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Bis{[1-(quinolin-2-ylmethylenehydrazono)ethyl]-η^5-cyclopentadienyl}iron(II)

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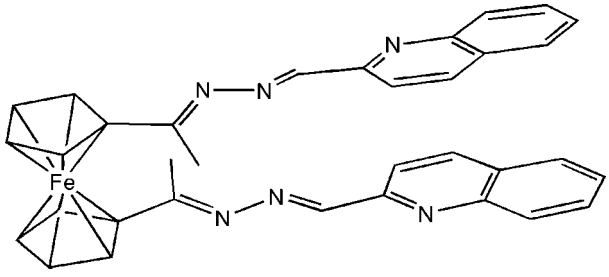
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.057; wR factor = 0.169; data-to-parameter ratio = 12.9.

The title complex, $[Fe(C_{17}H_{14}N_3)_2]$, was prepared by the reaction of 1,1′-diacetylferrocenedihydrazone with 2-quinolinecarboxaldehyde. The title compound adopts a Z configuration, in which the two quinoline groups from the two side chains are perfectly planar and nearly parallel.

Related literature

For related literature, see: Abuhijleh & Woods (1992); Allen (2002); Constable (1992); Duan *et al.* (1994); Takusagawa & Koetzle (1979); Tian *et al.* (1996); Togni & Hayashi (1995); Constable (1994).



Experimental

Crystal data

$[Fe(C_{17}H_{14}N_3)_2]$
M_r = 576.47
Triclinic, $P\overline{1}$
a = 9.5310 (19) Å
b = 14.174 (3) Å
c = 20.849 (4) Å
α = 86.93 (3)°
β = 86.54 (3)°
γ = 84.92 (3)°
V = 2797.1 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.894, T_{max} = 0.924
12350 measured reflections
9614 independent reflections
6494 reflections with $I > 2\sigma(I)$
R_{int} = 0.0875

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.169
S = 1.08
9614 reflections
743 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2475).

References

Abuhijleh, A. L. & Woods, C. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1249–1252.
Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2001). *SAINT and SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Constable, E. C. (1992). *Tetrahedron*, **48**, 10013–10059.
Constable, E. C. (1994). *Prog. Inorg. Chem.* **42**, 67–69.
Duan, C. Y., Xia, X. B., Zhu, L. G., You, X. Z., Yang, Y. & Wang, H. Q. (1994). *Chin. J. Chem.* **12**, 321–327.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.
Takusagawa, F. & Koetzle, T. F. (1979). *Acta Cryst.* B**35**, 2888–2896.
Tian, Y. P., Duan, C. Y., Lu, Z. L., You, X. Z. & Huang, X. Y. (1996). *J. Coord. Chem.* **38**, 219–226.
Togni, A. & Hayashi, T. (1995). *General Overview in Ferrocenes*. Weinheim: VCH.

supplementary materials

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Bis{[1-(quinolin-2-ylmethylenehydrazono)ethyl]-η^5-cyclopentadienyl}iron(II)

J. Zhou, L.-P. Zheng, C.-L. Chen and M.-X. Li

Comment

There is considerable interest in ferrocene-based ligands dueing to their potential application in many and diverse areas of chemistry (Togni & Hayashi, 1995). In addition, ferrocene-containing ligand are versatile ligands which can give rise to different geometries upon coordination to transition metal ions, dependent on the number and distribution of the donor sites and the coordination requirements of the metal (Constable, 1992; Constable, 1994).

The title compound, (I), is an easy-to-prepare ferrocenyl-containing imine-based bis-tridentate system. The average Fe—C_{ring} distance is 2.034 Å, in agreement with the value 2.04 Å of the free ferrocene. The C—C distances (1.4123 Å, average) and C—C—C angles (107.99 °, average) of the ferrocenyl units are all similar to those reported in the literature (Abuhijleh & Woods, 1992; Takusagawa & Koetzle 1979; Allen, & Kennard 1993). The cyclopentadienylrings are perfectly planar and nearly parallel with a dihedral angle of 2.1 ° at Fe1. The two pyridoquinoline groups attached to cyclopentadienyl ring adopt *cis* configuration corresponding to ferrocenyl. In the two side chains, the bond distances of N2—C10, N3—C11, N4—C23 and N5—C25 are 1.247 (4),1.286 (4), 1.288 (4), and 1.248 (4) Å, respectively. All of the C—N and C—C bond lengths are intermediate between formal single and double bonds. The measured N—N bond distances (N2—N3 = 1.396 (3) Å, N4—N5 = 1.406 (3) Å) are also intermediate between single and double bonds, pointing to extensive electron delocalization over the entire molecular skeleton (Duan *et al.*, 1994; Tian *et al.*, 1996).

Experimental

All reagents were commercially available and of analytical grade. The title compound was synthesized by the reaction of 1,1'-diacetylferrocenedihydrazone (1.2 g, 4 mmol) with 2-quinolinecarboxaldehyde (0.32 g, 8 mmol) in ethanol (15 ml). Five drops of acetic acid were added to the reaction solution as catalyst. After refluxing for 4 h, the solution was allowed to cool to room temperature, a dark-red precipitate was filtered, washed with ethanol, and dried *in vacuo* (yield 90%).

Refinement

All H atoms were positioned geometrically and refined as riding with C—H = 0.93 − 0.98Å and with U_{iso}(H) = 1.2U_{eq}(C) or1.5U_{eq} (methyl C).

Figures

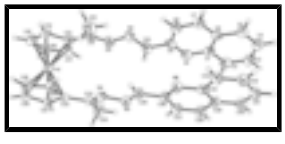


Fig. 1. The molecular structure of (I), showing atom displacement ellipsoids drawn at the 50% probability level.

Bis{[1-(quinolin-2-ylmethylenehydrazono)ethyl]-η^5-cyclopentadienyl}iron(II)

Crystal data

$[Fe(C_{17}H_{14}N_3)_2]$	$Z = 4$
$M_r = 576.47$	$F_{000} = 1200$
Triclinic, $P\overline{1}$	$D_x = 1.369$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.5310$ (19) Å	Cell parameters from 396 reflections
$b = 14.174$ (3) Å	$\theta = 3.4$–27.7°
$c = 20.849$ (4) Å	$\mu = 0.57$ mm^{-1}
$\alpha = 86.93$ (3)°	$T = 293$ (2) K
$\beta = 86.54$ (3)°	Irregular, red
$\gamma = 84.92$ (3)°	0.20 × 0.18 × 0.14 mm
$V = 2797.1$ (10) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	9614 independent reflections
Radiation source: fine-focus sealed tube	6494 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.088$
$T = 293$(2) K	$\theta_{max} = 25.0^\circ$
0.3° wide ω scans	$\theta_{min} = 3.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -11 \rightarrow 11$
$T_{min} = 0.894$, $T_{max} = 0.924$	$k = -16 \rightarrow 16$
12350 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.169$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
9614 reflections	$\Delta\rho_{max} = 1.19$ e Å^{-3}
743 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Fe1	0.98277 (4)	0.30512 (3)	0.411550 (18)	0.05024 (12)
Fe2	0.36478 (4)	0.60868 (3)	0.301205 (17)	0.04885 (12)
N1	1.3011 (3)	0.10489 (17)	0.74760 (11)	0.0582 (7)
N2	1.0406 (3)	0.15162 (18)	0.63580 (12)	0.0656 (8)
N3	1.0123 (3)	0.2273 (2)	0.59149 (12)	0.0679 (8)
N4	1.2728 (3)	0.13166 (18)	0.47873 (11)	0.0615 (7)
N5	1.3665 (3)	0.11010 (19)	0.52807 (11)	0.0638 (7)
N6	1.4081 (3)	−0.09841 (18)	0.62752 (12)	0.0650 (7)
N7	0.9526 (2)	0.25644 (15)	0.12609 (10)	0.0474 (6)
N8	0.8267 (2)	0.44948 (16)	0.21873 (10)	0.0500 (6)
N9	0.7077 (2)	0.46631 (17)	0.25942 (10)	0.0509 (6)
N10	0.4655 (3)	0.49048 (18)	0.13866 (11)	0.0579 (7)
N11	0.5767 (3)	0.47477 (18)	0.09280 (11)	0.0593 (7)
N12	0.6870 (3)	0.27633 (17)	0.00311 (11)	0.0560 (7)
C1	1.3411 (3)	0.0433 (2)	0.79661 (13)	0.0539 (8)
C2	1.4578 (3)	0.0598 (2)	0.82998 (16)	0.0683 (9)
H2A	1.5060	0.1130	0.8190	0.082*
C3	1.5024 (4)	−0.0020 (2)	0.87906 (16)	0.0734 (10)
H3A	1.5818	0.0097	0.9002	0.088*
C4	1.4327 (4)	−0.0808 (2)	0.89774 (16)	0.0680 (9)
H4A	1.4632	−0.1209	0.9318	0.082*
C5	1.3194 (3)	−0.0991 (2)	0.86604 (14)	0.0602 (9)
H5A	1.2724	−0.1526	0.8781	0.072*
C6	1.2716 (3)	−0.0378 (2)	0.81472 (12)	0.0500 (7)
C7	1.1551 (3)	−0.0551 (2)	0.77985 (14)	0.0618 (9)
H7A	1.1051	−0.1078	0.7903	0.074*
C8	1.1180 (4)	0.0060 (2)	0.73119 (14)	0.0642 (9)
H8A	1.0424	−0.0048	0.7071	0.077*
C9	1.1927 (3)	0.0866 (2)	0.71627 (12)	0.0519 (8)
C10	1.1513 (4)	0.1558 (2)	0.66412 (13)	0.0613 (9)
H10A	1.2092	0.2039	0.6520	0.074*
C11	0.9336 (3)	0.2070 (2)	0.54707 (14)	0.0611 (9)
C12	0.8850 (5)	0.1122 (3)	0.54017 (19)	0.1035 (14)

H12A	0.8858	0.0775	0.5810	0.155*
H12B	0.9468	0.0786	0.5095	0.155*
H12C	0.7909	0.1189	0.5255	0.155*
C13	0.8918 (3)	0.2837 (2)	0.50157 (14)	0.0637 (9)
C14	0.7912 (3)	0.2802 (3)	0.45176 (16)	0.0762 (11)
H14A	0.7365	0.2270	0.4440	0.091*
C15	0.7845 (4)	0.3689 (3)	0.41886 (18)	0.0845 (12)
H15A	0.7258	0.3875	0.3825	0.101*
C16	0.8751 (5)	0.4256 (3)	0.44423 (18)	0.0893 (13)
H16A	0.8913	0.4906	0.4290	0.107*
C17	0.9407 (4)	0.3749 (2)	0.49468 (15)	0.0759 (11)
H17A	1.0115	0.3983	0.5206	0.091*
C18	1.0873 (3)	0.1848 (2)	0.37868 (14)	0.0634 (9)
H18A	1.0712	0.1199	0.3939	0.076*
C19	1.0187 (4)	0.2375 (3)	0.32838 (15)	0.0743 (10)
H19A	0.9456	0.2149	0.3034	0.089*
C20	1.0687 (4)	0.3261 (3)	0.32020 (15)	0.0751 (11)
H20A	1.0377	0.3764	0.2888	0.090*
C21	1.1716 (3)	0.3318 (3)	0.36578 (14)	0.0701 (10)
H21A	1.2252	0.3864	0.3715	0.084*
C22	1.1818 (3)	0.2425 (2)	0.40305 (13)	0.0582 (8)
C23	1.2747 (3)	0.2176 (2)	0.45544 (13)	0.0584 (9)
C24	1.3611 (4)	0.2902 (3)	0.47669 (19)	0.0965 (13)
H24A	1.4291	0.2611	0.5054	0.145*
H24B	1.3013	0.3379	0.4985	0.145*
H24C	1.4093	0.3190	0.4399	0.145*
C25	1.3536 (3)	0.0293 (2)	0.55350 (15)	0.0660 (9)
H25A	1.2858	−0.0061	0.5386	0.079*
C26	1.4394 (3)	−0.0132 (2)	0.60572 (14)	0.0586 (8)
C27	1.5442 (3)	0.0352 (2)	0.62839 (15)	0.0664 (9)
H27A	1.5620	0.0951	0.6111	0.080*
C28	1.6206 (4)	−0.0069 (2)	0.67661 (15)	0.0701 (10)
H28A	1.6914	0.0243	0.6930	0.084*
C29	1.5926 (3)	−0.0980 (2)	0.70168 (14)	0.0588 (8)
C30	1.6675 (4)	−0.1473 (3)	0.75219 (16)	0.0780 (11)
H30A	1.7405	−0.1201	0.7701	0.094*
C31	1.6310 (4)	−0.2351 (3)	0.77407 (16)	0.0852 (12)
H31A	1.6798	−0.2670	0.8072	0.102*
C32	1.5241 (4)	−0.2772 (3)	0.74835 (17)	0.0839 (12)
H32A	1.5017	−0.3369	0.7642	0.101*
C33	1.4513 (4)	−0.2325 (2)	0.70005 (15)	0.0725 (10)
H33A	1.3794	−0.2616	0.6828	0.087*
C34	1.4846 (3)	−0.1417 (2)	0.67599 (14)	0.0607 (9)
C35	1.0598 (3)	0.2266 (2)	0.08375 (12)	0.0485 (7)
C36	1.0570 (4)	0.1386 (2)	0.05603 (14)	0.0635 (9)
H36A	0.9833	0.1011	0.0675	0.076*
C37	1.1609 (4)	0.1077 (3)	0.01252 (15)	0.0782 (11)
H37A	1.1587	0.0491	−0.0052	0.094*
C38	1.2696 (4)	0.1637 (3)	−0.00524 (15)	0.0792 (11)

H38A	1.3392	0.1428	−0.0357	0.095*
C39	1.2766 (3)	0.2489 (3)	0.02104 (14)	0.0652 (9)
H39A	1.3517	0.2849	0.0090	0.078*
C40	1.1719 (3)	0.2829 (2)	0.06606 (12)	0.0481 (7)
C41	1.1721 (3)	0.3701 (2)	0.09530 (13)	0.0526 (8)
H41A	1.2465	0.4079	0.0862	0.063*
C42	1.0645 (3)	0.3988 (2)	0.13653 (12)	0.0465 (7)
H42A	1.0631	0.4568	0.1554	0.056*
C43	0.9545 (3)	0.34014 (18)	0.15075 (12)	0.0415 (7)
C44	0.8362 (3)	0.3689 (2)	0.19416 (12)	0.0461 (7)
H44A	0.7662	0.3279	0.2042	0.055*
C45	0.6891 (3)	0.5537 (2)	0.27623 (12)	0.0469 (7)
C46	0.7822 (4)	0.6287 (2)	0.2558 (2)	0.0821 (11)
H46A	0.8392	0.6100	0.2183	0.123*
H46B	0.8420	0.6382	0.2899	0.123*
H46C	0.7259	0.6866	0.2458	0.123*
C47	0.5704 (3)	0.5781 (2)	0.32088 (13)	0.0532 (8)
C48	0.4840 (3)	0.5132 (2)	0.35484 (13)	0.0578 (8)
H48A	0.4921	0.4441	0.3518	0.069*
C49	0.3862 (3)	0.5676 (3)	0.39574 (14)	0.0726 (11)
H49A	0.3127	0.5420	0.4248	0.087*
C50	0.4084 (4)	0.6631 (3)	0.38588 (16)	0.0777 (11)
H50A	0.3535	0.7157	0.4069	0.093*
C51	0.5216 (3)	0.6717 (2)	0.33993 (15)	0.0643 (9)
H51A	0.5602	0.7308	0.3239	0.077*
C52	0.2599 (3)	0.5326 (2)	0.24211 (13)	0.0595 (8)
H52A	0.2702	0.4635	0.2390	0.071*
C53	0.1644 (3)	0.5841 (3)	0.28416 (16)	0.0719 (10)
H53A	0.0967	0.5566	0.3155	0.086*
C54	0.1821 (3)	0.6806 (3)	0.27400 (16)	0.0775 (11)
H54A	0.1291	0.7322	0.2969	0.093*
C55	0.2897 (3)	0.6912 (2)	0.22543 (15)	0.0675 (9)
H55A	0.3246	0.7512	0.2087	0.081*
C56	0.3384 (3)	0.5991 (2)	0.20470 (13)	0.0528 (8)
C57	0.4505 (3)	0.5766 (2)	0.15611 (12)	0.0511 (8)
C58	0.5361 (4)	0.6542 (2)	0.13042 (16)	0.0751 (10)
H58A	0.6280	0.6279	0.1158	0.113*
H58B	0.5452	0.6972	0.1637	0.113*
H58C	0.4904	0.6878	0.0951	0.113*
C59	0.5885 (3)	0.3914 (2)	0.07385 (13)	0.0564 (8)
H59A	0.5261	0.3486	0.0911	0.068*
C60	0.6974 (3)	0.3601 (2)	0.02566 (12)	0.0494 (7)
C61	0.8061 (3)	0.4182 (2)	0.00656 (14)	0.0570 (8)
H61A	0.8091	0.4770	0.0240	0.068*
C62	0.9048 (3)	0.3869 (2)	−0.03714 (14)	0.0610 (9)
H62A	0.9782	0.4240	−0.0499	0.073*
C63	0.8995 (3)	0.2979 (2)	−0.06452 (13)	0.0538 (8)
C64	0.9970 (4)	0.2602 (3)	−0.11112 (15)	0.0734 (10)
H64A	1.0726	0.2941	−0.1259	0.088*

C65	0.9827 (4)	0.1745 (3)	−0.13520 (16)	0.0841 (12)
H65A	1.0468	0.1515	−0.1673	0.101*
C66	0.8743 (5)	0.1214 (3)	−0.11252 (18)	0.0925 (13)
H66A	0.8674	0.0620	−0.1283	0.111*
C67	0.7779 (4)	0.1554 (2)	−0.06750 (16)	0.0761 (11)
H67A	0.7043	0.1195	−0.0528	0.091*
C68	0.7880 (3)	0.2446 (2)	−0.04266 (13)	0.0560 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0442 (2)	0.0551 (3)	0.0514 (2)	−0.00429 (19)	−0.00468 (18)	−0.00073 (19)
Fe2	0.0343 (2)	0.0612 (3)	0.0498 (2)	0.00557 (19)	0.00104 (17)	−0.01042 (18)
N1	0.0591 (15)	0.0533 (15)	0.0621 (14)	−0.0063 (12)	0.0059 (12)	−0.0113 (12)
N2	0.0710 (18)	0.0668 (17)	0.0564 (14)	−0.0017 (14)	0.0052 (13)	0.0040 (13)
N3	0.0697 (18)	0.0751 (18)	0.0568 (14)	0.0018 (14)	0.0031 (13)	−0.0029 (13)
N4	0.0522 (15)	0.0698 (17)	0.0588 (14)	0.0100 (13)	−0.0002 (12)	0.0013 (13)
N5	0.0555 (15)	0.0730 (17)	0.0602 (15)	0.0058 (13)	−0.0061 (12)	0.0056 (13)
N6	0.0628 (16)	0.0660 (17)	0.0638 (15)	0.0041 (14)	−0.0022 (13)	0.0013 (13)
N7	0.0443 (13)	0.0473 (13)	0.0500 (12)	−0.0024 (11)	−0.0002 (10)	−0.0006 (10)
N8	0.0370 (12)	0.0559 (15)	0.0562 (13)	0.0003 (11)	0.0024 (10)	−0.0063 (11)
N9	0.0402 (13)	0.0571 (15)	0.0536 (13)	0.0028 (11)	0.0027 (10)	−0.0042 (11)
N10	0.0502 (14)	0.0643 (16)	0.0600 (14)	−0.0064 (12)	0.0021 (12)	−0.0135 (12)
N11	0.0594 (15)	0.0658 (16)	0.0529 (13)	−0.0039 (13)	0.0037 (12)	−0.0146 (12)
N12	0.0545 (15)	0.0557 (15)	0.0592 (13)	−0.0097 (12)	0.0007 (12)	−0.0127 (11)
C1	0.0497 (17)	0.0547 (17)	0.0583 (16)	−0.0042 (14)	0.0017 (14)	−0.0173 (14)
C2	0.064 (2)	0.061 (2)	0.083 (2)	−0.0146 (16)	−0.0005 (17)	−0.0128 (17)
C3	0.065 (2)	0.077 (2)	0.081 (2)	−0.0055 (18)	−0.0172 (17)	−0.0163 (19)
C4	0.070 (2)	0.064 (2)	0.0706 (19)	−0.0003 (17)	−0.0110 (17)	−0.0082 (16)
C5	0.0587 (19)	0.0528 (18)	0.0694 (18)	−0.0065 (15)	0.0015 (16)	−0.0091 (15)
C6	0.0504 (17)	0.0489 (17)	0.0504 (15)	−0.0027 (14)	0.0058 (13)	−0.0114 (13)
C7	0.0614 (19)	0.063 (2)	0.0613 (17)	−0.0118 (16)	0.0016 (15)	−0.0053 (15)
C8	0.068 (2)	0.070 (2)	0.0568 (17)	−0.0145 (17)	−0.0047 (15)	−0.0116 (16)
C9	0.0576 (18)	0.0503 (17)	0.0473 (15)	−0.0055 (15)	0.0104 (13)	−0.0105 (13)
C10	0.078 (2)	0.0547 (18)	0.0500 (16)	0.0001 (17)	0.0071 (16)	−0.0101 (14)
C11	0.0469 (17)	0.076 (2)	0.0570 (17)	−0.0022 (16)	0.0173 (14)	−0.0005 (16)
C12	0.122 (3)	0.096 (3)	0.100 (3)	−0.053 (3)	−0.024 (2)	0.023 (2)
C13	0.0545 (18)	0.071 (2)	0.0607 (17)	0.0098 (16)	0.0105 (15)	−0.0008 (16)
C14	0.0403 (18)	0.108 (3)	0.077 (2)	0.0015 (18)	0.0005 (16)	0.007 (2)
C15	0.058 (2)	0.099 (3)	0.088 (2)	0.031 (2)	−0.0005 (18)	0.006 (2)
C16	0.112 (3)	0.059 (2)	0.093 (3)	0.017 (2)	−0.006 (2)	−0.0040 (19)
C17	0.103 (3)	0.060 (2)	0.0641 (19)	0.003 (2)	−0.0027 (19)	−0.0131 (16)
C18	0.0594 (19)	0.072 (2)	0.0589 (17)	0.0025 (17)	−0.0063 (15)	−0.0130 (15)
C19	0.063 (2)	0.105 (3)	0.0563 (17)	0.004 (2)	−0.0150 (15)	−0.0211 (18)
C20	0.063 (2)	0.108 (3)	0.0522 (17)	−0.007 (2)	−0.0078 (15)	0.0181 (18)
C21	0.0515 (18)	0.099 (2)	0.0596 (18)	−0.0184 (17)	−0.0109 (15)	0.0233 (17)
C22	0.0386 (16)	0.084 (2)	0.0503 (15)	−0.0015 (15)	0.0055 (13)	0.0007 (15)
C23	0.0408 (16)	0.081 (2)	0.0504 (16)	0.0012 (15)	0.0006 (13)	0.0071 (15)

C24	0.081 (2)	0.104 (3)	0.109 (3)	−0.029 (2)	−0.040 (2)	0.025 (2)
C25	0.0582 (19)	0.073 (2)	0.0654 (19)	0.0086 (17)	−0.0102 (15)	−0.0068 (17)
C26	0.0562 (18)	0.0540 (18)	0.0632 (18)	0.0053 (15)	0.0028 (15)	−0.0046 (15)
C27	0.064 (2)	0.063 (2)	0.0694 (19)	0.0049 (17)	−0.0006 (16)	−0.0008 (16)
C28	0.065 (2)	0.077 (2)	0.0679 (19)	0.0021 (18)	−0.0048 (17)	−0.0133 (17)
C29	0.0535 (18)	0.0636 (19)	0.0561 (16)	0.0133 (15)	0.0017 (14)	−0.0076 (15)
C30	0.070 (2)	0.096 (3)	0.066 (2)	0.010 (2)	−0.0028 (17)	−0.0091 (19)
C31	0.090 (3)	0.097 (3)	0.0592 (19)	0.026 (2)	0.0013 (19)	0.0193 (19)
C32	0.083 (3)	0.080 (2)	0.080 (2)	0.014 (2)	0.016 (2)	0.015 (2)
C33	0.070 (2)	0.075 (2)	0.068 (2)	0.0038 (18)	0.0034 (17)	0.0071 (17)
C34	0.0533 (18)	0.065 (2)	0.0597 (17)	0.0109 (16)	0.0083 (15)	−0.0009 (15)
C35	0.0491 (16)	0.0493 (16)	0.0465 (14)	0.0002 (13)	−0.0069 (13)	0.0003 (12)
C36	0.075 (2)	0.0506 (18)	0.0646 (18)	0.0009 (16)	−0.0040 (16)	−0.0084 (15)
C37	0.091 (3)	0.074 (2)	0.069 (2)	0.018 (2)	−0.0085 (19)	−0.0270 (17)
C38	0.070 (2)	0.105 (3)	0.0583 (18)	0.018 (2)	0.0071 (17)	−0.0169 (19)
C39	0.0515 (18)	0.090 (2)	0.0515 (16)	0.0012 (17)	0.0084 (14)	−0.0039 (16)
C40	0.0385 (15)	0.0585 (17)	0.0454 (14)	0.0042 (13)	−0.0036 (12)	0.0035 (13)
C41	0.0413 (15)	0.0593 (18)	0.0581 (16)	−0.0109 (14)	−0.0060 (13)	0.0020 (14)
C42	0.0434 (15)	0.0456 (15)	0.0508 (14)	−0.0010 (13)	−0.0073 (12)	−0.0047 (12)
C43	0.0351 (14)	0.0432 (15)	0.0455 (13)	0.0039 (12)	−0.0058 (11)	−0.0019 (12)
C44	0.0358 (14)	0.0497 (17)	0.0524 (15)	−0.0026 (13)	−0.0024 (12)	−0.0011 (13)
C45	0.0343 (14)	0.0605 (18)	0.0461 (14)	−0.0012 (13)	−0.0051 (11)	−0.0055 (13)
C46	0.051 (2)	0.066 (2)	0.127 (3)	−0.0081 (17)	0.026 (2)	−0.020 (2)
C47	0.0348 (15)	0.074 (2)	0.0510 (15)	−0.0013 (14)	−0.0045 (12)	−0.0119 (14)
C48	0.0435 (16)	0.076 (2)	0.0508 (15)	0.0051 (15)	0.0003 (13)	0.0015 (15)
C49	0.0543 (19)	0.116 (3)	0.0448 (16)	0.005 (2)	0.0026 (14)	−0.0062 (18)
C50	0.064 (2)	0.103 (3)	0.0679 (19)	0.004 (2)	−0.0014 (17)	−0.0393 (19)
C51	0.0436 (17)	0.073 (2)	0.0782 (19)	−0.0010 (16)	0.0004 (15)	−0.0345 (17)
C52	0.0408 (16)	0.079 (2)	0.0602 (17)	−0.0095 (15)	−0.0073 (14)	−0.0104 (16)
C53	0.0327 (16)	0.112 (3)	0.0702 (19)	0.0010 (18)	0.0019 (14)	−0.0101 (19)
C54	0.0469 (18)	0.102 (3)	0.078 (2)	0.0347 (19)	−0.0074 (16)	−0.011 (2)
C55	0.062 (2)	0.068 (2)	0.0683 (19)	0.0180 (17)	−0.0063 (16)	−0.0009 (16)
C56	0.0454 (16)	0.0632 (19)	0.0482 (15)	0.0069 (14)	−0.0067 (13)	−0.0007 (14)
C57	0.0479 (16)	0.0605 (19)	0.0448 (14)	0.0002 (14)	−0.0083 (12)	−0.0023 (13)
C58	0.085 (2)	0.063 (2)	0.073 (2)	−0.0018 (19)	0.0150 (18)	−0.0002 (17)
C59	0.0501 (17)	0.066 (2)	0.0554 (16)	−0.0117 (15)	−0.0018 (14)	−0.0098 (15)
C60	0.0511 (16)	0.0502 (17)	0.0481 (14)	−0.0090 (14)	−0.0052 (13)	−0.0036 (13)
C61	0.0616 (19)	0.0487 (17)	0.0615 (17)	−0.0097 (15)	−0.0026 (15)	−0.0040 (14)
C62	0.0548 (18)	0.0611 (19)	0.0662 (18)	−0.0108 (15)	0.0009 (15)	0.0114 (15)
C63	0.0566 (18)	0.0554 (18)	0.0473 (15)	0.0008 (15)	0.0003 (13)	0.0035 (13)
C64	0.067 (2)	0.087 (2)	0.0606 (18)	0.0074 (19)	0.0121 (16)	0.0067 (18)
C65	0.094 (3)	0.090 (3)	0.0621 (19)	0.021 (2)	0.0111 (19)	−0.0158 (19)
C66	0.117 (3)	0.072 (2)	0.088 (2)	0.012 (2)	0.002 (2)	−0.032 (2)
C67	0.086 (3)	0.061 (2)	0.083 (2)	−0.0094 (19)	0.007 (2)	−0.0239 (18)
C68	0.0608 (19)	0.0553 (18)	0.0522 (16)	−0.0037 (15)	−0.0052 (14)	−0.0050 (14)

Geometric parameters (Å, °)

Fe1—C14	2.015 (3)	C24—H24A	0.9600

Fe1—C19	2.022 (3)	C24—H24B	0.9600
Fe1—C15	2.022 (3)	C24—H24C	0.9600
Fe1—C22	2.024 (3)	C25—C26	1.472 (4)
Fe1—C18	2.027 (3)	C25—H25A	0.9300
Fe1—C13	2.038 (3)	C26—C27	1.379 (5)
Fe1—C16	2.041 (4)	C27—C28	1.358 (4)
Fe1—C21	2.042 (3)	C27—H27A	0.9300
Fe1—C17	2.042 (3)	C28—C29	1.408 (5)
Fe1—C20	2.045 (3)	C28—H28A	0.9300
Fe2—C48	2.023 (3)	C29—C34	1.395 (5)
Fe2—C53	2.027 (3)	C29—C30	1.425 (4)
Fe2—C47	2.030 (3)	C30—C31	1.368 (5)
Fe2—C54	2.034 (3)	C30—H30A	0.9300
Fe2—C51	2.035 (3)	C31—C32	1.375 (6)
Fe2—C52	2.040 (3)	C31—H31A	0.9300
Fe2—C55	2.041 (3)	C32—C33	1.355 (5)
Fe2—C49	2.042 (3)	C32—H32A	0.9300
Fe2—C50	2.043 (3)	C33—C34	1.412 (5)
Fe2—C56	2.056 (3)	C33—H33A	0.9300
N1—C9	1.307 (4)	C35—C36	1.405 (4)
N1—C1	1.357 (4)	C35—C40	1.409 (4)
N2—C10	1.247 (4)	C36—C37	1.361 (4)
N2—N3	1.396 (3)	C36—H36A	0.9300
N3—C11	1.286 (4)	C37—C38	1.381 (5)
N4—C23	1.288 (4)	C37—H37A	0.9300
N4—N5	1.406 (3)	C38—C39	1.361 (5)
N5—C25	1.248 (4)	C38—H38A	0.9300
N6—C26	1.321 (4)	C39—C40	1.399 (4)
N6—C34	1.368 (4)	C39—H39A	0.9300
N7—C43	1.320 (3)	C40—C41	1.408 (4)
N7—C35	1.363 (3)	C41—C42	1.347 (4)
N8—C44	1.270 (3)	C41—H41A	0.9300
N8—N9	1.386 (3)	C42—C43	1.403 (4)
N9—C45	1.299 (3)	C42—H42A	0.9300
N10—C57	1.286 (4)	C43—C44	1.446 (4)
N10—N11	1.395 (3)	C44—H44A	0.9300
N11—C59	1.260 (4)	C45—C47	1.451 (4)
N12—C60	1.315 (4)	C45—C46	1.473 (4)
N12—C68	1.377 (4)	C46—H46A	0.9600
C1—C2	1.390 (4)	C46—H46B	0.9600
C1—C6	1.401 (4)	C46—H46C	0.9600
C2—C3	1.373 (4)	C47—C48	1.422 (4)
C2—H2A	0.9300	C47—C51	1.434 (4)
C3—C4	1.376 (5)	C48—C49	1.427 (4)
C3—H3A	0.9300	C48—H48A	0.9800
C4—C5	1.350 (4)	C49—C50	1.391 (5)
C4—H4A	0.9300	C49—H49A	0.9800
C5—C6	1.413 (4)	C50—C51	1.408 (5)
C5—H5A	0.9300	C50—H50A	0.9800

C6—C7	1.409 (4)	C51—H51A	0.9800
C7—C8	1.342 (4)	C52—C53	1.409 (4)
C7—H7A	0.9300	C52—C56	1.426 (4)
C8—C9	1.410 (4)	C52—H52A	0.9800
C8—H8A	0.9300	C53—C54	1.397 (5)
C9—C10	1.473 (4)	C53—H53A	0.9800
C10—H10A	0.9300	C54—C55	1.409 (5)
C11—C13	1.449 (4)	C54—H54A	0.9800
C11—C12	1.476 (5)	C55—C56	1.427 (4)
C12—H12A	0.9600	C55—H55A	0.9800
C12—H12B	0.9600	C56—C57	1.453 (4)
C12—H12C	0.9600	C57—C58	1.485 (4)
C13—C17	1.409 (5)	C58—H58A	0.9600
C13—C14	1.461 (5)	C58—H58B	0.9600
C14—C15	1.398 (5)	C58—H58C	0.9600
C14—H14A	0.9800	C59—C60	1.457 (4)
C15—C16	1.376 (6)	C59—H59A	0.9300
C15—H15A	0.9800	C60—C61	1.405 (4)
C16—C17	1.391 (5)	C61—C62	1.333 (4)
C16—H16A	0.9800	C61—H61A	0.9300
C17—H17A	0.9800	C62—C63	1.418 (4)
C18—C22	1.402 (4)	C62—H62A	0.9300
C18—C19	1.413 (4)	C63—C64	1.397 (4)
C18—H18A	0.9800	C63—C68	1.398 (4)
C19—C20	1.381 (5)	C64—C65	1.359 (5)
C19—H19A	0.9800	C64—H64A	0.9300
C20—C21	1.417 (4)	C65—C66	1.378 (6)
C20—H20A	0.9800	C65—H65A	0.9300
C21—C22	1.448 (4)	C66—C67	1.350 (5)
C21—H21A	0.9800	C66—H66A	0.9300
C22—C23	1.456 (4)	C67—C68	1.406 (4)
C23—C24	1.477 (5)	C67—H67A	0.9300
C14—Fe1—C19	110.07 (16)	C20—C21—C22	107.4 (3)
C14—Fe1—C15	40.52 (14)	C20—C21—Fe1	69.83 (18)
C19—Fe1—C15	111.23 (15)	C22—C21—Fe1	68.48 (17)
C14—Fe1—C22	140.26 (14)	C20—C21—H21A	126.3
C19—Fe1—C22	68.36 (13)	C22—C21—H21A	126.3
C15—Fe1—C22	179.16 (14)	Fe1—C21—H21A	126.3
C14—Fe1—C18	111.32 (15)	C18—C22—C21	107.2 (3)
C19—Fe1—C18	40.85 (13)	C18—C22—C23	126.8 (3)
C15—Fe1—C18	139.62 (16)	C21—C22—C23	125.9 (3)
C22—Fe1—C18	40.51 (13)	C18—C22—Fe1	69.87 (17)
C14—Fe1—C13	42.26 (13)	C21—C22—Fe1	69.79 (17)
C19—Fe1—C13	139.51 (15)	C23—C22—Fe1	126.1 (2)
C15—Fe1—C13	68.70 (14)	N4—C23—C22	115.0 (3)
C22—Fe1—C13	112.10 (12)	N4—C23—C24	126.2 (3)
C18—Fe1—C13	111.88 (13)	C22—C23—C24	118.8 (3)
C14—Fe1—C16	68.07 (17)	C23—C24—H24A	109.5
C19—Fe1—C16	138.74 (15)	C23—C24—H24B	109.5

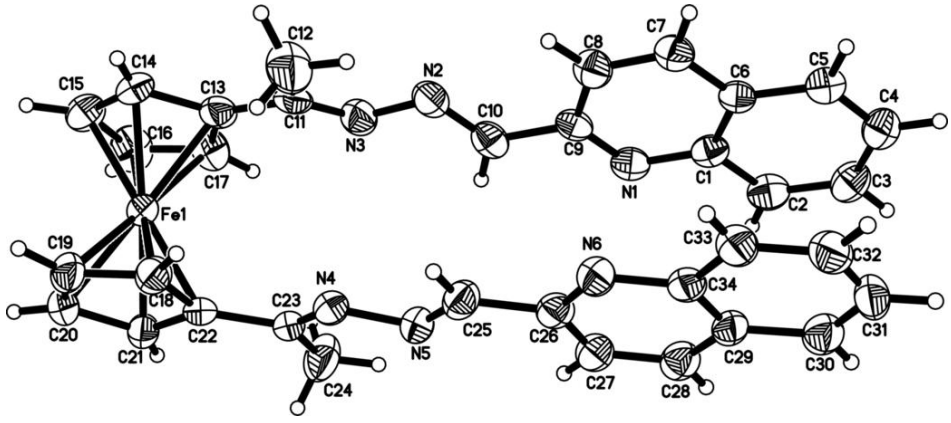
C15—Fe1—C16	39.59 (16)	H24A—C24—H24B	109.5
C22—Fe1—C16	140.28 (16)	C23—C24—H24C	109.5
C18—Fe1—C16	179.21 (16)	H24A—C24—H24C	109.5
C13—Fe1—C16	68.04 (14)	H24B—C24—H24C	109.5
C14—Fe1—C21	176.67 (12)	N5—C25—C26	123.9 (3)
C19—Fe1—C21	67.60 (15)	N5—C25—H25A	118.1
C15—Fe1—C21	137.47 (15)	C26—C25—H25A	118.1
C22—Fe1—C21	41.73 (12)	N6—C26—C27	124.5 (3)
C18—Fe1—C21	68.66 (14)	N6—C26—C25	115.1 (3)
C13—Fe1—C21	141.03 (13)	C27—C26—C25	120.4 (3)
C16—Fe1—C21	111.92 (17)	C28—C27—C26	118.3 (3)
C14—Fe1—C17	68.79 (16)	C28—C27—H27A	120.8
C19—Fe1—C17	178.31 (14)	C26—C27—H27A	120.8
C15—Fe1—C17	67.08 (16)	C27—C28—C29	119.9 (3)
C22—Fe1—C17	113.32 (14)	C27—C28—H28A	120.1
C18—Fe1—C17	140.57 (13)	C29—C28—H28A	120.1
C13—Fe1—C17	40.40 (14)	C34—C29—C28	118.0 (3)
C16—Fe1—C17	39.83 (14)	C34—C29—C30	118.4 (3)
C21—Fe1—C17	113.48 (16)	C28—C29—C30	123.6 (3)
C14—Fe1—C20	136.13 (14)	C31—C30—C29	119.3 (4)
C19—Fe1—C20	39.69 (15)	C31—C30—H30A	120.3
C15—Fe1—C20	110.05 (15)	C29—C30—H30A	120.3
C22—Fe1—C20	69.15 (13)	C30—C31—C32	121.6 (3)
C18—Fe1—C20	68.33 (14)	C30—C31—H31A	119.2
C13—Fe1—C20	178.40 (14)	C32—C31—H31A	119.2
C16—Fe1—C20	111.73 (16)	C33—C32—C31	120.6 (4)
C21—Fe1—C20	40.57 (13)	C33—C32—H32A	119.7
C17—Fe1—C20	140.34 (16)	C31—C32—H32A	119.7
C48—Fe2—C53	119.97 (14)	C32—C33—C34	119.9 (4)
C48—Fe2—C47	41.07 (12)	C32—C33—H33A	120.0
C53—Fe2—C47	157.88 (14)	C34—C33—H33A	120.0
C48—Fe2—C54	155.22 (14)	N6—C34—C29	121.5 (3)
C53—Fe2—C54	40.25 (15)	N6—C34—C33	118.3 (3)
C47—Fe2—C54	161.54 (15)	C29—C34—C33	120.2 (3)
C48—Fe2—C51	69.32 (13)	N7—C35—C36	119.3 (3)
C53—Fe2—C51	157.35 (13)	N7—C35—C40	121.5 (3)
C47—Fe2—C51	41.31 (12)	C36—C35—C40	119.2 (3)
C54—Fe2—C51	123.29 (15)	C37—C36—C35	120.7 (3)
C48—Fe2—C52	106.44 (13)	C37—C36—H36A	119.7
C53—Fe2—C52	40.53 (12)	C35—C36—H36A	119.7
C47—Fe2—C52	123.90 (12)	C36—C37—C38	119.8 (3)
C54—Fe2—C52	68.16 (14)	C36—C37—H37A	120.1
C51—Fe2—C52	161.55 (12)	C38—C37—H37A	120.1
C48—Fe2—C55	162.21 (12)	C39—C38—C37	121.1 (3)
C53—Fe2—C55	68.00 (15)	C39—C38—H38A	119.4
C47—Fe2—C55	126.57 (13)	C37—C38—H38A	119.4
C54—Fe2—C55	40.45 (13)	C38—C39—C40	120.7 (3)
C51—Fe2—C55	109.78 (14)	C38—C39—H39A	119.7
C52—Fe2—C55	68.48 (14)	C40—C39—H39A	119.7

C48—Fe2—C49	41.11 (12)	C39—C40—C41	123.9 (3)
C53—Fe2—C49	104.73 (14)	C39—C40—C35	118.4 (3)
C47—Fe2—C49	68.32 (12)	C41—C40—C35	117.7 (2)
C54—Fe2—C49	119.55 (14)	C42—C41—C40	119.9 (3)
C51—Fe2—C49	67.77 (15)	C42—C41—H41A	120.1
C52—Fe2—C49	121.57 (15)	C40—C41—H41A	120.1
C55—Fe2—C49	156.24 (13)	C41—C42—C43	119.4 (3)
C48—Fe2—C50	68.77 (14)	C41—C42—H42A	120.3
C53—Fe2—C50	120.35 (14)	C43—C42—H42A	120.3
C47—Fe2—C50	68.56 (13)	N7—C43—C42	122.7 (2)
C54—Fe2—C50	106.01 (15)	N7—C43—C44	116.3 (2)
C51—Fe2—C50	40.40 (13)	C42—C43—C44	121.0 (2)
C52—Fe2—C50	156.41 (14)	N8—C44—C43	120.8 (3)
C55—Fe2—C50	122.83 (15)	N8—C44—H44A	119.6
C49—Fe2—C50	39.81 (15)	C43—C44—H44A	119.6
C48—Fe2—C56	124.43 (12)	N9—C45—C47	117.2 (3)
C53—Fe2—C56	68.17 (13)	N9—C45—C46	125.3 (3)
C47—Fe2—C56	110.66 (11)	C47—C45—C46	117.5 (3)
C54—Fe2—C56	68.21 (13)	C45—C46—H46A	109.5
C51—Fe2—C56	125.92 (13)	C45—C46—H46B	109.5
C52—Fe2—C56	40.74 (12)	H46A—C46—H46B	109.5
C55—Fe2—C56	40.76 (12)	C45—C46—H46C	109.5
C49—Fe2—C56	159.55 (14)	H46A—C46—H46C	109.5
C50—Fe2—C56	160.37 (15)	H46B—C46—H46C	109.5
C9—N1—C1	117.8 (3)	C48—C47—C51	107.8 (3)
C10—N2—N3	113.9 (3)	C48—C47—C45	126.0 (3)
C11—N3—N2	113.1 (3)	C51—C47—C45	126.2 (3)
C23—N4—N5	113.1 (3)	C48—C47—Fe2	69.19 (16)
C25—N5—N4	111.6 (3)	C51—C47—Fe2	69.52 (17)
C26—N6—C34	117.8 (3)	C45—C47—Fe2	128.01 (19)
C43—N7—C35	118.9 (2)	C47—C48—C49	106.8 (3)
C44—N8—N9	113.8 (2)	C47—C48—Fe2	69.74 (16)
C45—N9—N8	112.6 (2)	C49—C48—Fe2	70.16 (17)
C57—N10—N11	112.6 (2)	C47—C48—H48A	126.6
C59—N11—N10	112.8 (3)	C49—C48—H48A	126.6
C60—N12—C68	117.7 (3)	Fe2—C48—H48A	126.6
N1—C1—C2	119.1 (3)	C50—C49—C48	109.1 (3)
N1—C1—C6	123.0 (3)	C50—C49—Fe2	70.13 (19)
C2—C1—C6	117.8 (3)	C48—C49—Fe2	68.73 (16)
C3—C2—C1	120.6 (3)	C50—C49—H49A	125.4
C3—C2—H2A	119.7	C48—C49—H49A	125.4
C1—C2—H2A	119.7	Fe2—C49—H49A	125.4
C2—C3—C4	121.7 (3)	C49—C50—C51	108.6 (3)
C2—C3—H3A	119.2	C49—C50—Fe2	70.05 (19)
C4—C3—H3A	119.2	C51—C50—Fe2	69.49 (18)
C5—C4—C3	119.2 (3)	C49—C50—H50A	125.7
C5—C4—H4A	120.4	C51—C50—H50A	125.7
C3—C4—H4A	120.4	Fe2—C50—H50A	125.7
C4—C5—C6	120.7 (3)	C50—C51—C47	107.6 (3)

C4—C5—H5A	119.7	C50—C51—Fe2	70.11 (19)
C6—C5—H5A	119.7	C47—C51—Fe2	69.17 (17)
C1—C6—C7	117.6 (3)	C50—C51—H51A	126.2
C1—C6—C5	120.0 (3)	C47—C51—H51A	126.2
C7—C6—C5	122.4 (3)	Fe2—C51—H51A	126.2
C8—C7—C6	118.6 (3)	C53—C52—C56	107.6 (3)
C8—C7—H7A	120.7	C53—C52—Fe2	69.24 (19)
C6—C7—H7A	120.7	C56—C52—Fe2	70.21 (17)
C7—C8—C9	120.5 (3)	C53—C52—H52A	126.2
C7—C8—H8A	119.8	C56—C52—H52A	126.2
C9—C8—H8A	119.8	Fe2—C52—H52A	126.2
N1—C9—C8	122.6 (3)	C54—C53—C52	108.9 (3)
N1—C9—C10	116.1 (3)	C54—C53—Fe2	70.13 (19)
C8—C9—C10	121.3 (3)	C52—C53—Fe2	70.23 (17)
N2—C10—C9	121.7 (3)	C54—C53—H53A	125.6
N2—C10—H10A	119.1	C52—C53—H53A	125.6
C9—C10—H10A	119.1	Fe2—C53—H53A	125.6
N3—C11—C13	116.3 (3)	C53—C54—C55	108.3 (3)
N3—C11—C12	124.3 (3)	C53—C54—Fe2	69.62 (18)
C13—C11—C12	119.4 (3)	C55—C54—Fe2	70.05 (17)
C11—C12—H12A	109.5	C53—C54—H54A	125.8
C11—C12—H12B	109.5	C55—C54—H54A	125.8
H12A—C12—H12B	109.5	Fe2—C54—H54A	125.8
C11—C12—H12C	109.5	C54—C55—C56	107.9 (3)
H12A—C12—H12C	109.5	C54—C55—Fe2	69.50 (18)
H12B—C12—H12C	109.5	C56—C55—Fe2	70.16 (16)
C17—C13—C11	128.1 (3)	C54—C55—H55A	126.0
C17—C13—C14	106.0 (3)	C56—C55—H55A	126.0
C11—C13—C14	126.0 (3)	Fe2—C55—H55A	126.0
C17—C13—Fe1	69.96 (19)	C52—C56—C55	107.2 (3)
C11—C13—Fe1	125.3 (2)	C52—C56—C57	126.2 (3)
C14—C13—Fe1	68.01 (17)	C55—C56—C57	126.6 (3)
C15—C14—C13	106.5 (3)	C52—C56—Fe2	69.05 (16)
C15—C14—Fe1	70.0 (2)	C55—C56—Fe2	69.08 (17)
C13—C14—Fe1	69.72 (18)	C57—C56—Fe2	125.5 (2)
C15—C14—H14A	126.7	N10—C57—C56	116.4 (3)
C13—C14—H14A	126.7	N10—C57—C58	125.7 (3)
Fe1—C14—H14A	126.7	C56—C57—C58	117.9 (3)
C16—C15—C14	109.8 (3)	C57—C58—H58A	109.5
C16—C15—Fe1	70.9 (2)	C57—C58—H58B	109.5
C14—C15—Fe1	69.47 (18)	H58A—C58—H58B	109.5
C16—C15—H15A	125.1	C57—C58—H58C	109.5
C14—C15—H15A	125.1	H58A—C58—H58C	109.5
Fe1—C15—H15A	125.1	H58B—C58—H58C	109.5
C15—C16—C17	108.5 (4)	N11—C59—C60	121.7 (3)
C15—C16—Fe1	69.5 (2)	N11—C59—H59A	119.1
C17—C16—Fe1	70.2 (2)	C60—C59—H59A	119.1
C15—C16—H16A	125.7	N12—C60—C61	123.9 (3)
C17—C16—H16A	125.7	N12—C60—C59	116.1 (3)

Fe1—C16—H16A	125.7	C61—C60—C59	120.0 (3)
C16—C17—C13	109.2 (3)	C62—C61—C60	118.4 (3)
C16—C17—Fe1	70.0 (2)	C62—C61—H61A	120.8
C13—C17—Fe1	69.64 (18)	C60—C61—H61A	120.8
C16—C17—H17A	125.4	C61—C62—C63	121.0 (3)
C13—C17—H17A	125.4	C61—C62—H62A	119.5
Fe1—C17—H17A	125.4	C63—C62—H62A	119.5
C22—C18—C19	107.7 (3)	C64—C63—C68	118.3 (3)
C22—C18—Fe1	69.62 (18)	C64—C63—C62	124.9 (3)
C19—C18—Fe1	69.39 (19)	C68—C63—C62	116.8 (3)
C22—C18—H18A	126.2	C65—C64—C63	120.9 (3)
C19—C18—H18A	126.2	C65—C64—H64A	119.6
Fe1—C18—H18A	126.2	C63—C64—H64A	119.6
C20—C19—C18	109.9 (3)	C64—C65—C66	120.6 (3)
C20—C19—Fe1	71.0 (2)	C64—C65—H65A	119.7
C18—C19—Fe1	69.76 (18)	C66—C65—H65A	119.7
C20—C19—H19A	125.1	C67—C66—C65	120.3 (4)
C18—C19—H19A	125.1	C67—C66—H66A	119.9
Fe1—C19—H19A	125.1	C65—C66—H66A	119.9
C19—C20—C21	107.8 (3)	C66—C67—C68	120.4 (4)
C19—C20—Fe1	69.29 (19)	C66—C67—H67A	119.8
C21—C20—Fe1	69.60 (17)	C68—C67—H67A	119.8
C19—C20—H20A	126.1	N12—C68—C63	122.2 (3)
C21—C20—H20A	126.1	N12—C68—C67	118.3 (3)
Fe1—C20—H20A	126.1	C63—C68—C67	119.5 (3)

Fig. 1


C12
C14
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C21
C24
C27
C28