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Bis[2-(butyliminomethyl)-4-chlorophenolato]iron(II)

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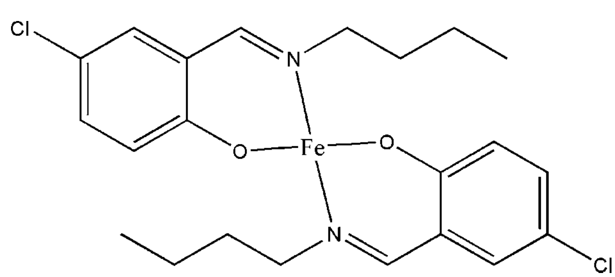
Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.009 Å; *R* factor = 0.065; *wR* factor = 0.201; data-to-parameter ratio = 15.8.

In the title compound, $[Fe(C_{11}H_{13}ClNO)_2]$, the Fe^{II} atom is four-coordinated in a square-planar geometry by the O and N atoms of two 2-(butyliminomethyl)-4-chlorophenolate Schiff base ligands.

Related literature

For related structures, see: Chen & Wang (2006); Chen *et al.* (2007); Ran *et al.* (2006); Ye *et al.* (2007); Zhu *et al.* (2003).



Experimental

Crystal data

$[Fe(C_{11}H_{13}ClNO)_2]$
M_r = 477.20
Triclinic, $P\overline{1}$
a = 10.059 (2) Å
b = 10.100 (2) Å
c = 11.569 (3) Å
α = 97.093 (3)°
β = 90.800 (2)°
γ = 105.755 (3)°
V = 1121.2 (4) $Å^3$
Z = 2
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 298 (2) K
0.32 × 0.32 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.755, T_{max} = 0.780
4427 measured reflections
4174 independent reflections
3009 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.201
S = 1.06
4174 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.80 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Fe1—O2	1.890 (4)	Fe1—N2	2.001 (4)
Fe1—O1	1.907 (4)	Fe1—N1	2.010 (4)
O2—Fe1—O1	176.03 (18)	O2—Fe1—N1	87.76 (17)
O2—Fe1—N2	91.69 (17)	O1—Fe1—N1	90.95 (16)
O1—Fe1—N2	90.18 (16)	N2—Fe1—N1	170.71 (16)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: SJ2502).

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supporting information

Acta Cryst. (2008). E**64**, m837 [doi:10.1107/S1600536808015080]

Bis[2-(butyliminomethyl)-4-chlorophenolato]iron(II)

Dong-Sheng Xia, Wu Chen, Li-Li Jiang and Qing-Fu Zeng

S1. Comment

As part of our ongoing interest in the structure of iron complexes (Zhu *et al.*, 2003), we report herein the crystal structure of the title compound, a new iron(II) complex, (I), Fig. 1, derived from the Schiff base ligand 2-(butyliminomethyl)-4-chlorophenol.

The Fe^{II} atom in (I) is four-coordinated by two O and two N atoms from two Schiff base ligands, forming a square-planar geometry. The dihedral angle between the two benzene rings is 8.2 (3) °. The coordinate bond distances and angles (Table 1) are comparable to the values observed in other similar iron(II) complexes (Chen & Wang, 2006; Chen *et al.*, 2007; Ran *et al.*, 2006; Ye *et al.*, 2007).

S2. Experimental

5-Chlorosalicylaldehyde (31.2 mg, 0.2 mmol), butylamine (14.6 mg, 0.2 mmol), and $FeCl_2$ (12.6 mg, 0.1 mmol) were dissolved in methanol (30 ml). The mixture was stirred for 30 min at room temperature in an atmosphere of argon. The resulting solution was left in air for a few days, yielding brown crystals.

S3. Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å, and with U_{iso}(H) set at 1.2U_{eq}(C) and 1.5U_{eq}(methyl C).

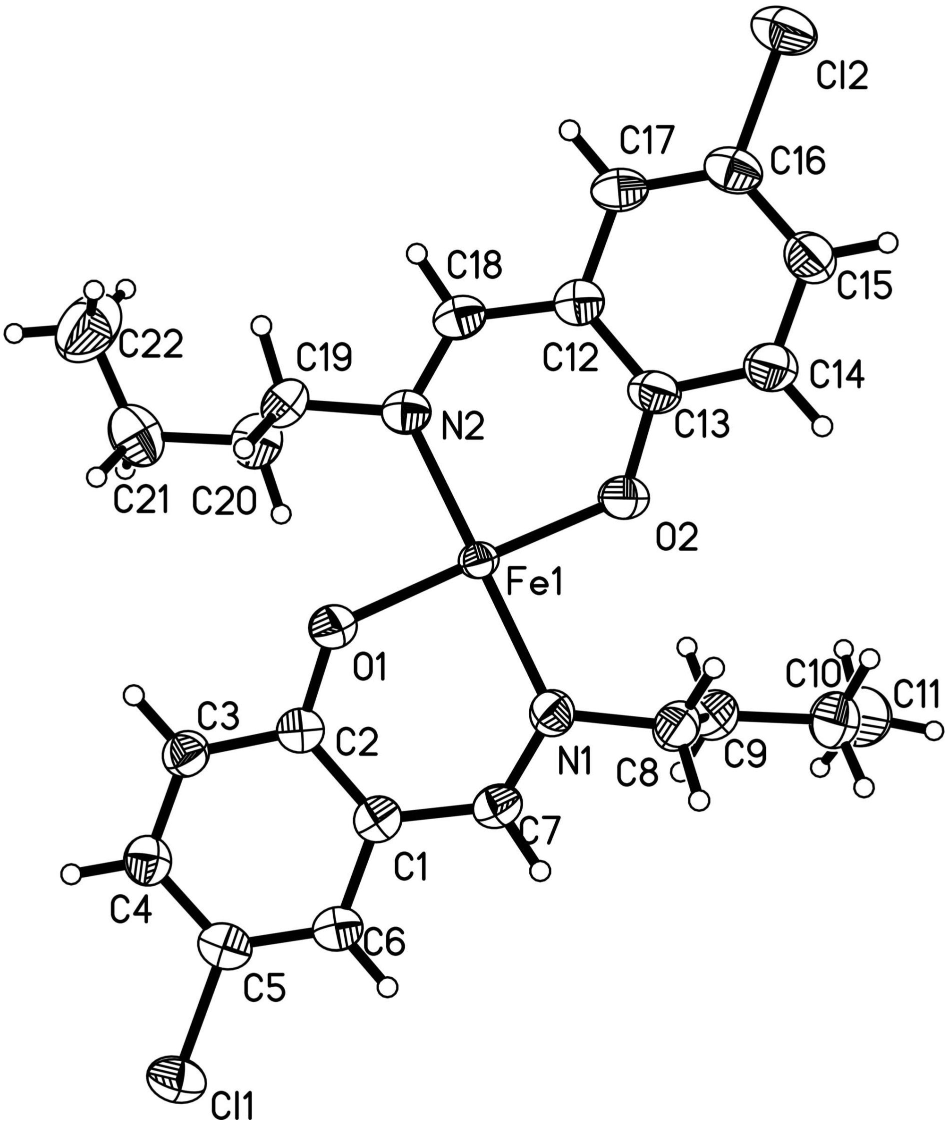

Figure 1

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

Bis[2-(butyliminomethyl)-4-chlorophenolato]iron(II)

Crystal data

$[Fe(C_{11}H_{13}ClNO)_2]$	$Z = 2$
$M_r = 477.20$	$F(000) = 496$
Triclinic, $P\overline{1}$	$D_x = 1.414$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.059$ (2) Å	Cell parameters from 2122 reflections
$b = 10.100$ (2) Å	$\theta = 2.3$–$24.5°$
$c = 11.569$ (3) Å	$\mu = 0.93$ mm^{-1}
$\alpha = 97.093$ (3)°	$T = 298$ K
$\beta = 90.800$ (2)°	Block, brown
$\gamma = 105.755$ (3)°	0.32 × 0.32 × 0.28 mm
$V = 1121.2$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.755, T_{max} = 0.781
4427 measured reflections
4174 independent reflections
3009 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.5°, θ_{min} = 1.8°
$h = 0 \rightarrow 12$
$k = -12 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.201$
$S = 1.06$
4174 reflections
265 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
$w = 1/[\sigma^2(F_o^2) + (0.1206P)^2 + 0.3449P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (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 $F^2 > \sigma(F^2)$ 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	0.88207 (6)	0.05266 (6)	0.59267 (5)	0.0378 (3)
Cl1	1.28816 (16)	0.67927 (15)	0.38259 (15)	0.0708 (5)
Cl2	0.43021 (19)	−0.54688 (18)	0.80626 (17)	0.0875 (6)
N1	1.0140 (4)	0.2108 (5)	0.6944 (3)	0.0510 (10)
N2	0.7290 (4)	−0.0862 (4)	0.4948 (4)	0.0505 (10)
O1	0.9611 (4)	0.1217 (4)	0.4557 (3)	0.0585 (9)
O2	0.8151 (5)	−0.0192 (4)	0.7305 (3)	0.0742 (12)
C1	1.0932 (5)	0.3499 (5)	0.5383 (4)	0.0489 (12)
C2	1.0296 (5)	0.2505 (5)	0.4429 (4)	0.0474 (11)
C3	1.0436 (6)	0.2901 (6)	0.3317 (5)	0.0546 (13)
H3	0.9990	0.2270	0.2683	0.065*
C4	1.1218 (6)	0.4204 (6)	0.3124 (5)	0.0554 (13)
H4	1.1309	0.4439	0.2371	0.067*
C5	1.1865 (5)	0.5153 (5)	0.4071 (5)	0.0542 (13)
C6	1.1748 (5)	0.4835 (5)	0.5187 (5)	0.0508 (12)

H6	1.2195	0.5484	0.5810	0.061*
C7	1.0854 (5)	0.3227 (5)	0.6570 (4)	0.0500 (12)
H7	1.1369	0.3927	0.7128	0.060*
C8	1.0251 (6)	0.2141 (6)	0.8225 (4)	0.0620 (14)
H8A	1.1163	0.2703	0.8520	0.074*
H8B	1.0137	0.1207	0.8410	0.074*
C9	0.9166 (7)	0.2733 (6)	0.8810 (5)	0.0685 (16)
H9A	0.9317	0.3682	0.8652	0.082*
H9B	0.8263	0.2205	0.8469	0.082*
C10	0.9164 (8)	0.2719 (8)	1.0105 (5)	0.089 (2)
H10A	1.0081	0.3198	1.0446	0.107*
H10B	0.8947	0.1766	1.0268	0.107*
C11	0.8128 (9)	0.3404 (8)	1.0668 (6)	0.103 (3)
H11A	0.8260	0.4303	1.0423	0.154*
H11B	0.8259	0.3502	1.1501	0.154*
H11C	0.7207	0.2842	1.0436	0.154*
C12	0.6426 (5)	−0.2250 (5)	0.6502 (5)	0.0516 (12)
C13	0.7240 (6)	−0.1362 (6)	0.7427 (5)	0.0597 (14)
C14	0.7078 (7)	−0.1759 (7)	0.8555 (6)	0.0753 (18)
H14	0.7590	−0.1169	0.9183	0.090*
C15	0.6177 (7)	−0.3004 (6)	0.8748 (5)	0.0718 (17)
H15	0.6090	−0.3253	0.9497	0.086*
C16	0.5405 (6)	−0.3874 (6)	0.7816 (6)	0.0632 (15)
C17	0.5499 (5)	−0.3530 (6)	0.6707 (5)	0.0571 (13)
H17	0.4963	−0.4126	0.6093	0.069*
C18	0.6473 (5)	−0.1940 (5)	0.5322 (5)	0.0528 (13)
H18	0.5860	−0.2570	0.4773	0.063*
C19	0.7085 (6)	−0.0779 (6)	0.3698 (4)	0.0551 (13)
H19A	0.6551	−0.1679	0.3313	0.066*
H19B	0.7976	−0.0547	0.3350	0.066*
C20	0.6344 (7)	0.0292 (6)	0.3507 (5)	0.0688 (16)
H20A	0.6864	0.1186	0.3913	0.083*
H20B	0.5442	0.0044	0.3835	0.083*
C21	0.6166 (8)	0.0414 (8)	0.2213 (6)	0.084 (2)
H21A	0.5821	0.1212	0.2149	0.100*
H21B	0.7070	0.0598	0.1885	0.100*
C22	0.5237 (12)	−0.0799 (10)	0.1499 (7)	0.132 (4)
H22A	0.5594	−0.1588	0.1514	0.198*
H22B	0.5178	−0.0608	0.0711	0.198*
H22C	0.4334	−0.0993	0.1808	0.198*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0373 (4)	0.0346 (4)	0.0378 (4)	0.0053 (3)	0.0030 (3)	0.0005 (2)
Cl1	0.0655 (9)	0.0538 (8)	0.0906 (11)	0.0085 (7)	0.0047 (8)	0.0182 (7)
Cl2	0.0835 (12)	0.0614 (10)	0.1079 (13)	−0.0007 (8)	0.0180 (10)	0.0201 (9)
N1	0.046 (2)	0.058 (3)	0.047 (2)	0.013 (2)	0.0061 (18)	0.0053 (19)

N2	0.048 (2)	0.045 (2)	0.059 (3)	0.015 (2)	0.0049 (19)	0.0032 (19)
O1	0.064 (2)	0.050 (2)	0.053 (2)	0.0039 (18)	0.0052 (17)	0.0005 (16)
O2	0.085 (3)	0.059 (2)	0.057 (2)	−0.012 (2)	0.013 (2)	−0.0011 (18)
C1	0.043 (3)	0.052 (3)	0.055 (3)	0.019 (2)	0.002 (2)	0.003 (2)
C2	0.044 (3)	0.046 (3)	0.054 (3)	0.016 (2)	0.001 (2)	0.006 (2)
C3	0.061 (3)	0.049 (3)	0.052 (3)	0.014 (3)	−0.002 (2)	0.004 (2)
C4	0.060 (3)	0.055 (3)	0.056 (3)	0.022 (3)	0.001 (3)	0.012 (2)
C5	0.046 (3)	0.048 (3)	0.074 (4)	0.020 (2)	0.010 (3)	0.010 (3)
C6	0.047 (3)	0.045 (3)	0.061 (3)	0.016 (2)	0.001 (2)	0.002 (2)
C7	0.041 (3)	0.052 (3)	0.055 (3)	0.014 (2)	0.002 (2)	−0.003 (2)
C8	0.060 (3)	0.070 (4)	0.051 (3)	0.012 (3)	−0.002 (3)	0.002 (3)
C9	0.078 (4)	0.062 (4)	0.062 (3)	0.017 (3)	0.003 (3)	0.000 (3)
C10	0.110 (6)	0.088 (5)	0.059 (4)	0.011 (4)	0.009 (4)	0.002 (3)
C11	0.114 (6)	0.098 (6)	0.089 (5)	0.025 (5)	0.036 (5)	−0.012 (4)
C12	0.047 (3)	0.050 (3)	0.059 (3)	0.018 (2)	0.007 (2)	0.002 (2)
C13	0.060 (3)	0.047 (3)	0.065 (3)	0.004 (3)	0.018 (3)	0.002 (3)
C14	0.085 (5)	0.063 (4)	0.065 (4)	0.001 (3)	0.016 (3)	0.002 (3)
C15	0.086 (4)	0.062 (4)	0.065 (4)	0.014 (3)	0.016 (3)	0.013 (3)
C16	0.056 (3)	0.051 (3)	0.082 (4)	0.014 (3)	0.018 (3)	0.011 (3)
C17	0.043 (3)	0.048 (3)	0.077 (4)	0.011 (2)	0.002 (3)	0.001 (3)
C18	0.046 (3)	0.047 (3)	0.064 (3)	0.016 (2)	0.002 (2)	−0.004 (2)
C19	0.057 (3)	0.057 (3)	0.051 (3)	0.021 (3)	−0.004 (2)	−0.005 (2)
C20	0.075 (4)	0.070 (4)	0.070 (4)	0.036 (3)	0.004 (3)	0.004 (3)
C21	0.087 (5)	0.090 (5)	0.091 (5)	0.043 (4)	0.016 (4)	0.034 (4)
C22	0.186 (11)	0.106 (7)	0.102 (7)	0.049 (7)	−0.044 (7)	−0.002 (5)

Geometric parameters (Å, º)

Fe1—O2	1.890 (4)	C10—C11	1.513 (10)
Fe1—O1	1.907 (4)	C10—H10A	0.9700
Fe1—N2	2.001 (4)	C10—H10B	0.9700
Fe1—N1	2.010 (4)	C11—H11A	0.9600
Cl1—C5	1.753 (5)	C11—H11B	0.9600
Cl2—C16	1.749 (6)	C11—H11C	0.9600
N1—C7	1.291 (7)	C12—C13	1.399 (7)
N1—C8	1.480 (6)	C12—C17	1.422 (7)
N2—C18	1.299 (7)	C12—C18	1.438 (7)
N2—C19	1.474 (6)	C13—C14	1.410 (8)
O1—C2	1.324 (6)	C14—C15	1.381 (8)
O2—C13	1.309 (6)	C14—H14	0.9300
C1—C2	1.412 (7)	C15—C16	1.383 (9)
C1—C6	1.423 (7)	C15—H15	0.9300
C1—C7	1.432 (7)	C16—C17	1.368 (8)
C2—C3	1.392 (7)	C17—H17	0.9300
C3—C4	1.384 (7)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.506 (7)
C4—C5	1.388 (8)	C19—H19A	0.9700
C4—H4	0.9300	C19—H19B	0.9700

C5—C6	1.368 (7)	C20—C21	1.529 (8)
C6—H6	0.9300	C20—H20A	0.9700
C7—H7	0.9300	C20—H20B	0.9700
C8—C9	1.510 (8)	C21—C22	1.470 (10)
C8—H8A	0.9700	C21—H21A	0.9700
C8—H8B	0.9700	C21—H21B	0.9700
C9—C10	1.500 (8)	C22—H22A	0.9600
C9—H9A	0.9700	C22—H22B	0.9600
C9—H9B	0.9700	C22—H22C	0.9600

O2—Fe1—O1	176.03 (18)	H10A—C10—H10B	107.9
O2—Fe1—N2	91.69 (17)	C10—C11—H11A	109.5
O1—Fe1—N2	90.18 (16)	C10—C11—H11B	109.5
O2—Fe1—N1	87.76 (17)	H11A—C11—H11B	109.5
O1—Fe1—N1	90.95 (16)	C10—C11—H11C	109.5
N2—Fe1—N1	170.71 (16)	H11A—C11—H11C	109.5
C7—N1—C8	114.2 (4)	H11B—C11—H11C	109.5
C7—N1—Fe1	123.9 (4)	C13—C12—C17	120.1 (5)
C8—N1—Fe1	121.6 (3)	C13—C12—C18	123.1 (5)
C18—N2—C19	114.8 (5)	C17—C12—C18	116.8 (5)
C18—N2—Fe1	124.0 (4)	O2—C13—C12	123.9 (5)
C19—N2—Fe1	121.1 (3)	O2—C13—C14	118.1 (5)
C2—O1—Fe1	128.2 (3)	C12—C13—C14	118.0 (5)
C13—O2—Fe1	129.4 (4)	C15—C14—C13	121.6 (6)
C2—C1—C6	120.0 (5)	C15—C14—H14	119.2
C2—C1—C7	123.5 (5)	C13—C14—H14	119.2
C6—C1—C7	116.5 (5)	C14—C15—C16	119.2 (6)
O1—C2—C3	119.6 (4)	C14—C15—H15	120.4
O1—C2—C1	122.4 (5)	C16—C15—H15	120.4
C3—C2—C1	118.0 (5)	C17—C16—C15	121.7 (5)
C4—C3—C2	122.1 (5)	C17—C16—Cl2	119.4 (5)
C4—C3—H3	119.0	C15—C16—Cl2	118.9 (5)
C2—C3—H3	119.0	C16—C17—C12	119.3 (5)
C3—C4—C5	119.0 (5)	C16—C17—H17	120.4
C3—C4—H4	120.5	C12—C17—H17	120.4
C5—C4—H4	120.5	N2—C18—C12	126.2 (5)
C6—C5—C4	121.7 (5)	N2—C18—H18	116.9
C6—C5—Cl1	119.2 (4)	C12—C18—H18	116.9
C4—C5—Cl1	119.0 (4)	N2—C19—C20	111.7 (4)
C5—C6—C1	119.1 (5)	N2—C19—H19A	109.3
C5—C6—H6	120.4	C20—C19—H19A	109.3
C1—C6—H6	120.4	N2—C19—H19B	109.3
N1—C7—C1	126.6 (5)	C20—C19—H19B	109.3
N1—C7—H7	116.7	H19A—C19—H19B	107.9
C1—C7—H7	116.7	C19—C20—C21	112.0 (5)
N1—C8—C9	111.1 (5)	C19—C20—H20A	109.2
N1—C8—H8A	109.4	C21—C20—H20A	109.2
C9—C8—H8A	109.4	C19—C20—H20B	109.2

N1—C8—H8B	109.4	C21—C20—H20B	109.2
C9—C8—H8B	109.4	H20A—C20—H20B	107.9
H8A—C8—H8B	108.0	C22—C21—C20	116.1 (6)
C10—C9—C8	113.9 (6)	C22—C21—H21A	108.3
C10—C9—H9A	108.8	C20—C21—H21A	108.3
C8—C9—H9A	108.8	C22—C21—H21B	108.3
C10—C9—H9B	108.8	C20—C21—H21B	108.3
C8—C9—H9B	108.8	H21A—C21—H21B	107.4
H9A—C9—H9B	107.7	C21—C22—H22A	109.5
C9—C10—C11	112.3 (7)	C21—C22—H22B	109.5
C9—C10—H10A	109.2	H22A—C22—H22B	109.5
C11—C10—H10A	109.2	C21—C22—H22C	109.5
C9—C10—H10B	109.2	H22A—C22—H22C	109.5
C11—C10—H10B	109.2	H22B—C22—H22C	109.5