36A	0.9460	0.0117	0.8806	0.073*

H36B	1.0515	0.0823	0.8317	0.073*
C37	1.0300 (4)	−0.1014 (3)	0.7987 (2)	0.0467 (9)
C38	0.9776 (5)	−0.2134 (4)	0.8207 (3)	0.0614 (11)
H38	0.9019	−0.2159	0.8522	0.074*
C39	1.0363 (6)	−0.3212 (4)	0.7965 (3)	0.0774 (14)
H39	1.0000	−0.3959	0.8115	0.093*
C40	1.1473 (6)	−0.3183 (5)	0.7507 (3)	0.0885 (17)
H40	1.1868	−0.3910	0.7343	0.106*
C41	1.2012 (6)	−0.2080 (5)	0.7286 (3)	0.0886 (17)
H41	1.2770	−0.2062	0.6971	0.106*
C42	1.1431 (5)	−0.1001 (4)	0.7529 (3)	0.0686 (13)
H42	1.1806	−0.0257	0.7382	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe	0.0438 (3)	0.0289 (3)	0.0396 (3)	0.0075 (2)	0.0040 (2)	0.00545 (19)
O1	0.0523 (16)	0.0539 (16)	0.0604 (18)	0.0033 (13)	0.0096 (14)	0.0044 (14)
O2	0.0623 (17)	0.0343 (13)	0.0516 (16)	0.0088 (12)	−0.0008 (13)	0.0056 (11)
O3	0.0483 (15)	0.0395 (14)	0.0496 (15)	0.0072 (11)	0.0036 (12)	0.0044 (12)
N1	0.0534 (19)	0.0324 (15)	0.0471 (18)	0.0086 (14)	0.0039 (15)	0.0072 (13)
N2	0.059 (2)	0.0386 (16)	0.0424 (17)	0.0098 (15)	0.0091 (15)	0.0054 (14)
N3	0.0519 (19)	0.0393 (17)	0.0439 (18)	0.0114 (15)	0.0047 (15)	0.0027 (14)
C1	0.054 (2)	0.0336 (19)	0.065 (3)	0.0123 (18)	−0.006 (2)	0.0040 (18)
C2	0.050 (2)	0.0339 (19)	0.068 (3)	0.0071 (17)	−0.004 (2)	0.0069 (19)
C3	0.051 (3)	0.061 (3)	0.095 (4)	0.006 (2)	0.002 (3)	0.012 (3)
C4	0.058 (3)	0.060 (3)	0.117 (5)	−0.004 (2)	−0.010 (3)	0.017 (3)
C5	0.068 (3)	0.047 (3)	0.105 (4)	0.008 (2)	−0.029 (3)	−0.002 (3)
C6	0.069 (3)	0.041 (2)	0.079 (3)	0.021 (2)	−0.014 (2)	−0.001 (2)
C7	0.066 (3)	0.0358 (19)	0.046 (2)	0.0175 (19)	0.000 (2)	0.0028 (16)
C8	0.066 (3)	0.039 (2)	0.047 (2)	0.0129 (18)	0.0143 (19)	0.0051 (17)
C9	0.063 (3)	0.041 (2)	0.047 (2)	0.0123 (19)	0.016 (2)	0.0061 (17)
C10	0.072 (3)	0.055 (3)	0.058 (3)	0.004 (2)	0.017 (2)	0.015 (2)
C11	0.093 (4)	0.058 (3)	0.069 (3)	−0.011 (3)	0.023 (3)	−0.001 (2)
C12	0.105 (4)	0.041 (2)	0.083 (3)	0.010 (3)	0.039 (3)	0.009 (2)
C13	0.103 (4)	0.053 (3)	0.088 (4)	0.033 (3)	0.022 (3)	0.027 (3)
C14	0.076 (3)	0.055 (3)	0.068 (3)	0.016 (2)	0.005 (2)	0.017 (2)
C15	0.055 (2)	0.0370 (19)	0.050 (2)	0.0077 (17)	0.0059 (18)	0.0103 (17)
C16	0.048 (2)	0.037 (2)	0.055 (2)	0.0049 (17)	0.0079 (19)	0.0098 (17)
C17	0.059 (3)	0.045 (2)	0.062 (3)	0.0129 (19)	0.006 (2)	0.0025 (19)
C18	0.071 (3)	0.052 (3)	0.082 (3)	0.025 (2)	0.006 (3)	0.006 (2)
C19	0.067 (3)	0.062 (3)	0.086 (4)	0.027 (2)	−0.002 (3)	0.019 (3)
C20	0.070 (3)	0.059 (3)	0.060 (3)	0.008 (2)	0.001 (2)	0.015 (2)
C21	0.069 (3)	0.045 (2)	0.044 (2)	0.008 (2)	0.007 (2)	0.0100 (17)
C22	0.085 (3)	0.054 (3)	0.057 (3)	0.018 (2)	0.022 (2)	0.003 (2)
C23	0.051 (2)	0.058 (3)	0.060 (3)	0.005 (2)	0.010 (2)	0.007 (2)
C24	0.100 (4)	0.097 (4)	0.097 (4)	−0.036 (4)	0.018 (3)	−0.018 (3)
C25	0.127 (6)	0.127 (6)	0.166 (8)	−0.064 (5)	0.045 (6)	−0.003 (6)

C26	0.106 (5)	0.149 (7)	0.136 (7)	−0.017 (5)	0.061 (5)	0.042 (5)
C27	0.097 (4)	0.136 (6)	0.074 (4)	0.012 (4)	0.034 (3)	0.014 (4)
C28	0.071 (3)	0.072 (3)	0.061 (3)	0.002 (2)	0.018 (2)	−0.003 (2)
C29	0.055 (2)	0.0351 (19)	0.047 (2)	0.0031 (17)	0.0041 (18)	0.0047 (16)
C30	0.047 (2)	0.044 (2)	0.046 (2)	0.0031 (17)	0.0070 (18)	0.0132 (17)
C31	0.049 (2)	0.060 (3)	0.065 (3)	0.007 (2)	0.002 (2)	0.010 (2)
C32	0.056 (3)	0.073 (3)	0.082 (3)	−0.004 (2)	−0.009 (2)	0.012 (3)
C33	0.068 (3)	0.060 (3)	0.074 (3)	−0.009 (2)	−0.011 (2)	−0.003 (2)
C34	0.069 (3)	0.045 (2)	0.066 (3)	−0.002 (2)	0.004 (2)	0.001 (2)
C35	0.065 (3)	0.0331 (19)	0.051 (2)	0.0102 (18)	0.009 (2)	0.0040 (17)
C36	0.073 (3)	0.048 (2)	0.062 (3)	0.023 (2)	−0.008 (2)	0.005 (2)
C37	0.050 (2)	0.041 (2)	0.051 (2)	0.0124 (17)	0.0021 (18)	0.0083 (17)
C38	0.066 (3)	0.052 (2)	0.071 (3)	0.011 (2)	0.018 (2)	0.017 (2)
C39	0.089 (4)	0.040 (2)	0.106 (4)	0.012 (2)	0.004 (3)	0.023 (2)
C40	0.103 (4)	0.071 (3)	0.097 (4)	0.048 (3)	0.014 (3)	0.006 (3)
C41	0.082 (4)	0.097 (4)	0.101 (4)	0.043 (3)	0.038 (3)	0.025 (3)
C42	0.056 (3)	0.065 (3)	0.093 (3)	0.016 (2)	0.019 (2)	0.032 (3)

Geometric parameters (Å, º)

Fe—O3	1.883 (3)	C18—C19	1.382 (6)
Fe—O1	1.887 (3)	C18—H18	0.9300
Fe—O2	1.899 (2)	C19—C20	1.375 (6)
Fe—N2	1.934 (3)	C19—H19	0.9300
Fe—N1	1.936 (3)	C20—H20	0.9300
Fe—N3	1.948 (3)	C21—H21	0.9300
O1—C2	1.306 (4)	C22—C23	1.506 (6)
O2—C16	1.304 (4)	C22—H22A	0.9700
O3—C30	1.314 (4)	C22—H22B	0.9700
N1—C7	1.283 (5)	C23—C28	1.363 (6)
N1—C8	1.485 (5)	C23—C24	1.383 (6)
N2—C21	1.271 (4)	C24—C25	1.383 (9)
N2—C22	1.497 (5)	C24—H24	0.9300
N3—C35	1.279 (5)	C25—C26	1.372 (9)
N3—C36	1.488 (5)	C25—H25	0.9300
C1—C6	1.409 (6)	C26—C27	1.353 (8)
C1—C2	1.413 (6)	C26—H26	0.9300
C1—C7	1.444 (6)	C27—C28	1.373 (7)
C2—C3	1.406 (6)	C27—H27	0.9300
C3—C4	1.358 (6)	C28—H28	0.9300
C3—H3	0.9300	C29—C34	1.394 (5)
C4—C5	1.380 (7)	C29—C30	1.416 (5)
C4—H4	0.9300	C29—C35	1.440 (5)
C5—C6	1.373 (7)	C30—C31	1.413 (5)
C5—H5	0.9300	C31—C32	1.371 (6)
C6—H6	0.9300	C31—H31	0.9300
C7—H7	0.9300	C32—C33	1.396 (6)
C8—C9	1.520 (5)	C32—H32	0.9300

C8—H8A	0.9700	C33—C34	1.362 (6)
C8—H8B	0.9700	C33—H33	0.9300
C9—C10	1.369 (6)	C34—H34	0.9300
C9—C14	1.380 (5)	C35—H35	0.9300
C10—C11	1.402 (6)	C36—C37	1.499 (5)
C10—H10	0.9300	C36—H36A	0.9700
C11—C12	1.362 (7)	C36—H36B	0.9700
C11—H11	0.9300	C37—C42	1.375 (6)
C12—C13	1.354 (7)	C37—C38	1.385 (5)
C12—H12	0.9300	C38—C39	1.380 (6)
C13—C14	1.390 (6)	C38—H38	0.9300
C13—H13	0.9300	C39—C40	1.359 (7)
C14—H14	0.9300	C39—H39	0.9300
C15—C20	1.396 (5)	C40—C41	1.374 (7)
C15—C16	1.406 (5)	C40—H40	0.9300
C15—C21	1.436 (5)	C41—C42	1.378 (6)
C16—C17	1.418 (5)	C41—H41	0.9300
C17—C18	1.358 (6)	C42—H42	0.9300
C17—H17	0.9300		

O3—Fe—O1	173.53 (12)	C17—C18—C19	121.7 (4)
O3—Fe—O2	88.52 (11)	C17—C18—H18	119.1
O1—Fe—O2	89.71 (12)	C19—C18—H18	119.1
O3—Fe—N2	88.56 (12)	C20—C19—C18	118.6 (4)
O1—Fe—N2	85.23 (13)	C20—C19—H19	120.7
O2—Fe—N2	90.60 (12)	C18—C19—H19	120.7
O3—Fe—N1	91.87 (12)	C19—C20—C15	121.5 (4)
O1—Fe—N1	94.17 (13)	C19—C20—H20	119.3
O2—Fe—N1	84.64 (11)	C15—C20—H20	119.3
N2—Fe—N1	175.21 (12)	N2—C21—C15	125.5 (4)
O3—Fe—N3	90.66 (12)	N2—C21—H21	117.2
O1—Fe—N3	91.47 (13)	C15—C21—H21	117.2
O2—Fe—N3	176.53 (12)	N2—C22—C23	114.6 (3)
N2—Fe—N3	92.76 (12)	N2—C22—H22A	108.6
N1—Fe—N3	92.01 (12)	C23—C22—H22A	108.6
C2—O1—Fe	125.9 (3)	N2—C22—H22B	108.6
C16—O2—Fe	120.7 (2)	C23—C22—H22B	108.6
C30—O3—Fe	119.9 (2)	H22A—C22—H22B	107.6
C7—N1—C8	116.2 (3)	C28—C23—C24	118.8 (5)
C7—N1—Fe	122.3 (3)	C28—C23—C22	121.0 (4)
C8—N1—Fe	120.6 (2)	C24—C23—C22	120.1 (4)
C21—N2—C22	117.7 (3)	C23—C24—C25	119.2 (6)
C21—N2—Fe	122.0 (3)	C23—C24—H24	120.4
C22—N2—Fe	120.3 (2)	C25—C24—H24	120.4
C35—N3—C36	120.0 (3)	C26—C25—C24	121.0 (6)
C35—N3—Fe	122.2 (3)	C26—C25—H25	119.5
C36—N3—Fe	117.7 (2)	C24—C25—H25	119.5
C6—C1—C2	119.2 (4)	C27—C26—C25	119.3 (6)

C6—C1—C7	117.9 (4)	C27—C26—H26	120.3
C2—C1—C7	122.9 (4)	C25—C26—H26	120.3
O1—C2—C3	119.2 (4)	C26—C27—C28	120.2 (6)
O1—C2—C1	123.0 (4)	C26—C27—H27	119.9
C3—C2—C1	117.8 (4)	C28—C27—H27	119.9
C4—C3—C2	121.4 (5)	C23—C28—C27	121.5 (5)
C4—C3—H3	119.3	C23—C28—H28	119.3
C2—C3—H3	119.3	C27—C28—H28	119.3
C3—C4—C5	121.2 (5)	C34—C29—C30	119.9 (4)
C3—C4—H4	119.4	C34—C29—C35	120.1 (3)
C5—C4—H4	119.4	C30—C29—C35	119.9 (3)
C6—C5—C4	119.3 (5)	O3—C30—C31	119.1 (3)
C6—C5—H5	120.3	O3—C30—C29	123.5 (3)
C4—C5—H5	120.3	C31—C30—C29	117.4 (4)
C5—C6—C1	121.0 (5)	C32—C31—C30	120.6 (4)
C5—C6—H6	119.5	C32—C31—H31	119.7
C1—C6—H6	119.5	C30—C31—H31	119.7
N1—C7—C1	126.9 (4)	C31—C32—C33	121.7 (4)
N1—C7—H7	116.5	C31—C32—H32	119.1
C1—C7—H7	116.5	C33—C32—H32	119.1
N1—C8—C9	113.7 (3)	C34—C33—C32	118.3 (4)
N1—C8—H8A	108.8	C34—C33—H33	120.8
C9—C8—H8A	108.8	C32—C33—H33	120.8
N1—C8—H8B	108.8	C33—C34—C29	122.0 (4)
C9—C8—H8B	108.8	C33—C34—H34	119.0
H8A—C8—H8B	107.7	C29—C34—H34	119.0
C10—C9—C14	118.6 (4)	N3—C35—C29	125.5 (3)
C10—C9—C8	121.5 (4)	N3—C35—H35	117.3
C14—C9—C8	119.8 (4)	C29—C35—H35	117.3
C9—C10—C11	120.6 (4)	N3—C36—C37	117.2 (3)
C9—C10—H10	119.7	N3—C36—H36A	108.0
C11—C10—H10	119.7	C37—C36—H36A	108.0
C12—C11—C10	119.6 (5)	N3—C36—H36B	108.0
C12—C11—H11	120.2	C37—C36—H36B	108.0
C10—C11—H11	120.2	H36A—C36—H36B	107.2
C13—C12—C11	120.5 (4)	C42—C37—C38	118.4 (4)
C13—C12—H12	119.8	C42—C37—C36	119.3 (4)
C11—C12—H12	119.8	C38—C37—C36	122.2 (4)
C12—C13—C14	120.2 (5)	C39—C38—C37	120.8 (4)
C12—C13—H13	119.9	C39—C38—H38	119.6
C14—C13—H13	119.9	C37—C38—H38	119.6
C9—C14—C13	120.5 (5)	C40—C39—C38	120.0 (4)
C9—C14—H14	119.7	C40—C39—H39	120.0
C13—C14—H14	119.7	C38—C39—H39	120.0
C20—C15—C16	119.8 (4)	C39—C40—C41	120.1 (5)
C20—C15—C21	119.6 (4)	C39—C40—H40	119.9
C16—C15—C21	120.1 (3)	C41—C40—H40	119.9
O2—C16—C15	124.1 (3)	C40—C41—C42	120.1 (5)

O2—C16—C17	118.4 (3)	C40—C41—H41	120.0
C15—C16—C17	117.4 (3)	C42—C41—H41	120.0
C18—C17—C16	120.9 (4)	C37—C42—C41	120.7 (4)
C18—C17—H17	119.6	C37—C42—H42	119.7
C16—C17—H17	119.6	C41—C42—H42	119.7
O3—Fe—O1—C2	134.2 (9)	C14—C9—C10—C11	−1.3 (6)
O2—Fe—O1—C2	60.1 (3)	C8—C9—C10—C11	−177.3 (4)
N2—Fe—O1—C2	150.7 (3)	C9—C10—C11—C12	0.6 (7)
N1—Fe—O1—C2	−24.5 (3)	C10—C11—C12—C13	0.6 (7)
N3—Fe—O1—C2	−116.7 (3)	C11—C12—C13—C14	−1.0 (7)
O3—Fe—O2—C16	−46.1 (3)	C10—C9—C14—C13	0.9 (6)
O1—Fe—O2—C16	127.7 (3)	C8—C9—C14—C13	177.0 (4)
N2—Fe—O2—C16	42.4 (3)	C12—C13—C14—C9	0.2 (7)
N1—Fe—O2—C16	−138.1 (3)	Fe—O2—C16—C15	−28.7 (5)
N3—Fe—O2—C16	−122 (2)	Fe—O2—C16—C17	153.8 (3)
O1—Fe—O3—C30	63.8 (10)	C20—C15—C16—O2	179.7 (4)
O2—Fe—O3—C30	138.0 (3)	C21—C15—C16—O2	−8.4 (6)
N2—Fe—O3—C30	47.4 (3)	C20—C15—C16—C17	−2.7 (6)
N1—Fe—O3—C30	−137.4 (2)	C21—C15—C16—C17	169.1 (3)
N3—Fe—O3—C30	−45.4 (3)	O2—C16—C17—C18	179.8 (4)
O3—Fe—N1—C7	−158.8 (3)	C15—C16—C17—C18	2.2 (6)
O1—Fe—N1—C7	18.9 (3)	C16—C17—C18—C19	0.7 (7)
O2—Fe—N1—C7	−70.4 (3)	C17—C18—C19—C20	−3.0 (7)
N2—Fe—N1—C7	−63.8 (17)	C18—C19—C20—C15	2.3 (7)
N3—Fe—N1—C7	110.5 (3)	C16—C15—C20—C19	0.5 (6)
O3—Fe—N1—C8	9.6 (2)	C21—C15—C20—C19	−171.3 (4)
O1—Fe—N1—C8	−172.7 (2)	C22—N2—C21—C15	−169.7 (4)
O2—Fe—N1—C8	98.0 (2)	Fe—N2—C21—C15	8.2 (6)
N2—Fe—N1—C8	104.6 (16)	C20—C15—C21—N2	−168.4 (4)
N3—Fe—N1—C8	−81.1 (2)	C16—C15—C21—N2	19.7 (6)
O3—Fe—N2—C21	55.8 (3)	C21—N2—C22—C23	43.0 (5)
O1—Fe—N2—C21	−122.3 (3)	Fe—N2—C22—C23	−135.0 (3)
O2—Fe—N2—C21	−32.7 (3)	N2—C22—C23—C28	−128.0 (4)
N1—Fe—N2—C21	−39.3 (18)	N2—C22—C23—C24	53.2 (6)
N3—Fe—N2—C21	146.4 (3)	C28—C23—C24—C25	0.7 (9)
O3—Fe—N2—C22	−126.2 (3)	C22—C23—C24—C25	179.6 (6)
O1—Fe—N2—C22	55.6 (3)	C23—C24—C25—C26	−1.5 (12)
O2—Fe—N2—C22	145.3 (3)	C24—C25—C26—C27	1.2 (13)
N1—Fe—N2—C22	138.7 (16)	C25—C26—C27—C28	−0.2 (12)
N3—Fe—N2—C22	−35.6 (3)	C24—C23—C28—C27	0.2 (8)
O3—Fe—N3—C35	29.1 (3)	C22—C23—C28—C27	−178.6 (5)
O1—Fe—N3—C35	−144.7 (3)	C26—C27—C28—C23	−0.5 (9)
O2—Fe—N3—C35	105 (2)	Fe—O3—C30—C31	−144.6 (3)
N2—Fe—N3—C35	−59.4 (3)	Fe—O3—C30—C29	36.7 (4)
N1—Fe—N3—C35	121.0 (3)	C34—C29—C30—O3	178.5 (4)
O3—Fe—N3—C36	−147.6 (3)	C35—C29—C30—O3	2.1 (6)
O1—Fe—N3—C36	38.6 (3)	C34—C29—C30—C31	−0.2 (5)

O2—Fe—N3—C36	−71 (2)	C35—C29—C30—C31	−176.6 (4)
N2—Fe—N3—C36	123.9 (3)	O3—C30—C31—C32	−179.9 (4)
N1—Fe—N3—C36	−55.7 (3)	C29—C30—C31—C32	−1.1 (6)
Fe—O1—C2—C3	−163.3 (3)	C30—C31—C32—C33	0.9 (7)
Fe—O1—C2—C1	18.6 (5)	C31—C32—C33—C34	0.8 (7)
C6—C1—C2—O1	−179.8 (3)	C32—C33—C34—C29	−2.2 (7)
C7—C1—C2—O1	−0.1 (6)	C30—C29—C34—C33	2.0 (6)
C6—C1—C2—C3	2.1 (5)	C35—C29—C34—C33	178.4 (4)
C7—C1—C2—C3	−178.2 (3)	C36—N3—C35—C29	174.3 (4)
O1—C2—C3—C4	179.9 (4)	Fe—N3—C35—C29	−2.4 (5)
C1—C2—C3—C4	−1.9 (6)	C34—C29—C35—N3	162.9 (4)
C2—C3—C4—C5	0.1 (7)	C30—C29—C35—N3	−20.7 (6)
C3—C4—C5—C6	1.4 (7)	C35—N3—C36—C37	28.5 (6)
C4—C5—C6—C1	−1.2 (6)	Fe—N3—C36—C37	−154.7 (3)
C2—C1—C6—C5	−0.6 (6)	N3—C36—C37—C42	94.3 (5)
C7—C1—C6—C5	179.6 (3)	N3—C36—C37—C38	−89.2 (5)
C8—N1—C7—C1	−177.2 (3)	C42—C37—C38—C39	−0.7 (6)
Fe—N1—C7—C1	−8.3 (5)	C36—C37—C38—C39	−177.3 (4)
C6—C1—C7—N1	174.7 (3)	C37—C38—C39—C40	0.2 (7)
C2—C1—C7—N1	−5.1 (6)	C38—C39—C40—C41	0.1 (8)
C7—N1—C8—C9	−110.8 (4)	C39—C40—C41—C42	0.1 (9)
Fe—N1—C8—C9	80.2 (4)	C38—C37—C42—C41	0.9 (7)
N1—C8—C9—C10	−115.1 (4)	C36—C37—C42—C41	177.6 (4)
N1—C8—C9—C14	69.0 (5)	C40—C41—C42—C37	−0.7 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O3	0.97	2.34	2.830 (2)	111
C22—H22*B*···O1	0.97	2.52	2.978 (2)	109
C22—H22*B*···N3	0.97	2.59	3.018 (2)	107
C36—H36*B*···O1	0.97	2.29	2.938 (2)	123