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# Tris(1,10-phenanthroline-$\kappa^2N,N'$)iron(II) bis[(1,10-phenanthroline-$\kappa^2N,N'$)-tetrakis(thiocyanato-$\kappa N$)chromate(III)] acetonitrile trisolvate monohydrate

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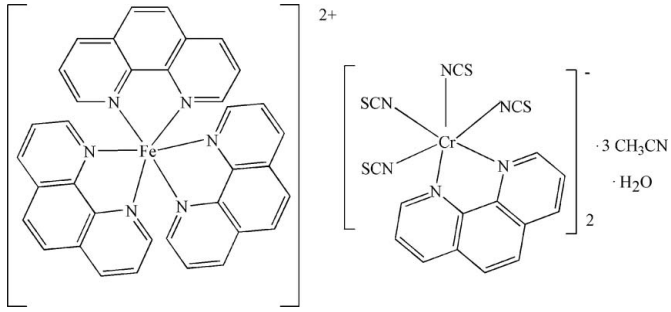
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.051; $wR$ factor = 0.135; data-to-parameter ratio = 15.9.

Single crystals of the title heterometallic compound, $[Fe(C_{12}H_8N_2)_3][Cr(NCS)_4(C_{12}H_8N_2)]_2\cdot3CH_3CN\cdot H_2O$ or $[Fe(Cphen)_3][Cr(NCS)_4(phen)]_2\cdot3CH_3CN\cdot H_2O$, were prepared using the one-pot open-air reaction of iron powder, Reineckes salt and 1,10-phenanthroline (phen) in acetonitrile. The asymetric unit consists of an $[Fe(phen)_3]^{2+}$ cation, two $[Cr(phen)(NCS)_4]^-$ anions, three acetonitrile solvent molecules and a water molecule. The Fe and Cr atoms both show a slightly distorted octahedral $FeN_6$ and $CrN_6$ coordination geometry with adjacent angles in the range 79.67 (12)–95.21 (12)°. No classical hydrogen bonding involving the water molecule is observed.

## Related literature

For background to direct synthesis, see: Makhankova (2011). For background to the use of Reineckes salt as a source of building blocks or metalloligands, see: Zhang *et al.* (2001); Cucos *et al.* (2006); Cherkasova & Gorunova (2003); Nikitina *et al.* (2009); Kolotilov *et al.* (2010). For Fe—N bond lengths in iron–phen derivatives, see: Alonso *et al.* (2005). For a related structure, see: Semenaka *et al.* (2011).




## Experimental

### Crystal data

$[Fe(C_{12}H_8N_2)_3][Cr(NCS)_4(C_{12}H_8N_2)]_2\cdot3C_2H_3N\cdot H_2O$
$M_r$ = 1666.69
Triclinic, $P\overline{1}$
$a$ = 12.641 (2) Å
$b$ = 16.681 (3) Å
$c$ = 20.692 (4) Å
$\alpha$ = 111.514 (5)°
$\beta$ = 107.291 (6)°
$\gamma$ = 92.231 (5)°
$V$ = 3821.5 (13) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.75 mm$^{-1}$
$T$ = 173 K
0.23 × 0.22 × 0.12 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.847, $T_{max}$ = 0.916
48046 measured reflections
15519 independent reflections
8993 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.078

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.135
$S$ = 0.99
15519 reflections
974 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2031).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m531–m532 [doi:10.1107/S1600536812012949]

# Tris(1,10-phenanthroline-$\kappa^2N,N'$)iron(II) bis[(1,10-phenanthroline-$\kappa^2N,N'$)tetrakis(thiocyanato-$\kappa N$)chromate(III)] acetonitrile trisolvate monohydrate

**Valentyna V. Semenaka, Oksana V. Nesterova, Volodymyr N. Kokozay and Volodymyr V. Bon**

## Comment

Recently we have reported that the Reineckes salt, $(NH)_4[Cr(NCS)_4(NH_3)_2]\cdot H_2O$, could be exploited as a source of building blocks or metalloligands in the direct synthesis of heterometallic Cu/Cr and Co/Cr compounds with amines and Schiff-base ligands (Nikitina *et al.*., 2009; Semenaka *et al.*., 2011). In the present work, we report that the reaction of iron powder, Reineckes salt and 1,10-phenanthroline (phen) in acetonitrile solution has afforded a single crystals of the novel heterometallic Fe/Cr compound. The asymetric unit of title compound consists of slightly distorted octahedral $[Fe(phen)_3]^{2+}$ cation and two $[Cr(phen)(NCS)_4]^-$ anion blocks as well as solvate acetonitrile and water molecules (Fig. 1). In complex cation iron centers are in elongated octahedral coordination environment with six nitrogen atoms phen ligands. The bond lengths of Fe–N vary in the range 1,959 (3) – 1,980 (3) Å which is in the range usually found in other iron-phen derivatives (Alonso *et al.*, 2005). The *cis* and *trans* N–Fe–N bond angles vary from 82,27 (12)° to 95.21 (12)° and from 172.90 (12)° to 174.04 (11)°, respectively. The Cr(III) ions have N6 donor set formed by two N atoms from phen, which are replaced NCS groups in initial anions of Reineckes salt, and two NCS-groups in the equatorial plane and by two another NCS-groups at the axial positions. The axial Cr–N bond lengths are vary from 1,962 (3) to 2,077 (3) Å. The *cis* and *trans* N–Cr–N bond angles vary from 79,80 (11)° to 94,97 (12)° and from 170,61 (12)° to 174,77 (12)°, respectively. The thiocyanate groups are almost linear, bond angles N–C–S are in a narrow range: from 178.1 (3) ° to 179.3 (4)°.

## Experimental

Iron powder (0.07 g, 1.25 mmol), $NH_4[Cr(NCS)_4(NH_3)_2]\cdot H_2O$ (0.443 g, 1.25 mmol), $NH_4NCS$ (0.190 g, 2.5 mmol), phen·$H_2O$ (0.496 g, 2.5 mmol) and acetonitrile (15 ml) were heated to 50–60° and stirred magnetically until total dissolution of the iron was observed (4,5 h). The resulting red solution was slowly evaporated at room temperature until dark-red crystals suitable for crystallographic study were formed. The crystals were filtered off, washed with dry $Pr^iOH$ and finally dried *in vacuo* at room temperature. Yield: 0.25 g. IR (KBr, $cm^{-1}$): 3048(sh), 3044(sh), 2314(w), 2066(*vs*), 1996(sh), 1645(sh), 1638(sh), 1635(*m*), 1599(*m*), 1578(*m*), 1554(sh), 1536(w), 1521(*m*), 1494(sh), 1472(sh), 1455(sh), 1424(*s*), 1409(sh), 1373(w), 1307(w), 1271(w), 1256(sh), 1223(sh), 1207(w), 1144(*m*), 1102(*m*), 1057(sh), 1039(sh), 990(*m*), 960(w), 942(sh), 915(sh), 876(w), 870(sh), 843(*s*), 798(*m*), 771(w), 737(sh), 719(*s*), 668(sh), 656(w), 620(w), 581(sh), 557(w), 626(w), 568(sh), 481(*m*), 451(sh), 433(w), 427(sh). The compound is sparingly soluble in dmso and dmf, insoluble in water and it is indefinitely stable in air.

## Refinement

All non-hydrogen atoms were located from the initial solution and refined with anisotropic thermal parameters. The hydrogen atoms were positioned geometrically and included into refinement using riding model approximation with $U_{iso}$

= $nU_{eq}$ of non-hydrogen carrier atom ($n$ = 1.5 for $CH_3$ groups and $n$ = 1.2 for remaining H-atoms)

### Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

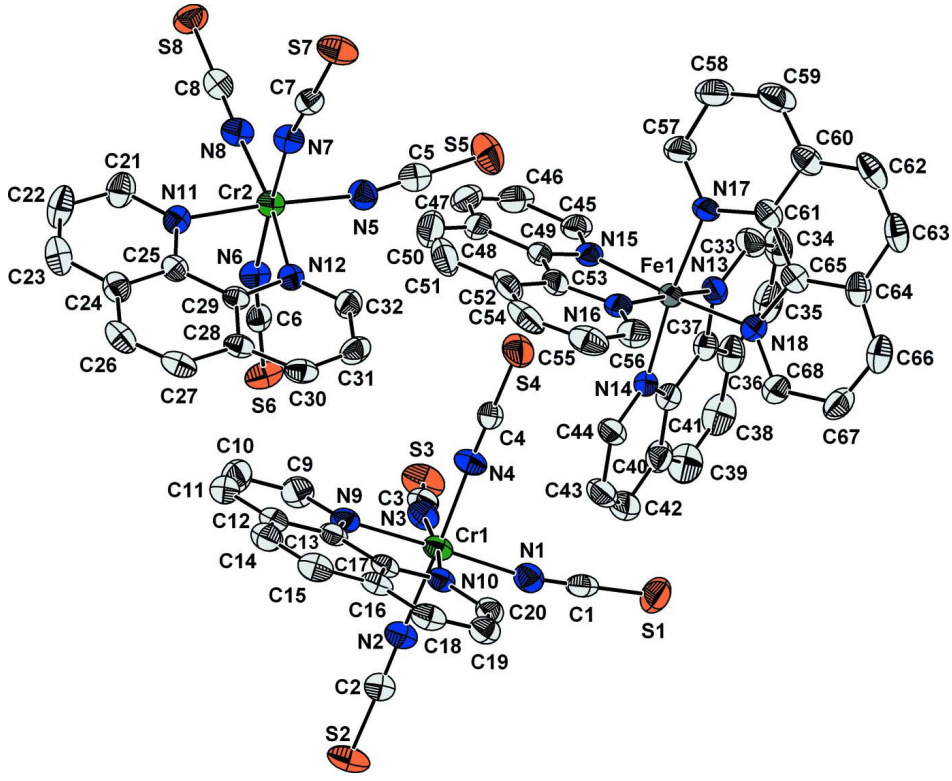


**Figure 1**

Crystal structure of the complex, showing the atom numbering, with 50% probability displacement ellipsoids. Solvent molecules are omitted for clarity.

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*Crystal data*

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$b$ = 16.681 (3) Å
$c$ = 20.692 (4) Å
$\alpha$ = 111.514 (5)°
$\beta$ = 107.291 (6)°
$\gamma$ = 92.231 (5)°
$V$ = 3821.5 (13) Å$^3$

$Z$ = 2
$F(000)$ = 1704
$D_x$ = 1.448 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4485 reflections
$\theta$ = 2.3–21.7°
$\mu$ = 0.75 mm$^{-1}$
$T$ = 173 K
Block, red
0.23 × 0.22 × 0.12 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.847, $T_{max}$ = 0.916
48046 measured reflections
15519 independent reflections
8993 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.078
$\theta_{max}$ = 26.4°, $\theta_{min}$ = 1.1°
$h$ = −15→15
$k$ = −20→20
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.135
$S$ = 0.99
15519 reflections
974 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.0054P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cr1 | 0.27228 (5) | 0.11974 (4) | 0.24479 (4) | 0.03091 (17) |
| Cr2 | 0.65438 (5) | 0.31815 (4) | 0.08754 (3) | 0.02873 (16) |
| Fe1 | 0.21655 (4) | 0.67016 (4) | 0.34300 (3) | 0.02632 (14) |
| S1 | 0.27329 (12) | 0.22111 (9) | 0.49075 (7) | 0.0579 (4) |
| S2 | 0.09452 (10) | −0.17085 (8) | 0.16961 (8) | 0.0536 (3) |
| S3 | 0.62676 (10) | 0.06152 (8) | 0.35925 (7) | 0.0531 (3) |
| S4 | 0.37743 (12) | 0.41344 (8) | 0.28415 (7) | 0.0530 (3) |
| S5 | 0.77068 (12) | 0.50790 (9) | 0.33991 (7) | 0.0604 (4) |
| S6 | 0.65109 (9) | 0.07691 (8) | 0.15795 (7) | 0.0441 (3) |
| S7 | 0.62707 (10) | 0.59283 (8) | 0.07321 (7) | 0.0491 (3) |
| S8 | 1.02840 (9) | 0.36578 (8) | 0.08940 (7) | 0.0451 (3) |
| N1 | 0.2488 (3) | 0.1575 (2) | 0.3417 (2) | 0.0376 (9) |
| N2 | 0.2035 (3) | −0.0022 (2) | 0.21591 (19) | 0.0371 (9) |
| N3 | 0.4240 (3) | 0.0943 (2) | 0.28350 (18) | 0.0356 (8) |
| N4 | 0.3298 (3) | 0.2410 (2) | 0.26495 (18) | 0.0358 (8) |
| N5 | 0.6900 (3) | 0.3873 (2) | 0.1943 (2) | 0.0371 (9) |

| | | | | |
|---|---|---|---|---|
| N6 | 0.6551 (3) | 0.2076 (2) | 0.10439 (18) | 0.0346 (8) |
| N7 | 0.6422 (3) | 0.4265 (2) | 0.07093 (18) | 0.0341 (8) |
| N8 | 0.8136 (3) | 0.3295 (2) | 0.09225 (18) | 0.0354 (8) |
| N9 | 0.2783 (3) | 0.0844 (2) | 0.13939 (18) | 0.0309 (8) |
| N10 | 0.1155 (3) | 0.1396 (2) | 0.19199 (17) | 0.0285 (7) |
| N11 | 0.6017 (3) | 0.2448 (2) | −0.02542 (17) | 0.0300 (8) |
| N12 | 0.4819 (3) | 0.2997 (2) | 0.06400 (17) | 0.0277 (7) |
| N13 | 0.3234 (3) | 0.6688 (2) | 0.43423 (17) | 0.0318 (8) |
| N14 | 0.1557 (3) | 0.5523 (2) | 0.33057 (17) | 0.0277 (7) |
| N15 | 0.3167 (3) | 0.6249 (2) | 0.28571 (18) | 0.0304 (8) |
| N16 | 0.1125 (3) | 0.6567 (2) | 0.24675 (18) | 0.0303 (8) |
| N17 | 0.2766 (3) | 0.7928 (2) | 0.36711 (18) | 0.0318 (8) |
| N18 | 0.1187 (3) | 0.7270 (2) | 0.39894 (17) | 0.0294 (8) |
| C1 | 0.2574 (3) | 0.1841 (3) | 0.4040 (3) | 0.0363 (10) |
| C2 | 0.1576 (3) | −0.0722 (3) | 0.1971 (2) | 0.0335 (10) |
| C3 | 0.5093 (3) | 0.0804 (3) | 0.3150 (2) | 0.0363 (10) |
| C4 | 0.3482 (3) | 0.3134 (3) | 0.2722 (2) | 0.0304 (9) |
| C5 | 0.7241 (3) | 0.4381 (3) | 0.2550 (3) | 0.0359 (10) |
| C6 | 0.6516 (3) | 0.1528 (3) | 0.1264 (2) | 0.0298 (9) |
| C7 | 0.6361 (3) | 0.4963 (3) | 0.0724 (2) | 0.0294 (9) |
| C8 | 0.9035 (3) | 0.3456 (3) | 0.0913 (2) | 0.0323 (10) |
| C9 | 0.3598 (3) | 0.0550 (3) | 0.1145 (2) | 0.0423 (11) |
| H9 | 0.4260 | 0.0487 | 0.1478 | 0.051* |
| C10 | 0.3528 (4) | 0.0328 (3) | 0.0414 (3) | 0.0476 (12) |
| H10 | 0.4130 | 0.0112 | 0.0254 | 0.057* |
| C11 | 0.2582 (4) | 0.0423 (3) | −0.0073 (2) | 0.0411 (11) |
| H11 | 0.2530 | 0.0281 | −0.0572 | 0.049* |
| C12 | 0.1700 (3) | 0.0730 (3) | 0.0169 (2) | 0.0346 (10) |
| C13 | 0.1840 (3) | 0.0932 (2) | 0.0913 (2) | 0.0301 (9) |
| C14 | 0.0672 (4) | 0.0842 (3) | −0.0288 (2) | 0.0390 (11) |
| H14 | 0.0572 | 0.0716 | −0.0792 | 0.047* |
| C15 | −0.0159 (3) | 0.1123 (3) | −0.0024 (2) | 0.0382 (11) |
| H15 | −0.0832 | 0.1192 | −0.0343 | 0.046* |
| C16 | −0.0044 (3) | 0.1321 (2) | 0.0735 (2) | 0.0315 (10) |
| C17 | 0.0967 (3) | 0.1231 (2) | 0.1195 (2) | 0.0279 (9) |
| C18 | −0.0874 (3) | 0.1580 (3) | 0.1043 (2) | 0.0362 (10) |
| H18 | −0.1578 | 0.1636 | 0.0746 | 0.043* |
| C19 | −0.0685 (3) | 0.1754 (3) | 0.1769 (2) | 0.0379 (10) |
| H19 | −0.1248 | 0.1944 | 0.1982 | 0.045* |
| C20 | 0.0349 (3) | 0.1652 (2) | 0.2197 (2) | 0.0344 (10) |
| H20 | 0.0475 | 0.1769 | 0.2702 | 0.041* |
| C21 | 0.6622 (4) | 0.2196 (3) | −0.0695 (2) | 0.0428 (11) |
| H21 | 0.7415 | 0.2367 | −0.0487 | 0.051* |
| C22 | 0.6150 (4) | 0.1688 (3) | −0.1451 (3) | 0.0525 (13) |
| H22 | 0.6616 | 0.1519 | −0.1747 | 0.063* |
| C23 | 0.5010 (4) | 0.1438 (3) | −0.1760 (3) | 0.0482 (12) |
| H23 | 0.4679 | 0.1079 | −0.2271 | 0.058* |
| C24 | 0.4338 (4) | 0.1714 (3) | −0.1322 (2) | 0.0360 (10) |
| C25 | 0.4875 (3) | 0.2212 (2) | −0.0566 (2) | 0.0288 (9) |

| | | | | |
|---|---|---|---|---|
| C26 | 0.3135 (4) | 0.1526 (3) | −0.1594 (2) | 0.0413 (11) |
| H26 | 0.2757 | 0.1178 | −0.2102 | 0.050* |
| C27 | 0.2526 (4) | 0.1829 (3) | −0.1146 (2) | 0.0392 (11) |
| H27 | 0.1729 | 0.1705 | −0.1347 | 0.047* |
| C28 | 0.3064 (3) | 0.2338 (2) | −0.0370 (2) | 0.0311 (9) |
| C29 | 0.4245 (3) | 0.2515 (2) | −0.0088 (2) | 0.0263 (9) |
| C30 | 0.2486 (3) | 0.2690 (3) | 0.0123 (2) | 0.0359 (10) |
| H30 | 0.1688 | 0.2601 | −0.0049 | 0.043* |
| C31 | 0.3074 (3) | 0.3161 (3) | 0.0850 (2) | 0.0388 (11) |
| H31 | 0.2687 | 0.3394 | 0.1190 | 0.047* |
| C32 | 0.4244 (3) | 0.3298 (3) | 0.1094 (2) | 0.0343 (10) |
| H32 | 0.4643 | 0.3619 | 0.1604 | 0.041* |
| C33 | 0.4073 (3) | 0.7303 (3) | 0.4874 (2) | 0.0407 (11) |
| H33 | 0.4205 | 0.7846 | 0.4835 | 0.049* |
| C34 | 0.4762 (4) | 0.7181 (3) | 0.5483 (2) | 0.0498 (13) |
| H34 | 0.5352 | 0.7634 | 0.5849 | 0.060* |
| C35 | 0.4589 (4) | 0.6411 (4) | 0.5554 (2) | 0.0526 (13) |
| H35 | 0.5064 | 0.6325 | 0.5966 | 0.063* |
| C36 | 0.3710 (4) | 0.5746 (3) | 0.5017 (2) | 0.0428 (11) |
| C37 | 0.3056 (3) | 0.5923 (3) | 0.4424 (2) | 0.0316 (9) |
| C38 | 0.3420 (4) | 0.4927 (3) | 0.5040 (3) | 0.0514 (13) |
| H38 | 0.3865 | 0.4796 | 0.5436 | 0.062* |
| C39 | 0.2537 (5) | 0.4335 (3) | 0.4520 (3) | 0.0540 (13) |
| H39 | 0.2361 | 0.3799 | 0.4558 | 0.065* |
| C40 | 0.1863 (4) | 0.4501 (3) | 0.3911 (2) | 0.0407 (11) |
| C41 | 0.2133 (3) | 0.5289 (3) | 0.3860 (2) | 0.0304 (9) |
| C42 | 0.0900 (4) | 0.3932 (3) | 0.3352 (3) | 0.0492 (13) |
| H42 | 0.0659 | 0.3392 | 0.3362 | 0.059* |
| C43 | 0.0321 (4) | 0.4165 (3) | 0.2800 (2) | 0.0456 (12) |
| H43 | −0.0332 | 0.3787 | 0.2424 | 0.055* |
| C44 | 0.0675 (4) | 0.4948 (3) | 0.2780 (2) | 0.0372 (10) |
| H44 | 0.0272 | 0.5081 | 0.2376 | 0.045* |
| C45 | 0.4222 (3) | 0.6122 (3) | 0.3077 (3) | 0.0388 (11) |
| H45 | 0.4587 | 0.6254 | 0.3585 | 0.047* |
| C46 | 0.4818 (4) | 0.5801 (3) | 0.2591 (3) | 0.0531 (14) |
| H46 | 0.5564 | 0.5702 | 0.2768 | 0.064* |
| C47 | 0.4325 (5) | 0.5629 (3) | 0.1860 (3) | 0.0582 (15) |
| H47 | 0.4731 | 0.5422 | 0.1528 | 0.070* |
| C48 | 0.3220 (4) | 0.5761 (3) | 0.1604 (3) | 0.0462 (12) |
| C49 | 0.2676 (4) | 0.6073 (2) | 0.2123 (2) | 0.0326 (10) |
| C50 | 0.2600 (6) | 0.5605 (3) | 0.0852 (3) | 0.0634 (16) |
| H50 | 0.2954 | 0.5399 | 0.0489 | 0.076* |
| C51 | 0.1544 (6) | 0.5741 (3) | 0.0648 (3) | 0.0615 (16) |
| H51 | 0.1162 | 0.5625 | 0.0145 | 0.074* |
| C52 | 0.0969 (5) | 0.6058 (3) | 0.1170 (2) | 0.0466 (12) |
| C53 | 0.1562 (4) | 0.6232 (2) | 0.1911 (2) | 0.0347 (10) |
| C54 | −0.0145 (5) | 0.6198 (3) | 0.1000 (3) | 0.0519 (14) |
| H54 | −0.0592 | 0.6069 | 0.0504 | 0.062* |
| C55 | −0.0581 (4) | 0.6523 (3) | 0.1554 (3) | 0.0479 (12) |

| | | | | |
|---|---|---|---|---|
| H55 | −0.1337 | 0.6622 | 0.1444 | 0.057* |
| C56 | 0.0075 (3) | 0.6712 (3) | 0.2281 (2) | 0.0383 (11) |
| H56 | −0.0243 | 0.6954 | 0.2659 | 0.046* |
| C57 | 0.3560 (4) | 0.8248 (3) | 0.3485 (3) | 0.0436 (11) |
| H57 | 0.3877 | 0.7853 | 0.3159 | 0.052* |
| C58 | 0.3943 (4) | 0.9148 (3) | 0.3754 (3) | 0.0540 (13) |
| H58 | 0.4510 | 0.9353 | 0.3610 | 0.065* |
| C59 | 0.3506 (4) | 0.9725 (3) | 0.4218 (3) | 0.0509 (13) |
| H59 | 0.3770 | 1.0334 | 0.4402 | 0.061* |
| C60 | 0.2657 (3) | 0.9420 (3) | 0.4428 (2) | 0.0377 (10) |
| C61 | 0.2327 (3) | 0.8515 (3) | 0.4135 (2) | 0.0310 (9) |
| C62 | 0.2158 (4) | 0.9964 (3) | 0.4924 (2) | 0.0450 (12) |
| H62 | 0.2395 | 1.0579 | 0.5135 | 0.054* |
| C63 | 0.1353 (4) | 0.9622 (3) | 0.5098 (2) | 0.0428 (11) |
| H63 | 0.1036 | 0.9999 | 0.5434 | 0.051* |
| C64 | 0.0968 (3) | 0.8696 (3) | 0.4785 (2) | 0.0350 (10) |
| C65 | 0.1474 (3) | 0.8161 (3) | 0.4315 (2) | 0.0304 (9) |
| C66 | 0.0108 (4) | 0.8297 (3) | 0.4916 (2) | 0.0458 (12) |
| H66 | −0.0265 | 0.8639 | 0.5230 | 0.055* |
| C67 | −0.0190 (4) | 0.7413 (3) | 0.4589 (2) | 0.0450 (12) |
| H67 | −0.0775 | 0.7135 | 0.4673 | 0.054* |
| C68 | 0.0361 (3) | 0.6915 (3) | 0.4129 (2) | 0.0379 (10) |
| H68 | 0.0141 | 0.6298 | 0.3907 | 0.045* |
| N21 | 0.9342 (4) | 0.8805 (3) | 0.3236 (3) | 0.0737 (14) |
| C70 | 0.6627 (4) | 0.7663 (3) | 0.3096 (3) | 0.0519 (13) |
| N20 | 0.6003 (4) | 0.8084 (3) | 0.3261 (3) | 0.0895 (17) |
| N19 | 0.9140 (5) | 0.2258 (4) | 0.3444 (3) | 0.0921 (18) |
| C69 | 0.7423 (4) | 0.7123 (3) | 0.2876 (3) | 0.0703 (16) |
| H69A | 0.7475 | 0.6677 | 0.3082 | 0.106* |
| H69B | 0.8162 | 0.7487 | 0.3059 | 0.106* |
| H69C | 0.7175 | 0.6839 | 0.2336 | 0.106* |
| C74 | 0.8294 (6) | 0.2449 (4) | 0.3437 (3) | 0.078 (2) |
| C75 | 0.7198 (6) | 0.2697 (4) | 0.3412 (4) | 0.105 (3) |
| H75A | 0.6719 | 0.2521 | 0.2898 | 0.158* |
| H75B | 0.7285 | 0.3332 | 0.3672 | 0.158* |
| H75C | 0.6851 | 0.2405 | 0.3651 | 0.158* |
| C78 | 0.9856 (6) | 1.0175 (4) | 0.3033 (3) | 0.105 (3) |
| H78A | 1.0594 | 1.0493 | 0.3388 | 0.158* |
| H78B | 0.9288 | 1.0552 | 0.3099 | 0.158* |
| H78C | 0.9876 | 1.0002 | 0.2530 | 0.158* |
| C77 | 0.9574 (4) | 0.9401 (4) | 0.3151 (3) | 0.0577 (15) |
| O1 | 0.0464 (10) | 0.5593 (6) | 0.5096 (4) | 0.250 (5) |
| H1O | 0.065 (13) | 0.589 (9) | 0.5548 (17) | 0.376* |
| H2O | −0.001 (11) | 0.585 (10) | 0.490 (7) | 0.376* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cr1 | 0.0235 (3) | 0.0264 (4) | 0.0375 (4) | 0.0009 (3) | 0.0060 (3) | 0.0105 (3) |
| Cr2 | 0.0239 (3) | 0.0303 (4) | 0.0328 (4) | 0.0069 (3) | 0.0082 (3) | 0.0142 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Fe1 | 0.0257 (3) | 0.0230 (3) | 0.0286 (3) | 0.0021 (2) | 0.0103 (3) | 0.0076 (3) |
| S1 | 0.0837 (10) | 0.0521 (9) | 0.0546 (8) | 0.0133 (7) | 0.0436 (8) | 0.0232 (7) |
| S2 | 0.0506 (8) | 0.0322 (7) | 0.0728 (9) | −0.0058 (6) | 0.0107 (7) | 0.0243 (7) |
| S3 | 0.0345 (7) | 0.0514 (8) | 0.0649 (9) | 0.0073 (6) | −0.0027 (6) | 0.0289 (7) |
| S4 | 0.0887 (10) | 0.0291 (7) | 0.0478 (8) | 0.0071 (6) | 0.0297 (7) | 0.0174 (6) |
| S5 | 0.0675 (9) | 0.0559 (9) | 0.0355 (7) | 0.0033 (7) | 0.0024 (6) | 0.0060 (7) |
| S6 | 0.0362 (6) | 0.0504 (8) | 0.0618 (8) | 0.0098 (5) | 0.0209 (6) | 0.0363 (7) |
| S7 | 0.0433 (7) | 0.0339 (7) | 0.0687 (9) | 0.0040 (5) | 0.0086 (6) | 0.0272 (7) |
| S8 | 0.0311 (6) | 0.0551 (8) | 0.0519 (7) | 0.0036 (5) | 0.0177 (6) | 0.0217 (6) |
| N1 | 0.033 (2) | 0.036 (2) | 0.037 (2) | 0.0016 (16) | 0.0077 (18) | 0.0109 (19) |
| N2 | 0.031 (2) | 0.030 (2) | 0.046 (2) | 0.0031 (16) | 0.0094 (17) | 0.0133 (19) |
| N3 | 0.029 (2) | 0.034 (2) | 0.035 (2) | 0.0020 (16) | 0.0022 (17) | 0.0109 (18) |
| N4 | 0.0296 (19) | 0.031 (2) | 0.039 (2) | −0.0029 (16) | 0.0026 (16) | 0.0126 (18) |
| N5 | 0.036 (2) | 0.038 (2) | 0.034 (2) | 0.0043 (17) | 0.0089 (18) | 0.0132 (19) |
| N6 | 0.0309 (19) | 0.034 (2) | 0.043 (2) | 0.0087 (16) | 0.0124 (17) | 0.0190 (19) |
| N7 | 0.0314 (19) | 0.036 (2) | 0.034 (2) | 0.0055 (16) | 0.0067 (16) | 0.0164 (18) |
| N8 | 0.0265 (19) | 0.035 (2) | 0.043 (2) | 0.0063 (16) | 0.0072 (17) | 0.0175 (18) |
| N9 | 0.0203 (17) | 0.030 (2) | 0.038 (2) | 0.0013 (15) | 0.0074 (16) | 0.0109 (17) |
| N10 | 0.0224 (17) | 0.0243 (19) | 0.034 (2) | 0.0016 (14) | 0.0069 (15) | 0.0082 (16) |
| N11 | 0.0310 (19) | 0.030 (2) | 0.034 (2) | 0.0117 (15) | 0.0126 (16) | 0.0151 (17) |
| N12 | 0.0289 (18) | 0.0254 (19) | 0.031 (2) | 0.0070 (15) | 0.0108 (16) | 0.0124 (16) |
| N13 | 0.0271 (18) | 0.030 (2) | 0.032 (2) | 0.0050 (15) | 0.0102 (16) | 0.0053 (17) |
| N14 | 0.0282 (18) | 0.0273 (19) | 0.0263 (18) | 0.0027 (15) | 0.0106 (15) | 0.0081 (16) |
| N15 | 0.035 (2) | 0.0222 (19) | 0.039 (2) | 0.0055 (15) | 0.0183 (17) | 0.0126 (17) |
| N16 | 0.035 (2) | 0.0231 (19) | 0.036 (2) | 0.0023 (15) | 0.0148 (17) | 0.0134 (16) |
| N17 | 0.0312 (19) | 0.0223 (19) | 0.039 (2) | 0.0005 (15) | 0.0130 (17) | 0.0078 (17) |
| N18 | 0.0296 (18) | 0.033 (2) | 0.0282 (19) | 0.0064 (15) | 0.0106 (15) | 0.0138 (17) |
| C1 | 0.030 (2) | 0.028 (2) | 0.053 (3) | 0.0021 (19) | 0.017 (2) | 0.016 (2) |
| C2 | 0.029 (2) | 0.032 (3) | 0.040 (3) | 0.0062 (19) | 0.009 (2) | 0.017 (2) |
| C3 | 0.032 (2) | 0.034 (3) | 0.036 (3) | −0.003 (2) | 0.005 (2) | 0.013 (2) |
| C4 | 0.033 (2) | 0.031 (3) | 0.025 (2) | 0.0026 (19) | 0.0085 (18) | 0.010 (2) |
| C5 | 0.031 (2) | 0.036 (3) | 0.044 (3) | 0.008 (2) | 0.010 (2) | 0.021 (2) |
| C6 | 0.020 (2) | 0.035 (3) | 0.030 (2) | 0.0070 (18) | 0.0094 (18) | 0.007 (2) |
| C7 | 0.020 (2) | 0.038 (3) | 0.029 (2) | 0.0034 (18) | 0.0046 (18) | 0.016 (2) |
| C8 | 0.031 (2) | 0.030 (2) | 0.032 (2) | 0.0085 (19) | 0.0026 (19) | 0.014 (2) |
| C9 | 0.026 (2) | 0.048 (3) | 0.047 (3) | 0.006 (2) | 0.010 (2) | 0.014 (2) |
| C10 | 0.037 (3) | 0.054 (3) | 0.050 (3) | 0.009 (2) | 0.020 (2) | 0.014 (3) |
| C11 | 0.041 (3) | 0.037 (3) | 0.042 (3) | 0.000 (2) | 0.016 (2) | 0.010 (2) |
| C12 | 0.035 (2) | 0.024 (2) | 0.038 (3) | −0.0030 (19) | 0.011 (2) | 0.007 (2) |
| C13 | 0.024 (2) | 0.022 (2) | 0.037 (2) | −0.0023 (17) | 0.0084 (19) | 0.007 (2) |
| C14 | 0.042 (3) | 0.033 (3) | 0.038 (3) | −0.001 (2) | 0.008 (2) | 0.015 (2) |
| C15 | 0.033 (2) | 0.034 (3) | 0.047 (3) | 0.004 (2) | 0.004 (2) | 0.023 (2) |
| C16 | 0.027 (2) | 0.021 (2) | 0.041 (3) | −0.0006 (17) | 0.0040 (19) | 0.012 (2) |
| C17 | 0.023 (2) | 0.019 (2) | 0.037 (2) | 0.0018 (16) | 0.0060 (18) | 0.0090 (19) |
| C18 | 0.023 (2) | 0.030 (3) | 0.052 (3) | 0.0047 (18) | 0.005 (2) | 0.018 (2) |
| C19 | 0.026 (2) | 0.033 (3) | 0.051 (3) | 0.0045 (19) | 0.014 (2) | 0.011 (2) |
| C20 | 0.031 (2) | 0.027 (2) | 0.042 (3) | 0.0032 (18) | 0.013 (2) | 0.008 (2) |
| C21 | 0.037 (3) | 0.052 (3) | 0.044 (3) | 0.018 (2) | 0.019 (2) | 0.018 (3) |
| C22 | 0.053 (3) | 0.069 (4) | 0.040 (3) | 0.027 (3) | 0.026 (3) | 0.017 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.059 (3) | 0.044 (3) | 0.033 (3) | 0.015 (2) | 0.015 (2) | 0.006 (2) |
| C24 | 0.042 (3) | 0.031 (3) | 0.032 (3) | 0.007 (2) | 0.009 (2) | 0.012 (2) |
| C25 | 0.031 (2) | 0.023 (2) | 0.033 (2) | 0.0071 (18) | 0.0100 (19) | 0.012 (2) |
| C26 | 0.045 (3) | 0.028 (3) | 0.035 (3) | 0.002 (2) | 0.000 (2) | 0.007 (2) |
| C27 | 0.031 (2) | 0.031 (3) | 0.046 (3) | −0.0037 (19) | 0.001 (2) | 0.015 (2) |
| C28 | 0.029 (2) | 0.023 (2) | 0.040 (3) | 0.0028 (18) | 0.008 (2) | 0.015 (2) |
| C29 | 0.029 (2) | 0.020 (2) | 0.030 (2) | 0.0035 (17) | 0.0094 (19) | 0.0111 (19) |
| C30 | 0.023 (2) | 0.033 (3) | 0.049 (3) | 0.0005 (19) | 0.009 (2) | 0.017 (2) |
| C31 | 0.032 (2) | 0.042 (3) | 0.052 (3) | 0.012 (2) | 0.024 (2) | 0.022 (2) |
| C32 | 0.032 (2) | 0.036 (3) | 0.033 (2) | 0.0055 (19) | 0.013 (2) | 0.011 (2) |
| C33 | 0.027 (2) | 0.039 (3) | 0.041 (3) | −0.003 (2) | 0.007 (2) | 0.003 (2) |
| C34 | 0.029 (3) | 0.063 (4) | 0.032 (3) | 0.001 (2) | 0.001 (2) | −0.001 (3) |
| C35 | 0.039 (3) | 0.082 (4) | 0.030 (3) | 0.022 (3) | 0.009 (2) | 0.016 (3) |
| C36 | 0.039 (3) | 0.055 (3) | 0.033 (3) | 0.019 (2) | 0.012 (2) | 0.014 (2) |
| C37 | 0.031 (2) | 0.033 (3) | 0.031 (2) | 0.0106 (19) | 0.0139 (19) | 0.011 (2) |
| C38 | 0.061 (3) | 0.064 (4) | 0.045 (3) | 0.033 (3) | 0.020 (3) | 0.035 (3) |
| C39 | 0.072 (4) | 0.051 (3) | 0.054 (3) | 0.026 (3) | 0.027 (3) | 0.032 (3) |
| C40 | 0.059 (3) | 0.036 (3) | 0.036 (3) | 0.013 (2) | 0.023 (2) | 0.017 (2) |
| C41 | 0.034 (2) | 0.030 (2) | 0.029 (2) | 0.0047 (19) | 0.0134 (19) | 0.012 (2) |
| C42 | 0.070 (3) | 0.031 (3) | 0.047 (3) | −0.003 (2) | 0.025 (3) | 0.012 (2) |
| C43 | 0.058 (3) | 0.034 (3) | 0.033 (3) | −0.011 (2) | 0.008 (2) | 0.008 (2) |
| C44 | 0.044 (3) | 0.029 (3) | 0.032 (2) | −0.005 (2) | 0.009 (2) | 0.007 (2) |
| C45 | 0.036 (3) | 0.026 (2) | 0.061 (3) | 0.0069 (19) | 0.027 (2) | 0.016 (2) |
| C46 | 0.051 (3) | 0.031 (3) | 0.094 (4) | 0.013 (2) | 0.048 (3) | 0.023 (3) |
| C47 | 0.080 (4) | 0.028 (3) | 0.088 (4) | 0.011 (3) | 0.067 (4) | 0.017 (3) |
| C48 | 0.066 (3) | 0.027 (3) | 0.055 (3) | 0.004 (2) | 0.041 (3) | 0.012 (2) |
| C49 | 0.049 (3) | 0.015 (2) | 0.039 (3) | 0.0032 (19) | 0.026 (2) | 0.0084 (19) |
| C50 | 0.106 (5) | 0.043 (3) | 0.055 (4) | 0.011 (3) | 0.053 (4) | 0.014 (3) |
| C51 | 0.116 (5) | 0.032 (3) | 0.035 (3) | 0.002 (3) | 0.032 (3) | 0.007 (2) |
| C52 | 0.079 (4) | 0.021 (2) | 0.031 (3) | −0.005 (2) | 0.012 (3) | 0.007 (2) |
| C53 | 0.051 (3) | 0.020 (2) | 0.035 (3) | 0.002 (2) | 0.019 (2) | 0.009 (2) |
| C54 | 0.076 (4) | 0.027 (3) | 0.031 (3) | −0.011 (2) | −0.009 (3) | 0.011 (2) |
| C55 | 0.050 (3) | 0.038 (3) | 0.050 (3) | −0.001 (2) | −0.001 (3) | 0.026 (3) |
| C56 | 0.035 (3) | 0.038 (3) | 0.041 (3) | 0.004 (2) | 0.008 (2) | 0.018 (2) |
| C57 | 0.043 (3) | 0.030 (3) | 0.064 (3) | 0.006 (2) | 0.030 (2) | 0.016 (2) |
| C58 | 0.052 (3) | 0.039 (3) | 0.078 (4) | 0.000 (2) | 0.030 (3) | 0.025 (3) |
| C59 | 0.051 (3) | 0.024 (3) | 0.073 (4) | 0.003 (2) | 0.020 (3) | 0.015 (3) |
| C60 | 0.036 (2) | 0.027 (3) | 0.043 (3) | 0.007 (2) | 0.009 (2) | 0.010 (2) |
| C61 | 0.031 (2) | 0.026 (2) | 0.033 (2) | 0.0090 (18) | 0.0069 (19) | 0.011 (2) |
| C62 | 0.046 (3) | 0.024 (3) | 0.045 (3) | 0.011 (2) | 0.004 (2) | 0.001 (2) |
| C63 | 0.046 (3) | 0.039 (3) | 0.033 (3) | 0.019 (2) | 0.011 (2) | 0.003 (2) |
| C64 | 0.034 (2) | 0.039 (3) | 0.031 (2) | 0.016 (2) | 0.012 (2) | 0.012 (2) |
| C65 | 0.030 (2) | 0.028 (2) | 0.031 (2) | 0.0089 (18) | 0.0063 (19) | 0.012 (2) |
| C66 | 0.051 (3) | 0.051 (3) | 0.039 (3) | 0.022 (2) | 0.023 (2) | 0.014 (3) |
| C67 | 0.045 (3) | 0.053 (3) | 0.051 (3) | 0.013 (2) | 0.031 (2) | 0.024 (3) |
| C68 | 0.039 (3) | 0.037 (3) | 0.041 (3) | 0.007 (2) | 0.020 (2) | 0.015 (2) |
| N21 | 0.066 (3) | 0.083 (4) | 0.068 (3) | −0.011 (3) | 0.011 (3) | 0.036 (3) |
| C70 | 0.042 (3) | 0.050 (3) | 0.065 (4) | 0.000 (3) | 0.014 (3) | 0.030 (3) |
| N20 | 0.083 (4) | 0.079 (4) | 0.135 (5) | 0.030 (3) | 0.064 (4) | 0.050 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N19 | 0.100 (5) | 0.093 (4) | 0.077 (4) | 0.000 (4) | 0.052 (4) | 0.011 (3) |
| C69 | 0.049 (3) | 0.068 (4) | 0.098 (5) | 0.004 (3) | 0.023 (3) | 0.039 (4) |
| C74 | 0.106 (6) | 0.053 (4) | 0.079 (4) | −0.007 (4) | 0.065 (5) | 0.006 (3) |
| C75 | 0.132 (6) | 0.056 (4) | 0.161 (7) | 0.021 (4) | 0.109 (6) | 0.032 (4) |
| C78 | 0.165 (7) | 0.057 (4) | 0.101 (5) | −0.020 (4) | 0.084 (5) | 0.011 (4) |
| C77 | 0.053 (3) | 0.069 (4) | 0.034 (3) | −0.014 (3) | 0.013 (2) | 0.005 (3) |
| O1 | 0.305 (13) | 0.339 (13) | 0.093 (5) | 0.207 (11) | 0.040 (7) | 0.076 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cr1—N4 | 1.969 (3) | C27—H27 | 0.9500 |
| Cr1—N3 | 1.975 (3) | C28—C30 | 1.398 (5) |
| Cr1—N2 | 1.978 (4) | C28—C29 | 1.407 (5) |
| Cr1—N1 | 1.986 (4) | C30—C31 | 1.363 (6) |
| Cr1—N10 | 2.064 (3) | C30—H30 | 0.9500 |
| Cr1—N9 | 2.066 (3) | C31—C32 | 1.393 (5) |
| Cr2—N7 | 1.963 (3) | C31—H31 | 0.9500 |
| Cr2—N5 | 1.977 (4) | C32—H32 | 0.9500 |
| Cr2—N8 | 1.984 (3) | C33—C34 | 1.392 (6) |
| Cr2—N6 | 1.999 (3) | C33—H33 | 0.9500 |
| Cr2—N12 | 2.071 (3) | C34—C35 | 1.361 (6) |
| Cr2—N11 | 2.078 (3) | C34—H34 | 0.9500 |
| Fe1—N16 | 1.959 (3) | C35—C36 | 1.402 (6) |
| Fe1—N15 | 1.972 (3) | C35—H35 | 0.9500 |
| Fe1—N13 | 1.976 (3) | C36—C37 | 1.399 (5) |
| Fe1—N18 | 1.977 (3) | C36—C38 | 1.423 (6) |
| Fe1—N17 | 1.978 (3) | C37—C41 | 1.425 (5) |
| Fe1—N14 | 1.978 (3) | C38—C39 | 1.342 (6) |
| S1—C1 | 1.615 (5) | C38—H38 | 0.9500 |
| S2—C2 | 1.616 (4) | C39—C40 | 1.424 (6) |
| S3—C3 | 1.608 (4) | C39—H39 | 0.9500 |
| S4—C4 | 1.606 (4) | C40—C41 | 1.395 (5) |
| S5—C5 | 1.619 (5) | C40—C42 | 1.410 (6) |
| S6—C6 | 1.623 (4) | C42—C43 | 1.357 (6) |
| S7—C7 | 1.612 (4) | C42—H42 | 0.9500 |
| S8—C8 | 1.616 (4) | C43—C44 | 1.382 (5) |
| N1—C1 | 1.168 (5) | C43—H43 | 0.9500 |
| N2—C2 | 1.153 (5) | C44—H44 | 0.9500 |
| N3—C3 | 1.163 (5) | C45—C46 | 1.397 (6) |
| N4—C4 | 1.166 (5) | C45—H45 | 0.9500 |
| N5—C5 | 1.163 (5) | C46—C47 | 1.366 (7) |
| N6—C6 | 1.166 (5) | C46—H46 | 0.9500 |
| N7—C7 | 1.160 (5) | C47—C48 | 1.396 (7) |
| N8—C8 | 1.166 (5) | C47—H47 | 0.9500 |
| N9—C9 | 1.318 (5) | C48—C49 | 1.398 (6) |
| N9—C13 | 1.359 (5) | C48—C50 | 1.437 (7) |
| N10—C20 | 1.324 (5) | C49—C53 | 1.412 (6) |
| N10—C17 | 1.364 (5) | C50—C51 | 1.330 (7) |
| N11—C21 | 1.324 (5) | C50—H50 | 0.9500 |
| N11—C25 | 1.368 (5) | C51—C52 | 1.432 (7) |

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| N12—C32 | 1.324 (5) | C51—H51 | 0.9500 |
| N12—C29 | 1.364 (5) | C52—C54 | 1.397 (7) |
| N13—C33 | 1.335 (5) | C52—C53 | 1.403 (6) |
| N13—C37 | 1.366 (5) | C54—C55 | 1.362 (6) |
| N14—C44 | 1.334 (5) | C54—H54 | 0.9500 |
| N14—C41 | 1.361 (5) | C55—C56 | 1.394 (6) |
| N15—C45 | 1.327 (5) | C55—H55 | 0.9500 |
| N15—C49 | 1.370 (5) | C56—H56 | 0.9500 |
| N16—C56 | 1.327 (5) | C57—C58 | 1.403 (6) |
| N16—C53 | 1.370 (5) | C57—H57 | 0.9500 |
| N17—C57 | 1.334 (5) | C58—C59 | 1.354 (6) |
| N17—C61 | 1.363 (5) | C58—H58 | 0.9500 |
| N18—C68 | 1.335 (5) | C59—C60 | 1.412 (6) |
| N18—C65 | 1.368 (5) | C59—H59 | 0.9500 |
| C9—C10 | 1.393 (6) | C60—C61 | 1.396 (5) |
| C9—H9 | 0.9500 | C60—C62 | 1.421 (6) |
| C10—C11 | 1.373 (6) | C61—C65 | 1.415 (5) |
| C10—H10 | 0.9500 | C62—C63 | 1.348 (6) |
| C11—C12 | 1.395 (6) | C62—H62 | 0.9500 |
| C11—H11 | 0.9500 | C63—C64 | 1.435 (6) |
| C12—C13 | 1.403 (5) | C63—H63 | 0.9500 |
| C12—C14 | 1.427 (6) | C64—C65 | 1.390 (5) |
| C13—C17 | 1.422 (5) | C64—C66 | 1.396 (6) |
| C14—C15 | 1.347 (6) | C66—C67 | 1.358 (6) |
| C14—H14 | 0.9500 | C66—H66 | 0.9500 |
| C15—C16 | 1.442 (5) | C67—C68 | 1.393 (6) |
| C15—H15 | 0.9500 | C67—H67 | 0.9500 |
| C16—C18 | 1.386 (5) | C68—H68 | 0.9500 |
| C16—C17 | 1.399 (5) | N21—C77 | 1.114 (6) |
| C18—C19 | 1.364 (6) | C70—N20 | 1.123 (6) |
| C18—H18 | 0.9500 | C70—C69 | 1.440 (7) |
| C19—C20 | 1.400 (5) | N19—C74 | 1.125 (8) |
| C19—H19 | 0.9500 | C69—H69A | 0.9800 |
| C20—H20 | 0.9500 | C69—H69B | 0.9800 |
| C21—C22 | 1.398 (6) | C69—H69C | 0.9800 |
| C21—H21 | 0.9500 | C74—C75 | 1.453 (9) |
| C22—C23 | 1.367 (6) | C75—H75A | 0.9800 |
| C22—H22 | 0.9500 | C75—H75B | 0.9800 |
| C23—C24 | 1.392 (6) | C75—H75C | 0.9800 |
| C23—H23 | 0.9500 | C78—C77 | 1.449 (7) |
| C24—C25 | 1.403 (5) | C78—H78A | 0.9800 |
| C24—C26 | 1.433 (6) | C78—H78B | 0.9800 |
| C25—C29 | 1.414 (5) | C78—H78C | 0.9800 |
| C26—C27 | 1.348 (6) | O1—H1O | 0.84 (2) |
| C26—H26 | 0.9500 | O1—H2O | 0.85 (2) |
| C27—C28 | 1.439 (6) | | |

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| N4—Cr1—N3 | 93.08 (13) | C28—C27—H27 | 119.5 |
| N4—Cr1—N2 | 174.49 (14) | C30—C28—C29 | 117.6 (4) |

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| N3—Cr1—N2 | 91.37 (14) | C30—C28—C27 | 124.1 (4) |
| N4—Cr1—N1 | 91.16 (14) | C29—C28—C27 | 118.3 (4) |
| N3—Cr1—N1 | 93.32 (14) | N12—C29—C28 | 121.9 (4) |
| N2—Cr1—N1 | 91.82 (14) | N12—C29—C25 | 117.9 (3) |
| N4—Cr1—N10 | 87.71 (13) | C28—C29—C25 | 120.2 (4) |
| N3—Cr1—N10 | 173.14 (14) | C31—C30—C28 | 119.6 (4) |
| N2—Cr1—N10 | 87.50 (13) | C31—C30—H30 | 120.2 |
| N1—Cr1—N10 | 93.48 (14) | C28—C30—H30 | 120.2 |
| N4—Cr1—N9 | 88.10 (13) | C30—C31—C32 | 119.7 (4) |
| N3—Cr1—N9 | 93.48 (13) | C30—C31—H31 | 120.2 |
| N2—Cr1—N9 | 88.38 (13) | C32—C31—H31 | 120.2 |
| N1—Cr1—N9 | 173.20 (13) | N12—C32—C31 | 122.3 (4) |
| N10—Cr1—N9 | 79.73 (13) | N12—C32—H32 | 118.8 |
| N7—Cr2—N5 | 89.11 (14) | C31—C32—H32 | 118.8 |
| N7—Cr2—N8 | 89.61 (13) | N13—C33—C34 | 122.6 (4) |
| N5—Cr2—N8 | 94.14 (14) | N13—C33—H33 | 118.7 |
| N7—Cr2—N6 | 175.77 (13) | C34—C33—H33 | 118.7 |
| N5—Cr2—N6 | 90.40 (14) | C35—C34—C33 | 119.9 (4) |
| N8—Cr2—N6 | 94.62 (13) | C35—C34—H34 | 120.0 |
| N7—Cr2—N12 | 88.04 (12) | C33—C34—H34 | 120.0 |
| N5—Cr2—N12 | 95.01 (13) | C34—C35—C36 | 119.9 (4) |
| N8—Cr2—N12 | 170.52 (13) | C34—C35—H35 | 120.0 |
| N6—Cr2—N12 | 87.81 (12) | C36—C35—H35 | 120.0 |
| N7—Cr2—N11 | 90.64 (13) | C37—C36—C35 | 116.5 (4) |
| N5—Cr2—N11 | 174.81 (13) | C37—C36—C38 | 118.2 (4) |
| N8—Cr2—N11 | 91.05 (13) | C35—C36—C38 | 125.3 (4) |
| N6—Cr2—N11 | 89.46 (13) | N13—C37—C36 | 124.0 (4) |
| N12—Cr2—N11 | 79.80 (12) | N13—C37—C41 | 115.8 (4) |
| N16—Fe1—N15 | 82.94 (14) | C36—C37—C41 | 120.2 (4) |
| N16—Fe1—N13 | 173.04 (13) | C39—C38—C36 | 121.9 (4) |
| N15—Fe1—N13 | 92.81 (13) | C39—C38—H38 | 119.0 |
| N16—Fe1—N18 | 95.12 (13) | C36—C38—H38 | 119.0 |
| N15—Fe1—N18 | 173.96 (13) | C38—C39—C40 | 120.7 (5) |
| N13—Fe1—N18 | 89.65 (13) | C38—C39—H39 | 119.7 |
| N16—Fe1—N17 | 92.39 (13) | C40—C39—H39 | 119.7 |
| N15—Fe1—N17 | 92.11 (13) | C41—C40—C42 | 116.1 (4) |
| N13—Fe1—N17 | 93.27 (13) | C41—C40—C39 | 119.1 (4) |
| N18—Fe1—N17 | 82.24 (13) | C42—C40—C39 | 124.7 (4) |
| N16—Fe1—N14 | 92.28 (13) | N14—C41—C40 | 124.7 (4) |
| N15—Fe1—N14 | 93.11 (12) | N14—C41—C37 | 115.5 (3) |
| N13—Fe1—N14 | 82.42 (13) | C40—C41—C37 | 119.8 (4) |
| N18—Fe1—N14 | 92.68 (13) | C43—C42—C40 | 119.3 (4) |
| N17—Fe1—N14 | 173.38 (13) | C43—C42—H42 | 120.3 |
| C1—N1—Cr1 | 166.9 (3) | C40—C42—H42 | 120.3 |
| C2—N2—Cr1 | 176.1 (3) | C42—C43—C44 | 120.5 (4) |
| C3—N3—Cr1 | 170.3 (3) | C42—C43—H43 | 119.7 |
| C4—N4—Cr1 | 170.4 (3) | C44—C43—H43 | 119.7 |
| C5—N5—Cr2 | 167.4 (3) | N14—C44—C43 | 122.8 (4) |
| C6—N6—Cr2 | 166.9 (3) | N14—C44—H44 | 118.6 |

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| C7—N7—Cr2 | 169.4 (3) | C43—C44—H44 | 118.6 |
| C8—N8—Cr2 | 170.1 (3) | N15—C45—C46 | 122.7 (5) |
| C9—N9—C13 | 118.1 (3) | N15—C45—H45 | 118.6 |
| C9—N9—Cr1 | 128.4 (3) | C46—C45—H45 | 118.6 |
| C13—N9—Cr1 | 113.5 (3) | C47—C46—C45 | 119.9 (5) |
| C20—N10—C17 | 118.6 (3) | C47—C46—H46 | 120.1 |
| C20—N10—Cr1 | 128.2 (3) | C45—C46—H46 | 120.1 |
| C17—N10—Cr1 | 113.2 (2) | C46—C47—C48 | 119.5 (4) |
| C21—N11—C25 | 117.5 (4) | C46—C47—H47 | 120.3 |
| C21—N11—Cr2 | 129.3 (3) | C48—C47—H47 | 120.3 |
| C25—N11—Cr2 | 113.1 (3) | C47—C48—C49 | 117.2 (5) |
| C32—N12—C29 | 118.8 (3) | C47—C48—C50 | 125.3 (5) |
| C32—N12—Cr2 | 128.5 (3) | C49—C48—C50 | 117.5 (5) |
| C29—N12—Cr2 | 112.7 (2) | N15—C49—C48 | 123.6 (4) |
| C33—N13—C37 | 117.0 (4) | N15—C49—C53 | 115.7 (4) |
| C33—N13—Fe1 | 130.0 (3) | C48—C49—C53 | 120.8 (4) |
| C37—N13—Fe1 | 113.0 (3) | C51—C50—C48 | 121.9 (5) |
| C44—N14—C41 | 116.5 (3) | C51—C50—H50 | 119.1 |
| C44—N14—Fe1 | 130.2 (3) | C48—C50—H50 | 119.1 |
| C41—N14—Fe1 | 113.3 (2) | C50—C51—C52 | 121.6 (5) |
| C45—N15—C49 | 117.1 (4) | C50—C51—H51 | 119.2 |
| C45—N15—Fe1 | 130.3 (3) | C52—C51—H51 | 119.2 |
| C49—N15—Fe1 | 112.6 (3) | C54—C52—C53 | 117.1 (4) |
| C56—N16—C53 | 117.1 (4) | C54—C52—C51 | 125.2 (5) |
| C56—N16—Fe1 | 129.9 (3) | C53—C52—C51 | 117.7 (5) |
| C53—N16—Fe1 | 112.9 (3) | N16—C53—C52 | 123.6 (4) |
| C57—N17—C61 | 117.1 (4) | N16—C53—C49 | 115.9 (4) |
| C57—N17—Fe1 | 130.0 (3) | C52—C53—C49 | 120.6 (4) |
| C61—N17—Fe1 | 112.7 (3) | C55—C54—C52 | 119.2 (4) |
| C68—N18—C65 | 117.0 (3) | C55—C54—H54 | 120.4 |
| C68—N18—Fe1 | 129.8 (3) | C52—C54—H54 | 120.4 |
| C65—N18—Fe1 | 113.0 (2) | C54—C55—C56 | 120.4 (5) |
| N1—C1—S1 | 178.2 (4) | C54—C55—H55 | 119.8 |
| N2—C2—S2 | 178.8 (4) | C56—C55—H55 | 119.8 |
| N3—C3—S3 | 179.4 (4) | N16—C56—C55 | 122.6 (4) |
| N4—C4—S4 | 178.2 (4) | N16—C56—H56 | 118.7 |
| N5—C5—S5 | 179.2 (4) | C55—C56—H56 | 118.7 |
| N6—C6—S6 | 178.1 (3) | N17—C57—C58 | 122.1 (4) |
| N7—C7—S7 | 179.2 (4) | N17—C57—H57 | 118.9 |
| N8—C8—S8 | 178.8 (4) | C58—C57—H57 | 118.9 |
| N9—C9—C10 | 122.6 (4) | C59—C58—C57 | 120.2 (4) |
| N9—C9—H9 | 118.7 | C59—C58—H58 | 119.9 |
| C10—C9—H9 | 118.7 | C57—C58—H58 | 119.9 |
| C11—C10—C9 | 119.5 (4) | C58—C59—C60 | 119.9 (4) |
| C11—C10—H10 | 120.2 | C58—C59—H59 | 120.1 |
| C9—C10—H10 | 120.2 | C60—C59—H59 | 120.1 |
| C10—C11—C12 | 119.5 (4) | C61—C60—C59 | 116.1 (4) |
| C10—C11—H11 | 120.2 | C61—C60—C62 | 119.2 (4) |
| C12—C11—H11 | 120.2 | C59—C60—C62 | 124.6 (4) |

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| C11—C12—C13 | 117.0 (4) | N17—C61—C60 | 124.5 (4) |
| C11—C12—C14 | 124.5 (4) | N17—C61—C65 | 116.1 (4) |
| C13—C12—C14 | 118.4 (4) | C60—C61—C65 | 119.4 (4) |
| N9—C13—C12 | 123.2 (4) | C63—C62—C60 | 121.1 (4) |
| N9—C13—C17 | 116.6 (3) | C63—C62—H62 | 119.5 |
| C12—C13—C17 | 120.2 (4) | C60—C62—H62 | 119.5 |
| C15—C14—C12 | 121.6 (4) | C62—C63—C64 | 121.0 (4) |
| C15—C14—H14 | 119.2 | C62—C63—H63 | 119.5 |
| C12—C14—H14 | 119.2 | C64—C63—H63 | 119.5 |
| C14—C15—C16 | 121.1 (4) | C65—C64—C66 | 117.6 (4) |
| C14—C15—H15 | 119.5 | C65—C64—C63 | 118.1 (4) |
| C16—C15—H15 | 119.5 | C66—C64—C63 | 124.3 (4) |
| C18—C16—C17 | 117.2 (4) | N18—C65—C64 | 123.4 (4) |
| C18—C16—C15 | 124.6 (4) | N18—C65—C61 | 115.4 (3) |
| C17—C16—C15 | 118.1 (4) | C64—C65—C61 | 121.2 (4) |
| N10—C17—C16 | 122.6 (4) | C67—C66—C64 | 119.3 (4) |
| N10—C17—C13 | 116.9 (3) | C67—C66—H66 | 120.3 |
| C16—C17—C13 | 120.6 (4) | C64—C66—H66 | 120.3 |
| C19—C18—C16 | 120.4 (4) | C66—C67—C68 | 120.1 (4) |
| C19—C18—H18 | 119.8 | C66—C67—H67 | 119.9 |
| C16—C18—H18 | 119.8 | C68—C67—H67 | 119.9 |
| C18—C19—C20 | 119.3 (4) | N18—C68—C67 | 122.5 (4) |
| C18—C19—H19 | 120.4 | N18—C68—H68 | 118.7 |
| C20—C19—H19 | 120.4 | C67—C68—H68 | 118.7 |
| N10—C20—C19 | 122.0 (4) | N20—C70—C69 | 179.3 (6) |
| N10—C20—H20 | 119.0 | C70—C69—H69A | 109.5 |
| C19—C20—H20 | 119.0 | C70—C69—H69B | 109.5 |
| N11—C21—C22 | 123.1 (4) | H69A—C69—H69B | 109.5 |
| N11—C21—H21 | 118.5 | C70—C69—H69C | 109.5 |
| C22—C21—H21 | 118.5 | H69A—C69—H69C | 109.5 |
| C23—C22—C21 | 119.4 (4) | H69B—C69—H69C | 109.5 |
| C23—C22—H22 | 120.3 | N19—C74—C75 | 178.8 (8) |
| C21—C22—H22 | 120.3 | C74—C75—H75A | 109.5 |
| C22—C23—C24 | 119.5 (4) | C74—C75—H75B | 109.5 |
| C22—C23—H23 | 120.3 | H75A—C75—H75B | 109.5 |
| C24—C23—H23 | 120.3 | C74—C75—H75C | 109.5 |
| C23—C24—C25 | 117.8 (4) | H75A—C75—H75C | 109.5 |
| C23—C24—C26 | 124.2 (4) | H75B—C75—H75C | 109.5 |
| C25—C24—C26 | 117.9 (4) | C77—C78—H78A | 109.5 |
| N11—C25—C24 | 122.7 (4) | C77—C78—H78B | 109.5 |
| N11—C25—C29 | 116.4 (4) | H78A—C78—H78B | 109.5 |
| C24—C25—C29 | 120.9 (4) | C77—C78—H78C | 109.5 |
| C27—C26—C24 | 121.7 (4) | H78A—C78—H78C | 109.5 |
| C27—C26—H26 | 119.2 | H78B—C78—H78C | 109.5 |
| C24—C26—H26 | 119.2 | N21—C77—C78 | 179.0 (7) |
| C26—C27—C28 | 121.0 (4) | H1O—O1—H2O | 105 (5) |
| C26—C27—H27 | 119.5 | | |

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| N4—Cr1—N1—C1 | −65.0 (15) | C20—N10—C17—C16 | 0.0 (5) |

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| N3—Cr1—N1—C1 | 28.2 (15) | Cr1—N10—C17—C16 | 179.7 (3) |
| N2—Cr1—N1—C1 | 119.7 (15) | C20—N10—C17—C13 | −178.1 (3) |
| N10—Cr1—N1—C1 | −152.7 (15) | Cr1—N10—C17—C13 | 1.6 (4) |
| N9—Cr1—N1—C1 | −148.7 (13) | C18—C16—C17—N10 | −0.7 (5) |
| N4—Cr1—N2—C2 | −30 (6) | C15—C16—C17—N10 | −179.6 (3) |
| N3—Cr1—N2—C2 | −173 (5) | C18—C16—C17—C13 | 177.3 (3) |
| N1—Cr1—N2—C2 | 93 (5) | C15—C16—C17—C13 | −1.6 (5) |
| N10—Cr1—N2—C2 | 0 (5) | N9—C13—C17—N10 | −0.4 (5) |
| N9—Cr1—N2—C2 | −80 (5) | C12—C13—C17—N10 | 178.7 (3) |
| N4—Cr1—N3—C3 | 104 (2) | N9—C13—C17—C16 | −178.5 (3) |
| N2—Cr1—N3—C3 | −79 (2) | C12—C13—C17—C16 | 0.6 (5) |
| N1—Cr1—N3—C3 | 13 (2) | C17—C16—C18—C19 | 1.4 (6) |
| N10—Cr1—N3—C3 | −159.7 (17) | C15—C16—C18—C19 | −179.9 (4) |
| N9—Cr1—N3—C3 | −168 (2) | C16—C18—C19—C20 | −1.3 (6) |
| N3—Cr1—N4—C4 | 177 (2) | C17—N10—C20—C19 | 0.1 (5) |
| N2—Cr1—N4—C4 | 33 (3) | Cr1—N10—C20—C19 | −179.5 (3) |
| N1—Cr1—N4—C4 | −90 (2) | C18—C19—C20—N10 | 0.5 (6) |
| N10—Cr1—N4—C4 | 4 (2) | C25—N11—C21—C22 | −1.5 (6) |
| N9—Cr1—N4—C4 | 83 (2) | Cr2—N11—C21—C22 | 179.1 (3) |
| N7—Cr2—N5—C5 | −45.6 (16) | N11—C21—C22—C23 | 0.3 (7) |
| N8—Cr2—N5—C5 | 43.9 (16) | C21—C22—C23—C24 | 1.9 (7) |
| N6—Cr2—N5—C5 | 138.6 (16) | C22—C23—C24—C25 | −2.6 (6) |
| N12—Cr2—N5—C5 | −133.6 (16) | C22—C23—C24—C26 | 177.0 (4) |
| N11—Cr2—N5—C5 | −132.9 (16) | C21—N11—C25—C24 | 0.7 (5) |
| N7—Cr2—N6—C6 | −61 (3) | Cr2—N11—C25—C24 | −179.9 (3) |
| N5—Cr2—N6—C6 | 22.6 (14) | C21—N11—C25—C29 | −177.9 (3) |
| N8—Cr2—N6—C6 | 116.8 (14) | Cr2—N11—C25—C29 | 1.6 (4) |
| N12—Cr2—N6—C6 | −72.4 (14) | C23—C24—C25—N11 | 1.4 (6) |
| N11—Cr2—N6—C6 | −152.2 (14) | C26—C24—C25—N11 | −178.2 (3) |
| N5—Cr2—N7—C7 | −9.2 (17) | C23—C24—C25—C29 | 179.9 (4) |
| N8—Cr2—N7—C7 | −103.3 (17) | C26—C24—C25—C29 | 0.3 (6) |
| N6—Cr2—N7—C7 | 74 (3) | C23—C24—C26—C27 | −178.2 (4) |
| N12—Cr2—N7—C7 | 85.8 (17) | C25—C24—C26—C27 | 1.4 (6) |
| N11—Cr2—N7—C7 | 165.6 (17) | C24—C26—C27—C28 | −1.7 (6) |
| N7—Cr2—N8—C8 | −11 (2) | C26—C27—C28—C30 | 178.5 (4) |
| N5—Cr2—N8—C8 | −100 (2) | C26—C27—C28—C29 | 0.3 (6) |
| N6—Cr2—N8—C8 | 169 (2) | C32—N12—C29—C28 | 0.6 (5) |
| N12—Cr2—N8—C8 | 65 (2) | Cr2—N12—C29—C28 | −177.9 (3) |
| N11—Cr2—N8—C8 | 80 (2) | C32—N12—C29—C25 | 179.0 (3) |
| N4—Cr1—N9—C9 | 93.9 (3) | Cr2—N12—C29—C25 | 0.5 (4) |
| N3—Cr1—N9—C9 | 0.9 (3) | C30—C28—C29—N12 | 1.3 (5) |
| N2—Cr1—N9—C9 | −90.4 (3) | C27—C28—C29—N12 | 179.6 (3) |
| N1—Cr1—N9—C9 | 177.8 (10) | C30—C28—C29—C25 | −177.0 (3) |
| N10—Cr1—N9—C9 | −178.1 (4) | C27—C28—C29—C25 | 1.3 (5) |
| N4—Cr1—N9—C13 | −86.6 (3) | N11—C25—C29—N12 | −1.4 (5) |
| N3—Cr1—N9—C13 | −179.6 (3) | C24—C25—C29—N12 | −180.0 (3) |
| N2—Cr1—N9—C13 | 89.2 (3) | N11—C25—C29—C28 | 177.0 (3) |
| N1—Cr1—N9—C13 | −2.7 (12) | C24—C25—C29—C28 | −1.5 (5) |
| N10—Cr1—N9—C13 | 1.4 (2) | C29—C28—C30—C31 | −2.1 (6) |

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| N4—Cr1—N10—C20 | −93.5 (3) | C27—C28—C30—C31 | 179.7 (4) |
| N3—Cr1—N10—C20 | 169.8 (10) | C28—C30—C31—C32 | 1.0 (6) |
| N2—Cr1—N10—C20 | 89.2 (3) | C29—N12—C32—C31 | −1.8 (6) |
| N1—Cr1—N10—C20 | −2.5 (3) | Cr2—N12—C32—C31 | 176.5 (3) |
| N9—Cr1—N10—C20 | 178.0 (3) | C30—C31—C32—N12 | 1.0 (6) |
| N4—Cr1—N10—C17 | 86.9 (3) | C37—N13—C33—C34 | 1.2 (6) |
| N3—Cr1—N10—C17 | −9.8 (12) | Fe1—N13—C33—C34 | −179.2 (3) |
| N2—Cr1—N10—C17 | −90.4 (3) | N13—C33—C34—C35 | −0.2 (7) |
| N1—Cr1—N10—C17 | 177.9 (3) | C33—C34—C35—C36 | −0.7 (7) |
| N9—Cr1—N10—C17 | −1.6 (2) | C34—C35—C36—C37 | 0.5 (6) |
| N7—Cr2—N11—C21 | 90.5 (3) | C34—C35—C36—C38 | −177.8 (4) |
| N5—Cr2—N11—C21 | 178 (61) | C33—N13—C37—C36 | −1.4 (6) |
| N8—Cr2—N11—C21 | 0.8 (3) | Fe1—N13—C37—C36 | 179.0 (3) |
| N6—Cr2—N11—C21 | −93.8 (3) | C33—N13—C37—C41 | 178.1 (3) |
| N12—Cr2—N11—C21 | 178.4 (4) | Fe1—N13—C37—C41 | −1.5 (4) |
| N7—Cr2—N11—C25 | −88.9 (3) | C35—C36—C37—N13 | 0.6 (6) |
| N5—Cr2—N11—C25 | −1.7 (16) | C38—C36—C37—N13 | 179.0 (4) |
| N8—Cr2—N11—C25 | −178.5 (3) | C35—C36—C37—C41 | −179.0 (4) |
| N6—Cr2—N11—C25 | 86.8 (3) | C38—C36—C37—C41 | −0.5 (6) |
| N12—Cr2—N11—C25 | −1.0 (2) | C37—C36—C38—C39 | −1.0 (7) |
| N7—Cr2—N12—C32 | −87.0 (3) | C35—C36—C38—C39 | 177.3 (5) |
| N5—Cr2—N12—C32 | 1.9 (3) | C36—C38—C39—C40 | 1.2 (7) |
| N8—Cr2—N12—C32 | −162.8 (7) | C38—C39—C40—C41 | 0.2 (7) |
| N6—Cr2—N12—C32 | 92.1 (3) | C38—C39—C40—C42 | −177.8 (5) |
| N11—Cr2—N12—C32 | −178.0 (3) | C44—N14—C41—C40 | 0.0 (6) |
| N7—Cr2—N12—C29 | 91.3 (3) | Fe1—N14—C41—C40 | 178.7 (3) |
| N5—Cr2—N12—C29 | −179.7 (3) | C44—N14—C41—C37 | −178.5 (3) |
| N8—Cr2—N12—C29 | 15.6 (9) | Fe1—N14—C41—C37 | 0.2 (4) |
| N6—Cr2—N12—C29 | −89.5 (3) | C42—C40—C41—N14 | −2.0 (6) |
| N11—Cr2—N12—C29 | 0.3 (2) | C39—C40—C41—N14 | 179.8 (4) |
| N16—Fe1—N13—C33 | 141.1 (10) | C42—C40—C41—C37 | 176.5 (4) |
| N15—Fe1—N13—C33 | 88.9 (4) | C39—C40—C41—C37 | −1.7 (6) |
| N18—Fe1—N13—C33 | −85.6 (4) | N13—C37—C41—N14 | 0.9 (5) |
| N17—Fe1—N13—C33 | −3.4 (4) | C36—C37—C41—N14 | −179.5 (4) |
| N14—Fe1—N13—C33 | −178.3 (4) | N13—C37—C41—C40 | −177.7 (4) |
| N16—Fe1—N13—C37 | −39.3 (12) | C36—C37—C41—C40 | 1.9 (6) |
| N15—Fe1—N13—C37 | −91.5 (3) | C41—C40—C42—C43 | 1.6 (6) |
| N18—Fe1—N13—C37 | 94.0 (3) | C39—C40—C42—C43 | 179.7 (4) |
| N17—Fe1—N13—C37 | 176.2 (3) | C40—C42—C43—C44 | 0.5 (7) |
| N14—Fe1—N13—C37 | 1.2 (3) | C41—N14—C44—C43 | 2.4 (6) |
| N16—Fe1—N14—C44 | −6.8 (4) | Fe1—N14—C44—C43 | −176.0 (3) |
| N15—Fe1—N14—C44 | −89.9 (4) | C42—C43—C44—N14 | −2.7 (7) |
| N13—Fe1—N14—C44 | 177.7 (4) | C49—N15—C45—C46 | −1.6 (5) |
| N18—Fe1—N14—C44 | 88.4 (3) | Fe1—N15—C45—C46 | −179.3 (3) |
| N17—Fe1—N14—C44 | 128.1 (11) | N15—C45—C46—C47 | 1.9 (6) |
| N16—Fe1—N14—C41 | 174.7 (3) | C45—C46—C47—C48 | −1.3 (7) |
| N15—Fe1—N14—C41 | 91.7 (3) | C46—C47—C48—C49 | 0.5 (6) |
| N13—Fe1—N14—C41 | −0.7 (3) | C46—C47—C48—C50 | −179.8 (4) |
| N18—Fe1—N14—C41 | −90.0 (3) | C45—N15—C49—C48 | 0.8 (5) |

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| N17—Fe1—N14—C41 | −50.4 (13) | Fe1—N15—C49—C48 | 178.9 (3) |
| N16—Fe1—N15—C45 | 177.4 (3) | C45—N15—C49—C53 | −178.8 (3) |
| N13—Fe1—N15—C45 | −8.1 (3) | Fe1—N15—C49—C53 | −0.8 (4) |
| N18—Fe1—N15—C45 | 105.9 (13) | C47—C48—C49—N15 | −0.2 (6) |
| N17—Fe1—N15—C45 | 85.3 (3) | C50—C48—C49—N15 | −180.0 (4) |
| N14—Fe1—N15—C45 | −90.6 (3) | C47—C48—C49—C53 | 179.4 (4) |
| N16—Fe1—N15—C49 | −0.3 (2) | C50—C48—C49—C53 | −0.4 (6) |
| N13—Fe1—N15—C49 | 174.2 (3) | C47—C48—C50—C51 | 179.6 (5) |
| N18—Fe1—N15—C49 | −71.9 (14) | C49—C48—C50—C51 | −0.7 (7) |
| N17—Fe1—N15—C49 | −92.4 (3) | C48—C50—C51—C52 | 0.6 (8) |
| N14—Fe1—N15—C49 | 91.6 (3) | C50—C51—C52—C54 | −178.4 (5) |
| N15—Fe1—N16—C56 | 178.0 (3) | C50—C51—C52—C53 | 0.6 (7) |
| N13—Fe1—N16—C56 | 125.3 (10) | C56—N16—C53—C52 | 1.5 (5) |
| N18—Fe1—N16—C56 | −7.8 (3) | Fe1—N16—C53—C52 | 178.6 (3) |
| N17—Fe1—N16—C56 | −90.2 (3) | C56—N16—C53—C49 | −179.2 (3) |
| N14—Fe1—N16—C56 | 85.1 (3) | Fe1—N16—C53—C49 | −2.1 (4) |
| N15—Fe1—N16—C53 | 1.3 (2) | C54—C52—C53—N16 | −3.4 (6) |
| N13—Fe1—N16—C53 | −51.4 (11) | C51—C52—C53—N16 | 177.5 (4) |
| N18—Fe1—N16—C53 | 175.6 (2) | C54—C52—C53—C49 | 177.4 (4) |
| N17—Fe1—N16—C53 | 93.2 (3) | C51—C52—C53—C49 | −1.7 (6) |
| N14—Fe1—N16—C53 | −91.5 (3) | N15—C49—C53—N16 | 1.9 (5) |
| N16—Fe1—N17—C57 | −83.2 (4) | C48—C49—C53—N16 | −177.7 (3) |
| N15—Fe1—N17—C57 | −0.2 (4) | N15—C49—C53—C52 | −178.8 (3) |
| N13—Fe1—N17—C57 | 92.7 (4) | C48—C49—C53—C52 | 1.6 (6) |
| N18—Fe1—N17—C57 | −178.1 (4) | C53—C52—C54—C55 | 2.5 (6) |
| N14—Fe1—N17—C57 | 141.9 (11) | C51—C52—C54—C55 | −178.4 (4) |
| N16—Fe1—N17—C61 | 101.1 (3) | C52—C54—C55—C56 | −0.1 (6) |
| N15—Fe1—N17—C61 | −175.9 (3) | C53—N16—C56—C55 | 1.1 (6) |
| N13—Fe1—N17—C61 | −83.0 (3) | Fe1—N16—C56—C55 | −175.4 (3) |
| N18—Fe1—N17—C61 | 6.2 (3) | C54—C55—C56—N16 | −1.8 (6) |
| N14—Fe1—N17—C61 | −33.8 (13) | C61—N17—C57—C58 | 0.5 (6) |
| N16—Fe1—N18—C68 | 86.4 (3) | Fe1—N17—C57—C58 | −175.1 (3) |
| N15—Fe1—N18—C68 | 157.4 (12) | N17—C57—C58—C59 | −0.1 (7) |
| N13—Fe1—N18—C68 | −88.5 (3) | C57—C58—C59—C60 | −0.4 (7) |
| N17—Fe1—N18—C68 | 178.1 (4) | C58—C59—C60—C61 | 0.5 (7) |
| N14—Fe1—N18—C68 | −6.1 (3) | C58—C59—C60—C62 | 178.5 (5) |
| N16—Fe1—N18—C65 | −98.4 (3) | C57—N17—C61—C60 | −0.4 (6) |
| N15—Fe1—N18—C65 | −27.5 (14) | Fe1—N17—C61—C60 | 175.9 (3) |
| N13—Fe1—N18—C65 | 86.6 (3) | C57—N17—C61—C65 | 179.0 (4) |
| N17—Fe1—N18—C65 | −6.7 (2) | Fe1—N17—C61—C65 | −4.8 (4) |
| N14—Fe1—N18—C65 | 169.0 (3) | C59—C60—C61—N17 | −0.1 (6) |
| Cr1—N1—C1—S1 | −6 (14) | C62—C60—C61—N17 | −178.2 (4) |
| Cr1—N2—C2—S2 | 108 (22) | C59—C60—C61—C65 | −179.4 (4) |
| Cr1—N3—C3—S3 | −12 (36) | C62—C60—C61—C65 | 2.4 (6) |
| Cr1—N4—C4—S4 | 164 (11) | C61—C60—C62—C63 | −1.8 (6) |
| Cr2—N5—C5—S5 | −173 (100) | C59—C60—C62—C63 | −179.8 (4) |
| Cr2—N6—C6—S6 | −102 (11) | C60—C62—C63—C64 | −0.5 (7) |
| Cr2—N7—C7—S7 | −167 (100) | C62—C63—C64—C65 | 2.0 (6) |
| Cr2—N8—C8—S8 | −146 (16) | C62—C63—C64—C66 | −177.3 (4) |

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| C13—N9—C9—C10 | 0.0 (6) | C68—N18—C65—C64 | 1.3 (5) |
| Cr1—N9—C9—C10 | 179.5 (3) | Fe1—N18—C65—C64 | −174.5 (3) |
| N9—C9—C10—C11 | 0.6 (7) | C68—N18—C65—C61 | −178.1 (3) |
| C9—C10—C11—C12 | −0.8 (6) | Fe1—N18—C65—C61 | 6.1 (4) |
| C10—C11—C12—C13 | 0.4 (6) | C66—C64—C65—N18 | −1.3 (6) |
| C10—C11—C12—C14 | −179.0 (4) | C63—C64—C65—N18 | 179.3 (3) |
| C9—N9—C13—C12 | −0.5 (5) | C66—C64—C65—C61 | 178.0 (4) |
| Cr1—N9—C13—C12 | 179.9 (3) | C63—C64—C65—C61 | −1.3 (6) |
| C9—N9—C13—C17 | 178.6 (3) | N17—C61—C65—N18 | −0.9 (5) |
| Cr1—N9—C13—C17 | −1.0 (4) | C60—C61—C65—N18 | 178.5 (3) |
| C11—C12—C13—N9 | 0.3 (6) | N17—C61—C65—C64 | 179.7 (4) |
| C14—C12—C13—N9 | 179.7 (3) | C60—C61—C65—C64 | −0.9 (6) |
| C11—C12—C13—C17 | −178.7 (3) | C65—C64—C66—C67 | 0.6 (6) |
| C14—C12—C13—C17 | 0.7 (5) | C63—C64—C66—C67 | 179.9 (4) |
| C11—C12—C14—C15 | 178.5 (4) | C64—C66—C67—C68 | 0.1 (7) |
| C13—C12—C14—C15 | −0.9 (6) | C65—N18—C68—C67 | −0.5 (6) |
| C12—C14—C15—C16 | −0.1 (6) | Fe1—N18—C68—C67 | 174.5 (3) |
| C14—C15—C16—C18 | −177.4 (4) | C66—C67—C68—N18 | −0.2 (7) |
| C14—C15—C16—C17 | 1.4 (6) | | |