metal-organic compounds

Chloridobis{*N*-[(dimethylamino)-dimethylsilyl]-2,6-dimethylanilido-$\kappa^2 N, N'$}iron(III)

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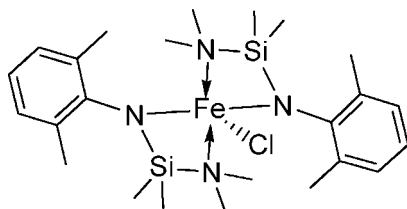Correspondence e-mail: sdbai@sxu.edu.cn

The title iron(III) compound, [Fe(C$_{12}$H$_{21}$N$_2$Si)$_2$Cl], is monomeric. The Fe atom is *N,N′*-chelated by the *N*-silylated anilide ligand. The two ligands around the Fe atom are arranged *trans* to each other. The Fe—N$_{amino}$ bond is longer than the Fe—N$_{anilide}$ bond by about 0.37 Å. The molecule displays a pseudo-twofold rotation. The five–coordinate Fe atom demonstrates a highly distorted trigonal–bipyramidal geometry.

Related literature

For related chelate iron(III) compounds and their applications, involving, for example, porphyrin, bypyridine, amidinate as well as guanidinate, see: Rath *et al.* (2004); Schunemann *et al.* (1999); Collomb *et al.* (1999); O'Keefe *et al.* (2002); Foley *et al.* (2000). For related zinc compounds with analogous analido ligands, see: Schumann *et al.* (2000).

Experimental

Crystal data

[Fe(C$_{12}$H$_{21}$N$_2$Si)$_2$Cl]	V = 5580.1 (16) Å^3
M_r = 534.10	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 34.213 (5) Å	μ = 0.74 mm^{-1}
b = 9.3555 (14) Å	T = 293 (2) K
c = 20.769 (4) Å	0.30 × 0.25 × 0.20 mm
β = 122.924 (5)°	

Data collection

Bruker SMART area-detector diffractometer	11193 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	4880 independent reflections
	4359 reflections with $I > 2\sigma(I)$
T_{min} = 0.808, T_{max} = 0.866	R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038	301 parameters
$wR(F^2)$ = 0.102	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
4880 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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supplementary materials

Chloridobis{*N*-[(dimethylamino)dimethylsilyl]-2,6-dimethylanilido-*κ*²*N*,*N*'}iron(III)

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Comment

The study of iron(III) amides with the monodentate ligands was relatively less because it was generally believed that a "mismatch" between the "hard" amido ligand and the "soft" late transition metal center rendered the corresponding *M*—N bond relatively unstable. Iron(III) ion could be stablized by the chelate ligands, such as porphyrin (Rath *et al.*, 2004; Schunemann *et al.*, 1999), bypyridine (Collomb *et al.*, 1999) and amidinate (O'Keefe *et al.*, 2002) as well as guanidinate (Foley *et al.*, 2000).

The title compound is supported by the *N*–silylated anilido ligand with a pendant amino group. It is the first example of iron(III) ion coordinated by an N—Si—N chelating moiety. It is monomeric and contains two *N*–silylated anilido ligands, which are arranged in *trans*– to each other and obey the *pseudo–C₂* symmetrical operation. Such arrangement makes Fe atom right in the triangular planes of N1···N3···Cl1 and N2···N4···Cl1. The five–coordinate iron(III) center demonstrates a highly distorted trigonal bipyramid geometry (N2 and N4 - apical atoms), which is closely similar to the amidinate and guanidinate iron(III) compounds, but significantly different from the tetragonal pyramid geometry in the porphyrin derivatives. The Fe center is chelated, with an average N—Fe—N bite angle of 74.29 (7)°. The corresponding N—Si—N of the ligand is constrained to be about 95.49 (9)°. The two values are quite different from those in the related amidinate and guanidinate Fe(III) compounds bearing the same geometry, N—Fe—N being about 66° and N—C—N being larger than 111°. The mean Fe—N$_{anilido}$ bond is 1.9409 (18)Å, whereas the mean Fe—N$_{amino}$ bond is 2.3126 (19)Å in the title compound. In the reported amidinate and guanidinate iron(III) compounds, the Fe—N bonds are ranging in the scope of 2.0~2.1Å. It suggests that the N—Si—N group is more flexible in coordination chemistry, than the N—C—N chelating unit.

Experimental

FeCl₃ (0.21 g, 1.29 mmol) was added into the solution of [LiN(Si*Me*₂N*Me*₂)(2,6–*Me*₂C₆H₃)]₂ (0.59 g, 1.29 mmol) in *Et*₂O (25 ml) at 273 K. The reaction mixture was warmed to room temperature and kept stirring for 12 h. It was dried in vacuum to remove all volatiles and the residue was extracted with CH₂Cl₂ (25 ml). Concentration of the filtrate under reduced pressure gave the black solid. Recrystallization of the solid in toluene yielded the title compound as black crystals (yield 0.41 g, 60%).

Refinement

The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each methyl group was allowed to rotate freely about its C–C bond. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).
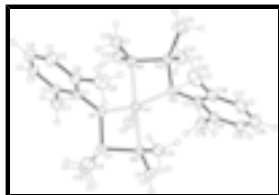
supplementary materials

Figures

Fig. 1. The molecular structure, showing the atom–numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

Chloridobis{*N*-[(dimethylamino)dimethylsilyl]-2,6-dimethylanilido- $\kappa^2 N,N'$}iron(III)

Crystal data

$[\text{Fe}(\text{C}_{12}\text{H}_{21}\text{N}_2\text{Si})_2\text{Cl}]$	$F_{000} = 2280$
$M_r = 534.10$	$D_x = 1.271$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 7222 reflections
$a = 34.213$ (5) Å	$\theta = 2.3–27.6°$
$b = 9.3555$ (14) Å	$\mu = 0.74$ mm^{-1}
$c = 20.769$ (4) Å	$T = 293$ (2) K
$\beta = 122.924$ (5)°	Prism, black
$V = 5580.1$ (16) Å^3	$0.30 \times 0.25 \times 0.20$ mm
$Z = 8$	

Data collection

Bruker SMART area-detector diffractometer	4880 independent reflections
Radiation source: Fine–focus sealed tube	4359 reflections with $I > 2\sigma(I)$
Monochromator: Graphite	$R_{int} = 0.031$
$T = 293(2)$ K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.0°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -40 \rightarrow 33$
$T_{min} = 0.808$, $T_{max} = 0.866$	$k = -11 \rightarrow 11$
11193 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: Difmap
Least-squares matrix: Full	Hydrogen site location: Geom
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 4.0594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
4880 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}

301 parameters

$\Delta\rho_{min} = -0.25$ e Å^{-3}

Primary atom site location: Direct

Extinction correction: none

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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	0.152240 (10)	0.34361 (3)	0.065107 (16)	0.03404 (12)
Cl1	0.22982 (2)	0.30852 (7)	0.13642 (4)	0.05195 (17)
Si1	0.14458 (2)	0.46111 (7)	0.18176 (3)	0.04116 (17)
Si2	0.12728 (2)	0.23365 (7)	−0.07896 (3)	0.04149 (17)
N1	0.12489 (6)	0.31269 (19)	0.12496 (10)	0.0340 (4)
N2	0.15405 (6)	0.5619 (2)	0.11810 (10)	0.0406 (4)
N3	0.12899 (6)	0.3964 (2)	−0.04016 (10)	0.0378 (4)
N4	0.13464 (7)	0.1293 (2)	−0.00134 (11)	0.0429 (5)
C1	0.10023 (8)	0.1984 (2)	0.13210 (11)	0.0353 (5)
C2	0.12431 (9)	0.0830 (3)	0.18117 (12)	0.0436 (5)
C3	0.09884 (11)	−0.0285 (3)	0.18479 (15)	0.0602 (7)
H3	0.1146	−0.1061	0.2165	0.072*
C4	0.05127 (12)	−0.0272 (3)	0.14302 (17)	0.0735 (9)
H4	0.0349	−0.1021	0.1471	0.088*
C5	0.02808 (10)	0.0852 (4)	0.09519 (17)	0.0655 (8)
H5	−0.0043	0.0856	0.0664	0.079*
C6	0.05161 (8)	0.1980 (3)	0.08872 (14)	0.0454 (6)
C7	0.17639 (9)	0.0764 (3)	0.22785 (15)	0.0592 (7)
H7A	0.1884	0.1382	0.2716	0.089*
H7B	0.1880	0.1067	0.1971	0.089*
H7C	0.1862	−0.0200	0.2449	0.089*
C8	0.02459 (9)	0.3161 (3)	0.03210 (17)	0.0633 (8)
H8A	−0.0076	0.2892	0.0003	0.095*
H8B	0.0369	0.3318	0.0007	0.095*
H8C	0.0273	0.4022	0.0594	0.095*
C9	0.10149 (11)	0.5424 (3)	0.19894 (18)	0.0663 (8)
H9A	0.0733	0.5628	0.1507	0.099*
H9B	0.1140	0.6295	0.2275	0.099*
H9C	0.0950	0.4770	0.2276	0.099*
C10	0.20056 (10)	0.4460 (3)	0.27514 (14)	0.0636 (8)

H10A	0.1963	0.3900	0.3096	0.095*
H10B	0.2114	0.5396	0.2963	0.095*
H10C	0.2231	0.4004	0.2680	0.095*
C11	0.19600 (10)	0.6507 (3)	0.15052 (17)	0.0588 (7)
H11A	0.1986	0.6870	0.1098	0.088*
H11B	0.2229	0.5940	0.1846	0.088*
H11C	0.1939	0.7290	0.1783	0.088*
C12	0.11329 (10)	0.6484 (3)	0.06259 (14)	0.0519 (6)
H12A	0.1105	0.7291	0.0884	0.078*
H12B	0.0856	0.5911	0.0406	0.078*
H12C	0.1173	0.6814	0.0227	0.078*
C13	0.12223 (9)	0.5265 (3)	−0.07968 (12)	0.0423 (5)
C14	0.16070 (10)	0.6008 (3)	−0.07176 (14)	0.0513 (6)
C15	0.15268 (13)	0.7255 (3)	−0.11318 (18)	0.0683 (8)
H15	0.1779	0.7744	−0.1081	0.082*
C16	0.10921 (15)	0.7785 (3)	−0.16087 (19)	0.0781 (10)
H16	0.1047	0.8606	−0.1894	0.094*
C17	0.07203 (13)	0.7101 (3)	−0.16673 (16)	0.0698 (9)
H17	0.0424	0.7488	−0.1981	0.084*
C18	0.07738 (9)	0.5847 (3)	−0.12716 (13)	0.0518 (6)
C19	0.20951 (10)	0.5485 (4)	−0.02041 (18)	0.0703 (8)
H19A	0.2145	0.4681	−0.0438	0.106*
H19B	0.2146	0.5202	0.0280	0.106*
H19C	0.2308	0.6236	−0.0124	0.106*
C20	0.03569 (10)	0.5156 (4)	−0.13425 (16)	0.0689 (8)
H20A	0.0120	0.5862	−0.1486	0.103*
H20B	0.0444	0.4740	−0.0859	0.103*
H20C	0.0240	0.4424	−0.1728	0.103*
C21	0.17490 (11)	0.1969 (4)	−0.09351 (19)	0.0697 (8)
H21A	0.1721	0.2593	−0.1325	0.105*
H21B	0.1731	0.0993	−0.1092	0.105*
H21C	0.2043	0.2130	−0.0464	0.105*
C22	0.07192 (11)	0.1936 (4)	−0.17116 (15)	0.0676 (8)
H22A	0.0464	0.1994	−0.1642	0.101*
H22B	0.0734	0.0991	−0.1878	0.101*
H22C	0.0674	0.2618	−0.2092	0.101*
C23	0.17204 (12)	0.0207 (3)	0.03273 (17)	0.0708 (9)
H23A	0.1764	−0.0137	0.0798	0.106*
H23B	0.2005	0.0628	0.0430	0.106*
H23C	0.1635	−0.0575	−0.0024	0.106*
C24	0.09130 (11)	0.0623 (3)	−0.01730 (16)	0.0653 (8)
H24A	0.0824	−0.0128	−0.0542	0.098*
H24B	0.0670	0.1328	−0.0373	0.098*
H24C	0.0962	0.0233	0.0293	0.098*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Fe1	0.03341 (19)	0.0380 (2)	0.02983 (18)	0.00023 (12)	0.01659 (14)	0.00240 (12)
Cl1	0.0352 (3)	0.0610 (4)	0.0520 (4)	0.0044 (3)	0.0187 (3)	0.0056 (3)
Si1	0.0515 (4)	0.0366 (4)	0.0383 (3)	−0.0044 (3)	0.0262 (3)	−0.0041 (3)
Si2	0.0463 (4)	0.0460 (4)	0.0349 (3)	−0.0003 (3)	0.0238 (3)	−0.0015 (3)
N1	0.0364 (10)	0.0324 (10)	0.0327 (9)	−0.0003 (7)	0.0184 (8)	0.0014 (7)
N2	0.0453 (11)	0.0340 (10)	0.0378 (10)	−0.0027 (8)	0.0195 (9)	−0.0011 (8)
N3	0.0398 (10)	0.0421 (11)	0.0309 (9)	0.0008 (8)	0.0188 (8)	0.0046 (8)
N4	0.0540 (12)	0.0366 (11)	0.0417 (10)	−0.0031 (9)	0.0283 (10)	−0.0028 (8)
C1	0.0443 (13)	0.0349 (12)	0.0311 (10)	−0.0026 (9)	0.0235 (10)	−0.0021 (9)
C2	0.0594 (15)	0.0361 (13)	0.0357 (11)	−0.0013 (11)	0.0262 (11)	0.0001 (10)
C3	0.090 (2)	0.0411 (15)	0.0479 (14)	−0.0125 (14)	0.0362 (15)	0.0017 (12)
C4	0.094 (2)	0.066 (2)	0.0643 (18)	−0.0380 (18)	0.0450 (18)	−0.0039 (16)
C5	0.0549 (16)	0.082 (2)	0.0620 (17)	−0.0256 (15)	0.0330 (14)	−0.0072 (16)
C6	0.0433 (13)	0.0517 (15)	0.0446 (13)	−0.0067 (11)	0.0261 (11)	−0.0054 (11)
C7	0.0598 (17)	0.0522 (17)	0.0521 (15)	0.0127 (13)	0.0217 (13)	0.0133 (12)
C8	0.0403 (15)	0.072 (2)	0.0651 (18)	0.0058 (13)	0.0207 (13)	0.0056 (15)
C9	0.093 (2)	0.0542 (18)	0.0779 (19)	0.0006 (15)	0.0636 (19)	−0.0101 (15)
C10	0.0754 (19)	0.0621 (18)	0.0380 (13)	−0.0143 (15)	0.0210 (13)	−0.0044 (12)
C11	0.0670 (18)	0.0471 (16)	0.0627 (17)	−0.0190 (13)	0.0355 (15)	−0.0070 (13)
C12	0.0638 (17)	0.0430 (15)	0.0462 (14)	0.0108 (12)	0.0281 (13)	0.0065 (11)
C13	0.0580 (15)	0.0417 (14)	0.0306 (11)	0.0025 (11)	0.0263 (11)	0.0014 (9)
C14	0.0726 (18)	0.0434 (14)	0.0493 (14)	−0.0058 (13)	0.0406 (14)	−0.0016 (11)
C15	0.114 (3)	0.0445 (17)	0.0706 (19)	−0.0082 (17)	0.066 (2)	0.0001 (14)
C16	0.131 (3)	0.0469 (18)	0.067 (2)	0.010 (2)	0.060 (2)	0.0141 (15)
C17	0.093 (2)	0.0611 (19)	0.0468 (15)	0.0274 (17)	0.0328 (16)	0.0147 (14)
C18	0.0639 (16)	0.0548 (16)	0.0344 (12)	0.0122 (13)	0.0251 (12)	0.0048 (11)
C19	0.0643 (18)	0.073 (2)	0.079 (2)	−0.0185 (16)	0.0427 (17)	0.0017 (16)
C20	0.0528 (16)	0.090 (2)	0.0506 (15)	0.0207 (16)	0.0198 (13)	0.0096 (15)
C21	0.086 (2)	0.069 (2)	0.084 (2)	0.0023 (16)	0.0652 (19)	−0.0030 (16)
C22	0.070 (2)	0.072 (2)	0.0424 (14)	−0.0015 (15)	0.0191 (14)	−0.0119 (14)
C23	0.100 (2)	0.0492 (17)	0.0574 (16)	0.0246 (16)	0.0392 (17)	0.0058 (13)
C24	0.088 (2)	0.0653 (19)	0.0614 (16)	−0.0338 (16)	0.0529 (16)	−0.0209 (14)

Geometric parameters (Å, °)

Fe1—N3	1.9406 (17)	C10—H10A	0.9600
Fe1—N1	1.9412 (18)	C10—H10B	0.9600
Fe1—Cl1	2.2523 (7)	C10—H10C	0.9600
Fe1—N2	2.3050 (19)	C11—H11A	0.9600
Fe1—N4	2.3203 (19)	C11—H11B	0.9600
Si1—N1	1.7058 (18)	C11—H11C	0.9600
Si1—N2	1.791 (2)	C12—H12A	0.9600
Si1—C10	1.847 (3)	C12—H12B	0.9600
Si1—C9	1.858 (3)	C12—H12C	0.9600
Si2—N3	1.709 (2)	C13—C18	1.407 (3)
Si2—N4	1.782 (2)	C13—C14	1.417 (4)
Si2—C21	1.844 (3)	C14—C15	1.386 (4)
Si2—C22	1.858 (3)	C14—C19	1.493 (4)
N1—C1	1.419 (3)	C15—C16	1.355 (5)

N2—C11	1.467 (3)	C15—H15	0.9300
N2—C12	1.477 (3)	C16—C17	1.369 (5)
N3—C13	1.415 (3)	C16—H16	0.9300
N4—C24	1.472 (3)	C17—C18	1.386 (4)
N4—C23	1.478 (3)	C17—H17	0.9300
C1—C6	1.396 (3)	C18—C20	1.499 (4)
C1—C2	1.404 (3)	C19—H19A	0.9600
C2—C3	1.387 (4)	C19—H19B	0.9600
C2—C7	1.497 (4)	C19—H19C	0.9600
C3—C4	1.366 (4)	C20—H20A	0.9600
C3—H3	0.9300	C20—H20B	0.9600
C4—C5	1.366 (4)	C20—H20C	0.9600
C4—H4	0.9300	C21—H21A	0.9600
C5—C6	1.377 (4)	C21—H21B	0.9600
C5—H5	0.9300	C21—H21C	0.9600
C6—C8	1.508 (4)	C22—H22A	0.9600
C7—H7A	0.9600	C22—H22B	0.9600
C7—H7B	0.9600	C22—H22C	0.9600
C7—H7C	0.9600	C23—H23A	0.9600
C8—H8A	0.9600	C23—H23B	0.9600
C8—H8B	0.9600	C23—H23C	0.9600
C8—H8C	0.9600	C24—H24A	0.9600
C9—H9A	0.9600	C24—H24B	0.9600
C9—H9B	0.9600	C24—H24C	0.9600
C9—H9C	0.9600		
N3—Fe1—N1	135.57 (8)	H9A—C9—H9C	109.5
N3—Fe1—Cl1	113.14 (6)	H9B—C9—H9C	109.5
N1—Fe1—Cl1	111.29 (6)	Si1—C10—H10A	109.5
N3—Fe1—N2	101.58 (7)	Si1—C10—H10B	109.5
N1—Fe1—N2	73.95 (7)	H10A—C10—H10B	109.5
Cl1—Fe1—N2	95.68 (5)	Si1—C10—H10C	109.5
N3—Fe1—N4	74.63 (7)	H10A—C10—H10C	109.5
N1—Fe1—N4	101.10 (7)	H10B—C10—H10C	109.5
Cl1—Fe1—N4	95.59 (5)	N2—C11—H11A	109.5
N2—Fe1—N4	168.71 (7)	N2—C11—H11B	109.5
N1—Si1—N2	94.59 (9)	H11A—C11—H11B	109.5
N1—Si1—C10	117.27 (12)	N2—C11—H11C	109.5
N2—Si1—C10	108.36 (11)	H11A—C11—H11C	109.5
N1—Si1—C9	114.20 (12)	H11B—C11—H11C	109.5
N2—Si1—C9	114.01 (12)	N2—C12—H12A	109.5
C10—Si1—C9	107.93 (15)	N2—C12—H12B	109.5
N3—Si2—N4	96.30 (9)	H12A—C12—H12B	109.5
N3—Si2—C21	115.89 (13)	N2—C12—H12C	109.5
N4—Si2—C21	110.08 (13)	H12A—C12—H12C	109.5
N3—Si2—C22	114.84 (12)	H12B—C12—H12C	109.5
N4—Si2—C22	112.69 (13)	C18—C13—N3	120.8 (2)
C21—Si2—C22	106.86 (15)	C18—C13—C14	118.8 (2)
C1—N1—Si1	125.09 (14)	N3—C13—C14	120.4 (2)
C1—N1—Fe1	134.44 (14)	C15—C14—C13	118.9 (3)

Si1—N1—Fe1	100.08 (9)	C15—C14—C19	119.1 (3)
C11—N2—C12	108.7 (2)	C13—C14—C19	122.0 (2)
C11—N2—Si1	118.92 (16)	C16—C15—C14	122.0 (3)
C12—N2—Si1	113.07 (16)	C16—C15—H15	119.0
C11—N2—Fe1	119.09 (16)	C14—C15—H15	119.0
C12—N2—Fe1	110.11 (14)	C15—C16—C17	119.5 (3)
Si1—N2—Fe1	85.25 (8)	C15—C16—H16	120.3
C13—N3—Si2	122.68 (14)	C17—C16—H16	120.3
C13—N3—Fe1	135.24 (15)	C16—C17—C18	121.7 (3)
Si2—N3—Fe1	101.10 (9)	C16—C17—H17	119.1
C24—N4—C23	108.6 (2)	C18—C17—H17	119.1
C24—N4—Si2	113.57 (17)	C17—C18—C13	119.1 (3)
C23—N4—Si2	117.99 (17)	C17—C18—C20	119.7 (3)
C24—N4—Fe1	113.94 (16)	C13—C18—C20	121.3 (2)
C23—N4—Fe1	115.57 (16)	C14—C19—H19A	109.5
Si2—N4—Fe1	85.87 (8)	C14—C19—H19B	109.5
C6—C1—C2	119.3 (2)	H19A—C19—H19B	109.5
C6—C1—N1	120.2 (2)	C14—C19—H19C	109.5
C2—C1—N1	120.5 (2)	H19A—C19—H19C	109.5
C3—C2—C1	118.7 (2)	H19B—C19—H19C	109.5
C3—C2—C7	119.7 (2)	C18—C20—H20A	109.5
C1—C2—C7	121.6 (2)	C18—C20—H20B	109.5
C4—C3—C2	121.7 (3)	H20A—C20—H20B	109.5
C4—C3—H3	119.1	C18—C20—H20C	109.5
C2—C3—H3	119.1	H20A—C20—H20C	109.5
C5—C4—C3	119.3 (3)	H20B—C20—H20C	109.5
C5—C4—H4	120.4	Si2—C21—H21A	109.5
C3—C4—H4	120.4	Si2—C21—H21B	109.5
C4—C5—C6	121.4 (3)	H21A—C21—H21B	109.5
C4—C5—H5	119.3	Si2—C21—H21C	109.5
C6—C5—H5	119.3	H21A—C21—H21C	109.5
C5—C6—C1	119.6 (2)	H21B—C21—H21C	109.5
C5—C6—C8	119.6 (2)	Si2—C22—H22A	109.5
C1—C6—C8	120.8 (2)	Si2—C22—H22B	109.5
C2—C7—H7A	109.5	H22A—C22—H22B	109.5
C2—C7—H7B	109.5	Si2—C22—H22C	109.5
H7A—C7—H7B	109.5	H22A—C22—H22C	109.5
C2—C7—H7C	109.5	H22B—C22—H22C	109.5
H7A—C7—H7C	109.5	N4—C23—H23A	109.5
H7B—C7—H7C	109.5	N4—C23—H23B	109.5
C6—C8—H8A	109.5	H23A—C23—H23B	109.5
C6—C8—H8B	109.5	N4—C23—H23C	109.5
H8A—C8—H8B	109.5	H23A—C23—H23C	109.5
C6—C8—H8C	109.5	H23B—C23—H23C	109.5
H8A—C8—H8C	109.5	N4—C24—H24A	109.5
H8B—C8—H8C	109.5	N4—C24—H24B	109.5
Si1—C9—H9A	109.5	H24A—C24—H24B	109.5
Si1—C9—H9B	109.5	N4—C24—H24C	109.5
H9A—C9—H9B	109.5	H24A—C24—H24C	109.5

| Si1—C9—H9C | 109.5 | H24B—C24—H24C | 109.5 |

Fig. 1