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[5,10,15,20-Tetrakis(4-methoxyphenyl)-porphyrinato- κ^4N,N',N'',N'''](trifluoromethanesulfonato- κO)iron(III)

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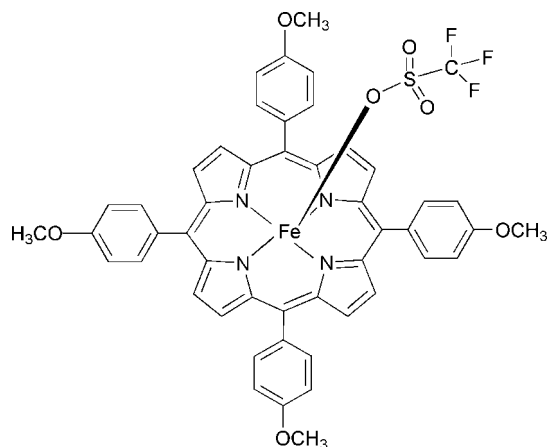
Received 9 December 2010; accepted 10 January 2011

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.055; wR factor = 0.155; data-to-parameter ratio = 14.0.

The title compound, $[\text{Fe}(\text{CF}_3\text{O}_3\text{S})(\text{C}_{48}\text{H}_{36}\text{N}_4\text{O}_4)]$, is a five-coordinate iron(III) porphyrin complex with a trifluoromethanesulfonate anion as an axial ligand. The Fe^{III} atom is displaced by 0.40 (1) Å towards the trifluoromethanesulfonate anion from the 24-atom mean plane of the porphyrin. The average $\text{Fe}-\text{N}_p$ distance is 2.044 (2) Å and the $\text{Fe}-\text{O}$ distance is 2.001 (2) Å.

Related literature

For the structures of related porphyrin ('picket-fence', tetraphenylporphyrin, octaethylporphyrin) derivatives, see: González & Wilson (1994); Gismelseed *et al.* (1990); Xu *et al.* (2008).



Experimental

Crystal data

| | |
|--|---|
| $[\text{Fe}(\text{CF}_3\text{O}_3\text{S})(\text{C}_{48}\text{H}_{36}\text{N}_4\text{O}_4)]$ | $\gamma = 103.483 (3)^\circ$ |
| $M_r = 937.73$ | $V = 2083.2 (4) \text{ \AA}^3$ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 12.5265 (14) \text{ \AA}$ | Mo $K\alpha$ radiation |
| $b = 13.2725 (16) \text{ \AA}$ | $\mu = 0.49 \text{ mm}^{-1}$ |
| $c = 14.0220 (17) \text{ \AA}$ | $T = 100 \text{ K}$ |
| $\alpha = 90.080 (2)^\circ$ | $0.49 \times 0.38 \times 0.19 \text{ mm}$ |
| $\beta = 112.534 (2)^\circ$ | |

Data collection

| | |
|---|--|
| Bruker SMART APEX CCD diffractometer | 25055 measured reflections |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2001) | 8187 independent reflections |
| $T_{\min} = 0.797$, $T_{\max} = 0.913$ | 6693 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.048$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.055$ | 586 parameters |
| $wR(F^2) = 0.155$ | H-atom parameters constrained |
| $S = 1.00$ | $\Delta\rho_{\max} = 1.62 \text{ e \AA}^{-3}$ |
| 8187 reflections | $\Delta\rho_{\min} = -0.83 \text{ e \AA}^{-3}$ |

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; 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: BV2171).

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supporting information

Acta Cryst. (2011). E67, m268 [doi:10.1107/S1600536811001395]

[5,10,15,20-Tetrakis(4-methoxyphenyl)porphyrinato- κ^4N,N',N'',N'''](trifluoromethanesulfonato- κO)iron(III)

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S1. Comment

In this paper, we report the structure of the five-coordinate compound (5,10,15,20-tetrakis(4-methoxyphenyl)porphyrinato) (trifluoromethanesulfonato)iron(III). Other trifluoromethanesulfonato iron porphyrin derivatives have been reported previously: The (T_{piv}PP)Fe(OSO₂CF₃)(H₂O) compound is six-coordinate at Fe, and the (TPP)Fe(OSO₂CF₃) and (OEP)Fe(OSO₂CF₃) compounds are five-coordinate at Fe (González *et al.* 1994, Gismelseed *et al.* 1990, and Xu *et al.* 2008).

The molecular structure of (5,10,15,20-tetrakis(4-methoxyphenyl)porphyrinato)(trifluoromethanesulfonato)iron(III) is shown in Fig. 1. The porphyrin core of the compound is slightly saddle shaped. The iron atom is displaced by 0.40 (1) Å from the 24-atom mean porphyrin plane toward the trifluoromethanesulfonate anion. The trifluoromethanesulfonate anion binds to the iron center through one of its sulfonato oxygen atoms. The average Fe—N_p distance is 2.044 (2) Å and the Fe—O distance is 2.001 (2) Å. The bond angle of the Fe—O—S linkage is 137.11 (13)°.

S2. Experimental

To a toluene solution (20 ml) of (T(*p*-OMe)PP)FeCl (0.025 g, 0.030 mmol) was added silver trifluoromethanesulfonate (0.009 g, 0.033 mmol) (purchased from Aldrich Chemical Company and used as received) under N₂. After stirring for 2 h, the resulting mixture was filtered and dried under vacuum. A suitable purple prism-shaped crystal was grown by slow evaporation of a dichloromethane-hexane (1:1) solution of the complex at room temperature under N₂.

S3. Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.95 Å for aromatic carbons, 0.98 Å for methyl carbons and were refined using a riding model with $U_{\text{iso}} = 1.2 U_{\text{eq}}(\text{C})$ for phenyl H atoms, $U_{\text{iso}} = 1.5 U_{\text{eq}}(\text{C})$ for methyl H atoms.

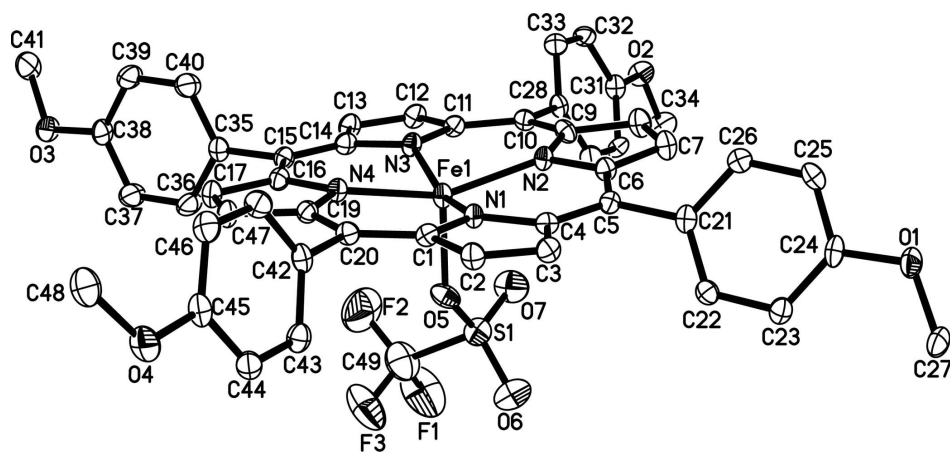


Figure 1

The molecular structure of (T(*p*-OMe)PP)Fe(OSO₂CF₃). Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

[5,10,15,20-Tetrakis(4-methoxyphenyl)porphyrinato-κ⁴N,N',N'',N'''](trifluoromethanesulfonato-κO)iron(III)

Crystal data

[Fe(CF₃O₃S)(C₄₈H₃₆N₄O₄)]

$M_r = 937.73$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 12.5265$ (14) Å

$b = 13.2725$ (16) Å

$c = 14.0220$ (17) Å

$\alpha = 90.080$ (2)°

$\beta = 112.534$ (2)°

$\gamma = 103.483$ (3)°

$V = 2083.2$ (4) Å³

$Z = 2$

$F(000) = 966$

$D_x = 1.495$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5786 reflections

$\theta = 2.4$ – 28.2 °

$\mu = 0.49$ mm⁻¹

$T = 100$ K

Prism, purple

$0.49 \times 0.38 \times 0.19$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2001)

$T_{\min} = 0.797$, $T_{\max} = 0.913$

25055 measured reflections

8187 independent reflections

6693 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 1.6$ °

$h = -15 \rightarrow 15$

$k = -16 \rightarrow 16$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.155$

$S = 1.00$

8187 reflections

586 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 3.420P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.62$ e Å⁻³

$\Delta\rho_{\min} = -0.83$ e Å⁻³

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|---------------|----------------------------------|
| Fe1 | 0.42277 (4) | 0.30132 (3) | 0.34621 (3) | 0.01581 (13) |
| S1 | 0.59702 (8) | 0.21512 (7) | 0.26618 (7) | 0.0276 (2) |
| F1 | 0.6429 (3) | 0.2189 (3) | 0.1011 (2) | 0.0762 (10) |
| F2 | 0.4999 (3) | 0.2899 (3) | 0.0886 (2) | 0.0750 (9) |
| F3 | 0.4704 (2) | 0.1228 (2) | 0.0792 (2) | 0.0661 (8) |
| O1 | 0.7771 (2) | 0.05917 (18) | 0.96773 (17) | 0.0244 (5) |
| O2 | 1.09252 (19) | 0.81551 (17) | 0.47718 (18) | 0.0250 (5) |
| O3 | 0.0686 (2) | 0.55562 (17) | -0.26646 (17) | 0.0251 (5) |
| O4 | -0.27784 (19) | -0.19225 (17) | 0.18668 (18) | 0.0257 (5) |
| O5 | 0.4856 (2) | 0.21102 (17) | 0.27749 (17) | 0.0240 (5) |
| O6 | 0.6331 (3) | 0.1210 (2) | 0.2908 (2) | 0.0445 (7) |
| O7 | 0.6838 (2) | 0.3117 (2) | 0.3069 (2) | 0.0397 (7) |
| N1 | 0.3634 (2) | 0.19301 (19) | 0.42998 (18) | 0.0146 (5) |
| N2 | 0.5656 (2) | 0.36534 (19) | 0.48099 (18) | 0.0154 (5) |
| N3 | 0.4583 (2) | 0.43788 (19) | 0.28462 (19) | 0.0166 (5) |
| N4 | 0.2496 (2) | 0.27372 (19) | 0.24044 (19) | 0.0152 (5) |
| C1 | 0.2525 (2) | 0.1225 (2) | 0.3977 (2) | 0.0157 (6) |
| C2 | 0.2513 (3) | 0.0513 (2) | 0.4738 (2) | 0.0182 (6) |
| H2 | 0.1857 | -0.0039 | 0.4703 | 0.022* |
| C3 | 0.3616 (3) | 0.0774 (2) | 0.5521 (2) | 0.0177 (6) |
| H3 | 0.3878 | 0.0429 | 0.6130 | 0.021* |
| C4 | 0.4310 (3) | 0.1665 (2) | 0.5259 (2) | 0.0157 (6) |
| C5 | 0.5448 (2) | 0.2237 (2) | 0.5926 (2) | 0.0150 (6) |
| C6 | 0.6047 (3) | 0.3192 (2) | 0.5722 (2) | 0.0165 (6) |
| C7 | 0.7186 (3) | 0.3820 (2) | 0.6418 (2) | 0.0216 (7) |
| H7 | 0.7639 | 0.3685 | 0.7101 | 0.026* |
| C8 | 0.7494 (3) | 0.4639 (2) | 0.5924 (2) | 0.0225 (7) |
| H8 | 0.8206 | 0.5184 | 0.6196 | 0.027* |
| C9 | 0.6556 (3) | 0.4539 (2) | 0.4916 (2) | 0.0181 (6) |
| C10 | 0.6606 (3) | 0.5193 (2) | 0.4154 (2) | 0.0167 (6) |
| C11 | 0.5679 (3) | 0.5114 (2) | 0.3185 (2) | 0.0168 (6) |
| C12 | 0.5725 (3) | 0.5767 (2) | 0.2385 (2) | 0.0198 (6) |
| H12 | 0.6381 | 0.6319 | 0.2418 | 0.024* |
| C13 | 0.4656 (3) | 0.5449 (2) | 0.1569 (2) | 0.0205 (7) |
| H13 | 0.4422 | 0.5741 | 0.0925 | 0.025* |
| C14 | 0.3944 (3) | 0.4595 (2) | 0.1855 (2) | 0.0177 (6) |
| C15 | 0.2784 (3) | 0.4063 (2) | 0.1219 (2) | 0.0170 (6) |
| C16 | 0.2111 (3) | 0.3202 (2) | 0.1490 (2) | 0.0171 (6) |
| C17 | 0.0911 (3) | 0.2663 (2) | 0.0841 (2) | 0.0197 (6) |
| H17 | 0.0449 | 0.2821 | 0.0171 | 0.024* |
| C18 | 0.0557 (3) | 0.1886 (2) | 0.1362 (2) | 0.0193 (6) |
| H18 | -0.0204 | 0.1403 | 0.1129 | 0.023* |
| C19 | 0.1546 (3) | 0.1926 (2) | 0.2334 (2) | 0.0160 (6) |
| C20 | 0.1537 (3) | 0.1212 (2) | 0.3061 (2) | 0.0162 (6) |
| C21 | 0.6062 (2) | 0.1789 (2) | 0.6907 (2) | 0.0166 (6) |

| | | | | |
|------|-------------|-------------|-------------|------------|
| C22 | 0.6269 (3) | 0.0815 (2) | 0.6880 (2) | 0.0175 (6) |
| H22 | 0.6016 | 0.0429 | 0.6227 | 0.021* |
| C23 | 0.6839 (3) | 0.0380 (2) | 0.7783 (2) | 0.0187 (6) |
| H23 | 0.6977 | -0.0290 | 0.7745 | 0.022* |
| C24 | 0.7202 (3) | 0.0945 (2) | 0.8742 (2) | 0.0195 (6) |
| C25 | 0.6996 (3) | 0.1914 (2) | 0.8791 (2) | 0.0197 (6) |
| H25 | 0.7243 | 0.2295 | 0.9446 | 0.024* |
| C26 | 0.6427 (3) | 0.2337 (2) | 0.7888 (2) | 0.0183 (6) |
| H26 | 0.6282 | 0.3004 | 0.7930 | 0.022* |
| C27 | 0.8137 (3) | -0.0341 (3) | 0.9644 (3) | 0.0271 (7) |
| H27A | 0.7433 | -0.0918 | 0.9287 | 0.041* |
| H27B | 0.8565 | -0.0494 | 1.0353 | 0.041* |
| H27C | 0.8666 | -0.0252 | 0.9269 | 0.041* |
| C28 | 0.7758 (3) | 0.5982 (2) | 0.4346 (2) | 0.0161 (6) |
| C29 | 0.8714 (3) | 0.5651 (2) | 0.4319 (2) | 0.0202 (7) |
| H29 | 0.8638 | 0.4926 | 0.4216 | 0.024* |
| C30 | 0.9782 (3) | 0.6349 (2) | 0.4436 (2) | 0.0186 (6) |
| H30 | 1.0421 | 0.6105 | 0.4396 | 0.022* |
| C31 | 0.9904 (3) | 0.7403 (2) | 0.4613 (2) | 0.0189 (6) |
| C32 | 0.8951 (3) | 0.7751 (2) | 0.4638 (2) | 0.0195 (6) |
| H32 | 0.9031 | 0.8475 | 0.4750 | 0.023* |
| C33 | 0.7883 (3) | 0.7046 (2) | 0.4499 (2) | 0.0201 (6) |
| H33 | 0.7232 | 0.7290 | 0.4509 | 0.024* |
| C34 | 1.1835 (3) | 0.7814 (3) | 0.4578 (3) | 0.0332 (8) |
| H34A | 1.2115 | 0.7313 | 0.5066 | 0.050* |
| H34B | 1.2505 | 0.8415 | 0.4671 | 0.050* |
| H34C | 1.1507 | 0.7483 | 0.3866 | 0.050* |
| C35 | 0.2212 (3) | 0.4458 (2) | 0.0198 (2) | 0.0177 (6) |
| C36 | 0.2233 (3) | 0.4045 (3) | -0.0703 (3) | 0.0267 (7) |
| H36 | 0.2605 | 0.3491 | -0.0673 | 0.032* |
| C37 | 0.1721 (3) | 0.4426 (3) | -0.1642 (3) | 0.0287 (8) |
| H37 | 0.1745 | 0.4134 | -0.2250 | 0.034* |
| C38 | 0.1172 (3) | 0.5235 (2) | -0.1702 (2) | 0.0212 (7) |
| C39 | 0.1138 (3) | 0.5647 (3) | -0.0813 (3) | 0.0290 (8) |
| H39 | 0.0766 | 0.6200 | -0.0843 | 0.035* |
| C40 | 0.1649 (3) | 0.5252 (3) | 0.0127 (3) | 0.0278 (8) |
| H40 | 0.1610 | 0.5533 | 0.0733 | 0.033* |
| C41 | 0.0405 (3) | 0.6529 (3) | -0.2709 (3) | 0.0325 (8) |
| H41A | -0.0270 | 0.6479 | -0.2504 | 0.049* |
| H41B | 0.0189 | 0.6728 | -0.3418 | 0.049* |
| H41C | 0.1100 | 0.7057 | -0.2235 | 0.049* |
| C42 | 0.0408 (3) | 0.0381 (2) | 0.2828 (2) | 0.0174 (6) |
| C43 | 0.0337 (3) | -0.0649 (2) | 0.2547 (2) | 0.0204 (7) |
| H43 | 0.1031 | -0.0833 | 0.2560 | 0.024* |
| C44 | -0.0729 (3) | -0.1404 (2) | 0.2252 (2) | 0.0211 (7) |
| H44 | -0.0765 | -0.2102 | 0.2062 | 0.025* |
| C45 | -0.1751 (3) | -0.1142 (2) | 0.2231 (2) | 0.0193 (6) |
| C46 | -0.1682 (3) | -0.0132 (3) | 0.2556 (2) | 0.0221 (7) |

| | | | | |
|------|-------------|-------------|------------|-------------|
| H46 | -0.2364 | 0.0047 | 0.2579 | 0.026* |
| C47 | -0.0604 (3) | 0.0612 (2) | 0.2847 (2) | 0.0213 (7) |
| H47 | -0.0559 | 0.1303 | 0.3067 | 0.026* |
| C48 | -0.3848 (3) | -0.1651 (3) | 0.1751 (3) | 0.0298 (8) |
| H48A | -0.3828 | -0.1472 | 0.2437 | 0.045* |
| H48B | -0.4533 | -0.2242 | 0.1391 | 0.045* |
| H48C | -0.3922 | -0.1051 | 0.1346 | 0.045* |
| C49 | 0.5495 (4) | 0.2124 (4) | 0.1254 (3) | 0.0484 (11) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Fe1 | 0.0136 (2) | 0.0161 (2) | 0.0146 (2) | 0.00055 (16) | 0.00399 (17) | 0.00446 (16) |
| S1 | 0.0271 (4) | 0.0292 (5) | 0.0285 (5) | 0.0072 (4) | 0.0128 (4) | 0.0045 (4) |
| F1 | 0.0607 (17) | 0.123 (3) | 0.0529 (17) | -0.0032 (17) | 0.0468 (15) | -0.0094 (17) |
| F2 | 0.102 (2) | 0.091 (2) | 0.0490 (17) | 0.052 (2) | 0.0317 (17) | 0.0329 (16) |
| F3 | 0.0576 (16) | 0.089 (2) | 0.0392 (15) | -0.0046 (15) | 0.0190 (13) | -0.0201 (14) |
| O1 | 0.0278 (12) | 0.0260 (12) | 0.0162 (11) | 0.0093 (10) | 0.0036 (9) | 0.0065 (9) |
| O2 | 0.0169 (11) | 0.0203 (12) | 0.0372 (14) | 0.0004 (9) | 0.0125 (10) | 0.0049 (10) |
| O3 | 0.0341 (13) | 0.0261 (12) | 0.0159 (11) | 0.0140 (10) | 0.0071 (10) | 0.0088 (9) |
| O4 | 0.0186 (11) | 0.0220 (12) | 0.0294 (13) | -0.0055 (9) | 0.0081 (10) | 0.0017 (10) |
| O5 | 0.0270 (12) | 0.0186 (11) | 0.0254 (12) | -0.0027 (9) | 0.0144 (10) | -0.0034 (9) |
| O6 | 0.0469 (16) | 0.0382 (16) | 0.0567 (19) | 0.0203 (13) | 0.0239 (15) | 0.0111 (14) |
| O7 | 0.0303 (13) | 0.0364 (15) | 0.0507 (17) | 0.0001 (11) | 0.0192 (13) | -0.0005 (13) |
| N1 | 0.0128 (11) | 0.0153 (12) | 0.0133 (12) | 0.0018 (9) | 0.0034 (10) | 0.0032 (10) |
| N2 | 0.0127 (11) | 0.0166 (12) | 0.0148 (12) | 0.0022 (10) | 0.0043 (10) | 0.0044 (10) |
| N3 | 0.0151 (12) | 0.0152 (12) | 0.0175 (13) | 0.0028 (10) | 0.0050 (10) | 0.0056 (10) |
| N4 | 0.0138 (11) | 0.0145 (12) | 0.0157 (12) | 0.0020 (10) | 0.0049 (10) | 0.0042 (10) |
| C1 | 0.0138 (13) | 0.0144 (14) | 0.0194 (15) | 0.0027 (11) | 0.0075 (12) | 0.0024 (12) |
| C2 | 0.0170 (14) | 0.0154 (15) | 0.0188 (15) | -0.0001 (12) | 0.0058 (12) | 0.0031 (12) |
| C3 | 0.0207 (15) | 0.0158 (15) | 0.0169 (15) | 0.0038 (12) | 0.0082 (12) | 0.0055 (12) |
| C4 | 0.0170 (14) | 0.0152 (14) | 0.0163 (15) | 0.0039 (12) | 0.0079 (12) | 0.0023 (11) |
| C5 | 0.0145 (13) | 0.0177 (15) | 0.0143 (14) | 0.0048 (11) | 0.0067 (11) | 0.0033 (11) |
| C6 | 0.0169 (14) | 0.0162 (15) | 0.0152 (15) | 0.0024 (12) | 0.0061 (12) | 0.0032 (11) |
| C7 | 0.0177 (15) | 0.0251 (17) | 0.0170 (15) | 0.0005 (13) | 0.0044 (12) | 0.0036 (13) |
| C8 | 0.0190 (15) | 0.0227 (16) | 0.0201 (16) | -0.0015 (13) | 0.0057 (13) | 0.0035 (13) |
| C9 | 0.0154 (14) | 0.0205 (15) | 0.0162 (15) | -0.0001 (12) | 0.0066 (12) | -0.0020 (12) |
| C10 | 0.0165 (14) | 0.0118 (14) | 0.0191 (15) | 0.0003 (11) | 0.0061 (12) | 0.0013 (11) |
| C11 | 0.0159 (14) | 0.0145 (14) | 0.0199 (15) | 0.0029 (11) | 0.0073 (12) | 0.0033 (12) |
| C12 | 0.0186 (15) | 0.0156 (15) | 0.0244 (17) | 0.0028 (12) | 0.0084 (13) | 0.0069 (12) |
| C13 | 0.0222 (15) | 0.0200 (16) | 0.0197 (16) | 0.0059 (13) | 0.0083 (13) | 0.0084 (12) |
| C14 | 0.0199 (14) | 0.0152 (14) | 0.0184 (15) | 0.0046 (12) | 0.0080 (12) | 0.0049 (12) |
| C15 | 0.0192 (14) | 0.0166 (15) | 0.0150 (15) | 0.0060 (12) | 0.0058 (12) | 0.0042 (12) |
| C16 | 0.0170 (14) | 0.0183 (15) | 0.0155 (15) | 0.0061 (12) | 0.0051 (12) | 0.0037 (12) |
| C17 | 0.0166 (14) | 0.0224 (16) | 0.0165 (15) | 0.0042 (12) | 0.0029 (12) | 0.0044 (12) |
| C18 | 0.0135 (13) | 0.0218 (16) | 0.0184 (16) | 0.0025 (12) | 0.0028 (12) | 0.0024 (12) |
| C19 | 0.0149 (14) | 0.0149 (14) | 0.0169 (15) | 0.0032 (11) | 0.0052 (12) | 0.0015 (11) |
| C20 | 0.0142 (13) | 0.0144 (14) | 0.0191 (15) | 0.0011 (11) | 0.0070 (12) | 0.0010 (12) |

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|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C21 | 0.0112 (13) | 0.0206 (15) | 0.0165 (15) | 0.0007 (11) | 0.0059 (11) | 0.0055 (12) |
| C22 | 0.0152 (14) | 0.0179 (15) | 0.0177 (15) | 0.0015 (12) | 0.0060 (12) | 0.0003 (12) |
| C23 | 0.0163 (14) | 0.0180 (15) | 0.0197 (16) | 0.0033 (12) | 0.0051 (12) | 0.0042 (12) |
| C24 | 0.0148 (14) | 0.0275 (17) | 0.0151 (15) | 0.0056 (12) | 0.0045 (12) | 0.0097 (13) |
| C25 | 0.0213 (15) | 0.0218 (16) | 0.0132 (15) | 0.0005 (12) | 0.0067 (12) | -0.0009 (12) |
| C26 | 0.0175 (14) | 0.0179 (15) | 0.0199 (16) | 0.0041 (12) | 0.0081 (12) | 0.0022 (12) |
| C27 | 0.0313 (18) | 0.0237 (17) | 0.0212 (17) | 0.0118 (14) | 0.0022 (14) | 0.0078 (14) |
| C28 | 0.0160 (14) | 0.0170 (15) | 0.0127 (14) | 0.0004 (12) | 0.0049 (11) | 0.0036 (11) |
| C29 | 0.0216 (15) | 0.0157 (15) | 0.0211 (16) | 0.0026 (12) | 0.0074 (13) | 0.0031 (12) |
| C30 | 0.0169 (14) | 0.0170 (15) | 0.0240 (16) | 0.0075 (12) | 0.0085 (12) | 0.0053 (12) |
| C31 | 0.0168 (14) | 0.0190 (15) | 0.0183 (15) | 0.0001 (12) | 0.0068 (12) | 0.0059 (12) |
| C32 | 0.0214 (15) | 0.0131 (14) | 0.0228 (16) | 0.0029 (12) | 0.0083 (13) | 0.0009 (12) |
| C33 | 0.0203 (15) | 0.0199 (16) | 0.0214 (16) | 0.0048 (12) | 0.0098 (13) | 0.0022 (12) |
| C34 | 0.0259 (17) | 0.0298 (19) | 0.048 (2) | 0.0055 (15) | 0.0195 (17) | 0.0093 (16) |
| C35 | 0.0160 (14) | 0.0154 (14) | 0.0179 (15) | 0.0001 (11) | 0.0048 (12) | 0.0038 (12) |
| C36 | 0.0357 (19) | 0.0292 (18) | 0.0211 (17) | 0.0199 (15) | 0.0108 (14) | 0.0073 (14) |
| C37 | 0.041 (2) | 0.0329 (19) | 0.0177 (17) | 0.0203 (16) | 0.0114 (15) | 0.0047 (14) |
| C38 | 0.0235 (15) | 0.0219 (16) | 0.0162 (15) | 0.0056 (13) | 0.0057 (13) | 0.0072 (12) |
| C39 | 0.0392 (19) | 0.0282 (18) | 0.0219 (17) | 0.0206 (16) | 0.0074 (15) | 0.0066 (14) |
| C40 | 0.041 (2) | 0.0302 (18) | 0.0161 (16) | 0.0180 (16) | 0.0099 (15) | 0.0048 (14) |
| C41 | 0.044 (2) | 0.0240 (18) | 0.0218 (18) | 0.0121 (16) | 0.0031 (16) | 0.0075 (14) |
| C42 | 0.0145 (13) | 0.0190 (15) | 0.0138 (14) | -0.0007 (12) | 0.0031 (11) | 0.0036 (12) |
| C43 | 0.0189 (15) | 0.0219 (16) | 0.0194 (16) | 0.0050 (12) | 0.0066 (12) | 0.0065 (12) |
| C44 | 0.0216 (15) | 0.0150 (15) | 0.0212 (16) | 0.0019 (12) | 0.0043 (13) | 0.0038 (12) |
| C45 | 0.0160 (14) | 0.0200 (15) | 0.0163 (15) | -0.0025 (12) | 0.0045 (12) | 0.0060 (12) |
| C46 | 0.0162 (14) | 0.0267 (17) | 0.0230 (16) | 0.0027 (13) | 0.0090 (13) | 0.0028 (13) |
| C47 | 0.0206 (15) | 0.0184 (15) | 0.0234 (17) | 0.0023 (12) | 0.0087 (13) | 0.0019 (13) |
| C48 | 0.0178 (15) | 0.0306 (19) | 0.0331 (19) | -0.0042 (14) | 0.0074 (14) | -0.0001 (15) |
| C49 | 0.050 (3) | 0.062 (3) | 0.035 (2) | 0.009 (2) | 0.022 (2) | 0.004 (2) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|----------|-----------|
| Fe1—O5 | 2.001 (2) | C18—C19 | 1.439 (4) |
| Fe1—N3 | 2.038 (2) | C18—H18 | 0.9500 |
| Fe1—N1 | 2.043 (2) | C19—C20 | 1.394 (4) |
| Fe1—N2 | 2.047 (2) | C20—C42 | 1.498 (4) |
| Fe1—N4 | 2.049 (2) | C21—C22 | 1.381 (4) |
| S1—O7 | 1.422 (3) | C21—C26 | 1.410 (4) |
| S1—O6 | 1.424 (3) | C22—C23 | 1.395 (4) |
| S1—O5 | 1.452 (2) | C22—H22 | 0.9500 |
| S1—C49 | 1.828 (4) | C23—C24 | 1.395 (4) |
| F1—C49 | 1.324 (5) | C23—H23 | 0.9500 |
| F2—C49 | 1.328 (6) | C24—C25 | 1.376 (5) |
| F3—C49 | 1.331 (5) | C25—C26 | 1.387 (4) |
| O1—C24 | 1.375 (4) | C25—H25 | 0.9500 |
| O1—C27 | 1.423 (4) | C26—H26 | 0.9500 |
| O2—C31 | 1.366 (3) | C27—H27A | 0.9800 |
| O2—C34 | 1.433 (4) | C27—H27B | 0.9800 |

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|-----------|-------------|-------------|-----------|
| O3—C38 | 1.367 (4) | C27—H27C | 0.9800 |
| O3—C41 | 1.411 (4) | C28—C29 | 1.381 (4) |
| O4—C45 | 1.365 (3) | C28—C33 | 1.390 (4) |
| O4—C48 | 1.418 (4) | C29—C30 | 1.389 (4) |
| N1—C4 | 1.384 (4) | C29—H29 | 0.9500 |
| N1—C1 | 1.386 (3) | C30—C31 | 1.383 (4) |
| N2—C6 | 1.383 (4) | C30—H30 | 0.9500 |
| N2—C9 | 1.388 (4) | C31—C32 | 1.389 (4) |
| N3—C14 | 1.382 (4) | C32—C33 | 1.385 (4) |
| N3—C11 | 1.391 (4) | C32—H32 | 0.9500 |
| N4—C19 | 1.377 (4) | C33—H33 | 0.9500 |
| N4—C16 | 1.388 (4) | C34—H34A | 0.9800 |
| C1—C20 | 1.398 (4) | C34—H34B | 0.9800 |
| C1—C2 | 1.428 (4) | C34—H34C | 0.9800 |
| C2—C3 | 1.359 (4) | C35—C40 | 1.382 (5) |
| C2—H2 | 0.9500 | C35—C36 | 1.389 (4) |
| C3—C4 | 1.434 (4) | C36—C37 | 1.380 (5) |
| C3—H3 | 0.9500 | C36—H36 | 0.9500 |
| C4—C5 | 1.398 (4) | C37—C38 | 1.390 (5) |
| C5—C6 | 1.405 (4) | C37—H37 | 0.9500 |
| C5—C21 | 1.497 (4) | C38—C39 | 1.380 (5) |
| C6—C7 | 1.434 (4) | C39—C40 | 1.391 (5) |
| C7—C8 | 1.350 (4) | C39—H39 | 0.9500 |
| C7—H7 | 0.9500 | C40—H40 | 0.9500 |
| C8—C9 | 1.431 (4) | C41—H41A | 0.9800 |
| C8—H8 | 0.9500 | C41—H41B | 0.9800 |
| C9—C10 | 1.388 (4) | C41—H41C | 0.9800 |
| C10—C11 | 1.393 (4) | C42—C47 | 1.381 (4) |
| C10—C28 | 1.500 (4) | C42—C43 | 1.395 (4) |
| C11—C12 | 1.430 (4) | C43—C44 | 1.382 (4) |
| C12—C13 | 1.357 (4) | C43—H43 | 0.9500 |
| C12—H12 | 0.9500 | C44—C45 | 1.392 (5) |
| C13—C14 | 1.430 (4) | C44—H44 | 0.9500 |
| C13—H13 | 0.9500 | C45—C46 | 1.388 (5) |
| C14—C15 | 1.390 (4) | C46—C47 | 1.385 (4) |
| C15—C16 | 1.399 (4) | C46—H46 | 0.9500 |
| C15—C35 | 1.493 (4) | C47—H47 | 0.9500 |
| C16—C17 | 1.431 (4) | C48—H48A | 0.9800 |
| C17—C18 | 1.354 (4) | C48—H48B | 0.9800 |
| C17—H17 | 0.9500 | C48—H48C | 0.9800 |
| O5—Fe1—N3 | 100.90 (10) | C23—C22—H22 | 119.0 |
| O5—Fe1—N1 | 97.98 (9) | C22—C23—C24 | 119.0 (3) |
| N3—Fe1—N1 | 161.10 (10) | C22—C23—H23 | 120.5 |
| O5—Fe1—N2 | 104.03 (10) | C24—C23—H23 | 120.5 |
| N3—Fe1—N2 | 88.27 (10) | O1—C24—C25 | 116.0 (3) |
| N1—Fe1—N2 | 87.93 (9) | O1—C24—C23 | 123.8 (3) |
| O5—Fe1—N4 | 100.32 (10) | C25—C24—C23 | 120.2 (3) |

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| N3—Fe1—N4 | 88.03 (10) | C24—C25—C26 | 120.2 (3) |
| N1—Fe1—N4 | 87.84 (9) | C24—C25—H25 | 119.9 |
| N2—Fe1—N4 | 155.63 (10) | C26—C25—H25 | 119.9 |
| O7—S1—O6 | 118.73 (17) | C25—C26—C21 | 120.8 (3) |
| O7—S1—O5 | 113.57 (15) | C25—C26—H26 | 119.6 |
| O6—S1—O5 | 111.28 (15) | C21—C26—H26 | 119.6 |
| O7—S1—C49 | 105.08 (19) | O1—C27—H27A | 109.5 |
| O6—S1—C49 | 104.7 (2) | O1—C27—H27B | 109.5 |
| O5—S1—C49 | 101.26 (18) | H27A—C27—H27B | 109.5 |
| C24—O1—C27 | 117.0 (2) | O1—C27—H27C | 109.5 |
| C31—O2—C34 | 115.8 (3) | H27A—C27—H27C | 109.5 |
| C38—O3—C41 | 116.9 (3) | H27B—C27—H27C | 109.5 |
| C45—O4—C48 | 116.9 (3) | C29—C28—C33 | 118.5 (3) |
| S1—O5—Fe1 | 137.11 (13) | C29—C28—C10 | 119.2 (3) |
| C4—N1—C1 | 105.7 (2) | C33—C28—C10 | 122.3 (3) |
| C4—N1—Fe1 | 126.53 (18) | C28—C29—C30 | 121.9 (3) |
| C1—N1—Fe1 | 127.30 (19) | C28—C29—H29 | 119.1 |
| C6—N2—C9 | 106.1 (2) | C30—C29—H29 | 119.1 |
| C6—N2—Fe1 | 126.95 (19) | C31—C30—C29 | 119.1 (3) |
| C9—N2—Fe1 | 125.77 (19) | C31—C30—H30 | 120.5 |
| C14—N3—C11 | 105.4 (2) | C29—C30—H30 | 120.5 |
| C14—N3—Fe1 | 125.80 (19) | O2—C31—C30 | 124.1 (3) |
| C11—N3—Fe1 | 125.9 (2) | O2—C31—C32 | 116.1 (3) |
| C19—N4—C16 | 105.7 (2) | C30—C31—C32 | 119.8 (3) |
| C19—N4—Fe1 | 127.4 (2) | C33—C32—C31 | 120.3 (3) |
| C16—N4—Fe1 | 125.57 (18) | C33—C32—H32 | 119.8 |
| N1—C1—C20 | 126.1 (3) | C31—C32—H32 | 119.8 |
| N1—C1—C2 | 110.1 (2) | C32—C33—C28 | 120.4 (3) |
| C20—C1—C2 | 123.8 (3) | C32—C33—H33 | 119.8 |
| C3—C2—C1 | 107.1 (3) | C28—C33—H33 | 119.8 |
| C3—C2—H2 | 126.5 | O2—C34—H34A | 109.5 |
| C1—C2—H2 | 126.5 | O2—C34—H34B | 109.5 |
| C2—C3—C4 | 107.4 (3) | H34A—C34—H34B | 109.5 |
| C2—C3—H3 | 126.3 | O2—C34—H34C | 109.5 |
| C4—C3—H3 | 126.3 | H34A—C34—H34C | 109.5 |
| N1—C4—C5 | 125.6 (3) | H34B—C34—H34C | 109.5 |
| N1—C4—C3 | 109.6 (2) | C40—C35—C36 | 118.2 (3) |
| C5—C4—C3 | 124.5 (3) | C40—C35—C15 | 120.6 (3) |
| C4—C5—C6 | 123.9 (3) | C36—C35—C15 | 121.2 (3) |
| C4—C5—C21 | 117.4 (3) | C37—C36—C35 | 121.0 (3) |
| C6—C5—C21 | 118.6 (3) | C37—C36—H36 | 119.5 |
| N2—C6—C5 | 125.5 (3) | C35—C36—H36 | 119.5 |
| N2—C6—C7 | 109.5 (2) | C36—C37—C38 | 120.4 (3) |
| C5—C6—C7 | 125.0 (3) | C36—C37—H37 | 119.8 |
| C8—C7—C6 | 107.3 (3) | C38—C37—H37 | 119.8 |
| C8—C7—H7 | 126.3 | O3—C38—C39 | 124.7 (3) |
| C6—C7—H7 | 126.3 | O3—C38—C37 | 116.2 (3) |
| C7—C8—C9 | 107.8 (3) | C39—C38—C37 | 119.1 (3) |

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| C7—C8—H8 | 126.1 | C38—C39—C40 | 120.0 (3) |
| C9—C8—H8 | 126.1 | C38—C39—H39 | 120.0 |
| C10—C9—N2 | 126.5 (3) | C40—C39—H39 | 120.0 |
| C10—C9—C8 | 124.1 (3) | C35—C40—C39 | 121.3 (3) |
| N2—C9—C8 | 109.2 (3) | C35—C40—H40 | 119.3 |
| C9—C10—C11 | 124.1 (3) | C39—C40—H40 | 119.3 |
| C9—C10—C28 | 118.4 (3) | O3—C41—H41A | 109.5 |
| C11—C10—C28 | 117.3 (3) | O3—C41—H41B | 109.5 |
| N3—C11—C10 | 125.2 (3) | H41A—C41—H41B | 109.5 |
| N3—C11—C12 | 110.1 (3) | O3—C41—H41C | 109.5 |
| C10—C11—C12 | 124.7 (3) | H41A—C41—H41C | 109.5 |
| C13—C12—C11 | 107.0 (3) | H41B—C41—H41C | 109.5 |
| C13—C12—H12 | 126.5 | C47—C42—C43 | 118.0 (3) |
| C11—C12—H12 | 126.5 | C47—C42—C20 | 121.4 (3) |
| C12—C13—C14 | 107.5 (3) | C43—C42—C20 | 120.5 (3) |
| C12—C13—H13 | 126.2 | C44—C43—C42 | 120.8 (3) |
| C14—C13—H13 | 126.2 | C44—C43—H43 | 119.6 |
| N3—C14—C15 | 125.6 (3) | C42—C43—H43 | 119.6 |
| N3—C14—C13 | 110.0 (3) | C43—C44—C45 | 120.1 (3) |
| C15—C14—C13 | 124.4 (3) | C43—C44—H44 | 120.0 |
| C14—C15—C16 | 124.0 (3) | C45—C44—H44 | 120.0 |
| C14—C15—C35 | 117.7 (3) | O4—C45—C46 | 124.2 (3) |
| C16—C15—C35 | 118.2 (3) | O4—C45—C44 | 116.0 (3) |
| N4—C16—C15 | 125.9 (3) | C46—C45—C44 | 119.8 (3) |
| N4—C16—C17 | 110.0 (2) | C47—C46—C45 | 119.0 (3) |
| C15—C16—C17 | 124.1 (3) | C47—C46—H46 | 120.5 |
| C18—C17—C16 | 107.1 (3) | C45—C46—H46 | 120.5 |
| C18—C17—H17 | 126.4 | C42—C47—C46 | 122.2 (3) |
| C16—C17—H17 | 126.4 | C42—C47—H47 | 118.9 |
| C17—C18—C19 | 107.3 (3) | C46—C47—H47 | 118.9 |
| C17—C18—H18 | 126.3 | O4—C48—H48A | 109.5 |
| C19—C18—H18 | 126.3 | O4—C48—H48B | 109.5 |
| N4—C19—C20 | 126.2 (3) | H48A—C48—H48B | 109.5 |
| N4—C19—C18 | 109.8 (2) | O4—C48—H48C | 109.5 |
| C20—C19—C18 | 124.0 (3) | H48A—C48—H48C | 109.5 |
| C19—C20—C1 | 123.5 (3) | H48B—C48—H48C | 109.5 |
| C19—C20—C42 | 117.6 (3) | F1—C49—F2 | 109.3 (4) |
| C1—C20—C42 | 118.9 (3) | F1—C49—F3 | 107.7 (4) |
| C22—C21—C26 | 117.8 (3) | F2—C49—F3 | 108.5 (4) |
| C22—C21—C5 | 120.9 (3) | F1—C49—S1 | 109.3 (3) |
| C26—C21—C5 | 121.4 (3) | F2—C49—S1 | 111.9 (3) |
| C21—C22—C23 | 122.0 (3) | F3—C49—S1 | 110.1 (3) |
| C21—C22—H22 | 119.0 | | |
| O7—S1—O5—Fe1 | -6.4 (3) | C19—N4—C16—C15 | -180.0 (3) |
| O6—S1—O5—Fe1 | 130.7 (2) | Fe1—N4—C16—C15 | -12.1 (4) |
| C49—S1—O5—Fe1 | -118.5 (2) | C19—N4—C16—C17 | -0.7 (3) |
| N3—Fe1—O5—S1 | 54.0 (2) | Fe1—N4—C16—C17 | 167.1 (2) |

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|---------------|------------|-----------------|------------|
| N1—Fe1—O5—S1 | -126.8 (2) | C14—C15—C16—N4 | -1.7 (5) |
| N2—Fe1—O5—S1 | -36.9 (2) | C35—C15—C16—N4 | -179.8 (3) |
| N4—Fe1—O5—S1 | 144.0 (2) | C14—C15—C16—C17 | 179.1 (3) |
| O5—Fe1—N1—C4 | 84.0 (2) | C35—C15—C16—C17 | 1.1 (5) |
| N3—Fe1—N1—C4 | -98.4 (4) | N4—C16—C17—C18 | 1.1 (4) |
| N2—Fe1—N1—C4 | -19.9 (2) | C15—C16—C17—C18 | -179.6 (3) |
| N4—Fe1—N1—C4 | -175.9 (2) | C16—C17—C18—C19 | -1.0 (4) |
| O5—Fe1—N1—C1 | -87.3 (2) | C16—N4—C19—C20 | 177.3 (3) |
| N3—Fe1—N1—C1 | 90.3 (4) | Fe1—N4—C19—C20 | 9.8 (4) |
| N2—Fe1—N1—C1 | 168.8 (2) | C16—N4—C19—C18 | 0.1 (3) |
| N4—Fe1—N1—C1 | 12.8 (2) | Fe1—N4—C19—C18 | -167.5 (2) |
| O5—Fe1—N2—C6 | -81.0 (3) | C17—C18—C19—N4 | 0.6 (4) |
| N3—Fe1—N2—C6 | 178.2 (3) | C17—C18—C19—C20 | -176.7 (3) |
| N1—Fe1—N2—C6 | 16.7 (2) | N4—C19—C20—C1 | -0.5 (5) |
| N4—Fe1—N2—C6 | 96.9 (3) | C18—C19—C20—C1 | 176.4 (3) |
| O5—Fe1—N2—C9 | 84.7 (3) | N4—C19—C20—C42 | -179.5 (3) |
| N3—Fe1—N2—C9 | -16.1 (3) | C18—C19—C20—C42 | -2.6 (5) |
| N1—Fe1—N2—C9 | -177.6 (3) | N1—C1—C20—C19 | 0.2 (5) |
| N4—Fe1—N2—C9 | -97.5 (3) | C2—C1—C20—C19 | 178.3 (3) |
| O5—Fe1—N3—C14 | 76.4 (3) | N1—C1—C20—C42 | 179.2 (3) |
| N1—Fe1—N3—C14 | -101.2 (4) | C2—C1—C20—C42 | -2.7 (5) |
| N2—Fe1—N3—C14 | -179.6 (3) | C4—C5—C21—C22 | 57.5 (4) |
| N4—Fe1—N3—C14 | -23.7 (2) | C6—C5—C21—C22 | -121.8 (3) |
| O5—Fe1—N3—C11 | -81.4 (2) | C4—C5—C21—C26 | -121.4 (3) |
| N1—Fe1—N3—C11 | 101.0 (3) | C6—C5—C21—C26 | 59.4 (4) |
| N2—Fe1—N3—C11 | 22.6 (2) | C26—C21—C22—C23 | -1.1 (4) |
| N4—Fe1—N3—C11 | 178.5 (2) | C5—C21—C22—C23 | 180.0 (3) |
| O5—Fe1—N4—C19 | 84.7 (3) | C21—C22—C23—C24 | 0.4 (4) |
| N3—Fe1—N4—C19 | -174.6 (3) | C27—O1—C24—C25 | -171.8 (3) |
| N1—Fe1—N4—C19 | -13.1 (3) | C27—O1—C24—C23 | 8.4 (4) |
| N2—Fe1—N4—C19 | -93.2 (3) | C22—C23—C24—O1 | -180.0 (3) |
| O5—Fe1—N4—C16 | -80.6 (2) | C22—C23—C24—C25 | 0.2 (4) |
| N3—Fe1—N4—C16 | 20.2 (2) | O1—C24—C25—C26 | -180.0 (3) |
| N1—Fe1—N4—C16 | -178.3 (2) | C23—C24—C25—C26 | -0.2 (4) |
| N2—Fe1—N4—C16 | 101.6 (3) | C24—C25—C26—C21 | -0.6 (4) |
| C4—N1—C1—C20 | 178.0 (3) | C22—C21—C26—C25 | 1.2 (4) |
| Fe1—N1—C1—C20 | -9.3 (4) | C5—C21—C26—C25 | -179.9 (3) |
| C4—N1—C1—C2 | -0.3 (3) | C9—C10—C28—C29 | 72.0 (4) |
| Fe1—N1—C1—C2 | 172.4 (2) | C11—C10—C28—C29 | -103.4 (3) |
| N1—C1—C2—C3 | -0.6 (4) | C9—C10—C28—C33 | -111.3 (3) |
| C20—C1—C2—C3 | -179.0 (3) | C11—C10—C28—C33 | 73.3 (4) |
| C1—C2—C3—C4 | 1.2 (3) | C33—C28—C29—C30 | -0.2 (5) |
| C1—N1—C4—C5 | -172.5 (3) | C10—C28—C29—C30 | 176.6 (3) |
| Fe1—N1—C4—C5 | 14.7 (4) | C28—C29—C30—C31 | 1.7 (5) |
| C1—N1—C4—C3 | 1.1 (3) | C34—O2—C31—C30 | 9.9 (4) |
| Fe1—N1—C4—C3 | -171.7 (2) | C34—O2—C31—C32 | -170.2 (3) |
| C2—C3—C4—N1 | -1.5 (3) | C29—C30—C31—O2 | 177.9 (3) |
| C2—C3—C4—C5 | 172.2 (3) | C29—C30—C31—C32 | -2.0 (5) |

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| N1—C4—C5—C6 | 2.4 (5) | O2—C31—C32—C33 | -179.1 (3) |
| C3—C4—C5—C6 | -170.3 (3) | C30—C31—C32—C33 | 0.8 (5) |
| N1—C4—C5—C21 | -176.8 (3) | C31—C32—C33—C28 | 0.7 (5) |
| C3—C4—C5—C21 | 10.5 (4) | C29—C28—C33—C32 | -1.0 (4) |
| C9—N2—C6—C5 | -175.7 (3) | C10—C28—C33—C32 | -177.7 (3) |
| Fe1—N2—C6—C5 | -7.8 (4) | C14—C15—C35—C40 | -84.6 (4) |
| C9—N2—C6—C7 | 2.1 (3) | C16—C15—C35—C40 | 93.6 (4) |
| Fe1—N2—C6—C7 | 170.1 (2) | C14—C15—C35—C36 | 95.2 (4) |
| C4—C5—C6—N2 | -6.0 (5) | C16—C15—C35—C36 | -86.6 (4) |
| C21—C5—C6—N2 | 173.2 (3) | C40—C35—C36—C37 | 1.0 (5) |
| C4—C5—C6—C7 | 176.5 (3) | C15—C35—C36—C37 | -178.8 (3) |
| C21—C5—C6—C7 | -4.4 (5) | C35—C36—C37—C38 | -0.1 (5) |
| N2—C6—C7—C8 | -1.5 (4) | C41—O3—C38—C39 | 16.7 (5) |
| C5—C6—C7—C8 | 176.4 (3) | C41—O3—C38—C37 | -164.1 (3) |
| C6—C7—C8—C9 | 0.2 (4) | C36—C37—C38—O3 | -179.7 (3) |
| C6—N2—C9—C10 | 173.3 (3) | C36—C37—C38—C39 | -0.4 (5) |
| Fe1—N2—C9—C10 | 5.2 (5) | O3—C38—C39—C40 | 179.2 (3) |
| C6—N2—C9—C8 | -2.0 (3) | C37—C38—C39—C40 | 0.0 (5) |
| Fe1—N2—C9—C8 | -170.1 (2) | C36—C35—C40—C39 | -1.4 (5) |
| C7—C8—C9—C10 | -174.3 (3) | C15—C35—C40—C39 | 178.4 (3) |
| C7—C8—C9—N2 | 1.1 (4) | C38—C39—C40—C35 | 1.0 (5) |
| N2—C9—C10—C11 | 7.3 (5) | C19—C20—C42—C47 | -70.0 (4) |
| C8—C9—C10—C11 | -178.1 (3) | C1—C20—C42—C47 | 110.9 (3) |
| N2—C9—C10—C28 | -167.8 (3) | C19—C20—C42—C43 | 107.7 (3) |
| C8—C9—C10—C28 | 6.9 (5) | C1—C20—C42—C43 | -71.4 (4) |
| C14—N3—C11—C10 | 179.4 (3) | C47—C42—C43—C44 | 3.0 (4) |
| Fe1—N3—C11—C10 | -19.1 (4) | C20—C42—C43—C44 | -174.8 (3) |
| C14—N3—C11—C12 | -1.7 (3) | C42—C43—C44—C45 | -0.1 (5) |
| Fe1—N3—C11—C12 | 159.8 (2) | C48—O4—C45—C46 | 4.5 (4) |
| C9—C10—C11—N3 | 0.0 (5) | C48—O4—C45—C44 | -174.5 (3) |
| C28—C10—C11—N3 | 175.2 (3) | C43—C44—C45—O4 | 176.0 (3) |
| C9—C10—C11—C12 | -178.7 (3) | C43—C44—C45—C46 | -3.0 (5) |
| C28—C10—C11—C12 | -3.6 (5) | O4—C45—C46—C47 | -175.8 (3) |
| N3—C11—C12—C13 | 1.3 (4) | C44—C45—C46—C47 | 3.2 (5) |
| C10—C11—C12—C13 | -179.8 (3) | C43—C42—C47—C46 | -2.8 (5) |
| C11—C12—C13—C14 | -0.4 (4) | C20—C42—C47—C46 | 174.9 (3) |
| C11—N3—C14—C15 | -178.9 (3) | C45—C46—C47—C42 | -0.2 (5) |
| Fe1—N3—C14—C15 | 19.6 (4) | O7—S1—C49—F1 | 59.7 (4) |
| C11—N3—C14—C13 | 1.4 (3) | O6—S1—C49—F1 | -66.1 (4) |
| Fe1—N3—C14—C13 | -160.1 (2) | O5—S1—C49—F1 | 178.1 (3) |
| C12—C13—C14—N3 | -0.7 (4) | O7—S1—C49—F2 | -61.5 (3) |
| C12—C13—C14—C15 | 179.7 (3) | O6—S1—C49—F2 | 172.7 (3) |
| N3—C14—C15—C16 | -2.2 (5) | O5—S1—C49—F2 | 56.9 (3) |
| C13—C14—C15—C16 | 177.4 (3) | O7—S1—C49—F3 | 177.8 (3) |
| N3—C14—C15—C35 | 175.9 (3) | O6—S1—C49—F3 | 52.0 (4) |
| C13—C14—C15—C35 | -4.5 (5) | O5—S1—C49—F3 | -63.8 (4) |
