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# 2,2′-Bis(4-methoxyphenyl)-2,2′-bis(trimethylsilanyloxy)-2,2′-(ferrocene-1,1′-diyl)diacetonitrile

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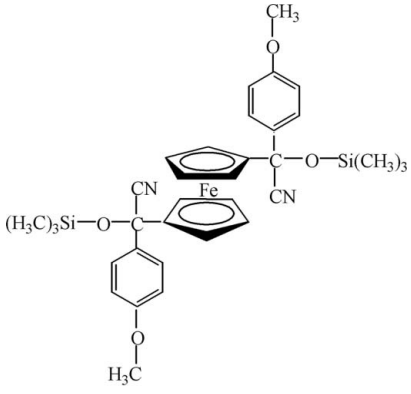
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.063; $wR$ factor = 0.204; data-to-parameter ratio = 17.2.

In the title compound, $[Fe(C_{17}H_{20}NO_2Si)_2]$, the Fe atom is situated on a crystallographic centre of inversion, leading to a perfectly staggered conformation of the Cp rings.

## Related literature

For related literature, see: Evans & Truesdale (1973); Evans *et al.* (1974); Lidy & Sundermeyer (1973); Dunitz *et al.* (1956); Fischer & Hüning (1987); Fleming & Woolias (1979); Gassman & Talley (1978); Groutas & Felker (1980); Rasmussen & Heilmann (1978); Zhou (1989).




## Experimental

### Crystal data

$[Fe(C_{17}H_{20}NO_2Si)_2]$
$M_r$ = 652.71
Triclinic, $P\overline{1}$
$a$ = 7.129 (2) Å
$b$ = 10.500 (4) Å
$c$ = 11.449 (4) Å
$\alpha$ = 95.613 (5)°
$\beta$ = 97.253 (6)°
$\gamma$ = 97.441 (6)°
$V$ = 837.3 (5) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.56 mm$^{-1}$
$T$ = 293 (2) K
0.24 × 0.14 × 0.12 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min}$ = 0.822, $T_{max}$ = 1.000
(expected range = 0.768–0.935)
4803 measured reflections
3367 independent reflections
2156 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.204
$S$ = 1.03
3367 reflections
196 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.98 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: IM2048).

## References

Bruker (1999) *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dunitz, J. D., Orgel, L. E. & Rich, A. (1956). *Acta Cryst.* **9**, 373–375.
Evans, D. A., Carroll, G. L. & Truesdale, L. K. (1974). *J. Org. Chem.* **39**, 914–917.
Evans, D. A. & Truesdale, L. K. (1973). *Tetrahedron Lett.* **49**, 4929–4932.
Fischer, K. & Hüning, S. (1987). *J. Org. Chem.* **52**, 564–569.
Fleming, L. & Woolias, M. (1979). *J. Chem. Soc. Perkin Trans. 1*, pp. 829–837.
Gassman, P. G. & Talley, J. J. (1978). *Tetrahedron Lett.* **40**, 3773–3776.
Groutas, W. C. & Felker, D. (1980). *Synthesis*, pp. 861–868.
Lidy, W. & Sundermeyer, W. (1973). *Chem. Ber.* **106**, 587–593.
Rasmussen, J. K. & Heilmann, S. M. (1978). *Synthesis*, pp. 219–221.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Zhou, G. D. (1989). *Foundations of Structural Chemistry*, 1st ed., p. 230. Beijing University Press.

# supplementary materials

*Acta Cryst.* (2008). E**64**, m123 [ **doi:10.1107/S1600536807064513** ]

# 2,2'-Bis(4-methoxyphenyl)-2,2'-bis(trimethylsilanyloxy)-2,2'-(ferrocene-1,1'-diyl)diacetonitrile

**X. Wang and H. Bao**

## Comment

Cyanohydrin trimethylsilyl ethers are useful in organic synthesis as they serve not only for the protection of carbonyl groups (Rasmussen *et al.*, 1978; Groutas *et al.*, 1980; Fischer *et al.*, 1987) but also as versatile intermediates (Gassman *et al.*, 1978; Evans *et al.*, 1974; Fleming *et al.*, 1979) in the synthesis of cyanohydrins, α,β-unsaturated nitriles and β-aminoalcohols. The general method for the preparation of cyanohydrin trimethylsilyl ethers is the addition of trimethylsilyl cyanide (TMSCN) to carbonyl compounds with the aid of a catalyst including Lewis acids, such as $ZnI_2$ (Evans *et al.*,1974) and $AlCl_3$ (Lidy *et al.*, 1973), as well as solubilized anionic species, such as $K^+CN^-$-18-Crown-6 and $^nBu_4N^+CN^-$ (Evans *et al.*,1973).

The molecular structure of the title compound, (I), shows the Fe atom on a crystallographic center of inversion and two Cp ligands with a cyanohydrin ether substituents. Because of the inversion symmetry the Cp ligands show a staggered conformation. The central tetrahedral C(6) atom is bound to C≡N, $(CH_3)_3SiO$ and $(CH_3O)C_6H_4$ groups in compound and is therefore a new stereogenic center which is formed during the reaction sequence. Due to the internal symmetry of the molecule Figure 1 shows the *R*,*S* diastereomer. There is no evidence for the formation of *R*,*R*- or S,*S*-diastereomers even from NMR spectra of the crude reaction product. The bond angle of C(6)–C(7)–N(1) is 178.9 (6)° showing *sp* hybridization for the C≡N carbon atom. The Si(1)—O(1)—C(6) bond angle measures to 131.6 (3)° which is significantly larger compared to that of a regular tetrahedron (109.5°). The influence of neighbouring C*sp* and C$sp^2$ atoms shorten the C(6)–C(1), C(6)–C(7) and C(6)–C(8) bond distances (1.511 (6) Å, 1.483 (7) Å and 1.531 (6), respectively) compared to normal C—C bond distances (app. 1.54 Å). It shows there may be a super conjugate effect in the molecule of the title compound.

## Experimental

Into a 100 ml 3-neck round-bottomed flask equipped with magnetic stirring bar, reflux condenser and $CaCl_2$ drying tube was placed 1.1 mmol (297 mg) bisacetylferrocene in 15 ml dry $CH_2Cl_2$ and 1 mmol (319 mg) $ZnI_2$. After stirring for 20 minutes, 4.4 mmol TMSCN (374 mg) were added and the was solution stirred for 10 h. During the reaction the progress of the reaction was monitored by TLC (benzene). After completion the solvent was evaporated under reduced pressure with the residue obtained being extracted with pentane. The solution was washed with saturated cold aqueous $NaHSO_3$ and dried over $Na_2SO_4$. Filtration and removal of the solvent under reduced pressure yielded the crude product which was recrystallized from ether/light petroleum (b.p. 60–90°) to obtain single crystals the title compound.

## Refinement

All the H atoms were positioned geometrically and refined using a riding model with C—H distances of 0.93–0.97° and $U_{iso}$(H) = 1.2$U_{eq}$ of the corresponding parent atom. The methyls at the terminal group have higher $U_{eq}$ than silicon atom in the central tetrahedral.

## Figures

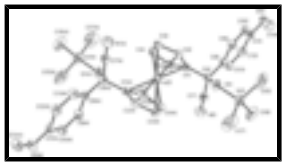


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary size.

## 2,2'-Bis(4-methoxyphenyl)-2,2'-bis(trimethylsilanyloxy)-2,2'-(ferrocene-1,1'- diyl)diacetonitrile

*Crystal data*

| | |
|---|---|
| $[Fe(C_{17}H_{20}NO_2Si)_2]$ | $Z = 1$ |
| $M_r = 652.71$ | $F_{000} = 344$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.295$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 7.129$ (2) Å | Cell parameters from 749 reflections |
| $b = 10.500$ (4) Å | $\theta = 2.5$–$25.4^\circ$ |
| $c = 11.449$ (4) Å | $\mu = 0.56$ mm$^{-1}$ |
| $\alpha = 95.613$ (5)° | $T = 293$ (2) K |
| $\beta = 97.253$ (6)° | Needle, yellow |
| $\gamma = 97.441$ (6)° | 0.24 × 0.14 × 0.12 mm |
| $V = 837.3$ (5) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3367 independent reflections |
| Radiation source: fine-focus sealed tube | 2156 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.030$ |
| $T = 293(2)$ K | $\theta_{max} = 26.4^\circ$ |
| φ and ω scans | $\theta_{min} = 1.8^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 1999) | $h = -7 \rightarrow 8$ |
| $T_{min} = 0.822$, $T_{max} = 1.000$ | $k = -10 \rightarrow 13$ |
| 4803 measured reflections | $l = -14 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | H-atom parameters constrained |
| $wR(F^2) = 0.204$ | $w = 1/[\sigma^2(F_o^2) + (0.111P)^2 + 0.2987P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 3367 reflections | $\Delta\rho_{max}$ = 0.98 e Å$^{-3}$ |
| 196 parameters | $\Delta\rho_{min}$ = −0.43 e Å$^{-3}$ |
| 21 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe2 | 1.0000 | 0.0000 | 0.0000 | 0.0414 (3) |
| Si1 | 1.0979 (2) | 0.43619 (14) | 0.25558 (15) | 0.0644 (5) |
| N1 | 0.6209 (8) | 0.2641 (6) | 0.0446 (5) | 0.0789 (15) |
| O1 | 1.0478 (5) | 0.2772 (3) | 0.2175 (3) | 0.0539 (9) |
| O2 | 0.6132 (6) | 0.1608 (4) | 0.6498 (3) | 0.0687 (11) |
| C1 | 0.9125 (6) | 0.0596 (4) | 0.1571 (4) | 0.0410 (10) |
| C2 | 1.0873 (7) | 0.0084 (5) | 0.1784 (4) | 0.0480 (11) |
| H2 | 1.2020 | 0.0520 | 0.2196 | 0.058* |
| C3 | 1.0536 (9) | −0.1225 (5) | 0.1245 (4) | 0.0597 (14) |
| H3 | 1.1433 | −0.1794 | 0.1250 | 0.072* |
| C4 | 0.8633 (10) | −0.1509 (5) | 0.0708 (4) | 0.0635 (16) |
| H4 | 0.8054 | −0.2297 | 0.0294 | 0.076* |
| C5 | 0.7750 (8) | −0.0411 (5) | 0.0897 (4) | 0.0532 (13) |
| H5 | 0.6483 | −0.0343 | 0.0630 | 0.064* |
| C6 | 0.8760 (6) | 0.1923 (4) | 0.2043 (4) | 0.0423 (10) |
| C7 | 0.7336 (8) | 0.2337 (5) | 0.1153 (4) | 0.0544 (13) |
| C8 | 0.7960 (6) | 0.1835 (4) | 0.3217 (4) | 0.0416 (10) |
| C9 | 0.9140 (7) | 0.1609 (5) | 0.4202 (4) | 0.0521 (12) |
| H9 | 1.0403 | 0.1511 | 0.4138 | 0.063* |
| C10 | 0.8494 (7) | 0.1524 (5) | 0.5273 (4) | 0.0538 (12) |
| H10 | 0.9319 | 0.1371 | 0.5924 | 0.065* |
| C11 | 0.6624 (7) | 0.1664 (5) | 0.5393 (4) | 0.0492 (12) |
| C12 | 0.5414 (7) | 0.1855 (5) | 0.4407 (4) | 0.0543 (12) |
| H12 | 0.4139 | 0.1919 | 0.4462 | 0.065* |
| C13 | 0.6097 (7) | 0.1950 (5) | 0.3340 (4) | 0.0503 (12) |
| H13 | 0.5272 | 0.2096 | 0.2686 | 0.060* |
| C14 | 0.4225 (9) | 0.1780 (7) | 0.6651 (5) | 0.0824 (19) |

| | | | | |
|---|---|---|---|---|
| H14A | 0.4054 | 0.1719 | 0.7463 | 0.124* |
| H14B | 0.3345 | 0.1121 | 0.6148 | 0.124* |
| H14C | 0.3989 | 0.2615 | 0.6446 | 0.124* |
| C15 | 1.2315 (13) | 0.4614 (8) | 0.4056 (7) | 0.122 (3) |
| H15A | 1.3430 | 0.4189 | 0.4066 | 0.183* |
| H15B | 1.1520 | 0.4262 | 0.4598 | 0.183* |
| H15C | 1.2695 | 0.5523 | 0.4291 | 0.183* |
| C16 | 0.8845 (10) | 0.5181 (7) | 0.2564 (7) | 0.098 (2) |
| H16A | 0.8091 | 0.4851 | 0.3136 | 0.146* |
| H16B | 0.8101 | 0.5025 | 0.1792 | 0.146* |
| H16C | 0.9232 | 0.6094 | 0.2770 | 0.146* |
| C17 | 1.2491 (13) | 0.4952 (9) | 0.1477 (8) | 0.133 (3) |
| H17A | 1.3593 | 0.4512 | 0.1500 | 0.200* |
| H17B | 1.2894 | 0.5865 | 0.1671 | 0.200* |
| H17C | 1.1776 | 0.4788 | 0.0695 | 0.200* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe2 | 0.0614 (7) | 0.0322 (5) | 0.0294 (5) | −0.0005 (4) | 0.0117 (4) | 0.0011 (3) |
| Si1 | 0.0751 (11) | 0.0402 (8) | 0.0728 (10) | −0.0016 (7) | 0.0095 (8) | −0.0043 (7) |
| N1 | 0.084 (4) | 0.087 (4) | 0.070 (3) | 0.018 (3) | 0.012 (3) | 0.025 (3) |
| O1 | 0.055 (2) | 0.0387 (17) | 0.066 (2) | −0.0051 (14) | 0.0222 (16) | −0.0050 (15) |
| O2 | 0.083 (3) | 0.082 (3) | 0.050 (2) | 0.017 (2) | 0.0323 (19) | 0.0128 (19) |
| C1 | 0.049 (3) | 0.040 (2) | 0.034 (2) | 0.0011 (19) | 0.0119 (19) | 0.0049 (18) |
| C2 | 0.066 (3) | 0.049 (3) | 0.030 (2) | 0.012 (2) | 0.007 (2) | 0.0025 (19) |
| C3 | 0.099 (5) | 0.047 (3) | 0.042 (3) | 0.025 (3) | 0.025 (3) | 0.011 (2) |
| C4 | 0.113 (5) | 0.034 (3) | 0.042 (3) | −0.008 (3) | 0.026 (3) | 0.003 (2) |
| C5 | 0.061 (3) | 0.050 (3) | 0.042 (2) | −0.016 (2) | 0.012 (2) | 0.003 (2) |
| C6 | 0.046 (3) | 0.039 (2) | 0.040 (2) | −0.0013 (19) | 0.014 (2) | −0.0024 (18) |
| C7 | 0.069 (3) | 0.054 (3) | 0.048 (3) | 0.017 (3) | 0.023 (3) | 0.017 (2) |
| C8 | 0.048 (3) | 0.038 (2) | 0.038 (2) | 0.0016 (19) | 0.009 (2) | −0.0005 (18) |
| C9 | 0.045 (3) | 0.060 (3) | 0.054 (3) | 0.012 (2) | 0.015 (2) | 0.002 (2) |
| C10 | 0.060 (3) | 0.061 (3) | 0.042 (3) | 0.013 (2) | 0.009 (2) | 0.004 (2) |
| C11 | 0.062 (3) | 0.044 (3) | 0.043 (2) | 0.003 (2) | 0.023 (2) | 0.000 (2) |
| C12 | 0.047 (3) | 0.063 (3) | 0.057 (3) | 0.013 (2) | 0.019 (2) | 0.007 (2) |
| C13 | 0.042 (3) | 0.062 (3) | 0.047 (3) | 0.008 (2) | 0.008 (2) | 0.007 (2) |
| C14 | 0.092 (5) | 0.092 (5) | 0.076 (4) | 0.016 (4) | 0.053 (4) | 0.018 (3) |
| C15 | 0.136 (5) | 0.096 (4) | 0.122 (5) | 0.017 (4) | −0.015 (4) | −0.007 (4) |
| C16 | 0.101 (4) | 0.079 (4) | 0.112 (4) | 0.022 (3) | 0.012 (3) | −0.001 (3) |
| C17 | 0.141 (5) | 0.118 (5) | 0.143 (5) | −0.004 (4) | 0.045 (4) | 0.023 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Fe2—C5 | 2.034 (5) | C4—H4 | 0.9300 |
| Fe2—C5$^{i}$ | 2.034 (5) | C5—H5 | 0.9300 |
| Fe2—C4 | 2.042 (5) | C6—C7 | 1.483 (7) |
| Fe2—C4$^{i}$ | 2.042 (5) | C6—C8 | 1.531 (6) |

| | | | |
|---|---|---|---|
| Fe2—C1 | 2.044 (4) | C8—C13 | 1.373 (6) |
| Fe2—C1$^{i}$ | 2.044 (4) | C8—C9 | 1.379 (6) |
| Fe2—C3 | 2.045 (5) | C9—C10 | 1.370 (6) |
| Fe2—C3$^{i}$ | 2.045 (5) | C9—H9 | 0.9300 |
| Fe2—C2 | 2.048 (4) | C10—C11 | 1.382 (7) |
| Fe2—C2$^{i}$ | 2.048 (4) | C10—H10 | 0.9300 |
| Si1—O1 | 1.663 (3) | C11—C12 | 1.378 (7) |
| Si1—C15 | 1.833 (7) | C12—C13 | 1.378 (6) |
| Si1—C17 | 1.841 (8) | C12—H12 | 0.9300 |
| Si1—C16 | 1.842 (7) | C13—H13 | 0.9300 |
| N1—C7 | 1.164 (7) | C14—H14A | 0.9600 |
| O1—C6 | 1.401 (5) | C14—H14B | 0.9600 |
| O2—C11 | 1.360 (5) | C14—H14C | 0.9600 |
| O2—C14 | 1.425 (7) | C15—H15A | 0.9600 |
| C1—C2 | 1.422 (7) | C15—H15B | 0.9600 |
| C1—C5 | 1.433 (6) | C15—H15C | 0.9600 |
| C1—C6 | 1.511 (6) | C16—H16A | 0.9600 |
| C2—C3 | 1.428 (7) | C16—H16B | 0.9600 |
| C2—H2 | 0.9300 | C16—H16C | 0.9600 |
| C3—C4 | 1.399 (8) | C17—H17A | 0.9600 |
| C3—H3 | 0.9300 | C17—H17B | 0.9600 |
| C4—C5 | 1.395 (8) | C17—H17C | 0.9600 |
| C5—Fe2—C5$^{i}$ | 180.0 (3) | C4—C3—Fe2 | 69.9 (3) |
| C5—Fe2—C4 | 40.0 (2) | C2—C3—Fe2 | 69.7 (3) |
| C5$^{i}$—Fe2—C4 | 140.0 (2) | C4—C3—H3 | 125.7 |
| C5—Fe2—C4$^{i}$ | 140.0 (2) | C2—C3—H3 | 125.7 |
| C5$^{i}$—Fe2—C4$^{i}$ | 40.0 (2) | Fe2—C3—H3 | 126.3 |
| C4—Fe2—C4$^{i}$ | 180.0 (3) | C5—C4—C3 | 108.5 (4) |
| C5—Fe2—C1 | 41.15 (17) | C5—C4—Fe2 | 69.7 (3) |
| C5$^{i}$—Fe2—C1 | 138.85 (17) | C3—C4—Fe2 | 70.1 (3) |
| C4—Fe2—C1 | 68.36 (18) | C5—C4—H4 | 125.8 |
| C4$^{i}$—Fe2—C1 | 111.64 (18) | C3—C4—H4 | 125.8 |
| C5—Fe2—C1$^{i}$ | 138.85 (17) | Fe2—C4—H4 | 126.0 |
| C5$^{i}$—Fe2—C1$^{i}$ | 41.15 (17) | C4—C5—C1 | 108.5 (5) |
| C4—Fe2—C1$^{i}$ | 111.64 (18) | C4—C5—Fe2 | 70.3 (3) |
| C4$^{i}$—Fe2—C1$^{i}$ | 68.36 (18) | C1—C5—Fe2 | 69.8 (2) |
| C1—Fe2—C1$^{i}$ | 180.00 (11) | C4—C5—H5 | 125.8 |
| C5—Fe2—C3 | 67.6 (2) | C1—C5—H5 | 125.8 |
| C5$^{i}$—Fe2—C3 | 112.4 (2) | Fe2—C5—H5 | 125.7 |
| C4—Fe2—C3 | 40.0 (2) | O1—C6—C7 | 109.7 (4) |
| C4$^{i}$—Fe2—C3 | 140.0 (2) | O1—C6—C1 | 108.4 (4) |
| C1—Fe2—C3 | 68.23 (19) | C7—C6—C1 | 107.3 (4) |
| C1$^{i}$—Fe2—C3 | 111.77 (19) | O1—C6—C8 | 112.2 (3) |
| C5—Fe2—C3$^{i}$ | 112.4 (2) | C7—C6—C8 | 110.0 (4) |
| C5$^{i}$—Fe2—C3$^{i}$ | 67.6 (2) | C1—C6—C8 | 108.9 (4) |

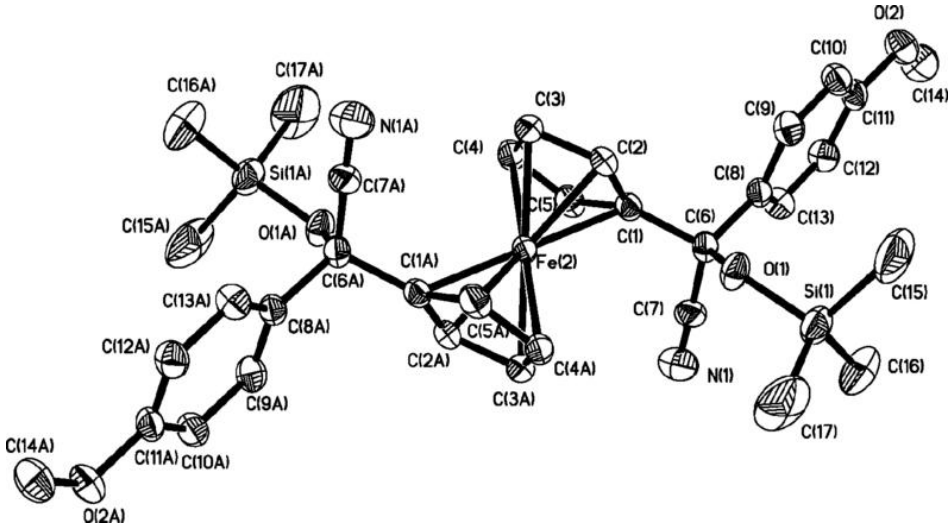
| | | | |
|---|---|---|---|
| C4—Fe2—C3$^{i}$ | 140.0 (2) | N1—C7—C6 | 178.9 (6) |
| C4$^{i}$—Fe2—C3$^{i}$ | 40.0 (2) | C13—C8—C9 | 117.6 (4) |
| C1—Fe2—C3$^{i}$ | 111.77 (19) | C13—C8—C6 | 123.2 (4) |
| C1$^{i}$—Fe2—C3$^{i}$ | 68.23 (19) | C9—C8—C6 | 119.2 (4) |
| C3—Fe2—C3$^{i}$ | 180.0 (4) | C10—C9—C8 | 121.5 (4) |
| C5—Fe2—C2 | 68.5 (2) | C10—C9—H9 | 119.3 |
| C5$^{i}$—Fe2—C2 | 111.5 (2) | C8—C9—H9 | 119.3 |
| C4—Fe2—C2 | 68.3 (2) | C9—C10—C11 | 120.5 (5) |
| C4$^{i}$—Fe2—C2 | 111.7 (2) | C9—C10—H10 | 119.8 |
| C1—Fe2—C2 | 40.67 (18) | C11—C10—H10 | 119.8 |
| C1$^{i}$—Fe2—C2 | 139.33 (18) | O2—C11—C12 | 125.1 (5) |
| C3—Fe2—C2 | 40.83 (19) | O2—C11—C10 | 116.2 (5) |
| C3$^{i}$—Fe2—C2 | 139.17 (19) | C12—C11—C10 | 118.7 (4) |
| C5—Fe2—C2$^{i}$ | 111.5 (2) | C13—C12—C11 | 120.0 (4) |
| C5$^{i}$—Fe2—C2$^{i}$ | 68.5 (2) | C13—C12—H12 | 120.0 |
| C4—Fe2—C2$^{i}$ | 111.7 (2) | C11—C12—H12 | 120.0 |
| C4$^{i}$—Fe2—C2$^{i}$ | 68.3 (2) | C8—C13—C12 | 121.8 (5) |
| C1—Fe2—C2$^{i}$ | 139.33 (18) | C8—C13—H13 | 119.1 |
| C1$^{i}$—Fe2—C2$^{i}$ | 40.67 (18) | C12—C13—H13 | 119.1 |
| C3—Fe2—C2$^{i}$ | 139.17 (19) | O2—C14—H14A | 109.5 |
| C3$^{i}$—Fe2—C2$^{i}$ | 40.83 (19) | O2—C14—H14B | 109.5 |
| C2—Fe2—C2$^{i}$ | 180.00 (7) | H14A—C14—H14B | 109.5 |
| O1—Si1—C15 | 107.0 (3) | O2—C14—H14C | 109.5 |
| O1—Si1—C17 | 105.0 (3) | H14A—C14—H14C | 109.5 |
| C15—Si1—C17 | 110.9 (4) | H14B—C14—H14C | 109.5 |
| O1—Si1—C16 | 113.7 (3) | Si1—C15—H15A | 109.5 |
| C15—Si1—C16 | 108.6 (4) | Si1—C15—H15B | 109.5 |
| C17—Si1—C16 | 111.7 (4) | H15A—C15—H15B | 109.5 |
| C6—O1—Si1 | 131.6 (3) | Si1—C15—H15C | 109.5 |
| C11—O2—C14 | 117.4 (4) | H15A—C15—H15C | 109.5 |
| C2—C1—C5 | 107.2 (4) | H15B—C15—H15C | 109.5 |
| C2—C1—C6 | 126.1 (4) | Si1—C16—H16A | 109.5 |
| C5—C1—C6 | 126.6 (4) | Si1—C16—H16B | 109.5 |
| C2—C1—Fe2 | 69.8 (2) | H16A—C16—H16B | 109.5 |
| C5—C1—Fe2 | 69.0 (2) | Si1—C16—H16C | 109.5 |
| C6—C1—Fe2 | 129.5 (3) | H16A—C16—H16C | 109.5 |
| C1—C2—C3 | 107.2 (4) | H16B—C16—H16C | 109.5 |
| C1—C2—Fe2 | 69.5 (2) | Si1—C17—H17A | 109.5 |
| C3—C2—Fe2 | 69.5 (3) | Si1—C17—H17B | 109.5 |
| C1—C2—H2 | 126.4 | H17A—C17—H17B | 109.5 |
| C3—C2—H2 | 126.4 | Si1—C17—H17C | 109.5 |
| Fe2—C2—H2 | 126.2 | H17A—C17—H17C | 109.5 |
| C4—C3—C2 | 108.6 (5) | H17B—C17—H17C | 109.5 |
| C15—Si1—O1—C6 | 108.2 (5) | C4$^{i}$—Fe2—C4—C5 | 17 (100) |
| C17—Si1—O1—C6 | −134.0 (5) | C1—Fe2—C4—C5 | 38.1 (3) |

| | | | |
|---|---|---|---|
| C16—Si1—O1—C6 | −11.6 (5) | C1$^{i}$—Fe2—C4—C5 | −141.9 (3) |
| C5—Fe2—C1—C2 | 118.6 (4) | C3—Fe2—C4—C5 | 119.6 (4) |
| C5$^{i}$—Fe2—C1—C2 | −61.4 (4) | C3$^{i}$—Fe2—C4—C5 | −60.4 (4) |
| C4—Fe2—C1—C2 | 81.5 (3) | C2—Fe2—C4—C5 | 82.0 (3) |
| C4$^{i}$—Fe2—C1—C2 | −98.5 (3) | C2$^{i}$—Fe2—C4—C5 | −98.0 (3) |
| C1$^{i}$—Fe2—C1—C2 | −51 (100) | C5—Fe2—C4—C3 | −119.6 (4) |
| C3—Fe2—C1—C2 | 38.2 (3) | C5$^{i}$—Fe2—C4—C3 | 60.4 (4) |
| C3$^{i}$—Fe2—C1—C2 | −141.8 (3) | C4$^{i}$—Fe2—C4—C3 | −102 (100) |
| C2$^{i}$—Fe2—C1—C2 | 180.0 | C1—Fe2—C4—C3 | −81.5 (3) |
| C5$^{i}$—Fe2—C1—C5 | 180.0 | C1$^{i}$—Fe2—C4—C3 | 98.5 (3) |
| C4—Fe2—C1—C5 | −37.1 (3) | C3$^{i}$—Fe2—C4—C3 | 180.0 |
| C4$^{i}$—Fe2—C1—C5 | 142.9 (3) | C2—Fe2—C4—C3 | −37.6 (3) |
| C1$^{i}$—Fe2—C1—C5 | −170 (100) | C2$^{i}$—Fe2—C4—C3 | 142.4 (3) |
| C3—Fe2—C1—C5 | −80.3 (3) | C3—C4—C5—C1 | 0.0 (5) |
| C3$^{i}$—Fe2—C1—C5 | 99.7 (3) | Fe2—C4—C5—C1 | −59.6 (3) |
| C2—Fe2—C1—C5 | −118.6 (4) | C3—C4—C5—Fe2 | 59.6 (3) |
| C2$^{i}$—Fe2—C1—C5 | 61.4 (4) | C2—C1—C5—C4 | 0.3 (5) |
| C5—Fe2—C1—C6 | −120.8 (5) | C6—C1—C5—C4 | −175.9 (4) |
| C5$^{i}$—Fe2—C1—C6 | 59.2 (5) | Fe2—C1—C5—C4 | 59.9 (3) |
| C4—Fe2—C1—C6 | −157.9 (5) | C2—C1—C5—Fe2 | −59.6 (3) |
| C4$^{i}$—Fe2—C1—C6 | 22.1 (5) | C6—C1—C5—Fe2 | 124.3 (4) |
| C1$^{i}$—Fe2—C1—C6 | 69 (100) | C5$^{i}$—Fe2—C5—C4 | −170 (100) |
| C3—Fe2—C1—C6 | 158.9 (5) | C4$^{i}$—Fe2—C5—C4 | 180.0 |
| C3$^{i}$—Fe2—C1—C6 | −21.1 (5) | C1—Fe2—C5—C4 | −119.4 (4) |
| C2—Fe2—C1—C6 | 120.7 (5) | C1$^{i}$—Fe2—C5—C4 | 60.6 (4) |
| C2$^{i}$—Fe2—C1—C6 | −59.3 (5) | C3—Fe2—C5—C4 | −37.2 (3) |
| C5—C1—C2—C3 | −0.4 (5) | C3$^{i}$—Fe2—C5—C4 | 142.8 (3) |
| C6—C1—C2—C3 | 175.8 (4) | C2—Fe2—C5—C4 | −81.4 (3) |
| Fe2—C1—C2—C3 | −59.5 (3) | C2$^{i}$—Fe2—C5—C4 | 98.6 (3) |
| C5—C1—C2—Fe2 | 59.1 (3) | C5$^{i}$—Fe2—C5—C1 | −50 (100) |
| C6—C1—C2—Fe2 | −124.7 (4) | C4—Fe2—C5—C1 | 119.4 (4) |
| C5—Fe2—C2—C1 | −38.4 (3) | C4$^{i}$—Fe2—C5—C1 | −60.6 (4) |
| C5$^{i}$—Fe2—C2—C1 | 141.6 (3) | C1$^{i}$—Fe2—C5—C1 | 180.0 |
| C4—Fe2—C2—C1 | −81.6 (3) | C3—Fe2—C5—C1 | 82.1 (3) |
| C4$^{i}$—Fe2—C2—C1 | 98.4 (3) | C3$^{i}$—Fe2—C5—C1 | −97.9 (3) |
| C1$^{i}$—Fe2—C2—C1 | 180.0 | C2—Fe2—C5—C1 | 38.0 (3) |
| C3—Fe2—C2—C1 | −118.5 (4) | C2$^{i}$—Fe2—C5—C1 | −142.0 (3) |
| C3$^{i}$—Fe2—C2—C1 | 61.5 (4) | Si1—O1—C6—C7 | 58.0 (5) |
| C2$^{i}$—Fe2—C2—C1 | 22 (100) | Si1—O1—C6—C1 | 174.9 (3) |
| C5—Fe2—C2—C3 | 80.1 (3) | Si1—O1—C6—C8 | −64.7 (5) |
| C5$^{i}$—Fe2—C2—C3 | −99.9 (3) | C2—C1—C6—O1 | 30.2 (6) |
| C4—Fe2—C2—C3 | 36.9 (3) | C5—C1—C6—O1 | −154.4 (4) |

| | | | |
|---|---|---|---|
| $C4^{i}$—Fe2—C2—C3 | −143.1 (3) | Fe2—C1—C6—O1 | −62.5 (5) |
| C1—Fe2—C2—C3 | 118.5 (4) | C2—C1—C6—C7 | 148.7 (4) |
| $C1^{i}$—Fe2—C2—C3 | −61.5 (4) | C5—C1—C6—C7 | −35.9 (6) |
| $C3^{i}$—Fe2—C2—C3 | 180.0 | Fe2—C1—C6—C7 | 56.0 (5) |
| $C2^{i}$—Fe2—C2—C3 | 140 (100) | C2—C1—C6—C8 | −92.2 (5) |
| C1—C2—C3—C4 | 0.4 (5) | C5—C1—C6—C8 | 83.2 (5) |
| Fe2—C2—C3—C4 | −59.2 (3) | Fe2—C1—C6—C8 | 175.1 (3) |
| C1—C2—C3—Fe2 | 59.6 (3) | O1—C6—C7—N1 | 137 (29) |
| C5—Fe2—C3—C4 | 37.2 (3) | C1—C6—C7—N1 | 19 (29) |
| $C5^{i}$—Fe2—C3—C4 | −142.8 (3) | C8—C6—C7—N1 | −99 (29) |
| $C4^{i}$—Fe2—C3—C4 | 180.0 | O1—C6—C8—C13 | 131.0 (5) |
| C1—Fe2—C3—C4 | 81.8 (3) | C7—C6—C8—C13 | 8.5 (6) |
| $C1^{i}$—Fe2—C3—C4 | −98.2 (3) | C1—C6—C8—C13 | −109.0 (5) |
| $C3^{i}$—Fe2—C3—C4 | 127 (100) | O1—C6—C8—C9 | −50.2 (6) |
| C2—Fe2—C3—C4 | 119.9 (4) | C7—C6—C8—C9 | −172.7 (4) |
| $C2^{i}$—Fe2—C3—C4 | −60.1 (4) | C1—C6—C8—C9 | 69.9 (5) |
| C5—Fe2—C3—C2 | −82.7 (3) | C13—C8—C9—C10 | −1.2 (7) |
| $C5^{i}$—Fe2—C3—C2 | 97.3 (3) | C6—C8—C9—C10 | 179.9 (4) |
| C4—Fe2—C3—C2 | −119.9 (4) | C8—C9—C10—C11 | 0.1 (8) |
| $C4^{i}$—Fe2—C3—C2 | 60.1 (4) | C14—O2—C11—C12 | −1.0 (8) |
| C1—Fe2—C3—C2 | −38.1 (3) | C14—O2—C11—C10 | 178.6 (5) |
| $C1^{i}$—Fe2—C3—C2 | 141.9 (3) | C9—C10—C11—O2 | −177.9 (5) |
| $C3^{i}$—Fe2—C3—C2 | 7(100) | C9—C10—C11—C12 | 1.8 (7) |
| $C2^{i}$—Fe2—C3—C2 | 180.0 | O2—C11—C12—C13 | 177.2 (5) |
| C2—C3—C4—C5 | −0.2 (5) | C10—C11—C12—C13 | −2.4 (8) |
| Fe2—C3—C4—C5 | −59.3 (3) | C9—C8—C13—C12 | 0.5 (7) |
| C2—C3—C4—Fe2 | 59.1 (3) | C6—C8—C13—C12 | 179.4 (4) |
| $C5^{i}$—Fe2—C4—C5 | 180.0 | C11—C12—C13—C8 | 1.3 (8) |

Symmetry codes: (i) −*x*+2, −*y*, −*z*.

**Fig. 1**


O(2)
C(10)
C(14)
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O(1)
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Si(1A)
C(7A)
C(15A)
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