Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Pentacarbonyl-1$\kappa^2C$,2$\kappa^3C$-(ferrocenyldiphenylphosphine-1$\kappa P$)[$\mu$-2-(4-methylphenyl)-2-azapropane-1,3-dithiolato-1:2$\kappa^4S,S'$:$S,S'$]diiron(I)(*Fe—Fe*)

**Yan-Feng Tang and Jin-Li Zhu***

School of Chemistry and Chemical Engineering, Nantong University, Natong 226007, People's Republic of China
Correspondence e-mail: jinlizhu@ntu.edu.cn

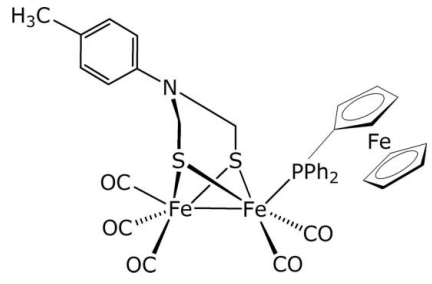
Received 26 September 2008; accepted 10 October 2008

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.048; $wR$ factor = 0.079; data-to-parameter ratio = 18.9.

The title compound, $[Fe_2(C_9H_{11}NS_2)\{Fe(C_5H_5)(C_{17}H_{14}P)\}(CO)_5]$, was prepared as an azadithiolato–iron model for the iron-only hydrogenase active site. The $Fe_2S_2$ unit exhibits a butterfly conformation and the ferrocenyldiphenylphosphine ligand is *trans* to the Fe—Fe bond. The Fe—Fe distance of 2.5160 (8) Å is longer than found in related model structures. Intramolecular C—H···S and intermolecular C—H···O hydrogen bonds are observed.

## Related literature

For general background, see: Cammack (1999); Evans & Pickett (2003); Nicolet *et al.* (1999); Peters *et al.* (1998). For related structures, see: Hou *et al.* (2006); Lawrence *et al.* (2001); Ott *et al.* (2004).




## Experimental

### Crystal data

$[Fe_3(C_5H_5)(C_9H_{11}NS_2)(C_{17}H_{14}P)(CO)_5]$
$M_r$ = 819.25
Monoclinic, $P2_1/c$
$a$ = 13.600 (2) Å
$b$ = 10.8964 (19) Å
$c$ = 23.396 (4) Å
$\beta$ = 94.741 (3)°
$V$ = 3455.2 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.45 mm$^{-1}$
$T$ = 298 (2) K
0.20 × 0.20 × 0.10 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.760, $T_{max}$ = 0.868
21457 measured reflections
8202 independent reflections
4258 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.070

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.079
$S$ = 0.80
8202 reflections
434 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Fe1—C13 | 1.750 (4) | Fe2—C11 | 1.761 (5) |
| Fe1—P1 | 2.2565 (10) | Fe2—C12 | 1.777 (5) |
| Fe1—S1 | 2.2762 (11) | Fe2—C10 | 1.813 (5) |
| Fe1—S2 | 2.2818 (11) | Fe2—S2 | 2.2546 (11) |
| Fe1—Fe2 | 2.5160 (8) | Fe2—S1 | 2.2867 (11) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C22—H22···O2$^{i}$ | 0.98 | 2.53 | 3.224 (5) | 128 |
| C24—H24···S2 | 0.98 | 2.72 | 3.561 (4) | 144 |

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: *SHELXL97*.

The authors thank the Science Foundation of Nantong Municipality (grant No. K2007011), the Science Foundation of Nantong University (grant Nos. 06Z017 and 06Z022) and the National Natural Science Foundation of China (grant No. 20276009) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2685).

## References

Bruker (1997). *SMART* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cammack, R. (1999). *Nature* (*London*), **297**, 214–215.
Evans, D. J. & Pickett, C. J. (2003). *Chem. Soc. Rev.* **32**, 268–275.
Hou, J., Peng, X. J., Liu, J. F., Gao, Y. L., Zhao, X., Gao, S. & Han, K. L. (2006). *Eur. J. Inorg. Chem.* pp. 4679–4686.
Lawrence, J. D., Li, H., Rauchfuss, T. B., Bénard, M. & Rohmer, M.-M. (2001). *Angew. Chem. Int. Ed.* **113**, 1818–1821.
Nicolet, Y., Piras, C., Legrand, P. C., Hatchikian, E. & Fontecilla-Camps, J. C. (1999). *Structure*, **7**, 13–23.
Ott, S., Borgström, M., Kritikos, M., Lomoth, R., Bergquist, J., Åkermark, B., Hammarström, L. & Sun, L. (2004). *Inorg. Chem.* **43**, 4683–4692.
Peters, J. W., Lanzilotta, W. N., Lemon, B. J. & Seefeldt, L. C. (1998). *Science*, **282**, 1853–1858.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supplementary materials

*Acta Cryst.* (2008). E**64**, m1423 [ **doi:10.1107/S1600536808032698** ]

# Pentacarbonyl-1$\kappa^2C$,2$\kappa^3C$-(ferrocenyldiphenylphosphine-1$\kappa P$)[$\mu$-2-(4-methylphenyl)-2-azapropane-1,3-dithiolato-1:2$\kappa^4S,S':S,S'$]diiron(I)(*Fe-Fe*)

**Y.-F. Tang and J.-L. Zhu**

## Comment

The iron-only hydrogenases are enzymes that can efficiently catalyze the reversible reaction of hydrogen production (Cammack, 1999; Evans & Pickett, 2003). The active site at which this reaction takes place is composed of a butterfly shaped $Fe_2S_2$ unit covalently linked to a conventional $Fe_4S_4$ cluster by a bridged cysteinyl thioether (Peters *et al.*, 1998; Nicolet *et al.*, 1999). We have prepared the title complex as a structural model for the iron-only hydrogenases active site. Herein we report its crystal structure.

The molecular structure of the title complex is shown in Fig.1 and selected bond distances are listed in Table 1. In the $Fe_2S_2$ unit, the Fe—Fe distance of 2.5160 (8) Å is slightly longer than those observed in related complexes (Lawrence *et al.*, 2001; Ott *et al.*, 2004). The $FcPPh_2$ (Fc is ferrocenyl and Ph is phenyl) ligand is in apical position (*trans* to Fe—Fe bond), with an Fe—P distance of 2.2565 (10) Å. The Fe1—C(≡O) distances are ~0.04 Å shorter than those found in a related complex (Hou *et al.*, 2006), consistent with an increase in the charge of Fe1 because one of the CO ligands was replaced by the $FcPPh_2$ ligand. The ferrocene unit is covalently linked to the $Fe_2S_2$ unit *via* the bridged diphenyl P atom, with an Fe1—P1—C23 angle of 118.32 (12)°. The N1 atom is displaced from the C5/C8/C9 plane by 0.168 (3) Å, and the sum of angles around N1 is 355.8°.

Intramolecular C—H···S and intermolecular C—H···O hydrogen bonds are observed.

## Experimental

The starting material $[Fe_2(\mu\text{-}SCH_2)_2(4\text{-}CH_3C_6H_4N)(CO)_6]$ was obtained in 50% yield according to the literature method (Hou *et al.*, 2006). The solution of $Me_3NO$ (120 mg, 1.06 mmol) was added to a red solution of $[Fe_2(\mu\text{-}SCH_2)_2(4\text{-}CH_3C_6H_4N)(CO)_6]$ (0.50 g, 1.05 mmol) with $FcPPh_2$ (0.39 g, 1.05 mmol) in $CH_3CN$ (100 ml) *via* syringe under a nitrogen atmosphere. The reaction mixture was stirred at ambient temperature until the TLC indicated there was no remaining carbonyl complex of starting material. The solvent was removed under vacuum and the resulted dark red residue was purified by column chromatography on silica gel eluting with $CH_2Cl_2$-hexane (1:5 *v/v*). A dark red solid was obtained from recrystallization in n-pentane-$CH_2Cl_2$. Single crystals of the title compound for X-ray analysis were grown from a $CH_2Cl_2$-hexane (1:5 *v/v*) solution by slow evaporation at ambient temperature.

## Refinement

H atoms were placed in geometrically calculated positions (C—H = 0.93–0.98 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$($C_{methyl}$)

## Figures

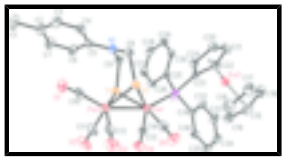


Fig. 1. The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level.

## Pentacarbonyl-1κ$^2$C,2κ$^3$C-(ferrocenyldiphenylphosphine-1κP)[μ-2-(4- methylphenyl)-2-azapropane-1,3-dithiolato- 1:2κ$^4$*S*,*S*':*S*,*S*']diiron(I)(Fe—Fe)

*Crystal data*

| | |
|---|---|
| $[Fe_3(C_5H_5)(C_9H_{11}NS_2)(C_{17}H_{14}P)(CO)_5]$ | $F_{000}$ = 1672 |
| $M_r$ = 819.25 | $D_x$ = 1.575 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 2549 reflections |
| $a$ = 13.600 (2) Å | θ = 2.4–22.0º |
| $b$ = 10.8964 (19) Å | μ = 1.45 mm$^{-1}$ |
| $c$ = 23.396 (4) Å | $T$ = 298 (2) K |
| β = 94.741 (3)º | Block, red |
| $V$ = 3455.2 (11) Å$^3$ | 0.20 × 0.20 × 0.10 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 8202 independent reflections |
| Radiation source: fine-focus sealed tube | 4258 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.070 |
| $T$ = 298(2) K | $\theta_{max}$ = 28.4º |
| φ and ω scans | $\theta_{min}$ = 1.5º |
| Absorption correction: multi-scan (SADABS; Bruker, 1997) | $h$ = −17→18 |
| $T_{min}$ = 0.760, $T_{max}$ = 0.868 | $k$ = −9→14 |
| 21457 measured reflections | $l$ = −31→30 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0157P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $wR(F^2)$ = 0.079 | $\Delta\rho_{max}$ = 0.66 e Å$^{-3}$ |
| $S$ = 0.80 | $\Delta\rho_{min}$ = −0.38 e Å$^{-3}$ |

8202 reflections
434 parameters

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^ > σ(*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 | 0.20737 (4) | 0.18453 (5) | 0.30929 (2) | 0.03252 (14) |
| Fe2 | 0.20176 (4) | 0.09491 (5) | 0.40808 (2) | 0.03988 (16) |
| Fe3 | 0.08083 (4) | 0.09519 (5) | 0.11522 (2) | 0.04244 (16) |
| S1 | 0.34466 (7) | 0.12772 (9) | 0.36528 (4) | 0.0387 (2) |
| S2 | 0.15575 (7) | −0.00994 (9) | 0.32718 (4) | 0.0382 (2) |
| P1 | 0.26239 (7) | 0.19707 (9) | 0.22109 (4) | 0.0316 (2) |
| O1 | 0.2115 (2) | −0.1033 (3) | 0.49363 (13) | 0.0791 (11) |
| O2 | 0.2652 (3) | 0.3021 (3) | 0.48103 (14) | 0.1006 (13) |
| O3 | −0.0037 (2) | 0.1481 (3) | 0.42412 (14) | 0.0962 (12) |
| O4 | 0.2502 (2) | 0.4345 (2) | 0.34576 (12) | 0.0634 (9) |
| O5 | 0.0021 (2) | 0.2479 (3) | 0.27912 (12) | 0.0661 (9) |
| N1 | 0.3407 (2) | −0.1259 (3) | 0.34951 (12) | 0.0409 (8) |
| C1 | 0.4517 (4) | −0.3802 (4) | 0.56016 (18) | 0.0874 (16) |
| H1A | 0.4496 | −0.4671 | 0.5535 | 0.131* |
| H1B | 0.4066 | −0.3592 | 0.5881 | 0.131* |
| H1C | 0.5173 | −0.3566 | 0.5741 | 0.131* |
| C2 | 0.4224 (3) | −0.3132 (4) | 0.50438 (17) | 0.0536 (11) |
| C3 | 0.3533 (3) | −0.3595 (4) | 0.46376 (18) | 0.0529 (11) |
| H3 | 0.3241 | −0.4348 | 0.4706 | 0.063* |
| C4 | 0.3255 (3) | −0.2992 (4) | 0.41345 (16) | 0.0459 (10) |
| H4 | 0.2792 | −0.3346 | 0.3870 | 0.055* |
| C5 | 0.3662 (3) | −0.1853 (4) | 0.40172 (16) | 0.0394 (9) |
| C6 | 0.4364 (3) | −0.1384 (4) | 0.44210 (17) | 0.0485 (11) |
| H6 | 0.4658 | −0.0634 | 0.4353 | 0.058* |
| C7 | 0.4635 (3) | −0.2009 (4) | 0.49226 (17) | 0.0579 (12) |
| H7 | 0.5107 | −0.1667 | 0.5186 | 0.069* |
| C8 | 0.2455 (3) | −0.1362 (3) | 0.31877 (16) | 0.0479 (11) |
| H8A | 0.2156 | −0.2121 | 0.3304 | 0.057* |
| H8B | 0.2551 | −0.1436 | 0.2783 | 0.057* |
| C9 | 0.3917 (3) | −0.0175 (3) | 0.33541 (15) | 0.0448 (10) |
| H9A | 0.3883 | −0.0103 | 0.2940 | 0.054* |

| | | | | |
|---|---|---|---|---|
| H9B | 0.4606 | −0.0266 | 0.3490 | 0.054* |
| C10 | 0.2131 (3) | −0.0291 (4) | 0.45986 (18) | 0.0539 (12) |
| C11 | 0.2391 (3) | 0.2194 (4) | 0.45270 (18) | 0.0651 (14) |
| C12 | 0.0758 (3) | 0.1262 (4) | 0.41723 (17) | 0.0561 (12) |
| C13 | 0.2339 (3) | 0.3362 (4) | 0.32971 (15) | 0.0385 (10) |
| C14 | 0.0838 (3) | 0.2218 (3) | 0.28947 (16) | 0.0431 (10) |
| C15 | 0.0207 (4) | 0.2515 (5) | 0.0789 (2) | 0.0749 (15) |
| H15 | 0.0568 | 0.3196 | 0.0630 | 0.090* |
| C16 | −0.0165 (4) | 0.1463 (5) | 0.0488 (2) | 0.0738 (15) |
| H16 | −0.0101 | 0.1287 | 0.0081 | 0.089* |
| C17 | −0.0633 (3) | 0.0727 (5) | 0.0861 (2) | 0.0736 (15) |
| H17 | −0.0958 | −0.0058 | 0.0766 | 0.088* |
| C18 | −0.0557 (3) | 0.1293 (5) | 0.1406 (2) | 0.0686 (14) |
| H18 | −0.0826 | 0.0979 | 0.1754 | 0.082* |
| C19 | −0.0044 (3) | 0.2407 (4) | 0.1355 (2) | 0.0662 (14) |
| H19 | 0.0115 | 0.2999 | 0.1664 | 0.079* |
| C20 | 0.1400 (3) | −0.0774 (4) | 0.12177 (17) | 0.0518 (11) |
| H20 | 0.1039 | −0.1546 | 0.1152 | 0.062* |
| C21 | 0.1848 (3) | −0.0097 (4) | 0.08032 (18) | 0.0551 (12) |
| H21 | 0.1854 | −0.0312 | 0.0397 | 0.066* |
| C22 | 0.2278 (3) | 0.0960 (4) | 0.10657 (15) | 0.0440 (10) |
| H22 | 0.2638 | 0.1598 | 0.0874 | 0.053* |
| C23 | 0.2103 (2) | 0.0944 (3) | 0.16603 (14) | 0.0331 (9) |
| C24 | 0.1549 (3) | −0.0139 (3) | 0.17502 (16) | 0.0429 (10) |
| H24 | 0.1310 | −0.0401 | 0.2115 | 0.051* |
| C25 | 0.3951 (2) | 0.1685 (3) | 0.22119 (14) | 0.0303 (8) |
| C26 | 0.4591 (3) | 0.2380 (3) | 0.25719 (15) | 0.0380 (9) |
| H26 | 0.4338 | 0.2998 | 0.2791 | 0.046* |
| C27 | 0.5593 (3) | 0.2175 (4) | 0.26120 (16) | 0.0471 (11) |
| H27 | 0.6011 | 0.2650 | 0.2857 | 0.056* |
| C28 | 0.5975 (3) | 0.1257 (4) | 0.22858 (17) | 0.0483 (11) |
| H28 | 0.6650 | 0.1103 | 0.2315 | 0.058* |
| C29 | 0.5357 (3) | 0.0582 (3) | 0.19212 (16) | 0.0455 (11) |
| H29 | 0.5618 | −0.0015 | 0.1693 | 0.055* |
| C30 | 0.4351 (3) | 0.0770 (3) | 0.18864 (15) | 0.0370 (9) |
| H30 | 0.3937 | 0.0283 | 0.1645 | 0.044* |
| C31 | 0.2548 (3) | 0.3488 (3) | 0.18691 (15) | 0.0343 (9) |
| C32 | 0.3189 (3) | 0.3814 (3) | 0.14616 (16) | 0.0477 (11) |
| H32 | 0.3677 | 0.3266 | 0.1371 | 0.057* |
| C33 | 0.3115 (3) | 0.4942 (4) | 0.11883 (17) | 0.0577 (12) |
| H33 | 0.3544 | 0.5141 | 0.0913 | 0.069* |
| C34 | 0.2412 (3) | 0.5761 (4) | 0.13229 (18) | 0.0591 (12) |
| H34 | 0.2364 | 0.6519 | 0.1140 | 0.071* |
| C35 | 0.1777 (3) | 0.5472 (4) | 0.17249 (18) | 0.0547 (12) |
| H35 | 0.1301 | 0.6034 | 0.1817 | 0.066* |
| C36 | 0.1843 (3) | 0.4339 (3) | 0.19954 (15) | 0.0427 (10) |
| H36 | 0.1405 | 0.4148 | 0.2267 | 0.051* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0317 (3) | 0.0340 (3) | 0.0323 (3) | −0.0013 (3) | 0.0052 (2) | −0.0022 (2) |
| Fe2 | 0.0415 (4) | 0.0483 (4) | 0.0305 (3) | −0.0029 (3) | 0.0065 (3) | −0.0030 (3) |
| Fe3 | 0.0349 (3) | 0.0523 (4) | 0.0393 (3) | 0.0000 (3) | −0.0020 (3) | −0.0046 (3) |
| S1 | 0.0357 (6) | 0.0427 (6) | 0.0374 (6) | −0.0044 (5) | 0.0019 (5) | 0.0000 (5) |
| S2 | 0.0405 (6) | 0.0395 (6) | 0.0343 (6) | −0.0058 (5) | 0.0014 (5) | 0.0002 (4) |
| P1 | 0.0296 (5) | 0.0336 (6) | 0.0319 (6) | 0.0006 (5) | 0.0038 (4) | −0.0019 (4) |
| O1 | 0.103 (3) | 0.087 (3) | 0.051 (2) | 0.012 (2) | 0.0248 (19) | 0.0228 (18) |
| O2 | 0.138 (3) | 0.099 (3) | 0.067 (3) | −0.033 (3) | 0.026 (2) | −0.042 (2) |
| O3 | 0.055 (2) | 0.151 (4) | 0.084 (3) | 0.020 (2) | 0.018 (2) | −0.018 (2) |
| O4 | 0.067 (2) | 0.046 (2) | 0.079 (2) | −0.0107 (16) | 0.0131 (17) | −0.0186 (16) |
| O5 | 0.0356 (18) | 0.080 (2) | 0.083 (2) | 0.0090 (16) | 0.0092 (17) | 0.0150 (17) |
| N1 | 0.049 (2) | 0.038 (2) | 0.036 (2) | 0.0013 (16) | 0.0032 (17) | 0.0055 (15) |
| C1 | 0.098 (4) | 0.094 (4) | 0.067 (4) | −0.003 (3) | −0.013 (3) | 0.034 (3) |
| C2 | 0.056 (3) | 0.057 (3) | 0.047 (3) | 0.001 (2) | 0.002 (2) | 0.018 (2) |
| C3 | 0.055 (3) | 0.047 (3) | 0.058 (3) | −0.009 (2) | 0.010 (2) | 0.012 (2) |
| C4 | 0.049 (3) | 0.044 (3) | 0.043 (3) | −0.006 (2) | −0.002 (2) | −0.001 (2) |
| C5 | 0.041 (2) | 0.040 (3) | 0.037 (2) | 0.004 (2) | 0.0059 (19) | 0.0015 (19) |
| C6 | 0.042 (3) | 0.049 (3) | 0.054 (3) | −0.007 (2) | −0.001 (2) | 0.014 (2) |
| C7 | 0.050 (3) | 0.062 (3) | 0.059 (3) | −0.004 (2) | −0.011 (2) | 0.008 (2) |
| C8 | 0.063 (3) | 0.035 (3) | 0.044 (3) | 0.001 (2) | −0.006 (2) | −0.0051 (19) |
| C9 | 0.044 (2) | 0.046 (3) | 0.046 (3) | 0.012 (2) | 0.014 (2) | 0.009 (2) |
| C10 | 0.045 (3) | 0.080 (4) | 0.039 (3) | 0.002 (2) | 0.016 (2) | −0.006 (2) |
| C11 | 0.072 (3) | 0.083 (4) | 0.043 (3) | −0.010 (3) | 0.022 (3) | −0.013 (3) |
| C12 | 0.056 (3) | 0.074 (3) | 0.039 (3) | 0.002 (3) | 0.005 (2) | −0.006 (2) |
| C13 | 0.032 (2) | 0.044 (3) | 0.040 (2) | 0.004 (2) | 0.0056 (18) | −0.004 (2) |
| C14 | 0.045 (3) | 0.037 (3) | 0.050 (3) | −0.006 (2) | 0.012 (2) | 0.0042 (19) |
| C15 | 0.073 (4) | 0.067 (4) | 0.082 (4) | 0.013 (3) | −0.011 (3) | 0.016 (3) |
| C16 | 0.065 (4) | 0.094 (5) | 0.058 (3) | 0.017 (3) | −0.021 (3) | −0.009 (3) |
| C17 | 0.038 (3) | 0.087 (4) | 0.093 (4) | −0.001 (3) | −0.016 (3) | −0.020 (3) |
| C18 | 0.035 (3) | 0.098 (4) | 0.073 (4) | 0.004 (3) | 0.005 (2) | −0.013 (3) |
| C19 | 0.045 (3) | 0.071 (4) | 0.080 (4) | 0.020 (3) | −0.012 (3) | −0.021 (3) |
| C20 | 0.055 (3) | 0.042 (3) | 0.056 (3) | −0.001 (2) | −0.011 (2) | −0.013 (2) |
| C21 | 0.047 (3) | 0.076 (3) | 0.042 (3) | 0.003 (2) | 0.002 (2) | −0.024 (2) |
| C22 | 0.038 (2) | 0.058 (3) | 0.036 (2) | −0.005 (2) | 0.0070 (19) | −0.006 (2) |
| C23 | 0.030 (2) | 0.037 (2) | 0.032 (2) | 0.0003 (18) | 0.0013 (17) | −0.0005 (18) |
| C24 | 0.046 (3) | 0.045 (3) | 0.036 (2) | −0.002 (2) | −0.001 (2) | −0.0014 (19) |
| C25 | 0.030 (2) | 0.032 (2) | 0.030 (2) | 0.0019 (17) | 0.0070 (17) | 0.0068 (16) |
| C26 | 0.037 (2) | 0.036 (2) | 0.042 (2) | −0.0003 (19) | 0.010 (2) | −0.0054 (18) |
| C27 | 0.036 (2) | 0.052 (3) | 0.052 (3) | −0.010 (2) | −0.003 (2) | 0.001 (2) |
| C28 | 0.025 (2) | 0.059 (3) | 0.061 (3) | 0.006 (2) | 0.004 (2) | 0.009 (2) |
| C29 | 0.039 (3) | 0.046 (3) | 0.053 (3) | 0.012 (2) | 0.015 (2) | 0.000 (2) |
| C30 | 0.037 (2) | 0.036 (2) | 0.038 (2) | 0.0036 (18) | 0.0033 (18) | 0.0005 (18) |
| C31 | 0.032 (2) | 0.035 (2) | 0.036 (2) | 0.0001 (17) | 0.0041 (18) | 0.0048 (17) |
| C32 | 0.042 (3) | 0.049 (3) | 0.053 (3) | 0.013 (2) | 0.007 (2) | 0.014 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C33 | 0.053 (3) | 0.065 (3) | 0.057 (3) | 0.006 (3) | 0.014 (2) | 0.027 (2) |
| C34 | 0.060 (3) | 0.050 (3) | 0.067 (3) | 0.008 (2) | −0.001 (3) | 0.023 (2) |
| C35 | 0.054 (3) | 0.045 (3) | 0.065 (3) | 0.021 (2) | 0.004 (2) | 0.009 (2) |
| C36 | 0.036 (2) | 0.050 (3) | 0.043 (2) | 0.008 (2) | 0.0061 (19) | 0.001 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Fe1—C13 | 1.750 (4) | C7—H7 | 0.93 |
| Fe1—C14 | 1.754 (4) | C8—H8A | 0.97 |
| Fe1—P1 | 2.2565 (10) | C8—H8B | 0.97 |
| Fe1—S1 | 2.2762 (11) | C9—H9A | 0.97 |
| Fe1—S2 | 2.2818 (11) | C9—H9B | 0.97 |
| Fe1—Fe2 | 2.5160 (8) | C15—C19 | 1.399 (5) |
| Fe2—C11 | 1.761 (5) | C15—C16 | 1.417 (6) |
| Fe2—C12 | 1.777 (5) | C15—H15 | 0.98 |
| Fe2—C10 | 1.813 (5) | C16—C17 | 1.379 (6) |
| Fe2—S2 | 2.2546 (11) | C16—H16 | 0.98 |
| Fe2—S1 | 2.2867 (11) | C17—C18 | 1.413 (6) |
| Fe3—C22 | 2.025 (4) | C17—H17 | 0.98 |
| Fe3—C18 | 2.030 (4) | C18—C19 | 1.410 (5) |
| Fe3—C16 | 2.034 (4) | C18—H18 | 0.98 |
| Fe3—C17 | 2.036 (4) | C19—H19 | 0.98 |
| Fe3—C24 | 2.038 (4) | C20—C21 | 1.398 (5) |
| Fe3—C21 | 2.040 (4) | C20—C24 | 1.425 (5) |
| Fe3—C23 | 2.041 (3) | C20—H20 | 0.98 |
| Fe3—C19 | 2.043 (4) | C21—C22 | 1.409 (5) |
| Fe3—C15 | 2.044 (4) | C21—H21 | 0.98 |
| Fe3—C20 | 2.047 (4) | C22—C23 | 1.431 (4) |
| S1—C9 | 1.864 (3) | C22—H22 | 0.98 |
| S2—C8 | 1.860 (4) | C23—C24 | 1.425 (4) |
| P1—C23 | 1.806 (3) | C24—H24 | 0.98 |
| P1—C25 | 1.832 (3) | C25—C26 | 1.385 (4) |
| P1—C31 | 1.836 (3) | C25—C30 | 1.392 (4) |
| O1—C10 | 1.132 (4) | C26—C27 | 1.376 (5) |
| O2—C11 | 1.157 (4) | C26—H26 | 0.93 |
| O3—C12 | 1.132 (4) | C27—C28 | 1.385 (5) |
| O4—C13 | 1.151 (4) | C27—H27 | 0.93 |
| O5—C14 | 1.153 (4) | C28—C29 | 1.363 (5) |
| N1—C5 | 1.400 (4) | C28—H28 | 0.93 |
| N1—C9 | 1.421 (4) | C29—C30 | 1.380 (5) |
| N1—C8 | 1.433 (4) | C29—H29 | 0.93 |
| C1—C2 | 1.519 (5) | C30—H30 | 0.93 |
| C1—H1A | 0.96 | C31—C36 | 1.382 (4) |
| C1—H1B | 0.96 | C31—C32 | 1.391 (4) |
| C1—H1C | 0.96 | C32—C33 | 1.386 (5) |
| C2—C3 | 1.376 (5) | C32—H32 | 0.93 |
| C2—C7 | 1.385 (5) | C33—C34 | 1.363 (5) |
| C3—C4 | 1.374 (5) | C33—H33 | 0.93 |
| C3—H3 | 0.93 | C34—C35 | 1.364 (5) |

| | | | |
|---|---|---|---|
| C4—C5 | 1.396 (5) | C34—H34 | 0.93 |
| C4—H4 | 0.93 | C35—C36 | 1.386 (4) |
| C5—C6 | 1.384 (5) | C35—H35 | 0.93 |
| C6—C7 | 1.381 (5) | C36—H36 | 0.93 |
| C6—H6 | 0.93 | | |
| C13—Fe1—C14 | 91.41 (17) | N1—C8—S2 | 117.6 (2) |
| C13—Fe1—P1 | 96.67 (12) | N1—C8—H8A | 107.9 |
| C14—Fe1—P1 | 97.31 (12) | S2—C8—H8A | 107.9 |
| C13—Fe1—S1 | 87.66 (12) | N1—C8—H8B | 107.9 |
| C14—Fe1—S1 | 159.67 (12) | S2—C8—H8B | 107.9 |
| P1—Fe1—S1 | 102.97 (4) | H8A—C8—H8B | 107.2 |
| C13—Fe1—S2 | 152.46 (12) | N1—C9—S1 | 115.4 (2) |
| C14—Fe1—S2 | 87.77 (12) | N1—C9—H9A | 108.4 |
| P1—Fe1—S2 | 110.75 (4) | S1—C9—H9A | 108.4 |
| S1—Fe1—S2 | 83.80 (4) | N1—C9—H9B | 108.4 |
| C13—Fe1—Fe2 | 97.87 (12) | S1—C9—H9B | 108.4 |
| C14—Fe1—Fe2 | 103.39 (12) | H9A—C9—H9B | 107.5 |
| P1—Fe1—Fe2 | 154.30 (4) | O1—C10—Fe2 | 173.4 (4) |
| S1—Fe1—Fe2 | 56.73 (3) | O2—C11—Fe2 | 178.3 (4) |
| S2—Fe1—Fe2 | 55.80 (3) | O3—C12—Fe2 | 178.3 (4) |
| C11—Fe2—C12 | 90.8 (2) | O4—C13—Fe1 | 176.7 (3) |
| C11—Fe2—C10 | 100.0 (2) | O5—C14—Fe1 | 176.7 (4) |
| C12—Fe2—C10 | 95.26 (18) | C19—C15—C16 | 107.3 (5) |
| C11—Fe2—S2 | 159.16 (15) | C19—C15—Fe3 | 69.9 (3) |
| C12—Fe2—S2 | 89.71 (14) | C16—C15—Fe3 | 69.3 (3) |
| C10—Fe2—S2 | 100.70 (14) | C19—C15—H15 | 126.3 |
| C11—Fe2—S1 | 85.74 (13) | C16—C15—H15 | 126.4 |
| C12—Fe2—S1 | 152.32 (14) | Fe3—C15—H15 | 126.4 |
| C10—Fe2—S1 | 112.39 (13) | C17—C16—C15 | 108.7 (5) |
| S2—Fe2—S1 | 84.18 (4) | C17—C16—Fe3 | 70.3 (3) |
| C11—Fe2—Fe1 | 102.51 (14) | C15—C16—Fe3 | 70.0 (3) |
| C12—Fe2—Fe1 | 97.99 (13) | C17—C16—H16 | 125.6 |
| C10—Fe2—Fe1 | 153.62 (13) | C15—C16—H16 | 125.7 |
| S2—Fe2—Fe1 | 56.83 (3) | Fe3—C16—H16 | 125.6 |
| S1—Fe2—Fe1 | 56.34 (3) | C16—C17—C18 | 108.3 (5) |
| C22—Fe3—C18 | 164.24 (18) | C16—C17—Fe3 | 70.1 (3) |
| C22—Fe3—C16 | 120.53 (19) | C18—C17—Fe3 | 69.5 (2) |
| C18—Fe3—C16 | 67.69 (19) | C16—C17—H17 | 126.0 |
| C22—Fe3—C17 | 153.86 (18) | C18—C17—H17 | 125.7 |
| C18—Fe3—C17 | 40.67 (16) | Fe3—C17—H17 | 125.8 |
| C16—Fe3—C17 | 39.61 (17) | C19—C18—C17 | 107.4 (4) |
| C22—Fe3—C24 | 68.59 (15) | C19—C18—Fe3 | 70.2 (2) |
| C18—Fe3—C24 | 108.54 (17) | C17—C18—Fe3 | 69.9 (2) |
| C16—Fe3—C24 | 159.7 (2) | C19—C18—H18 | 126.3 |
| C17—Fe3—C24 | 124.54 (19) | C17—C18—H18 | 126.3 |
| C22—Fe3—C21 | 40.55 (13) | Fe3—C18—H18 | 126.3 |
| C18—Fe3—C21 | 154.22 (19) | C15—C19—C18 | 108.4 (4) |
| C16—Fe3—C21 | 106.06 (18) | C15—C19—Fe3 | 70.0 (2) |
| C17—Fe3—C21 | 118.59 (18) | C18—C19—Fe3 | 69.3 (2) |

| | | | |
|---|---|---|---|
| C24—Fe3—C21 | 68.17 (16) | C15—C19—H19 | 125.9 |
| C22—Fe3—C23 | 41.20 (12) | C18—C19—H19 | 125.8 |
| C18—Fe3—C23 | 126.57 (17) | Fe3—C19—H19 | 126.0 |
| C16—Fe3—C23 | 157.2 (2) | C21—C20—C24 | 108.1 (4) |
| C17—Fe3—C23 | 162.63 (19) | C21—C20—Fe3 | 69.8 (2) |
| C24—Fe3—C23 | 40.89 (12) | C24—C20—Fe3 | 69.3 (2) |
| C21—Fe3—C23 | 68.77 (14) | C21—C20—H20 | 125.8 |
| C22—Fe3—C19 | 127.14 (18) | C24—C20—H20 | 126.0 |
| C18—Fe3—C19 | 40.50 (15) | Fe3—C20—H20 | 126.1 |
| C16—Fe3—C19 | 67.59 (18) | C20—C21—C22 | 108.5 (4) |
| C17—Fe3—C19 | 67.78 (18) | C20—C21—Fe3 | 70.2 (2) |
| C24—Fe3—C19 | 123.45 (18) | C22—C21—Fe3 | 69.1 (2) |
| C21—Fe3—C19 | 162.4 (2) | C20—C21—H21 | 125.9 |
| C23—Fe3—C19 | 110.29 (16) | C22—C21—H21 | 125.6 |
| C22—Fe3—C15 | 108.63 (18) | Fe3—C21—H21 | 125.7 |
| C18—Fe3—C15 | 67.97 (19) | C21—C22—C23 | 108.5 (3) |
| C16—Fe3—C15 | 40.67 (16) | C21—C22—Fe3 | 70.3 (2) |
| C17—Fe3—C15 | 67.7 (2) | C23—C22—Fe3 | 70.00 (19) |
| C24—Fe3—C15 | 158.38 (19) | C21—C22—H22 | 125.9 |
| C21—Fe3—C15 | 124.6 (2) | C23—C22—H22 | 125.6 |
| C23—Fe3—C15 | 122.80 (18) | Fe3—C22—H22 | 125.7 |
| C19—Fe3—C15 | 40.03 (16) | C24—C23—C22 | 106.6 (3) |
| C22—Fe3—C20 | 68.06 (16) | C24—C23—P1 | 126.1 (3) |
| C18—Fe3—C20 | 120.63 (19) | C22—C23—P1 | 126.8 (3) |
| C16—Fe3—C20 | 122.40 (18) | C24—C23—Fe3 | 69.4 (2) |
| C17—Fe3—C20 | 106.01 (18) | C22—C23—Fe3 | 68.8 (2) |
| C24—Fe3—C20 | 40.84 (13) | P1—C23—Fe3 | 132.96 (18) |
| C21—Fe3—C20 | 40.00 (14) | C23—C24—C20 | 108.2 (3) |
| C23—Fe3—C20 | 68.76 (14) | C23—C24—Fe3 | 69.7 (2) |
| C19—Fe3—C20 | 157.4 (2) | C20—C24—Fe3 | 69.9 (2) |
| C15—Fe3—C20 | 159.8 (2) | C23—C24—H24 | 125.9 |
| C9—S1—Fe1 | 107.79 (13) | C20—C24—H24 | 125.9 |
| C9—S1—Fe2 | 111.20 (12) | Fe3—C24—H24 | 125.9 |
| Fe1—S1—Fe2 | 66.93 (3) | C26—C25—C30 | 118.0 (3) |
| C8—S2—Fe2 | 108.94 (12) | C26—C25—P1 | 118.5 (3) |
| C8—S2—Fe1 | 116.93 (13) | C30—C25—P1 | 123.4 (3) |
| Fe2—S2—Fe1 | 67.37 (3) | C27—C26—C25 | 121.5 (3) |
| C23—P1—C25 | 102.96 (16) | C27—C26—H26 | 119.3 |
| C23—P1—C31 | 104.03 (16) | C25—C26—H26 | 119.3 |
| C25—P1—C31 | 100.01 (15) | C26—C27—C28 | 119.6 (4) |
| C23—P1—Fe1 | 118.32 (12) | C26—C27—H27 | 120.2 |
| C25—P1—Fe1 | 112.95 (11) | C28—C27—H27 | 120.2 |
| C31—P1—Fe1 | 116.22 (12) | C29—C28—C27 | 119.7 (4) |
| C5—N1—C9 | 119.7 (3) | C29—C28—H28 | 120.2 |
| C5—N1—C8 | 123.4 (3) | C27—C28—H28 | 120.2 |
| C9—N1—C8 | 112.7 (3) | C28—C29—C30 | 120.9 (4) |
| C2—C1—H1A | 109.5 | C28—C29—H29 | 119.5 |
| C2—C1—H1B | 109.5 | C30—C29—H29 | 119.5 |
| H1A—C1—H1B | 109.5 | C29—C30—C25 | 120.3 (4) |

| | | | |
|---|---|---|---|
| C2—C1—H1C | 109.5 | C29—C30—H30 | 119.9 |
| H1A—C1—H1C | 109.5 | C25—C30—H30 | 119.9 |
| H1B—C1—H1C | 109.5 | C36—C31—C32 | 117.4 (3) |
| C3—C2—C7 | 116.6 (4) | C36—C31—P1 | 121.7 (3) |
| C3—C2—C1 | 122.2 (4) | C32—C31—P1 | 120.8 (3) |
| C7—C2—C1 | 121.2 (4) | C33—C32—C31 | 121.1 (4) |
| C4—C3—C2 | 122.7 (4) | C33—C32—H32 | 119.4 |
| C4—C3—H3 | 118.7 | C31—C32—H32 | 119.4 |
| C2—C3—H3 | 118.7 | C34—C33—C32 | 120.0 (4) |
| C3—C4—C5 | 120.6 (4) | C34—C33—H33 | 120.0 |
| C3—C4—H4 | 119.7 | C32—C33—H33 | 120.0 |
| C5—C4—H4 | 119.7 | C33—C34—C35 | 120.3 (4) |
| C6—C5—C4 | 117.1 (4) | C33—C34—H34 | 119.9 |
| C6—C5—N1 | 122.2 (4) | C35—C34—H34 | 119.9 |
| C4—C5—N1 | 120.6 (4) | C34—C35—C36 | 120.0 (4) |
| C7—C6—C5 | 121.3 (4) | C34—C35—H35 | 120.0 |
| C7—C6—H6 | 119.4 | C36—C35—H35 | 120.0 |
| C5—C6—H6 | 119.4 | C31—C36—C35 | 121.3 (4) |
| C6—C7—C2 | 121.7 (4) | C31—C36—H36 | 119.4 |
| C6—C7—H7 | 119.1 | C35—C36—H36 | 119.4 |
| C2—C7—H7 | 119.1 | | |
| C13—Fe1—Fe2—C11 | −5.79 (19) | C20—Fe3—C18—C17 | −78.6 (3) |
| C14—Fe1—Fe2—C11 | −99.1 (2) | C16—C15—C19—C18 | 0.7 (5) |
| P1—Fe1—Fe2—C11 | 118.10 (17) | Fe3—C15—C19—C18 | −58.8 (3) |
| S1—Fe1—Fe2—C11 | 76.16 (16) | C16—C15—C19—Fe3 | 59.5 (3) |
| S2—Fe1—Fe2—C11 | −177.00 (16) | C17—C18—C19—C15 | −1.0 (5) |
| C13—Fe1—Fe2—C12 | 86.84 (18) | Fe3—C18—C19—C15 | 59.3 (3) |
| C14—Fe1—Fe2—C12 | −6.51 (19) | C17—C18—C19—Fe3 | −60.3 (3) |
| P1—Fe1—Fe2—C12 | −149.28 (16) | C22—Fe3—C19—C15 | 73.8 (3) |
| S1—Fe1—Fe2—C12 | 168.78 (14) | C18—Fe3—C19—C15 | −119.7 (4) |
| S2—Fe1—Fe2—C12 | −84.38 (14) | C16—Fe3—C19—C15 | −38.3 (3) |
| C13—Fe1—Fe2—C10 | −153.7 (3) | C17—Fe3—C19—C15 | −81.3 (3) |
| C14—Fe1—Fe2—C10 | 112.9 (3) | C24—Fe3—C19—C15 | 161.0 (3) |
| P1—Fe1—Fe2—C10 | −29.8 (3) | C21—Fe3—C19—C15 | 33.6 (7) |
| S1—Fe1—Fe2—C10 | −71.8 (3) | C23—Fe3—C19—C15 | 117.2 (3) |
| S2—Fe1—Fe2—C10 | 35.1 (3) | C20—Fe3—C19—C15 | −159.5 (4) |
| C13—Fe1—Fe2—S2 | 171.21 (12) | C22—Fe3—C19—C18 | −166.5 (3) |
| C14—Fe1—Fe2—S2 | 77.86 (13) | C16—Fe3—C19—C18 | 81.4 (3) |
| P1—Fe1—Fe2—S2 | −64.90 (8) | C17—Fe3—C19—C18 | 38.4 (3) |
| S1—Fe1—Fe2—S2 | −106.84 (4) | C24—Fe3—C19—C18 | −79.2 (3) |
| C13—Fe1—Fe2—S1 | −81.95 (12) | C21—Fe3—C19—C18 | 153.3 (5) |
| C14—Fe1—Fe2—S1 | −175.30 (13) | C23—Fe3—C19—C18 | −123.0 (3) |
| P1—Fe1—Fe2—S1 | 41.94 (8) | C15—Fe3—C19—C18 | 119.7 (4) |
| S2—Fe1—Fe2—S1 | 106.84 (4) | C20—Fe3—C19—C18 | −39.7 (6) |
| C13—Fe1—S1—C9 | −152.98 (16) | C22—Fe3—C20—C21 | −37.4 (2) |
| C14—Fe1—S1—C9 | 119.3 (4) | C18—Fe3—C20—C21 | 157.3 (3) |
| P1—Fe1—S1—C9 | −56.67 (12) | C16—Fe3—C20—C21 | 75.7 (3) |
| S2—Fe1—S1—C9 | 53.25 (12) | C17—Fe3—C20—C21 | 115.6 (3) |
| Fe2—Fe1—S1—C9 | 106.02 (12) | C24—Fe3—C20—C21 | −119.6 (3) |

| | | | |
|---|---|---|---|
| C13—Fe1—S1—Fe2 | 101.00 (11) | C23—Fe3—C20—C21 | −81.9 (2) |
| C14—Fe1—S1—Fe2 | 13.3 (4) | C19—Fe3—C20—C21 | −173.9 (4) |
| P1—Fe1—S1—Fe2 | −162.70 (4) | C15—Fe3—C20—C21 | 47.0 (6) |
| S2—Fe1—S1—Fe2 | −52.78 (3) | C22—Fe3—C20—C24 | 82.2 (2) |
| C11—Fe2—S1—C9 | 150.9 (2) | C18—Fe3—C20—C24 | −83.1 (3) |
| C12—Fe2—S1—C9 | −125.5 (3) | C16—Fe3—C20—C24 | −164.7 (3) |
| C10—Fe2—S1—C9 | 51.8 (2) | C17—Fe3—C20—C24 | −124.8 (3) |
| S2—Fe2—S1—C9 | −47.37 (13) | C21—Fe3—C20—C24 | 119.6 (3) |
| Fe1—Fe2—S1—C9 | −101.01 (13) | C23—Fe3—C20—C24 | 37.7 (2) |
| C11—Fe2—S1—Fe1 | −108.09 (16) | C19—Fe3—C20—C24 | −54.3 (5) |
| C12—Fe2—S1—Fe1 | −24.5 (3) | C15—Fe3—C20—C24 | 166.6 (5) |
| C10—Fe2—S1—Fe1 | 152.84 (15) | C24—C20—C21—C22 | −0.1 (5) |
| S2—Fe2—S1—Fe1 | 53.64 (3) | Fe3—C20—C21—C22 | 58.7 (3) |
| C11—Fe2—S2—C8 | 120.3 (4) | C24—C20—C21—Fe3 | −58.8 (3) |
| C12—Fe2—S2—C8 | −148.17 (19) | C22—Fe3—C21—C20 | 119.9 (4) |
| C10—Fe2—S2—C8 | −52.87 (18) | C18—Fe3—C21—C20 | −49.8 (5) |
| S1—Fe2—S2—C8 | 58.87 (13) | C16—Fe3—C21—C20 | −121.6 (3) |
| Fe1—Fe2—S2—C8 | 112.07 (13) | C17—Fe3—C21—C20 | −80.8 (3) |
| C11—Fe2—S2—Fe1 | 8.2 (4) | C24—Fe3—C21—C20 | 37.8 (2) |
| C12—Fe2—S2—Fe1 | 99.76 (14) | C23—Fe3—C21—C20 | 81.9 (2) |
| C10—Fe2—S2—Fe1 | −164.94 (13) | C19—Fe3—C21—C20 | 172.2 (5) |
| S1—Fe2—S2—Fe1 | −53.20 (3) | C15—Fe3—C21—C20 | −162.2 (3) |
| C13—Fe1—S2—C8 | −119.6 (3) | C18—Fe3—C21—C22 | −169.7 (4) |
| C14—Fe1—S2—C8 | 151.61 (18) | C16—Fe3—C21—C22 | 118.5 (3) |
| P1—Fe1—S2—C8 | 54.64 (14) | C17—Fe3—C21—C22 | 159.3 (3) |
| S1—Fe1—S2—C8 | −46.91 (14) | C24—Fe3—C21—C22 | −82.1 (3) |
| Fe2—Fe1—S2—C8 | −100.52 (14) | C23—Fe3—C21—C22 | −38.0 (2) |
| C13—Fe1—S2—Fe2 | −19.1 (3) | C19—Fe3—C21—C22 | 52.3 (7) |
| C14—Fe1—S2—Fe2 | −107.87 (12) | C15—Fe3—C21—C22 | 77.9 (3) |
| P1—Fe1—S2—Fe2 | 155.17 (4) | C20—Fe3—C21—C22 | −119.9 (4) |
| S1—Fe1—S2—Fe2 | 53.61 (3) | C20—C21—C22—C23 | 0.4 (5) |
| C13—Fe1—P1—C23 | −153.80 (18) | Fe3—C21—C22—C23 | 59.8 (3) |
| C14—Fe1—P1—C23 | −61.51 (18) | C20—C21—C22—Fe3 | −59.4 (3) |
| S1—Fe1—P1—C23 | 117.07 (13) | C18—Fe3—C22—C21 | 163.4 (6) |
| S2—Fe1—P1—C23 | 28.86 (14) | C16—Fe3—C22—C21 | −78.7 (3) |
| Fe2—Fe1—P1—C23 | 82.08 (15) | C17—Fe3—C22—C21 | −44.7 (5) |
| C13—Fe1—P1—C25 | 85.87 (17) | C24—Fe3—C22—C21 | 81.0 (3) |
| C14—Fe1—P1—C25 | 178.16 (17) | C23—Fe3—C22—C21 | 119.3 (3) |
| S1—Fe1—P1—C25 | −3.25 (13) | C19—Fe3—C22—C21 | −162.5 (3) |
| S2—Fe1—P1—C25 | −91.46 (13) | C15—Fe3—C22—C21 | −121.8 (3) |
| Fe2—Fe1—P1—C25 | −38.24 (16) | C20—Fe3—C22—C21 | 36.9 (2) |
| C13—Fe1—P1—C31 | −28.89 (18) | C18—Fe3—C22—C23 | 44.1 (7) |
| C14—Fe1—P1—C31 | 63.40 (18) | C16—Fe3—C22—C23 | 162.0 (2) |
| S1—Fe1—P1—C31 | −118.01 (13) | C17—Fe3—C22—C23 | −164.0 (4) |
| S2—Fe1—P1—C31 | 153.78 (13) | C24—Fe3—C22—C23 | −38.3 (2) |
| Fe2—Fe1—P1—C31 | −153.00 (13) | C21—Fe3—C22—C23 | −119.3 (3) |
| C7—C2—C3—C4 | 0.1 (6) | C19—Fe3—C22—C23 | 78.2 (3) |
| C1—C2—C3—C4 | 179.4 (4) | C15—Fe3—C22—C23 | 118.9 (3) |
| C2—C3—C4—C5 | −0.9 (6) | C20—Fe3—C22—C23 | −82.4 (2) |

| | | | |
|---|---|---|---|
| C3—C4—C5—C6 | 1.4 (5) | C21—C22—C23—C24 | −0.6 (4) |
| C3—C4—C5—N1 | 177.6 (3) | Fe3—C22—C23—C24 | 59.4 (2) |
| C9—N1—C5—C6 | 3.7 (5) | C21—C22—C23—P1 | 171.5 (3) |
| C8—N1—C5—C6 | −151.7 (3) | Fe3—C22—C23—P1 | −128.5 (3) |
| C9—N1—C5—C4 | −172.3 (3) | C21—C22—C23—Fe3 | −60.0 (3) |
| C8—N1—C5—C4 | 32.3 (5) | C25—P1—C23—C24 | 109.2 (3) |
| C4—C5—C6—C7 | −1.1 (6) | C31—P1—C23—C24 | −146.8 (3) |
| N1—C5—C6—C7 | −177.2 (3) | Fe1—P1—C23—C24 | −16.1 (4) |
| C5—C6—C7—C2 | 0.3 (6) | C25—P1—C23—C22 | −61.3 (3) |
| C3—C2—C7—C6 | 0.2 (6) | C31—P1—C23—C22 | 42.6 (4) |
| C1—C2—C7—C6 | −179.0 (4) | Fe1—P1—C23—C22 | 173.3 (3) |
| C5—N1—C8—S2 | 98.7 (4) | C25—P1—C23—Fe3 | −155.9 (2) |
| C9—N1—C8—S2 | −58.1 (4) | C31—P1—C23—Fe3 | −51.9 (3) |
| Fe2—S2—C8—N1 | −20.0 (3) | Fe1—P1—C23—Fe3 | 78.7 (3) |
| Fe1—S2—C8—N1 | 53.6 (3) | C22—Fe3—C23—C24 | −118.2 (3) |
| C5—N1—C9—S1 | −84.2 (4) | C18—Fe3—C23—C24 | 75.4 (3) |
| C8—N1—C9—S1 | 73.6 (3) | C16—Fe3—C23—C24 | −161.7 (4) |
| Fe1—S1—C9—N1 | −79.0 (3) | C17—Fe3—C23—C24 | 37.8 (6) |
| Fe2—S1—C9—N1 | −7.5 (3) | C21—Fe3—C23—C24 | −80.8 (2) |
| C22—Fe3—C15—C19 | −126.1 (3) | C19—Fe3—C23—C24 | 118.1 (2) |
| C18—Fe3—C15—C19 | 37.5 (3) | C15—Fe3—C23—C24 | 161.0 (2) |
| C16—Fe3—C15—C19 | 118.4 (4) | C20—Fe3—C23—C24 | −37.7 (2) |
| C17—Fe3—C15—C19 | 81.6 (3) | C18—Fe3—C23—C22 | −166.4 (3) |
| C24—Fe3—C15—C19 | −47.4 (6) | C16—Fe3—C23—C22 | −43.4 (5) |
| C21—Fe3—C15—C19 | −168.2 (3) | C17—Fe3—C23—C22 | 156.0 (5) |
| C23—Fe3—C15—C19 | −82.8 (3) | C24—Fe3—C23—C22 | 118.2 (3) |
| C20—Fe3—C15—C19 | 157.0 (5) | C21—Fe3—C23—C22 | 37.5 (2) |
| C22—Fe3—C15—C16 | 115.5 (3) | C19—Fe3—C23—C22 | −123.7 (3) |
| C18—Fe3—C15—C16 | −80.9 (3) | C15—Fe3—C23—C22 | −80.8 (3) |
| C17—Fe3—C15—C16 | −36.9 (3) | C20—Fe3—C23—C22 | 80.5 (2) |
| C24—Fe3—C15—C16 | −165.8 (4) | C22—Fe3—C23—P1 | 121.1 (4) |
| C21—Fe3—C15—C16 | 73.3 (4) | C18—Fe3—C23—P1 | −45.3 (4) |
| C23—Fe3—C15—C16 | 158.8 (3) | C16—Fe3—C23—P1 | 77.7 (5) |
| C19—Fe3—C15—C16 | −118.4 (4) | C17—Fe3—C23—P1 | −82.9 (6) |
| C20—Fe3—C15—C16 | 38.6 (7) | C24—Fe3—C23—P1 | −120.7 (3) |
| C19—C15—C16—C17 | −0.1 (5) | C21—Fe3—C23—P1 | 158.6 (3) |
| Fe3—C15—C16—C17 | 59.8 (3) | C19—Fe3—C23—P1 | −2.6 (3) |
| C19—C15—C16—Fe3 | −59.9 (3) | C15—Fe3—C23—P1 | 40.3 (3) |
| C22—Fe3—C16—C17 | 157.2 (3) | C20—Fe3—C23—P1 | −158.4 (3) |
| C18—Fe3—C16—C17 | −37.8 (3) | C22—C23—C24—C20 | 0.5 (4) |
| C24—Fe3—C16—C17 | 45.4 (6) | P1—C23—C24—C20 | −171.6 (3) |
| C21—Fe3—C16—C17 | 115.7 (3) | Fe3—C23—C24—C20 | 59.5 (3) |
| C23—Fe3—C16—C17 | −171.0 (3) | C22—C23—C24—Fe3 | −59.0 (2) |
| C19—Fe3—C16—C17 | −81.8 (3) | P1—C23—C24—Fe3 | 128.9 (3) |
| C15—Fe3—C16—C17 | −119.5 (4) | C21—C20—C24—C23 | −0.2 (4) |
| C20—Fe3—C16—C17 | 75.3 (4) | Fe3—C20—C24—C23 | −59.4 (3) |
| C22—Fe3—C16—C15 | −83.3 (3) | C21—C20—C24—Fe3 | 59.1 (3) |
| C18—Fe3—C16—C15 | 81.7 (3) | C22—Fe3—C24—C23 | 38.56 (19) |
| C17—Fe3—C16—C15 | 119.5 (4) | C18—Fe3—C24—C23 | −124.9 (2) |

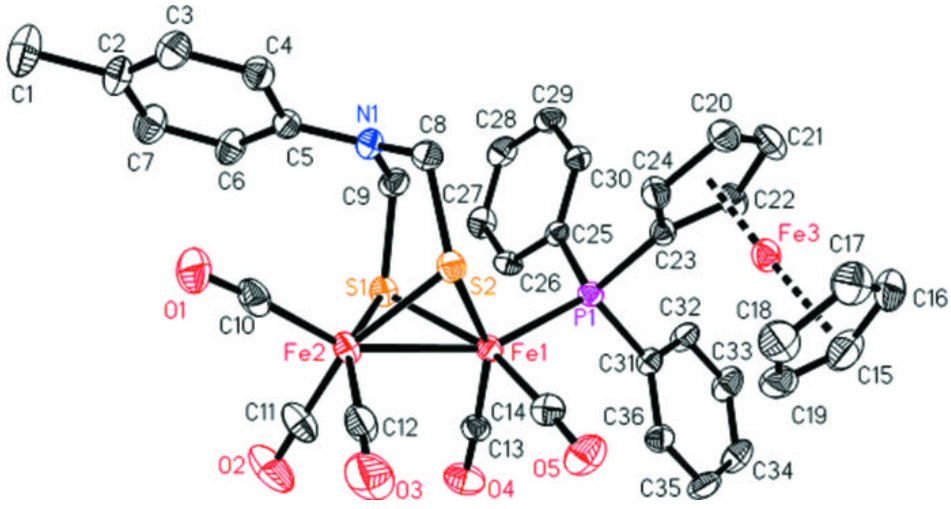
| | | | |
|---|---|---|---|
| C24—Fe3—C16—C15 | 164.9 (4) | C16—Fe3—C24—C23 | 159.4 (5) |
| C21—Fe3—C16—C15 | −124.8 (3) | C17—Fe3—C24—C23 | −167.2 (2) |
| C23—Fe3—C16—C15 | −51.5 (6) | C21—Fe3—C24—C23 | 82.3 (2) |
| C19—Fe3—C16—C15 | 37.7 (3) | C19—Fe3—C24—C23 | −82.6 (3) |
| C20—Fe3—C16—C15 | −165.2 (3) | C15—Fe3—C24—C23 | −48.1 (5) |
| C15—C16—C17—C18 | −0.6 (5) | C20—Fe3—C24—C23 | 119.3 (3) |
| Fe3—C16—C17—C18 | 59.1 (3) | C22—Fe3—C24—C20 | −80.8 (2) |
| C15—C16—C17—Fe3 | −59.7 (3) | C18—Fe3—C24—C20 | 115.7 (3) |
| C22—Fe3—C17—C16 | −49.2 (6) | C16—Fe3—C24—C20 | 40.1 (6) |
| C18—Fe3—C17—C16 | 119.5 (5) | C17—Fe3—C24—C20 | 73.5 (3) |
| C24—Fe3—C17—C16 | −162.6 (3) | C21—Fe3—C24—C20 | −37.0 (2) |
| C21—Fe3—C17—C16 | −80.5 (4) | C23—Fe3—C24—C20 | −119.3 (3) |
| C23—Fe3—C17—C16 | 168.3 (5) | C19—Fe3—C24—C20 | 158.0 (3) |
| C19—Fe3—C17—C16 | 81.2 (3) | C15—Fe3—C24—C20 | −167.4 (5) |
| C15—Fe3—C17—C16 | 37.8 (3) | C23—P1—C25—C26 | 176.8 (3) |
| C20—Fe3—C17—C16 | −121.8 (3) | C31—P1—C25—C26 | 69.7 (3) |
| C22—Fe3—C17—C18 | −168.7 (4) | Fe1—P1—C25—C26 | −54.5 (3) |
| C16—Fe3—C17—C18 | −119.5 (5) | C23—P1—C25—C30 | −6.0 (3) |
| C24—Fe3—C17—C18 | 77.9 (3) | C31—P1—C25—C30 | −113.1 (3) |
| C21—Fe3—C17—C18 | 160.0 (3) | Fe1—P1—C25—C30 | 122.8 (3) |
| C23—Fe3—C17—C18 | 48.8 (7) | C30—C25—C26—C27 | −0.3 (5) |
| C19—Fe3—C17—C18 | −38.3 (3) | P1—C25—C26—C27 | 177.1 (3) |
| C15—Fe3—C17—C18 | −81.7 (3) | C25—C26—C27—C28 | 0.1 (6) |
| C20—Fe3—C17—C18 | 118.6 (3) | C26—C27—C28—C29 | 1.2 (6) |
| C16—C17—C18—C19 | 1.0 (5) | C27—C28—C29—C30 | −2.2 (6) |
| Fe3—C17—C18—C19 | 60.5 (3) | C28—C29—C30—C25 | 2.1 (6) |
| C16—C17—C18—Fe3 | −59.6 (3) | C26—C25—C30—C29 | −0.8 (5) |
| C22—Fe3—C18—C19 | 43.4 (8) | P1—C25—C30—C29 | −178.0 (3) |
| C16—Fe3—C18—C19 | −81.1 (3) | C23—P1—C31—C36 | 104.2 (3) |
| C17—Fe3—C18—C19 | −118.0 (4) | C25—P1—C31—C36 | −149.6 (3) |
| C24—Fe3—C18—C19 | 120.2 (3) | Fe1—P1—C31—C36 | −27.7 (3) |
| C21—Fe3—C18—C19 | −161.8 (4) | C23—P1—C31—C32 | −74.4 (3) |
| C23—Fe3—C18—C19 | 78.3 (3) | C25—P1—C31—C32 | 31.8 (3) |
| C15—Fe3—C18—C19 | −37.1 (3) | Fe1—P1—C31—C32 | 153.6 (3) |
| C20—Fe3—C18—C19 | 163.4 (3) | C36—C31—C32—C33 | −0.8 (6) |
| C22—Fe3—C18—C17 | 161.4 (6) | P1—C31—C32—C33 | 177.8 (3) |
| C16—Fe3—C18—C17 | 36.9 (3) | C31—C32—C33—C34 | 0.9 (6) |
| C24—Fe3—C18—C17 | −121.8 (3) | C32—C33—C34—C35 | −0.2 (7) |
| C21—Fe3—C18—C17 | −43.8 (6) | C33—C34—C35—C36 | −0.4 (7) |
| C23—Fe3—C18—C17 | −163.8 (3) | C32—C31—C36—C35 | 0.2 (6) |
| C19—Fe3—C18—C17 | 118.0 (4) | P1—C31—C36—C35 | −178.5 (3) |
| C15—Fe3—C18—C17 | 80.9 (3) | C34—C35—C36—C31 | 0.4 (6) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22···O2$^{i}$ | 0.98 | 2.53 | 3.224 (5) | 128 |
| C24—H24···S2 | 0.98 | 2.72 | 3.561 (4) | 144 |

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2.

**Fig. 1**


C1
C2
C3
C4
C5
C6
C7
N1
C8
C9
C10
O1
S1
S2
Fe1
Fe2
C11
C12
C13
C14
O2
O3
O4
O5
C27
C28
C29
C30
C25
C26
P1
C20
C21
C22
C23
C24
Fe3
C17
C16
C15
C18
C19
C32
C33
C31
C36
C34
C35