Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[*N*,*N*′-Bis(salicylidene)benzene-1,2-diaminato]iron(II)

Yong-Hao Ye, Yue Han, Ting-Ting Chen and Chang-Hong Liu*

College of Plant Protection, Nanjing Agricultural University, Nanjing 210095, People's Republic of China, and State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: changhong_liu2223@yahoo.com.cn

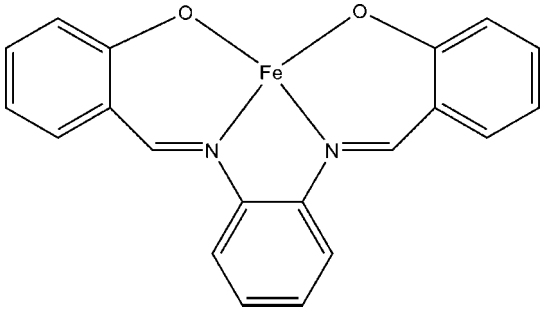
Received 30 May 2007; accepted 16 June 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.054; wR factor = 0.170; data-to-parameter ratio = 13.7.

The title complex (systematic name; {2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}iron(II)), [Fe($C_{20}H_{14}N_2O_2$)], is a mononuclear iron(II) complex with a distorted square-planar coordination geometry. The central Fe^{2+} ion is four-coordinated by two O and two N atoms from a Schiff base ligand, which is obtained by condensing 1,2-diaminobenzene and two equivalents of salicylaldehyde in acetonitrile.

Related literature

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



Experimental

Crystal data

Fe($C_{20}H_{14}N_2O_2$)]
M_r = 370.18
Orthorhombic, $P2_12_12_1$
a = 5.4675 (10) Å
b = 16.616 (4) Å
c = 17.310 (3) Å
V = 1572.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.759, T_{max} = 0.829
11948 measured reflections
3106 independent reflections
2404 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.170
S = 0.69
3106 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 1279 Friedel pairs
Flack parameter: −0.09 (4)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Analytical Test Fund for CHL at Nanjing University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2132).

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Liu, Z.-D., Tan, M.-Y. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m910–m911.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
You, Z.-L., Tang, L.-L. & Zhu, H.-L. (2005). *Acta Cryst.* E**61**, m36–m38.
You, Z.-L. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m1046–m1048.
You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m794–m796.
Zhu, H.-L., Xia, D.-S., Zeng, Q.-F., Wang, Z.-G. & Wang, D.-Q. (2003). *Acta Cryst.* E**59**, m1020–m1021.

 doi:10.1107/S1600536807029601

supplementary materials

Acta Cryst. (2007). E**63**, m1963 [**doi:10.1107/S1600536807029601**]

[*N*,*N*'-Bis(salicylidene)benzene-1,2-diaminato]iron(II)

Y.-H. Ye, Y. Han, T.-T. Chen and C.-H. Liu

Comment

Because of their interesting physical and biological properties, many iron complexes with amines or imines have structurally been studied (Liu, *et al.* 2004, You, *et al.* 2004*a*, 2004*b*, You, *et al.* 2005, Zhu, 2003*a*). When trying to synthesize iron(II) complexes with a Schiff base, condensed from salicylaldehyde and *N*-1,2-diaminobenzene, we isolated the title Fe(II) complex.

The title complex is a discrete iron(II) complex. The central iron(II) atom is four-coordinated by two oxygen atoms and two nitrogen atoms from a Schiff base ligand. The Schiff base acts as a tetradentate ligand. The iron(II) atom is in a distorted planar square coordination geometry.

Interestingly, all the atoms, including the hydrogen atoms, are in a plane with the mean deviation of 0.100 (2) /%A.

Experimental

All the solvents and chemicals were used as bought from Shanghai Chmical Company, Shanghai China, without further purification. 1,2-diaminobenzene and two equivalents of salicylaldehyde were dissolved in acetonitrile at room temperature with stirring. Five minutes later, equimolar $Fe(ClO_4)_2{\cdot}6H_2O$ in methanol was added to the above solution, giving a clear dark green solution. Large green crystals precipitated after the solution was stood still in air for three days. These crystals were filtered, washed with acetonitrile/methanol (v:v = 1:1) for three times, and dried in air. Yield: 93%.

When using $FeCl_2{\cdot}4H_2O$, $Fe(NO_3)_2{\cdot}6H_2O$, $FeSO_4{\cdot}7H_2O$, or $Fe(CH_3COO)_2{\cdot}2H_2O$ replaced $Fe(ClO_4)_2{\cdot}6H_2O$ in the above reaction, the same product was isolated with the yields 65%, 46%, 70%, and 41%, respectively.

Refinement

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

Figures

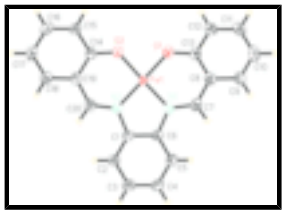


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

{2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}iron(II)

Crystal data

$Fe(C_{20}H_{14}N_2O_2)]$	F_{000} = 760
M_r = 370.18	D_x = 1.564 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 1882 reflections
a = 5.4675 (10) Å	θ = 2.2–24.8º
b = 16.616 (4) Å	μ = 0.98 mm^{-1}
c = 17.310 (3) Å	T = 298 (2) K
V = 1572.6 (5) Å^3	Block, green
Z = 4	0.30 × 0.20 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer	3106 independent reflections
Radiation source: fine-focus sealed tube	2404 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.069
T = 298(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→6
T_{min} = 0.759, T_{max} = 0.829	k = −20→20
11948 measured reflections	l = −21→21

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.1483P)^2 + 4.4994P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.170	$(\Delta/\sigma)_{max}$ = 0.003
S = 0.69	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
3106 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
226 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1279 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.09 (4)

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}
C1	1.1934 (12)	0.3423 (4)	0.1633 (4)	0.0426 (15)
C2	1.3846 (14)	0.3878 (4)	0.1349 (4)	0.0521 (17)
H2	1.4875	0.3673	0.0969	0.063*
C3	1.4207 (15)	0.4650 (4)	0.1642 (4)	0.060 (2)
H3	1.5508	0.4958	0.1462	0.072*
C4	1.2652 (16)	0.4965 (4)	0.2199 (4)	0.060 (2)
H4	1.2917	0.5481	0.2390	0.072*
C5	1.0714 (14)	0.4514 (4)	0.2471 (4)	0.0541 (18)
H5	0.9652	0.4730	0.2836	0.065*
C6	1.0350 (13)	0.3734 (4)	0.2197 (4)	0.0453 (15)
C7	0.7082 (12)	0.3363 (4)	0.3033 (4)	0.0490 (16)
H7	0.7374	0.3846	0.3289	0.059*
C8	0.5157 (12)	0.2872 (4)	0.3314 (4)	0.0488 (16)
C9	0.3786 (15)	0.3146 (5)	0.3949 (4)	0.0571 (18)
H9	0.4183	0.3635	0.4180	0.069*
C10	0.1874 (14)	0.2704 (5)	0.4231 (4)	0.067 (2)
H10	0.1015	0.2882	0.4662	0.080*
C11	0.1221 (15)	0.1991 (5)	0.3876 (5)	0.062 (2)
H11	−0.0125	0.1705	0.4057	0.075*
C12	0.2531 (14)	0.1696 (5)	0.3256 (4)	0.0567 (19)
H12	0.2087	0.1210	0.3031	0.068*
C13	0.4562 (12)	0.2135 (4)	0.2962 (3)	0.0443 (15)
C14	1.0161 (12)	0.0988 (4)	0.0916 (4)	0.0430 (14)
C15	0.9921 (14)	0.0188 (4)	0.0622 (4)	0.0526 (17)
H15	0.8568	−0.0117	0.0764	0.063*
C16	1.1597 (16)	−0.0137 (4)	0.0145 (4)	0.0582 (18)
H16	1.1385	−0.0664	−0.0023	0.070*
C17	1.3645 (16)	0.0293 (4)	−0.0106 (4)	0.0609 (19)
H17	1.4765	0.0065	−0.0445	0.073*
C18	1.3949 (14)	0.1061 (4)	0.0164 (4)	0.0556 (18)
H18	1.5315	0.1353	0.0010	0.067*
C19	1.2225 (12)	0.1426 (4)	0.0677 (4)	0.0479 (16)
C20	1.2689 (12)	0.2227 (5)	0.0936 (4)	0.0472 (14)
H20	1.4090	0.2482	0.0755	0.057*
Fe1	0.85107 (14)	0.22313 (5)	0.18970 (4)	0.0326 (2)
N1	0.8475 (11)	0.3190 (3)	0.2446 (3)	0.0423 (12)
N2	1.1281 (10)	0.2625 (3)	0.1408 (3)	0.0402 (11)
O1	0.5742 (9)	0.1826 (3)	0.2377 (3)	0.0512 (12)

O2	0.8516 (10)	0.1260 (3)	0.1390 (3)	0.0559 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (4)	0.040 (3)	0.037 (3)	0.000 (3)	−0.006 (3)	0.005 (3)
C2	0.059 (4)	0.047 (4)	0.050 (4)	−0.006 (3)	0.000 (3)	0.000 (3)
C3	0.075 (5)	0.052 (4)	0.054 (4)	−0.014 (4)	0.001 (4)	−0.001 (3)
C4	0.081 (5)	0.048 (4)	0.051 (4)	−0.013 (4)	0.002 (4)	−0.008 (3)
C5	0.059 (5)	0.049 (4)	0.055 (4)	0.002 (3)	0.006 (3)	−0.007 (3)
C6	0.049 (4)	0.041 (3)	0.046 (3)	−0.003 (3)	−0.007 (3)	0.002 (3)
C7	0.058 (4)	0.050 (3)	0.039 (3)	0.007 (3)	−0.001 (3)	−0.004 (3)
C8	0.049 (4)	0.053 (4)	0.044 (3)	0.006 (3)	0.001 (3)	0.007 (3)
C9	0.066 (5)	0.054 (4)	0.051 (4)	0.009 (4)	0.010 (4)	−0.003 (3)
C10	0.068 (5)	0.081 (6)	0.051 (4)	0.020 (5)	0.016 (4)	0.007 (4)
C11	0.049 (4)	0.068 (5)	0.069 (5)	0.009 (4)	0.014 (4)	0.015 (4)
C12	0.048 (4)	0.058 (4)	0.064 (5)	0.006 (3)	0.001 (3)	0.007 (4)
C13	0.041 (3)	0.045 (3)	0.047 (4)	0.011 (3)	0.002 (3)	0.008 (3)
C14	0.044 (4)	0.049 (4)	0.036 (3)	0.002 (3)	0.001 (3)	−0.003 (3)
C15	0.069 (5)	0.043 (3)	0.046 (4)	−0.005 (3)	0.004 (4)	−0.003 (3)
C16	0.080 (5)	0.044 (3)	0.051 (4)	0.014 (4)	−0.005 (4)	−0.005 (3)
C17	0.069 (5)	0.060 (4)	0.054 (4)	0.018 (4)	0.011 (4)	−0.009 (3)
C18	0.056 (5)	0.057 (4)	0.054 (4)	0.002 (3)	0.000 (3)	−0.012 (3)
C19	0.046 (4)	0.058 (4)	0.040 (3)	0.002 (3)	−0.003 (3)	0.001 (3)
C20	0.042 (3)	0.055 (4)	0.044 (3)	−0.006 (3)	−0.001 (3)	−0.002 (3)
Fe1	0.0365 (4)	0.0296 (4)	0.0318 (4)	0.0026 (4)	0.0019 (4)	0.0010 (3)
N1	0.047 (3)	0.040 (3)	0.040 (3)	0.010 (3)	−0.001 (3)	0.001 (2)
N2	0.042 (3)	0.042 (3)	0.037 (2)	−0.002 (2)	0.000 (2)	0.003 (2)
O1	0.050 (3)	0.046 (2)	0.057 (3)	−0.002 (2)	0.006 (2)	−0.001 (2)
O2	0.060 (3)	0.046 (2)	0.061 (3)	−0.008 (3)	0.013 (3)	−0.009 (2)

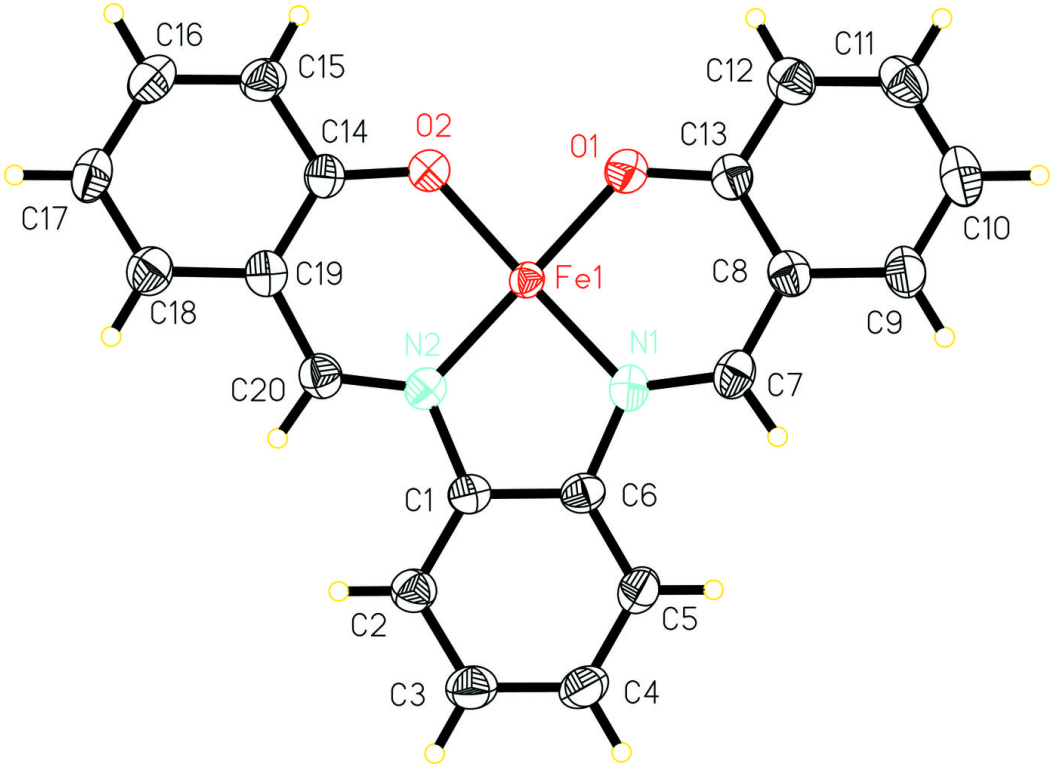
Geometric parameters (Å, °)

C1—C2	1.381 (9)	C11—H11	0.9300
C1—C6	1.403 (9)	C12—C13	1.423 (10)
C1—N2	1.427 (8)	C12—H12	0.9300
C2—C3	1.394 (10)	C13—O1	1.306 (7)
C2—H2	0.9300	C14—O2	1.299 (7)
C3—C4	1.388 (11)	C14—C19	1.405 (9)
C3—H3	0.9300	C14—C15	1.429 (9)
C4—C5	1.381 (10)	C15—C16	1.346 (10)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.395 (9)	C16—C17	1.398 (11)
C5—H5	0.9300	C16—H16	0.9300
C6—N1	1.433 (8)	C17—C18	1.368 (10)
C7—N1	1.302 (8)	C17—H17	0.9300
C7—C8	1.417 (9)	C18—C19	1.429 (9)
C7—H7	0.9300	C18—H18	0.9300
C8—C13	1.406 (9)	C19—C20	1.428 (10)

C8—C9	1.406 (9)	C20—N2	1.303 (8)
C9—C10	1.368 (11)	C20—H20	0.9300
C9—H9	0.9300	Fe1—O2	1.838 (4)
C10—C11	1.382 (12)	Fe1—O1	1.854 (5)
C10—H10	0.9300	Fe1—N2	1.855 (5)
C11—C12	1.379 (10)	Fe1—N1	1.856 (5)
C2—C1—C6	121.0 (6)	O1—C13—C12	117.5 (6)
C2—C1—N2	126.9 (6)	C8—C13—C12	118.1 (6)
C6—C1—N2	112.1 (6)	O2—C14—C19	124.2 (6)
C1—C2—C3	118.8 (7)	O2—C14—C15	119.0 (6)
C1—C2—H2	120.6	C19—C14—C15	116.8 (6)
C3—C2—H2	120.6	C16—C15—C14	121.9 (7)
C4—C3—C2	120.9 (7)	C16—C15—H15	119.0
C4—C3—H3	119.5	C14—C15—H15	119.0
C2—C3—H3	119.5	C15—C16—C17	122.0 (7)
C5—C4—C3	120.1 (7)	C15—C16—H16	119.0
C5—C4—H4	119.9	C17—C16—H16	119.0
C3—C4—H4	119.9	C18—C17—C16	117.9 (7)
C4—C5—C6	119.9 (7)	C18—C17—H17	121.0
C4—C5—H5	120.1	C16—C17—H17	121.0
C6—C5—H5	120.1	C17—C18—C19	121.8 (7)
C5—C6—C1	119.4 (6)	C17—C18—H18	119.1
C5—C6—N1	125.8 (6)	C19—C18—H18	119.1
C1—C6—N1	114.8 (5)	C14—C19—C20	122.2 (6)
N1—C7—C8	125.1 (6)	C14—C19—C18	119.5 (6)
N1—C7—H7	117.4	C20—C19—C18	118.3 (6)
C8—C7—H7	117.4	N2—C20—C19	124.5 (6)
C13—C8—C9	119.9 (6)	N2—C20—H20	117.8
C13—C8—C7	121.6 (6)	C19—C20—H20	117.8
C9—C8—C7	118.5 (7)	O2—Fe1—O1	84.0 (2)
C10—C9—C8	120.8 (7)	O2—Fe1—N2	95.2 (2)
C10—C9—H9	119.6	O1—Fe1—N2	179.2 (2)
C8—C9—H9	119.6	O2—Fe1—N1	177.7 (2)
C9—C10—C11	120.0 (7)	O1—Fe1—N1	94.2 (2)
C9—C10—H10	120.0	N2—Fe1—N1	86.5 (2)
C11—C10—H10	120.0	C7—N1—C6	121.0 (5)
C12—C11—C10	121.1 (8)	C7—N1—Fe1	126.5 (5)
C12—C11—H11	119.5	C6—N1—Fe1	112.3 (4)
C10—C11—H11	119.5	C20—N2—C1	119.7 (6)
C11—C12—C13	120.1 (7)	C20—N2—Fe1	126.1 (4)
C11—C12—H12	119.9	C1—N2—Fe1	114.1 (4)
C13—C12—H12	119.9	C13—O1—Fe1	127.4 (4)
O1—C13—C8	124.4 (6)	C14—O2—Fe1	127.5 (4)
C6—C1—C2—C3	1.1 (10)	C18—C19—C20—N2	−179.3 (6)
N2—C1—C2—C3	−179.8 (6)	C8—C7—N1—C6	178.8 (6)
C1—C2—C3—C4	−1.2 (11)	C8—C7—N1—Fe1	−6.6 (9)
C2—C3—C4—C5	0.0 (12)	C5—C6—N1—C7	−8.0 (10)
C3—C4—C5—C6	1.4 (12)	C1—C6—N1—C7	171.2 (6)

C4—C5—C6—C1	−1.5 (10)	C5—C6—N1—Fe1	176.7 (6)
C4—C5—C6—N1	177.7 (6)	C1—C6—N1—Fe1	−4.1 (7)
C2—C1—C6—C5	0.2 (10)	O2—Fe1—N1—C7	−33 (6)
N2—C1—C6—C5	−179.0 (6)	O1—Fe1—N1—C7	9.0 (5)
C2—C1—C6—N1	−179.0 (5)	N2—Fe1—N1—C7	−171.1 (5)
N2—C1—C6—N1	1.7 (8)	O2—Fe1—N1—C6	142 (6)
N1—C7—C8—C13	−0.6 (10)	O1—Fe1—N1—C6	−176.0 (4)
N1—C7—C8—C9	−179.1 (6)	N2—Fe1—N1—C6	3.9 (4)
C13—C8—C9—C10	0.1 (10)	C19—C20—N2—C1	179.6 (6)
C7—C8—C9—C10	178.6 (6)	C19—C20—N2—Fe1	4.2 (9)
C8—C9—C10—C11	−2.1 (11)	C2—C1—N2—C20	6.4 (9)
C9—C10—C11—C12	2.8 (12)	C6—C1—N2—C20	−174.4 (6)
C10—C11—C12—C13	−1.4 (11)	C2—C1—N2—Fe1	−177.7 (5)
C9—C8—C13—O1	−179.1 (6)	C6—C1—N2—Fe1	1.5 (6)
C7—C8—C13—O1	2.5 (10)	O2—Fe1—N2—C20	−6.0 (5)
C9—C8—C13—C12	1.3 (9)	O1—Fe1—N2—C20	−14 (18)
C7—C8—C13—C12	−177.1 (6)	N1—Fe1—N2—C20	172.5 (5)
C11—C12—C13—O1	179.7 (6)	O2—Fe1—N2—C1	178.5 (4)
C11—C12—C13—C8	−0.7 (10)	O1—Fe1—N2—C1	170 (67)
O2—C14—C15—C16	−178.2 (6)	N1—Fe1—N2—C1	−3.1 (4)
C19—C14—C15—C16	0.6 (10)	C8—C13—O1—Fe1	3.1 (9)
C14—C15—C16—C17	−1.4 (11)	C12—C13—O1—Fe1	−177.3 (5)
C15—C16—C17—C18	1.6 (12)	O2—Fe1—O1—C13	171.0 (5)
C16—C17—C18—C19	−1.0 (12)	N2—Fe1—O1—C13	179 (100)
O2—C14—C19—C20	−0.6 (10)	N1—Fe1—O1—C13	−7.4 (5)
C15—C14—C19—C20	−179.3 (6)	C19—C14—O2—Fe1	−3.3 (9)
O2—C14—C19—C18	178.7 (6)	C15—C14—O2—Fe1	175.5 (5)
C15—C14—C19—C18	0.0 (9)	O1—Fe1—O2—C14	−174.6 (6)
C17—C18—C19—C14	0.3 (11)	N2—Fe1—O2—C14	5.6 (6)
C17—C18—C19—C20	179.6 (7)	N1—Fe1—O2—C14	−132 (6)
C14—C19—C20—N2	0.0 (10)		

Fig. 1


C16
C15
C14
O2
O1
C13
C12
C11
C17
C10
C19
Fe1
C8
C18
C9
N2
N1
C20
C7
C1
C6
C2
C5
C3
C4