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# Benzyl 5-ferrocenyl-3-(4-methylphenyl)-2-pyrazoline-1-dithiocarboxylate

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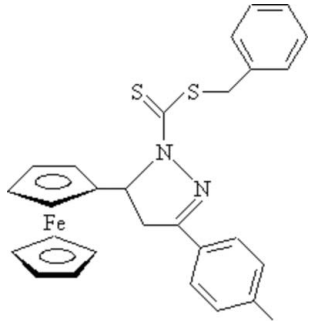
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.028; $wR$ factor = 0.088; data-to-parameter ratio = 18.5.

In the title compound, $[Fe(C_5H_5)(C_{23}H_{21}N_2S_2)]$, the cyclopentadienyl rings of the ferrocenyl unit deviate slightly from the eclipsed form. In the pyrazoline ring, the N atom bonded to *S*-benzyl dithiocarbazate exhibits unconventional $sp^2$-hybrid character in order to form an extended conjugated system. The pyrazoline ring displays an envelope conformation. The molecules are linked into chains along the *b* axis *via* C—H···S intermolecular hydrogen bonds.

## Related literature

For related literature, see: Fahrni *et al.* (2003); Huang & Katzenellenbogen (2000); Huang *et al.* (1998); Liu *et al.* (2007); Rivett *et al.* (1979); Shi *et al.* (2004); Sun *et al.* (2004); Wiley *et al.* (1958); Wilkinson *et al.* (1990).




## Experimental

### Crystal data

$[Fe(C_5H_5)(C_{23}H_{21}N_2S_2)]$
$M_r$ = 510.50
Triclinic, $P\overline{1}$
$a$ = 9.178 (1) Å
$b$ = 10.468 (2) Å
$c$ = 13.216 (2) Å
$\alpha$ = 99.37 (1)°
$\beta$ = 101.55 (2)°
$\gamma$ = 96.12 (1)°
$V$ = 1214.6 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.81 mm$^{-1}$
$T$ = 296 (2) K
0.33 × 0.31 × 0.28 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.776, $T_{max}$ = 0.805
10742 measured reflections
5528 independent reflections
5035 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.088
$S$ = 0.99
5528 reflections
299 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2002).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2048).

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# supplementary materials

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# Benzyl 5-ferrocenyl-3-(4-methylphenyl)-2-pyrazoline-1-dithiocarboxylate

**X.-L. Liu, B.-W. Tong, Y. Zhao, J. Ye and Y.-H. Liu**

## Comment

Pyrazoline derivatives are an important class of conjugated fluorescent dyes emitting blue fluorescence and have been extensively applied in the industry due to the high fluorescence quantum yield (Wilkinson *et al.*, 1990; Rivett *et al.*, 1979). For example, pyrazolines have been widely used as optical brightening agents for textiles, paper and fabrics and as a hole-conveying medium in photoconductive materials (Sun *et al.*, 2004; Huang & Katzenellenbogen, 2000; Wiley *et al.*, 1958). We found that ferrocene derivatives have good properties of fluorescence and coordination chemistry with many metal ions (Huang *et al.*, 1998; Shi *et al.*, 2004). Continuing our research (Liu *et al.*, 2007) we report the synthesis and structure of the title compound, (I).

In the structure of (I), the substituted ring (*Cps*) and unsubstituted ring (*Cp*) of the ferrocenyl moiety are slightly deprived from eclipsed form, with the five pseudo-torsion angles in the range 10.5 (2) — 10.9 (3)°. The distances from central Fe(II) ion to Cps center [*Cg*(1)] and to Cp center [*Cg*(2)] are 1.651 (3) Å and 1.656 (2) Å, respectively. The angle *Cg*(1)–Fe–*Cg*(2) is 177.9 (3)° and the central Fe(II) ion is located almost in the middle of the two cyclopentadiene rings which are not parallel because their dihedral angle is 2.3 (4)° (Fig. 1).

In the pyrazolinyl ring, the C=N and C–N bond lengths are in agreement with those found in similar structures (Fahrni *et al.*, 2003). However, the N–N bond length is longer than those found in the above-cited structures. But the bond distance of C21–N1 is shorter than a C–N single bond and slight longer than a C=N double bond. It might contribute to unclassical $sp^2$-hybrid N1 atom which is evident from the sum of the three angles around the N1 atom being 360° (Table 1) and that atoms C21, N1, N2 and C13 are co-planar. Furthemore, atoms S2, C21, N1, N2, C13 along with adjacent phenyl ring result in a large cojugated system.

In its packing diagram, the molecules of (I) are linked into two invers chains *via* C— H···S intermolecular hydrogen-bonds with C···S distance 3.583 (3) Å and C26—H26···S2 angle 142°, along the *b* axis (Fig. 2, Table 2).

## Experimental

The title compound was synthesized by refluxing an absolute ethanol solution of 1-(4-methylphenyl)-3-ferrocenylprop-2-en-1-one (3.30 g, 10 mmol) and *S*-benzyldithiocarbazate (1.98 g, 10 mmol) for 24 h. After refrigeration (278 K) of the solution for 10 h, yellow pricipite separated out and recrystallized from a mixture of 1,2-dichloroethane and petroleum ether (5:1 volume ratio) (3.1 g, yield 61%). The yellow crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane solution at 278 K.

### Refinement

All H atoms were fixed geometrically at ideal positions and allowed to ride on the parent atoms with C—H distances 0.96, 0.97, 0.98 and 0.93 Å for $CH_3$, $CH_2$, CH and aromatic CH groups, respectively, and with $U_{iso}$(H) values of 1.2 and 1.5 times $U_{eq}$(C) for the nonmethyl and methyl groups, respectively.

### Figures

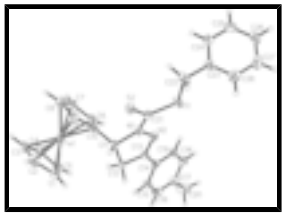

Fig. 1. The molecular structure of (I); displacement ellipsoids are drawn at 50% probability level.

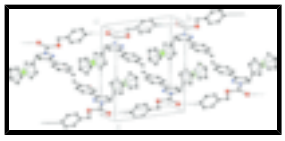

Fig. 2. Packing diagram of (I), C—H···S inter-molecular hydrogen bonds shown as dashed lines. The H atoms not involved in hyydrogen bonding have been omitted.

### Benzyl 5-ferrocenyl-3-(4-methylphenyl)-2-pyrazoline-1-dithiocarboxylate

*Crystal data*

| | |
|---|---|
| $[Fe(C_5H_5)(C_{23}H_{21}N_2S_2)]$ | $Z = 2$ |
| $M_r = 510.50$ | $F_{000} = 532.0$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.396$ Mg m$^{-3}$ |
| Hall symbol: - P 1 | Melting point: 345(2) K |
| $a = 9.178$ (1) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 10.468$ (2) Å | Cell parameters from 7052 reflections |
| $c = 13.216$ (2) Å | $\theta = 2.3$–$27.6$º |
| $\alpha = 99.37$ (1)º | $\mu = 0.81$ mm$^{-1}$ |
| $\beta = 101.55$ (2)º | $T = 296$ (2) K |
| $\gamma = 96.12$ (1)º | Block, yellow |
| $V = 1214.6$ (3) Å$^3$ | 0.33 × 0.31 × 0.28 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 5528 independent reflections |
| Radiation source: fine-focus sealed tube | 5035 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.019$ |
| $T = 296$(2) K | $\theta_{max} = 27.7$º |
| φ and ω scans | $\theta_{min} = 2.3$º |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $h = -10 \rightarrow 10$ |

$T_{min}$ = 0.776, $T_{max}$ = 0.805
10742 measured reflections

$k$ = −12→12
$l$ = −15→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.088
$S$ = 0.99
5528 reflections
299 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.4985P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Extinction correction: none

*Special details*

**Experimental**. Analysis calculated for $C_{18}H_{16}N_4OS_2$: C 65.87, H 5.13, N 5.49%; found: C 65.82, H 5.11, N 5.51%. IR (KBr, cm$^{-1}$): *v*(C=N), *v*(S=C) and *v*(N–N) 1559 (*m*), 1245 (*s*) and 1037 (w) cm$^{-1.}$ $^1$H NMR (600 MHz, $CDCl_3$,δ, p.p.m.): 7.23–7.76 (m, 9H, ArH), 6.04 (broad, 1H, CH), 4.50–4.47 (d, 1H, $CH_2$), 4.41–4.39 (d, 1H, $CH_2$), 4.15 (s, 5H, $C_5H_5$), 4.03 (s, 1H, $C_5H_4$), 4.12 (s, 1H, $C_5H_4$), 4.19 (s, 1H, $C_5H_4$), 4.71 (s, 1H, $C_5H_4$), 3.72 (s, 2H, $ArCH_2$), 2.41 (s, 3H, $CH_3$) p.p.m..

**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 $F^2 > 2$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 | 0.56551 (3) | −0.22018 (2) | 0.364537 (18) | 0.02183 (10) |
| S1 | 0.64012 (5) | 0.30267 (4) | 0.12369 (4) | 0.02864 (13) |
| S2 | 0.72753 (5) | 0.03133 (4) | 0.06920 (3) | 0.02501 (12) |
| N1 | 0.52328 (15) | 0.09334 (13) | 0.17619 (11) | 0.0209 (3) |
| N2 | 0.43248 (16) | 0.18040 (13) | 0.21361 (11) | 0.0219 (3) |
| C5 | 0.3598 (2) | −0.28594 (18) | 0.38988 (16) | 0.0310 (4) |
| H5 | 0.2866 | −0.2347 | 0.4034 | 0.037* |
| C4 | 0.4760 (2) | −0.31695 (18) | 0.46642 (16) | 0.0322 (4) |
| H4 | 0.4920 | −0.2897 | 0.5388 | 0.039* |
| C3 | 0.5633 (2) | −0.39647 (18) | 0.41353 (16) | 0.0342 (4) |
| H3 | 0.6465 | −0.4305 | 0.4452 | 0.041* |

| | | | | |
|---|---|---|---|---|
| C2 | 0.5017 (2) | −0.41532 (18) | 0.30377 (16) | 0.0351 (4) |
| H2 | 0.5376 | −0.4637 | 0.2509 | 0.042* |
| C1 | 0.3750 (2) | −0.34678 (18) | 0.28908 (16) | 0.0324 (4) |
| H1 | 0.3133 | −0.3427 | 0.2250 | 0.039* |
| C6 | 0.6003 (2) | −0.01980 (17) | 0.39096 (14) | 0.0262 (4) |
| H6 | 0.5385 | 0.0357 | 0.4175 | 0.031* |
| C7 | 0.7219 (2) | −0.06716 (19) | 0.45157 (15) | 0.0340 (4) |
| H7 | 0.7534 | −0.0483 | 0.5245 | 0.041* |
| C8 | 0.7865 (2) | −0.1481 (2) | 0.38121 (17) | 0.0365 (5) |
| H8 | 0.8680 | −0.1917 | 0.4001 | 0.044* |
| C9 | 0.7059 (2) | −0.15140 (18) | 0.27690 (15) | 0.0287 (4) |
| H9 | 0.7257 | −0.1972 | 0.2158 | 0.034* |
| C10 | 0.58923 (19) | −0.07210 (16) | 0.28218 (13) | 0.0218 (3) |
| C11 | 0.47914 (18) | −0.04276 (16) | 0.19133 (13) | 0.0212 (3) |
| H11 | 0.4742 | −0.1063 | 0.1271 | 0.025* |
| C12 | 0.32107 (19) | −0.03292 (16) | 0.21151 (14) | 0.0230 (4) |
| H12A | 0.2439 | −0.0746 | 0.1500 | 0.028* |
| H12B | 0.3063 | −0.0725 | 0.2708 | 0.028* |
| C13 | 0.31983 (18) | 0.11285 (16) | 0.23500 (12) | 0.0211 (3) |
| C14 | 0.20317 (18) | 0.17603 (17) | 0.27623 (13) | 0.0219 (3) |
| C15 | 0.0737 (2) | 0.10168 (18) | 0.28749 (14) | 0.0271 (4) |
| H15 | 0.0607 | 0.0111 | 0.2677 | 0.033* |
| C16 | −0.0357 (2) | 0.16144 (19) | 0.32793 (14) | 0.0309 (4) |
| H16 | −0.1212 | 0.1103 | 0.3349 | 0.037* |
| C17 | −0.0196 (2) | 0.2960 (2) | 0.35799 (14) | 0.0309 (4) |
| C18 | 0.1102 (2) | 0.37050 (18) | 0.34690 (14) | 0.0296 (4) |
| H18 | 0.1230 | 0.4611 | 0.3671 | 0.036* |
| C19 | 0.2197 (2) | 0.31208 (17) | 0.30645 (14) | 0.0260 (4) |
| H19 | 0.3048 | 0.3635 | 0.2993 | 0.031* |
| C20 | −0.1389 (2) | 0.3607 (3) | 0.40227 (19) | 0.0483 (6) |
| H20A | −0.2364 | 0.3153 | 0.3658 | 0.072* |
| H20B | −0.1313 | 0.4502 | 0.3934 | 0.072* |
| H20C | −0.1246 | 0.3576 | 0.4758 | 0.072* |
| C21 | 0.62648 (18) | 0.13289 (16) | 0.12474 (13) | 0.0210 (3) |
| C22 | 0.7966 (2) | 0.32849 (18) | 0.06058 (17) | 0.0356 (5) |
| H22A | 0.8841 | 0.2976 | 0.0978 | 0.043* |
| H22B | 0.7706 | 0.2810 | −0.0115 | 0.043* |
| C23 | 0.8295 (2) | 0.47341 (17) | 0.06311 (14) | 0.0263 (4) |
| C28 | 0.7407 (2) | 0.5341 (2) | −0.00745 (16) | 0.0370 (5) |
| H28 | 0.6566 | 0.4858 | −0.0549 | 0.044* |
| C27 | 0.7770 (3) | 0.6667 (2) | −0.00738 (18) | 0.0442 (5) |
| H27 | 0.7181 | 0.7062 | −0.0557 | 0.053* |
| C26 | 0.8997 (2) | 0.73954 (19) | 0.06398 (19) | 0.0405 (5) |
| H26 | 0.9246 | 0.8279 | 0.0636 | 0.049* |
| C25 | 0.9849 (2) | 0.6807 (2) | 0.13578 (19) | 0.0408 (5) |
| H25 | 1.0664 | 0.7300 | 0.1853 | 0.049* |
| C24 | 0.9504 (2) | 0.54858 (19) | 0.13486 (17) | 0.0344 (4) |
| H24 | 1.0097 | 0.5098 | 0.1834 | 0.041* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.02452 (15) | 0.02086 (15) | 0.02275 (15) | 0.00548 (10) | 0.00666 (11) | 0.00855 (10) |
| S1 | 0.0313 (2) | 0.0201 (2) | 0.0413 (3) | 0.00543 (17) | 0.0205 (2) | 0.00872 (19) |
| S2 | 0.0281 (2) | 0.0247 (2) | 0.0256 (2) | 0.00900 (17) | 0.01053 (18) | 0.00548 (17) |
| N1 | 0.0250 (7) | 0.0185 (7) | 0.0220 (7) | 0.0066 (5) | 0.0085 (6) | 0.0057 (5) |
| N2 | 0.0242 (7) | 0.0224 (7) | 0.0221 (7) | 0.0077 (6) | 0.0085 (6) | 0.0064 (6) |
| C5 | 0.0291 (9) | 0.0274 (9) | 0.0412 (11) | 0.0029 (7) | 0.0142 (8) | 0.0125 (8) |
| C4 | 0.0403 (11) | 0.0297 (10) | 0.0319 (10) | 0.0035 (8) | 0.0138 (8) | 0.0148 (8) |
| C3 | 0.0408 (11) | 0.0239 (9) | 0.0443 (12) | 0.0099 (8) | 0.0121 (9) | 0.0180 (8) |
| C2 | 0.0442 (11) | 0.0213 (9) | 0.0415 (11) | 0.0056 (8) | 0.0147 (9) | 0.0040 (8) |
| C1 | 0.0332 (10) | 0.0254 (9) | 0.0361 (11) | −0.0019 (8) | 0.0038 (8) | 0.0075 (8) |
| C6 | 0.0326 (9) | 0.0209 (8) | 0.0240 (9) | 0.0000 (7) | 0.0053 (7) | 0.0049 (7) |
| C7 | 0.0351 (10) | 0.0348 (10) | 0.0268 (10) | −0.0067 (8) | −0.0032 (8) | 0.0108 (8) |
| C8 | 0.0236 (9) | 0.0423 (11) | 0.0481 (12) | 0.0062 (8) | 0.0046 (8) | 0.0248 (10) |
| C9 | 0.0270 (9) | 0.0308 (10) | 0.0356 (10) | 0.0082 (7) | 0.0144 (8) | 0.0153 (8) |
| C10 | 0.0239 (8) | 0.0201 (8) | 0.0239 (9) | 0.0021 (6) | 0.0076 (7) | 0.0092 (7) |
| C11 | 0.0268 (9) | 0.0172 (8) | 0.0205 (8) | 0.0040 (6) | 0.0059 (7) | 0.0049 (6) |
| C12 | 0.0229 (8) | 0.0213 (8) | 0.0254 (9) | 0.0027 (6) | 0.0045 (7) | 0.0071 (7) |
| C13 | 0.0228 (8) | 0.0230 (8) | 0.0175 (8) | 0.0027 (7) | 0.0024 (6) | 0.0070 (6) |
| C14 | 0.0220 (8) | 0.0265 (9) | 0.0182 (8) | 0.0054 (7) | 0.0035 (6) | 0.0069 (7) |
| C15 | 0.0267 (9) | 0.0270 (9) | 0.0270 (9) | 0.0011 (7) | 0.0051 (7) | 0.0059 (7) |
| C16 | 0.0214 (9) | 0.0424 (11) | 0.0280 (9) | −0.0021 (8) | 0.0073 (7) | 0.0060 (8) |
| C17 | 0.0268 (9) | 0.0444 (11) | 0.0221 (9) | 0.0080 (8) | 0.0075 (7) | 0.0032 (8) |
| C18 | 0.0331 (10) | 0.0283 (9) | 0.0277 (9) | 0.0078 (8) | 0.0082 (8) | 0.0020 (7) |
| C19 | 0.0250 (9) | 0.0260 (9) | 0.0287 (9) | 0.0034 (7) | 0.0084 (7) | 0.0074 (7) |
| C20 | 0.0334 (11) | 0.0616 (15) | 0.0477 (13) | 0.0092 (10) | 0.0175 (10) | −0.0079 (11) |
| C21 | 0.0222 (8) | 0.0217 (8) | 0.0190 (8) | 0.0035 (6) | 0.0030 (6) | 0.0054 (6) |
| C22 | 0.0384 (11) | 0.0265 (10) | 0.0497 (12) | 0.0037 (8) | 0.0282 (9) | 0.0076 (9) |
| C23 | 0.0271 (9) | 0.0252 (9) | 0.0320 (10) | 0.0048 (7) | 0.0171 (8) | 0.0077 (7) |
| C28 | 0.0345 (10) | 0.0428 (12) | 0.0327 (11) | 0.0070 (9) | 0.0050 (8) | 0.0066 (9) |
| C27 | 0.0503 (13) | 0.0474 (13) | 0.0487 (13) | 0.0257 (11) | 0.0184 (10) | 0.0276 (10) |
| C26 | 0.0370 (11) | 0.0266 (10) | 0.0701 (15) | 0.0109 (8) | 0.0301 (11) | 0.0178 (10) |
| C25 | 0.0266 (10) | 0.0321 (11) | 0.0620 (14) | 0.0017 (8) | 0.0098 (9) | 0.0055 (10) |
| C24 | 0.0290 (10) | 0.0342 (10) | 0.0439 (11) | 0.0074 (8) | 0.0086 (8) | 0.0159 (9) |

*Geometric parameters (Å, °)*

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| Fe1—C8 | 2.0428 (19) | C10—C11 | 1.502 (2) |
| Fe1—C2 | 2.0452 (19) | C11—C12 | 1.538 (2) |
| Fe1—C1 | 2.0460 (19) | C11—H11 | 0.9800 |
| Fe1—C9 | 2.0474 (18) | C12—C13 | 1.509 (2) |
| Fe1—C6 | 2.0488 (17) | C12—H12A | 0.9700 |
| Fe1—C7 | 2.0487 (19) | C12—H12B | 0.9700 |
| Fe1—C5 | 2.0493 (18) | C13—C14 | 1.466 (2) |
| Fe1—C10 | 2.0510 (16) | C14—C15 | 1.397 (2) |
| Fe1—C3 | 2.0521 (18) | C14—C19 | 1.398 (2) |

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| Fe1—C4 | 2.0549 (18) | C15—C16 | 1.388 (3) |
| S1—C21 | 1.7708 (17) | C15—H15 | 0.9300 |
| S1—C22 | 1.8167 (18) | C16—C17 | 1.383 (3) |
| S2—C21 | 1.6608 (17) | C16—H16 | 0.9300 |
| N1—C21 | 1.340 (2) | C17—C18 | 1.399 (3) |
| N1—N2 | 1.3964 (19) | C17—C20 | 1.512 (3) |
| N1—C11 | 1.495 (2) | C18—C19 | 1.382 (3) |
| N2—C13 | 1.294 (2) | C18—H18 | 0.9300 |
| C5—C1 | 1.420 (3) | C19—H19 | 0.9300 |
| C5—C4 | 1.419 (3) | C20—H20A | 0.9600 |
| C5—H5 | 0.9300 | C20—H20B | 0.9600 |
| C4—C3 | 1.414 (3) | C20—H20C | 0.9600 |
| C4—H4 | 0.9300 | C22—C23 | 1.508 (2) |
| C3—C2 | 1.420 (3) | C22—H22A | 0.9700 |
| C3—H3 | 0.9300 | C22—H22B | 0.9700 |
| C2—C1 | 1.428 (3) | C23—C24 | 1.378 (3) |
| C2—H2 | 0.9300 | C23—C28 | 1.392 (3) |
| C1—H1 | 0.9300 | C28—C27 | 1.392 (3) |
| C6—C7 | 1.422 (3) | C28—H28 | 0.9300 |
| C6—C10 | 1.432 (2) | C27—C26 | 1.377 (3) |
| C6—H6 | 0.9300 | C27—H27 | 0.9300 |
| C7—C8 | 1.416 (3) | C26—C25 | 1.374 (3) |
| C7—H7 | 0.9300 | C26—H26 | 0.9300 |
| C8—C9 | 1.421 (3) | C25—C24 | 1.383 (3) |
| C8—H8 | 0.9300 | C25—H25 | 0.9300 |
| C9—C10 | 1.429 (2) | C24—H24 | 0.9300 |
| C9—H9 | 0.9300 | | |
| C8—Fe1—C2 | 116.95 (9) | C6—C7—Fe1 | 69.69 (10) |
| C8—Fe1—C1 | 151.92 (9) | C8—C7—H7 | 126.1 |
| C2—Fe1—C1 | 40.85 (8) | C6—C7—H7 | 126.1 |
| C8—Fe1—C9 | 40.66 (8) | Fe1—C7—H7 | 126.3 |
| C2—Fe1—C9 | 106.49 (8) | C7—C8—C9 | 108.51 (17) |
| C1—Fe1—C9 | 118.79 (8) | C7—C8—Fe1 | 69.98 (11) |
| C8—Fe1—C6 | 68.20 (8) | C9—C8—Fe1 | 69.85 (10) |
| C2—Fe1—C6 | 166.18 (8) | C7—C8—H8 | 125.7 |
| C1—Fe1—C6 | 129.18 (7) | C9—C8—H8 | 125.7 |
| C9—Fe1—C6 | 68.42 (7) | Fe1—C8—H8 | 126.0 |
| C8—Fe1—C7 | 40.49 (9) | C8—C9—C10 | 108.07 (17) |
| C2—Fe1—C7 | 151.03 (8) | C8—C9—Fe1 | 69.49 (11) |
| C1—Fe1—C7 | 166.78 (8) | C10—C9—Fe1 | 69.73 (9) |
| C9—Fe1—C7 | 68.41 (8) | C8—C9—H9 | 126.0 |
| C6—Fe1—C7 | 40.62 (8) | C10—C9—H9 | 126.0 |
| C8—Fe1—C5 | 164.95 (8) | Fe1—C9—H9 | 126.4 |
| C2—Fe1—C5 | 68.37 (8) | C9—C10—C6 | 107.23 (15) |
| C1—Fe1—C5 | 40.57 (8) | C9—C10—C11 | 127.04 (15) |
| C9—Fe1—C5 | 153.95 (8) | C6—C10—C11 | 125.67 (15) |
| C6—Fe1—C5 | 110.18 (7) | C9—C10—Fe1 | 69.46 (9) |
| C7—Fe1—C5 | 128.59 (8) | C6—C10—Fe1 | 69.47 (9) |
| C8—Fe1—C10 | 68.59 (7) | C11—C10—Fe1 | 128.36 (11) |

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| C2—Fe1—C10 | 127.05 (8) | N1—C11—C10 | 109.61 (13) |
| C1—Fe1—C10 | 108.77 (7) | N1—C11—C12 | 100.44 (12) |
| C9—Fe1—C10 | 40.81 (7) | C10—C11—C12 | 114.22 (14) |
| C6—Fe1—C10 | 40.88 (7) | N1—C11—H11 | 110.7 |
| C7—Fe1—C10 | 68.72 (7) | C10—C11—H11 | 110.7 |
| C5—Fe1—C10 | 120.71 (7) | C12—C11—H11 | 110.7 |
| C8—Fe1—C3 | 106.16 (8) | C13—C12—C11 | 102.75 (13) |
| C2—Fe1—C3 | 40.56 (8) | C13—C12—H12A | 111.2 |
| C1—Fe1—C3 | 68.31 (8) | C11—C12—H12A | 111.2 |
| C9—Fe1—C3 | 125.60 (8) | C13—C12—H12B | 111.2 |
| C6—Fe1—C3 | 152.81 (8) | C11—C12—H12B | 111.2 |
| C7—Fe1—C3 | 117.78 (8) | H12A—C12—H12B | 109.1 |
| C5—Fe1—C3 | 68.04 (8) | N2—C13—C14 | 121.50 (15) |
| C10—Fe1—C3 | 164.02 (8) | N2—C13—C12 | 113.60 (15) |
| C8—Fe1—C4 | 126.35 (8) | C14—C13—C12 | 124.88 (14) |
| C2—Fe1—C4 | 68.10 (8) | C15—C14—C19 | 118.43 (16) |
| C1—Fe1—C4 | 68.15 (8) | C15—C14—C13 | 120.79 (15) |
| C9—Fe1—C4 | 163.37 (8) | C19—C14—C13 | 120.77 (15) |
| C6—Fe1—C4 | 120.38 (8) | C16—C15—C14 | 120.77 (17) |
| C7—Fe1—C4 | 108.22 (8) | C16—C15—H15 | 119.6 |
| C5—Fe1—C4 | 40.46 (8) | C14—C15—H15 | 119.6 |
| C10—Fe1—C4 | 154.75 (7) | C17—C16—C15 | 120.92 (17) |
| C3—Fe1—C4 | 40.27 (8) | C17—C16—H16 | 119.5 |
| C21—S1—C22 | 101.89 (8) | C15—C16—H16 | 119.5 |
| C21—N1—N2 | 120.26 (13) | C16—C17—C18 | 118.34 (17) |
| C21—N1—C11 | 127.22 (14) | C16—C17—C20 | 120.75 (18) |
| N2—N1—C11 | 112.25 (12) | C18—C17—C20 | 120.91 (19) |
| C13—N2—N1 | 108.02 (13) | C19—C18—C17 | 121.25 (17) |
| C1—C5—C4 | 108.06 (17) | C19—C18—H18 | 119.4 |
| C1—C5—Fe1 | 69.59 (11) | C17—C18—H18 | 119.4 |
| C4—C5—Fe1 | 69.98 (11) | C18—C19—C14 | 120.30 (16) |
| C1—C5—H5 | 126.0 | C18—C19—H19 | 119.9 |
| C4—C5—H5 | 126.0 | C14—C19—H19 | 119.9 |
| Fe1—C5—H5 | 126.0 | C17—C20—H20A | 109.5 |
| C3—C4—C5 | 108.19 (17) | C17—C20—H20B | 109.5 |
| C3—C4—Fe1 | 69.76 (10) | H20A—C20—H20B | 109.5 |
| C5—C4—Fe1 | 69.56 (10) | C17—C20—H20C | 109.5 |
| C3—C4—H4 | 125.9 | H20A—C20—H20C | 109.5 |
| C5—C4—H4 | 125.9 | H20B—C20—H20C | 109.5 |
| Fe1—C4—H4 | 126.4 | N1—C21—S2 | 122.65 (13) |
| C4—C3—C2 | 108.20 (17) | N1—C21—S1 | 112.19 (12) |
| C4—C3—Fe1 | 69.97 (10) | S2—C21—S1 | 125.16 (10) |
| C2—C3—Fe1 | 69.46 (10) | C23—C22—S1 | 107.43 (12) |
| C4—C3—H3 | 125.9 | C23—C22—H22A | 110.2 |
| C2—C3—H3 | 125.9 | S1—C22—H22A | 110.2 |
| Fe1—C3—H3 | 126.2 | C23—C22—H22B | 110.2 |
| C3—C2—C1 | 107.78 (18) | S1—C22—H22B | 110.2 |
| C3—C2—Fe1 | 69.98 (11) | H22A—C22—H22B | 108.5 |
| C1—C2—Fe1 | 69.60 (10) | C24—C23—C28 | 118.41 (17) |

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| C3—C2—H2 | 126.1 | C24—C23—C22 | 120.43 (17) |
| C1—C2—H2 | 126.1 | C28—C23—C22 | 121.16 (18) |
| Fe1—C2—H2 | 125.9 | C23—C28—C27 | 120.40 (19) |
| C5—C1—C2 | 107.77 (18) | C23—C28—H28 | 119.8 |
| C5—C1—Fe1 | 69.84 (11) | C27—C28—H28 | 119.8 |
| C2—C1—Fe1 | 69.54 (11) | C26—C27—C28 | 120.19 (19) |
| C5—C1—H1 | 126.1 | C26—C27—H27 | 119.9 |
| C2—C1—H1 | 126.1 | C28—C27—H27 | 119.9 |
| Fe1—C1—H1 | 126.1 | C25—C26—C27 | 119.51 (18) |
| C7—C6—C10 | 108.33 (16) | C25—C26—H26 | 120.2 |
| C7—C6—Fe1 | 69.69 (10) | C27—C26—H26 | 120.2 |
| C10—C6—Fe1 | 69.64 (9) | C26—C25—C24 | 120.4 (2) |
| C7—C6—H6 | 125.8 | C26—C25—H25 | 119.8 |
| C10—C6—H6 | 125.8 | C24—C25—H25 | 119.8 |
| Fe1—C6—H6 | 126.4 | C23—C24—C25 | 121.06 (19) |
| C8—C7—C6 | 107.85 (17) | C23—C24—H24 | 119.5 |
| C8—C7—Fe1 | 69.53 (11) | C25—C24—H24 | 119.5 |
| C21—N1—N2—C13 | 163.81 (15) | C1—Fe1—C7—C6 | −43.9 (4) |
| C11—N1—N2—C13 | −10.50 (18) | C9—Fe1—C7—C6 | 81.61 (12) |
| C8—Fe1—C5—C1 | −151.8 (3) | C5—Fe1—C7—C6 | −75.37 (13) |
| C2—Fe1—C5—C1 | −38.01 (11) | C10—Fe1—C7—C6 | 37.61 (10) |
| C9—Fe1—C5—C1 | 45.3 (2) | C3—Fe1—C7—C6 | −158.46 (11) |
| C6—Fe1—C5—C1 | 127.27 (11) | C4—Fe1—C7—C6 | −115.72 (12) |
| C7—Fe1—C5—C1 | 169.42 (11) | C6—C7—C8—C9 | 0.0 (2) |
| C10—Fe1—C5—C1 | 83.21 (12) | Fe1—C7—C8—C9 | 59.42 (13) |
| C3—Fe1—C5—C1 | −81.85 (12) | C6—C7—C8—Fe1 | −59.37 (13) |
| C4—Fe1—C5—C1 | −119.19 (16) | C2—Fe1—C8—C7 | −156.34 (11) |
| C8—Fe1—C5—C4 | −32.6 (3) | C1—Fe1—C8—C7 | 171.85 (15) |
| C2—Fe1—C5—C4 | 81.18 (12) | C9—Fe1—C8—C7 | 119.58 (16) |
| C1—Fe1—C5—C4 | 119.19 (16) | C6—Fe1—C8—C7 | 37.76 (11) |
| C9—Fe1—C5—C4 | 164.52 (16) | C5—Fe1—C8—C7 | −49.0 (3) |
| C6—Fe1—C5—C4 | −113.54 (12) | C10—Fe1—C8—C7 | 81.88 (12) |
| C7—Fe1—C5—C4 | −71.39 (14) | C3—Fe1—C8—C7 | −114.07 (12) |
| C10—Fe1—C5—C4 | −157.60 (11) | C4—Fe1—C8—C7 | −74.70 (14) |
| C3—Fe1—C5—C4 | 37.34 (12) | C2—Fe1—C8—C9 | 84.08 (13) |
| C1—C5—C4—C3 | 0.1 (2) | C1—Fe1—C8—C9 | 52.3 (2) |
| Fe1—C5—C4—C3 | −59.26 (13) | C6—Fe1—C8—C9 | −81.83 (12) |
| C1—C5—C4—Fe1 | 59.39 (12) | C7—Fe1—C8—C9 | −119.58 (16) |
| C8—Fe1—C4—C3 | −70.49 (15) | C5—Fe1—C8—C9 | −168.6 (3) |
| C2—Fe1—C4—C3 | 37.61 (12) | C10—Fe1—C8—C9 | −37.70 (11) |
| C1—Fe1—C4—C3 | 81.79 (13) | C3—Fe1—C8—C9 | 126.35 (12) |
| C9—Fe1—C4—C3 | −36.3 (3) | C4—Fe1—C8—C9 | 165.72 (11) |
| C6—Fe1—C4—C3 | −154.57 (12) | C7—C8—C9—C10 | −0.2 (2) |
| C7—Fe1—C4—C3 | −111.74 (13) | Fe1—C8—C9—C10 | 59.26 (12) |
| C5—Fe1—C4—C3 | 119.51 (17) | C7—C8—C9—Fe1 | −59.50 (13) |
| C10—Fe1—C4—C3 | 169.66 (15) | C2—Fe1—C9—C8 | −112.38 (13) |
| C8—Fe1—C4—C5 | 170.00 (12) | C1—Fe1—C9—C8 | −154.87 (12) |
| C2—Fe1—C4—C5 | −81.90 (13) | C6—Fe1—C9—C8 | 81.23 (13) |
| C1—Fe1—C4—C5 | −37.72 (11) | C7—Fe1—C9—C8 | 37.40 (12) |

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| C9—Fe1—C4—C5 | −155.8 (2) | C5—Fe1—C9—C8 | 173.27 (16) |
| C6—Fe1—C4—C5 | 85.92 (13) | C10—Fe1—C9—C8 | 119.41 (16) |
| C7—Fe1—C4—C5 | 128.75 (12) | C3—Fe1—C9—C8 | −72.06 (15) |
| C10—Fe1—C4—C5 | 50.2 (2) | C4—Fe1—C9—C8 | −44.0 (3) |
| C3—Fe1—C4—C5 | −119.51 (17) | C8—Fe1—C9—C10 | −119.41 (16) |
| C5—C4—C3—C2 | 0.0 (2) | C2—Fe1—C9—C10 | 128.21 (11) |
| Fe1—C4—C3—C2 | −59.13 (13) | C1—Fe1—C9—C10 | 85.72 (12) |
| C5—C4—C3—Fe1 | 59.14 (13) | C6—Fe1—C9—C10 | −38.18 (10) |
| C8—Fe1—C3—C4 | 127.78 (12) | C7—Fe1—C9—C10 | −82.01 (11) |
| C2—Fe1—C3—C4 | −119.45 (17) | C5—Fe1—C9—C10 | 53.9 (2) |
| C1—Fe1—C3—C4 | −81.37 (13) | C3—Fe1—C9—C10 | 168.53 (10) |
| C9—Fe1—C3—C4 | 167.97 (11) | C4—Fe1—C9—C10 | −163.4 (2) |
| C6—Fe1—C3—C4 | 54.2 (2) | C8—C9—C10—C6 | 0.34 (19) |
| C7—Fe1—C3—C4 | 85.70 (13) | Fe1—C9—C10—C6 | 59.45 (11) |
| C5—Fe1—C3—C4 | −37.51 (12) | C8—C9—C10—C11 | 177.69 (16) |
| C10—Fe1—C3—C4 | −163.8 (2) | Fe1—C9—C10—C11 | −123.19 (16) |
| C8—Fe1—C3—C2 | −112.77 (13) | C8—C9—C10—Fe1 | −59.12 (12) |
| C1—Fe1—C3—C2 | 38.08 (12) | C7—C6—C10—C9 | −0.31 (19) |
| C9—Fe1—C3—C2 | −72.58 (14) | Fe1—C6—C10—C9 | −59.44 (11) |
| C6—Fe1—C3—C2 | 173.60 (15) | C7—C6—C10—C11 | −177.71 (15) |
| C7—Fe1—C3—C2 | −154.85 (12) | Fe1—C6—C10—C11 | 123.15 (16) |
| C5—Fe1—C3—C2 | 81.94 (13) | C7—C6—C10—Fe1 | 59.14 (12) |
| C10—Fe1—C3—C2 | −44.4 (3) | C8—Fe1—C10—C9 | 37.56 (12) |
| C4—Fe1—C3—C2 | 119.45 (17) | C2—Fe1—C10—C9 | −70.73 (14) |
| C4—C3—C2—C1 | −0.1 (2) | C1—Fe1—C10—C9 | −112.63 (12) |
| Fe1—C3—C2—C1 | −59.58 (13) | C6—Fe1—C10—C9 | 118.56 (15) |
| C4—C3—C2—Fe1 | 59.45 (13) | C7—Fe1—C10—C9 | 81.19 (12) |
| C8—Fe1—C2—C3 | 83.47 (13) | C5—Fe1—C10—C9 | −155.64 (11) |
| C1—Fe1—C2—C3 | −118.83 (17) | C3—Fe1—C10—C9 | −36.0 (3) |
| C9—Fe1—C2—C3 | 125.99 (12) | C4—Fe1—C10—C9 | 168.95 (16) |
| C6—Fe1—C2—C3 | −167.7 (3) | C8—Fe1—C10—C6 | −81.00 (12) |
| C7—Fe1—C2—C3 | 50.9 (2) | C2—Fe1—C10—C6 | 170.70 (11) |
| C5—Fe1—C2—C3 | −81.07 (12) | C1—Fe1—C10—C6 | 128.81 (11) |
| C10—Fe1—C2—C3 | 166.04 (11) | C9—Fe1—C10—C6 | −118.56 (15) |
| C4—Fe1—C2—C3 | −37.35 (12) | C7—Fe1—C10—C6 | −37.37 (11) |
| C8—Fe1—C2—C1 | −157.71 (12) | C5—Fe1—C10—C6 | 85.80 (12) |
| C9—Fe1—C2—C1 | −115.19 (12) | C3—Fe1—C10—C6 | −154.5 (3) |
| C6—Fe1—C2—C1 | −48.9 (4) | C4—Fe1—C10—C6 | 50.4 (2) |
| C7—Fe1—C2—C1 | 169.74 (15) | C8—Fe1—C10—C11 | 159.15 (17) |
| C5—Fe1—C2—C1 | 37.75 (12) | C2—Fe1—C10—C11 | 50.85 (18) |
| C10—Fe1—C2—C1 | −75.14 (14) | C1—Fe1—C10—C11 | 8.96 (17) |
| C3—Fe1—C2—C1 | 118.83 (17) | C9—Fe1—C10—C11 | 121.59 (19) |
| C4—Fe1—C2—C1 | 81.48 (12) | C6—Fe1—C10—C11 | −119.85 (19) |
| C4—C5—C1—C2 | −0.2 (2) | C7—Fe1—C10—C11 | −157.23 (17) |
| Fe1—C5—C1—C2 | 59.43 (13) | C5—Fe1—C10—C11 | −34.05 (18) |
| C4—C5—C1—Fe1 | −59.63 (13) | C3—Fe1—C10—C11 | 85.6 (3) |
| C3—C2—C1—C5 | 0.2 (2) | C4—Fe1—C10—C11 | −69.5 (2) |
| Fe1—C2—C1—C5 | −59.62 (12) | C21—N1—C11—C10 | 82.3 (2) |
| C3—C2—C1—Fe1 | 59.82 (13) | N2—N1—C11—C10 | −103.92 (15) |

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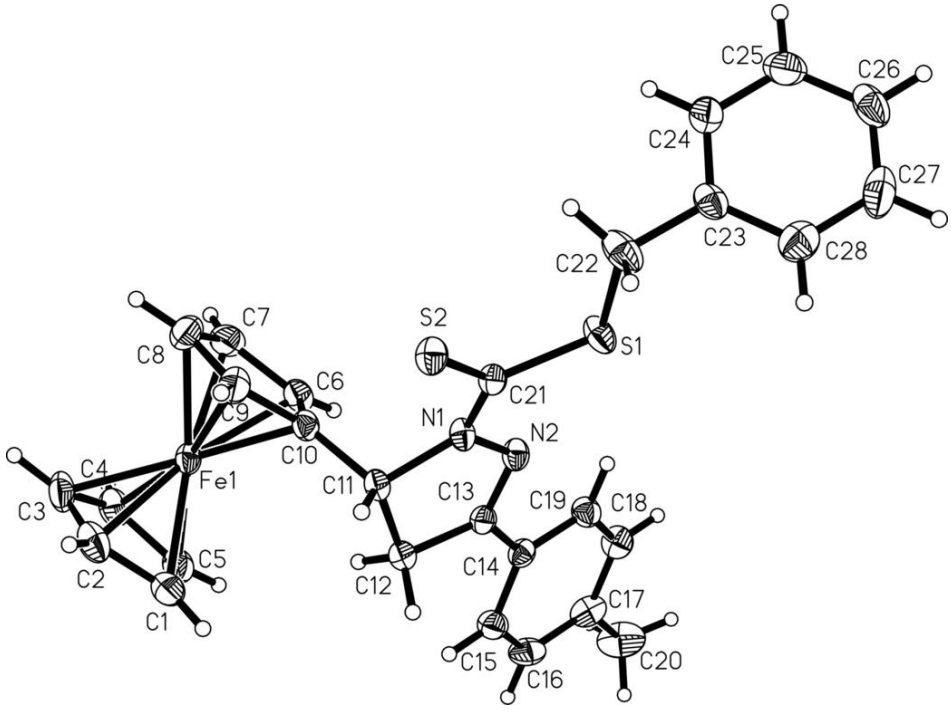
| C8—Fe1—C1—C5 | 164.87 (15) | C21—N1—C11—C12 | −157.18 (16) |
| C2—Fe1—C1—C5 | 118.94 (16) | N2—N1—C11—C12 | 16.65 (16) |
| C9—Fe1—C1—C5 | −159.12 (11) | C9—C10—C11—N1 | −104.11 (18) |
| C6—Fe1—C1—C5 | −74.48 (14) | C6—C10—C11—N1 | 72.8 (2) |
| C7—Fe1—C1—C5 | −38.9 (4) | Fe1—C10—C11—N1 | 163.79 (12) |
| C10—Fe1—C1—C5 | −115.62 (11) | C9—C10—C11—C12 | 144.09 (17) |
| C3—Fe1—C1—C5 | 81.13 (12) | C6—C10—C11—C12 | −39.0 (2) |
| C4—Fe1—C1—C5 | 37.62 (11) | Fe1—C10—C11—C12 | 52.0 (2) |
| C8—Fe1—C1—C2 | 45.9 (2) | N1—C11—C12—C13 | −15.48 (15) |
| C9—Fe1—C1—C2 | 81.94 (13) | C10—C11—C12—C13 | 101.72 (15) |
| C6—Fe1—C1—C2 | 166.58 (11) | N1—N2—C13—C14 | 179.95 (14) |
| C7—Fe1—C1—C2 | −157.8 (3) | N1—N2—C13—C12 | −1.10 (19) |
| C5—Fe1—C1—C2 | −118.94 (16) | C11—C12—C13—N2 | 11.39 (18) |
| C10—Fe1—C1—C2 | 125.44 (12) | C11—C12—C13—C14 | −169.70 (15) |
| C3—Fe1—C1—C2 | −37.81 (12) | N2—C13—C14—C15 | 172.56 (16) |
| C4—Fe1—C1—C2 | −81.33 (12) | C12—C13—C14—C15 | −6.3 (2) |
| C8—Fe1—C6—C7 | −37.65 (12) | N2—C13—C14—C19 | −8.2 (2) |
| C2—Fe1—C6—C7 | −152.3 (3) | C12—C13—C14—C19 | 172.93 (16) |
| C1—Fe1—C6—C7 | 168.21 (12) | C19—C14—C15—C16 | −0.1 (3) |
| C9—Fe1—C6—C7 | −81.56 (12) | C13—C14—C15—C16 | 179.08 (16) |
| C5—Fe1—C6—C7 | 126.32 (12) | C14—C15—C16—C17 | 0.1 (3) |
| C10—Fe1—C6—C7 | −119.67 (16) | C15—C16—C17—C18 | −0.2 (3) |
| C3—Fe1—C6—C7 | 45.3 (2) | C15—C16—C17—C20 | −179.84 (18) |
| C4—Fe1—C6—C7 | 82.72 (13) | C16—C17—C18—C19 | 0.3 (3) |
| C8—Fe1—C6—C10 | 82.03 (11) | C20—C17—C18—C19 | −179.98 (18) |
| C2—Fe1—C6—C10 | −32.7 (4) | C17—C18—C19—C14 | −0.4 (3) |
| C1—Fe1—C6—C10 | −72.12 (13) | C15—C14—C19—C18 | 0.3 (3) |
| C9—Fe1—C6—C10 | 38.12 (10) | C13—C14—C19—C18 | −178.90 (16) |
| C7—Fe1—C6—C10 | 119.67 (16) | N2—N1—C21—S2 | −174.50 (11) |
| C5—Fe1—C6—C10 | −114.01 (11) | C11—N1—C21—S2 | −1.1 (2) |
| C3—Fe1—C6—C10 | 164.99 (15) | N2—N1—C21—S1 | 5.40 (19) |
| C4—Fe1—C6—C10 | −157.61 (10) | C11—N1—C21—S1 | 178.78 (12) |
| C10—C6—C7—C8 | 0.2 (2) | C22—S1—C21—N1 | 175.13 (13) |
| Fe1—C6—C7—C8 | 59.27 (13) | C22—S1—C21—S2 | −4.97 (14) |
| C10—C6—C7—Fe1 | −59.11 (12) | C21—S1—C22—C23 | −175.12 (14) |
| C2—Fe1—C7—C8 | 47.6 (2) | S1—C22—C23—C24 | 102.92 (18) |
| C1—Fe1—C7—C8 | −163.0 (3) | S1—C22—C23—C28 | −78.0 (2) |
| C9—Fe1—C7—C8 | −37.54 (11) | C24—C23—C28—C27 | 2.2 (3) |
| C6—Fe1—C7—C8 | −119.15 (16) | C22—C23—C28—C27 | −176.87 (18) |
| C5—Fe1—C7—C8 | 165.48 (11) | C23—C28—C27—C26 | −1.2 (3) |
| C10—Fe1—C7—C8 | −81.54 (12) | C28—C27—C26—C25 | −0.7 (3) |
| C3—Fe1—C7—C8 | 82.39 (13) | C27—C26—C25—C24 | 1.7 (3) |
| C4—Fe1—C7—C8 | 125.13 (12) | C28—C23—C24—C25 | −1.2 (3) |
| C8—Fe1—C7—C6 | 119.15 (16) | C22—C23—C24—C25 | 177.82 (18) |
| C2—Fe1—C7—C6 | 166.76 (15) | C26—C25—C24—C23 | −0.7 (3) |

**Fig. 1**


C25
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C10
C4
Fe1
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C3
C5
C14
C2
C12
C17
C1
C15
C16
C20

**Fig. 2**