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# Trinuclear nickel coordination complexes of phenanthrene-9,10-dione dioxime

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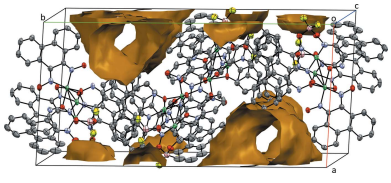
**CCDC references**: 1462814; 1462813

**Supporting information**: this article has supporting information at journals.iucr.org/e

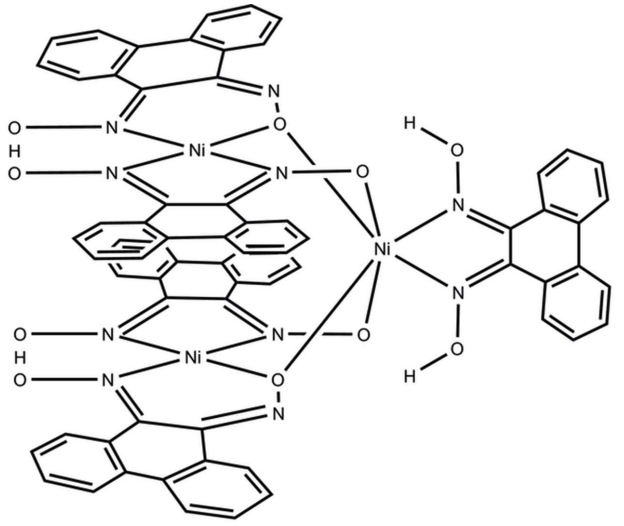
A trinuclear nickel complex of phenanthrene-9,10-dione dioxime ($H_2$pqd), namely bis[$\mu_2$-9,10-bis(oxidoimino)phenanthrene]bis[$\mu_2$-10-(oxidoimino)-phenanthrene-9-one oxime](phenanthrene-9,10-dione dioxime)trinickel(II) toluene disolvate, $[Ni_3(C_{14}H_8N_2O_2)_2(C_{14}H_9N_2O_2)_2(C_{14}H_{10}N_2O_2)]\cdot 2C_7H_8$, has been isolated and its crystal structure determined. This complex features three independent $Ni^{II}$ atoms that are arranged in a triangular fashion along with five supporting ligands. There are two square-planar $Ni^{II}$ atoms and a third pseudo-octahedral $Ni^{II}$ atom. While the square-planar $Ni^{II}$ atoms are stacked, there are no ligand bridges between them. Each square-planar $Ni^{II}$ atom, however, bridges with the pseudo-octahedral $Ni^{II}$ atom through Ni—N—O—Ni and Ni—O—Ni bonds. A fluoridoboration reaction of the proton-bridged species gave the analogous complex bis($\mu_2$-bis{[10-(oxidoimino)-9,10-dihydrophenanthren-9-ylidene]amino}difluoridoborato)(phenanthrene-9,10-dione dioxime)trinickel(II) dichloromethane trisolvate, $[Ni_3(C_{28}H_{16}BF_2N_4O_4)_2(C_{14}H_{10}N_2O_2)]\cdot 3CH_2Cl_2$, which shows the same binding structure, but features a widened Ni—Ni interaction between the square-planar $Ni^{II}$ atoms. The proton-bridged complex completes the macrocyclic coordination around the square-planar $Ni^{II}$ atoms by means of an O—H···O hydrogen bond. Both compounds feature O—H···N hydrogen bonds between the oxime and the N atoms attached to square-planar nickel atom. The nickel units show no direct interaction with their nearest neighbors in the extended lattice. Two $\pi$-stacking interactions between adjacent molecules are found: one with a centroid–centroid distance of 3.886 (2) Å and the other with a centroid–centroid distance of 4.256 (3) Å. In the latter case, although not aromatic, the distance to the centroid of the central phenanthrene ring is shorter, with a distance of 3.528 (3) Å. Toluene molecules occupy the solvent channels that are oriented along the *c* axis. In the fluoridoboronate structure, the solvent (DCM) was too badly disordered to be modelled, so its contribution was removed using SQUEEZE [Spek (2015). *Acta Cryst.* C**71**, 9–18].

## 1. Chemical context

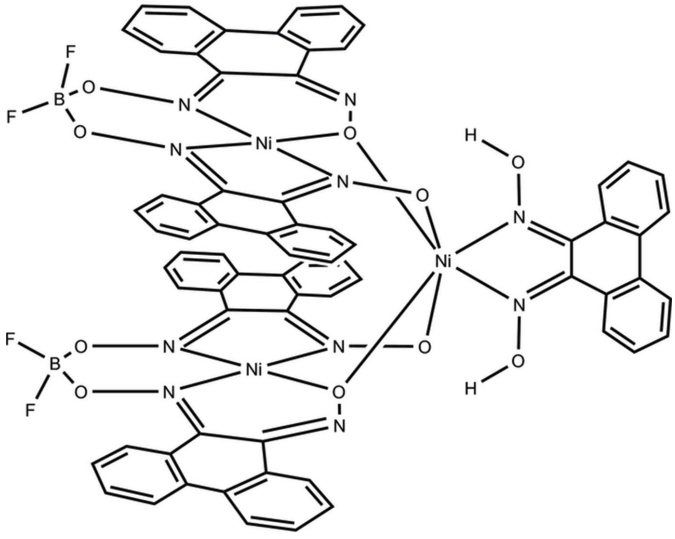
Oxime functional groups can coordinate to transition metal ions in a variety of ways, due to the presence of both nitrogen and oxygen donors. On account of the multitude of possible coordinations, these ligands, and particularly $\alpha$–$\beta$ dioximes, have the capability of forming bridging multinuclear complexes with many transition metals, including nickel (Chaudhuri, 2003). From the standpoint of single-molecule magnets, these multi-nuclear complexes play an important role due to their ability to facilitate spin-frustration in magnetic transition-metal clusters (Aromí & Brechin, 2006). Other nickel polynuclear compounds supported by oxime ligands have been reported (Jiang *et al.*, 2005; Biswas *et al.*, 2009).



Phenanthrenequinone dioxime ($pqdH_2$) is an $\alpha$–$\beta$ dioxime ligand that incorporates a constrained ring system. Similar to other dioximes, however, it exists as three separate stereoisomers (*E*–*E*, *E*–*Z*, and *Z*–*Z*), as confirmed by liquid chromatography – mass spectrometry. Interestingly, although this compound was synthesized over 100 years ago (Schmidt & Söll, 1907), no coordination complexes of this ligand have been structurally characterized to date.




(1)




(2)

## 2. Structural commentary

Fig. 1 shows the structure of $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$, (**1**). This complex consists of three $Ni^{II}$ atoms in a triangular arrangement, two of which are in a square-planar coordination environment, while the third is in a pseudo-octahedral coordination environment. The square-planar $Ni^{II}$ atoms (Ni1 and Ni2) consist of one *N*,*N*-coordinating and one *N*,*O*-coordinating ligand. These ligands form bridges with the pseudo-octahedral $Ni^{II}$ atom (Ni3) by means of their oxime O atoms.

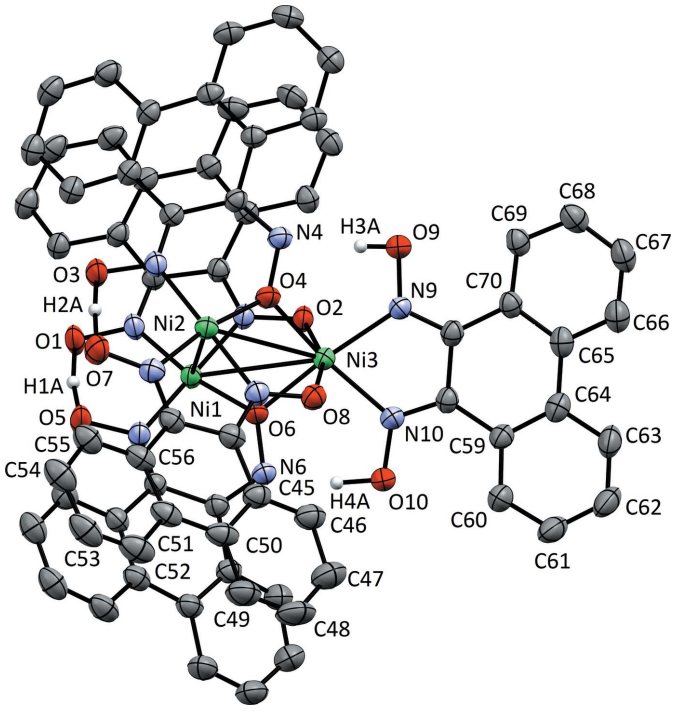



**Figure 1**
Displacement ellipsoid plot at the 50% probability level for $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$. H atoms (with the exception of hydrogen-bonded atoms) and solvent molecules have been omitted for clarity.

This arrangement permits the formation of Ni—N—O—Ni and Ni—O—Ni bridges between each square-planar $Ni^{II}$ atom and the pseudo-octahedral $Ni^{II}$ atom.

The structural features of the core ligation sphere warrant special attention. The $Ni_{sp}$—$Ni_{sp}$ distance is 3.3657 (9) Å, a distance that precludes the presence of any metal–metal bonding. However, the distances between each of these nickel moieties and the pseudo-octahedral $Ni^{II}$ atom are nearly identical [$Ni_{sp}$—$Ni_{oct}$ = 3.2697 (7), 3.2674 (7) Å]. The pseudo-octahedral nickel geometry deviates significantly from a perfect octahedral symmetry [O2—Ni3—O8 = 160.00 (9), O4—Ni3—N10 = 164.8 (1), N9—Ni3—O6 = 165.5 (1)°].

Fig. 2 shows the complete coordination geometry of the compound $[Ni_3(pqdH_2)(pqdBF_2)_2(pqd)_2]$, (**2**). The physical arrangement of the ligation sphere directly mimics that of (**1**). In this case, however, the steric bulk of the $BF_2$ groups forces an expansion of the stacked square-planar nickel units, resulting in an $Ni_{sp}$—$Ni_{sp}$ distance of 3.592 (1) Å. The distances between these units and the pseudo-octahedral $Ni^{II}$ atom, however, remain similar [$Ni_{sp}$—$Ni_{oct}$ = 3.274 (1), 3.255 (1) Å]. Overall, the entire structure retains all the other structural features that are present in the proton-bridged compound.

The phenanthrene backbones show pronounced twisting between their aromatic rings, which precludes conjugation across this unit. For the proton-bridged complex, the angle between mean planes within a single phenanthrene backbone ranges from 9.24 (19)° (between C45–C50 and C51–C56) to 15.44 (13)° (between C59–C64 and C65–C70). For the

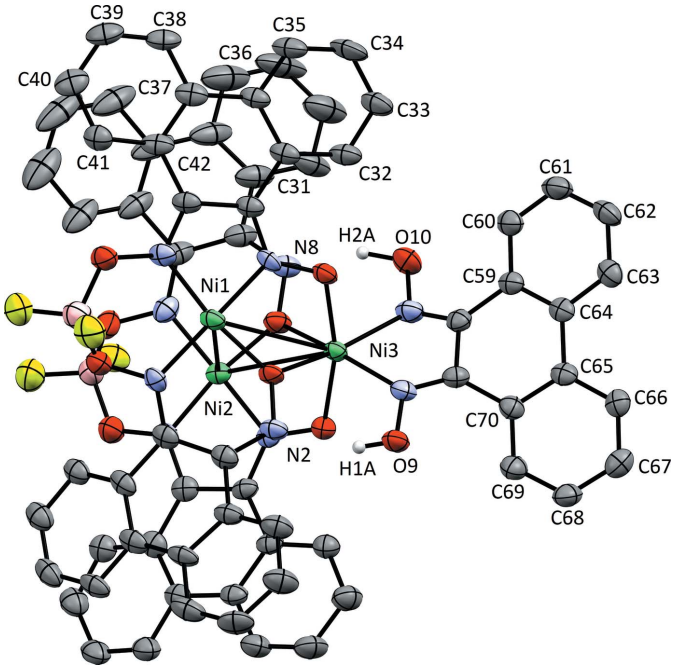



**Figure 2**
Displacement ellipsoid plot at the 50% probability level of $[Ni_3(H_2pqd)(BF_2pqd)_2(pqd)_2]$. H atoms (with the exception of hydrogen-bonded atoms) and solvent molecules have been omitted for clarity.

$BF_2$-bridged complex, there is a wider range of angles, with 5.2 (4)° (between C31–C36 and C37–C42) being the smallest, and 17.5 (3)° (between C59–C64 and C65–C70) being the largest.

**Table 1**
Hydrogen-bond geometry (Å, °) for (**1**).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O5 | 1.29 (6) | 1.13 (6) | 2.405 (4) | 169 (6) |
| O3—H2$A$···O7 | 1.17 (5) | 1.23 (5) | 2.402 (4) | 176 (5) |
| O9—H3$A$···N4 | 0.86 (6) | 1.82 (6) | 2.672 (4) | 175 (7) |
| O10—H4$A$···N6 | 1.04 (5) | 1.63 (5) | 2.657 (4) | 168 (4) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O9—H1$A$···N2 | 0.85 | 1.96 | 2.771 (6) | 158 |
| O10—H2$A$···N8 | 1.06 | 1.77 | 2.765 (6) | 155 |

## 3. Supramolecular features

The proton-bridged complex completes the macrocyclic coordination around the square-planar $Ni^{II}$ atoms by means of hydrogen bonds. Furthermore, the ligand that coordinates the pseudo-octahedral $Ni^{II}$ atom features hydrogen-bonding interactions (Table 1) between the oxime hydroxy groups and the ligands of the square-planar $Ni^{II}$ atoms. The nickel units show no direct interaction with their nearest neighbors in the extended lattice. Some $\pi$-stacking between adjacent molecules is, however, evident (Fig. 3). Two interactions were found, one with a centroid–centroid distance of 3.886 (2) Å (symmetry code: $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$) and the other with a centroid–centroid distance of 4.256 (3) Å (symmetry code: $-x, -y, 2-z$). In the latter case, although not aromatic, the distance to the centroid of the central ring of phenanthrene is shorter, with a distance of 3.528 (3) Å. Toluene molecules occupy the solvent channels that are oriented along the $c$ axis.

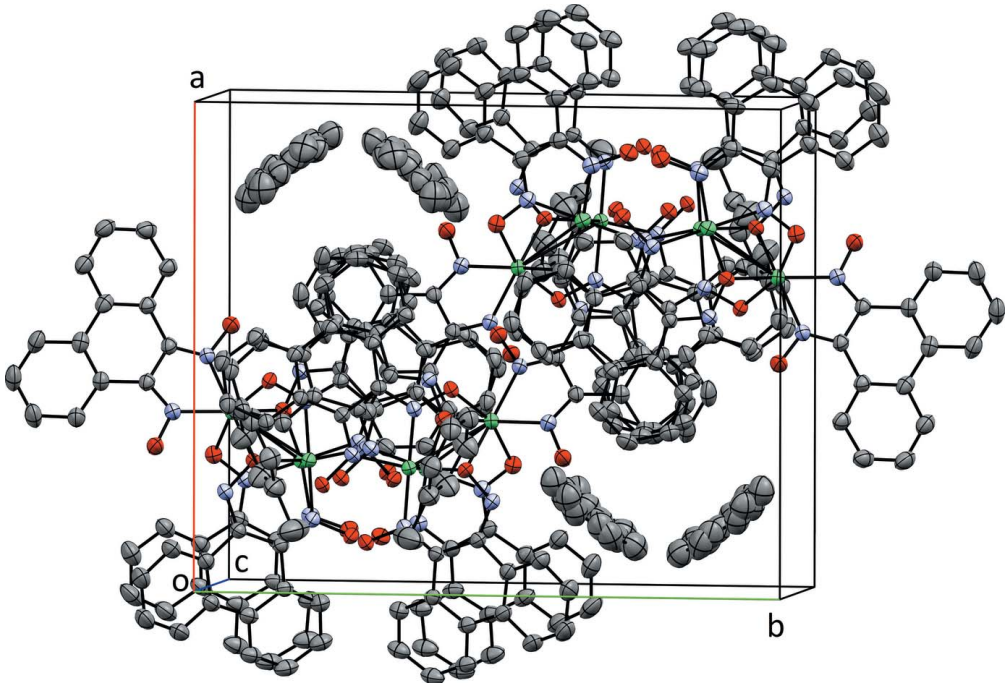



**Figure 3**
Packing diagram of $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$, viewed approximately down the $c$-axis direction.

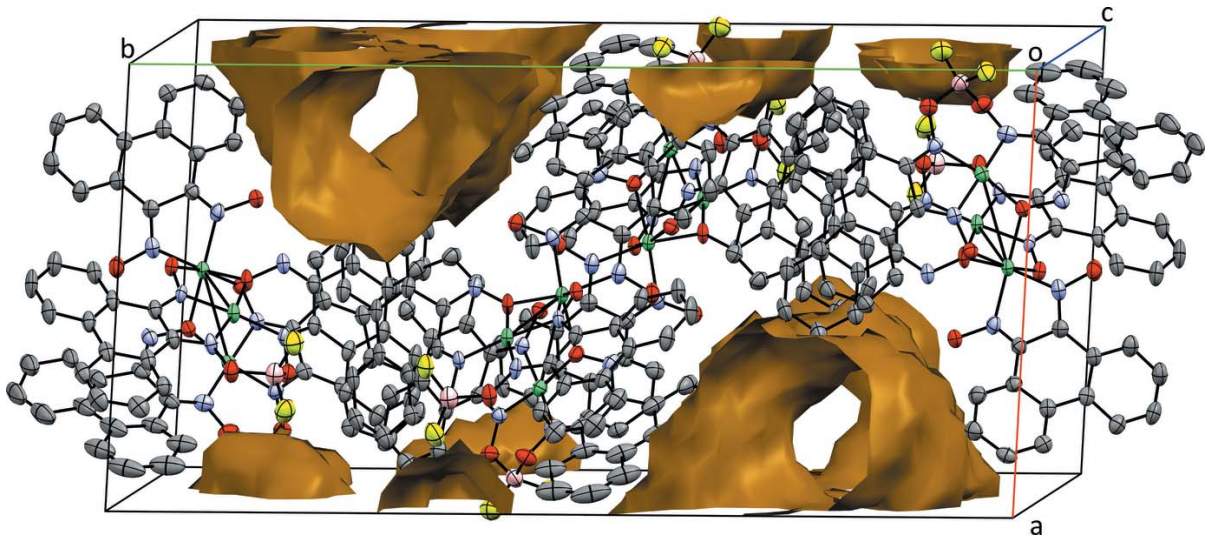



**Figure 4**
Packing diagram of $Ni_3(H_2pqd)(BF_2pqd)_2(pqd)_2$, viewed approximately down the *c*-axis direction. Voids presented in brown were calculated in *Mercury* (Macrae *et al.*, 2006) using a probe radius of 1.2 Å.

The $BF_2$-bridged complex completes the macrocyclic coordination around the square-planar $Ni^{II}$ atoms by means of covalent O—B—O bonds. However, the hydrogen-bonding interactions (Table 2) that lock the pseudo-octahedral $Ni^{II}$ atom remain in place. The nickel units show no direct interaction with their nearest neighbors in the extended lattice. A solvent channel oriented along the *c* axis is also evident (Fig. 4). However, the extreme disorder of the solvent does not permit the determination of a suitable model.

**Table 3**
Experimental details.

| | (**1**) | (**2**) |
|---|---|---|
| Crystal data | | |
| Chemical formula | $[Ni_3(C_{14}H_8N_2O_2)_2(C_{14}H_9N_2O_2)_2$-$(C_{14}H_{10}N_2O_2)]\cdot 2C_7H_8$ | $[Ni_3(C_{28}H_{16}BF_2N_4O_4)_2(C_{14}H_{10}N_2O_2)]\cdot$-$3CH_2Cl_2$ |
| $M_r$ | 1545.55 | 1456.88 |
| Crystal system, space group | Monoclinic, $P2_1/c$ | Monoclinic, $P2_1/c$ |
| Temperature (K) | 100 | 100 |
| *a*, *b*, *c* (Å) | 15.973 (3), 18.639 (3), 22.785 (4) | 15.6414 (8), 30.8358 (11), 14.7380 (8) |
| $\beta$ (°) | 101.757 (4) | 112.411 (6) |
| $V$ (Å$^3$) | 6641.1 (19) | 6571.5 (6) |
| $Z$ | 4 | 4 |
| Radiation type | Mo $K\alpha$ | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.92 | 1.67 |
| Crystal size (mm) | 0.16 × 0.11 × 0.11 | 0.29 × 0.07 × 0.04 |
| Data collection | | |
| Diffractometer | Rigaku Saturn724+ | Agilent SuperNova Dual Source diffractometer with an Atlas detector |
| Absorption correction | Multi-scan (*ABSCOR*; Higashi, 1995) | Multi-scan (*CrysAlis PRO*; Agilent, 2014) |
| $T_{min}$, $T_{max}$ | 0.799, 1.000 | 0.303, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 79592, 15260, 13993 | 25337, 13041, 8782 |
| $R_{int}$ | 0.054 | 0.060 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.650 | 0.626 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.067, 0.151, 1.21 | 0.077, 0.226, 1.03 |
| No. of reflections | 15260 | 13041 |
| No. of parameters | 1046 | 896 |
| No. of restraints | 291 | 0 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.56, −0.68 | 1.16, −0.83 |

Computer programs: *CrystalClear* (Rigaku Inc, 2008), *CrysAlis PRO* (Agilent, 2014), *SIR2004* (Burla *et al.*, 2005), *OLEX2* (Dolomanov *et al.*, 2009), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006), *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 1999).

## 4. Synthesis and crystallization

The parent ligand, $pqdH_2$ (0.75 g; 3.1 mmol), was dissolved in 100 ml of ethanol, to which nickel(II) acetate (0.33 g, 1.3 mmol) was added. A red precipitate began to form after approximately 30 min. The solution was then allowed to stir for 1 h, followed by cooling in a freezer and filtration of the crude product (yield: 272 mg, 0.2 mmol, 32%). The resulting product was dissolved in DMF solution and layered with toluene, resulting in the formation of crystals of $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$ after a period of 3–4 d. The crystals grew as red blocks with an asymmetric unit consisting of a complete $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$ molecule and two toluene solvent molecules.

The foregoing complex is stable enough to undergo a fluoridoboration reaction with boron trifluoride, thereby affording the compound $[Ni_3(H_2pqd)(BF_2pqd)_2(pqd)_2]$. $[Ni_3(H_2pqd)(Hpqd)_2(pqd)_2]$ was diluted in diethyl ether, thereby creating a slurry. One ml of 1.0 molar $BF_3$–$OEt_2$ (in ether) was then added and the mixture was allowed to react overnight. The resulting precipitate was then filtered off and washed thoroughly with EtOH and $Et_2O$. The resulting precipitate was then dissolved in dichloromethane (DCM) and filtered through Celite (yield: 43 mg, 30 µmol, 79%). Subsequently, a crop of red block-shaped crystals was grown by solvent evaporation over a period of one day.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. In proton-bridged structure (1), atoms H1*A*, H2*A* and H4*A* were found by assignment of difference map peaks and refined isotropically without geometrical constraints. The proton H3*A* was initially placed with the *SHELXL* HFIX 147 command (refinement on rotation) on O9, but was refined freely. Four distinct hydrogen-bonding interactions were evident in the trinuclear cluster. Finally, there were two O—H—O interactions between an oxime and oximato of each $[Ni(Hpqd)(pqd)]^-$ unit that could not be resolved due to rapid conversion to $[Ni(pqd)(Hpqd)]^-$. All the restraints that are reported were included for the modelling of the disordered toluene solvent molecules.

In the case of $BF_2$-bridged structure (2), atoms H1*A* and H2*A* were affixed to O9 and O10, respectively. They were then refined isotropically without rotational constraints. The SQUEEZE routine (Spek, 2015) as implemented in *PLATON* (Spek, 2009) was used to remove the electron density of three solvent DCM molecules per unit cell (calculated: 134 $e^-$; 593 $Å^3$).

## Acknowledgements

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# supporting information

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### Computing details

Data collection: *CrystalClear* (Rigaku Inc, 2008) for (1); *CrysAlis PRO* (Agilent, 2014) for (2). Cell refinement: *CrystalClear* (Rigaku Inc, 2008) for (1); *CrysAlis PRO* (Agilent, 2014) for (2). Data reduction: *CrystalClear* (Rigaku Inc, 2008) for (1); *CrysAlis PRO* (Agilent, 2014) for (2). Program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005) for (1); *OLEX2* (Dolomanov *et al.*, 2009) for (2). For both compounds, program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 1999).

### (1) Bis[$\mu_2$-9,10-bis(oxidoimino)phenanthrene]bis[$\mu_2$-10-(oxidoimino)phenanthrene-9-one oxime] (phenanthrene-9,10-dione dioxime)trinickel(II) toluene disolvate

*Crystal data*

$[Ni_3(C_{14}H_8N_2O_2)_2(C_{14}H_9N_2O_2)_2(C_{14}H_{10}N_2O_2)]\cdot 2C_7H_8$
$M_r$ = 1545.55
Monoclinic, $P2_1/c$
$a$ = 15.973 (3) Å
$b$ = 18.639 (3) Å
$c$ = 22.785 (4) Å
$\beta$ = 101.757 (4)°
$V$ = 6641.1 (19) Å$^3$
$Z$ = 4
$F(000)$ = 3192
$D_x$ = 1.546 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71069 Å
Cell parameters from 20424 reflections
$\theta$ = 1.3–31.1°
$\mu$ = 0.92 mm$^{-1}$
$T$ = 100 K
Block, red
0.16 × 0.11 × 0.11 mm

*Data collection*

Rigaku Saturn724+ (2x2 bin mode) diffractometer
Radiation source: Sealed Tube
Detector resolution: 28.5714 pixels mm$^{-1}$
dtprofit.ref scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
$T_{min}$ = 0.799, $T_{max}$ = 1.000
79592 measured reflections
15260 independent reflections
13993 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 1.8°
$h$ = −20→20
$k$ = −24→24
$l$ = −29→29

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.151
$S$ = 1.21
15260 reflections
1046 parameters
291 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 7.4732P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.56 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.68 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.3573 (2) | 0.26380 (17) | 0.77353 (15) | 0.0300 (7) | |
| C2 | 0.4143 (2) | 0.20289 (17) | 0.79218 (14) | 0.0287 (6) | |
| C3 | 0.5058 (2) | 0.21463 (17) | 0.81436 (14) | 0.0289 (7) | |
| C4 | 0.5622 (2) | 0.15956 (19) | 0.83987 (15) | 0.0341 (7) | |
| H4 | 0.5433 | 0.1123 | 0.8376 | 0.041* | |
| C5 | 0.6447 (2) | 0.1749 (2) | 0.86803 (16) | 0.0392 (8) | |
| H5 | 0.6811 | 0.1381 | 0.8850 | 0.047* | |
| C6 | 0.6738 (2) | 0.2450 (2) | 0.87123 (17) | 0.0423 (9) | |
| H6 | 0.7292 | 0.2554 | 0.8913 | 0.051* | |
| C7 | 0.6209 (2) | 0.2991 (2) | 0.84477 (17) | 0.0412 (8) | |
| H7 | 0.6418 | 0.3458 | 0.8465 | 0.049* | |
| C8 | 0.5364 (2) | 0.28614 (18) | 0.81521 (15) | 0.0318 (7) | |
| C9 | 0.4809 (2) | 0.34500 (17) | 0.78633 (15) | 0.0306 (7) | |
| C10 | 0.5151 (2) | 0.41244 (19) | 0.77676 (16) | 0.0371 (8) | |
| H10 | 0.5735 | 0.4200 | 0.7897 | 0.045* | |
| C11 | 0.4652 (2) | 0.46755 (19) | 0.74890 (17) | 0.0403 (8) | |
| H11 | 0.4897 | 0.5119 | 0.7442 | 0.048* | |
| C12 | 0.3783 (2) | 0.45710 (18) | 0.72779 (17) | 0.0388 (8) | |
| H12 | 0.3445 | 0.4941 | 0.7085 | 0.047* | |
| C13 | 0.3423 (2) | 0.39116 (17) | 0.73569 (16) | 0.0334 (7) | |
| H13 | 0.2841 | 0.3841 | 0.7212 | 0.040* | |
| C14 | 0.3922 (2) | 0.33465 (16) | 0.76530 (15) | 0.0294 (7) | |
| C15 | 0.3654 (2) | 0.24577 (17) | 0.93609 (14) | 0.0292 (7) | |
| C16 | 0.4342 (2) | 0.19229 (17) | 0.94884 (14) | 0.0283 (6) | |
| C17 | 0.5203 (2) | 0.21590 (17) | 0.98016 (14) | 0.0293 (7) | |
| C18 | 0.5819 (2) | 0.16511 (18) | 1.00548 (14) | 0.0327 (7) | |
| H18 | 0.5684 | 0.1165 | 1.0024 | 0.039* | |
| C19 | 0.6622 (2) | 0.1864 (2) | 1.03489 (15) | 0.0364 (8) | |
| H19 | 0.7032 | 0.1524 | 1.0507 | 0.044* | |
| C20 | 0.6815 (2) | 0.2591 (2) | 1.04065 (17) | 0.0410 (8) | |
| H20 | 0.7354 | 0.2738 | 1.0606 | 0.049* | |
| C21 | 0.6211 (2) | 0.3092 (2) | 1.01689 (16) | 0.0396 (8) | |
| H21 | 0.6345 | 0.3577 | 1.0218 | 0.048* | |
| C22 | 0.5392 (2) | 0.28906 (18) | 0.98522 (14) | 0.0317 (7) | |
| C23 | 0.4766 (2) | 0.34208 (17) | 0.95560 (15) | 0.0317 (7) | |
| C24 | 0.4995 (2) | 0.41366 (19) | 0.94928 (17) | 0.0386 (8) | |
| H24 | 0.5548 | 0.4282 | 0.9663 | 0.046* | |
| C25 | 0.4432 (3) | 0.4633 (2) | 0.91884 (18) | 0.0428 (9) | |
| H25 | 0.4599 | 0.5108 | 0.9166 | 0.051* | |

| | | | | |
|---|---|---|---|---|
| C26 | 0.3618 (2) | 0.44223 (19) | 0.89172 (17) | 0.0408 (8) |
| H26 | 0.3242 | 0.4751 | 0.8696 | 0.049* |
| C27 | 0.3360 (2) | 0.37214 (18) | 0.89741 (16) | 0.0363 (8) |
| H27 | 0.2809 | 0.3585 | 0.8790 | 0.044* |
| C28 | 0.3911 (2) | 0.32129 (17) | 0.93032 (15) | 0.0312 (7) |
| C29 | 0.0764 (2) | 0.10264 (17) | 0.76379 (14) | 0.0291 (7) |
| C30 | 0.1064 (2) | 0.03055 (17) | 0.75287 (15) | 0.0309 (7) |
| C31 | 0.0435 (2) | −0.02258 (18) | 0.72335 (15) | 0.0346 (7) |
| C32 | 0.0685 (2) | −0.0803 (2) | 0.69200 (18) | 0.0429 (9) |
| H32 | 0.1254 | −0.0851 | 0.6889 | 0.051* |
| C33 | 0.0088 (3) | −0.1305 (2) | 0.6655 (2) | 0.0529 (10) |
| H33 | 0.0255 | −0.1689 | 0.6445 | 0.064* |
| C34 | −0.0749 (3) | −0.1236 (2) | 0.6701 (2) | 0.0539 (11) |
| H34 | −0.1146 | −0.1579 | 0.6526 | 0.065* |
| C35 | −0.1009 (2) | −0.0668 (2) | 0.70016 (19) | 0.0472 (9) |
| H35 | −0.1581 | −0.0628 | 0.7026 | 0.057* |
| C36 | −0.0422 (2) | −0.01423 (19) | 0.72739 (16) | 0.0366 (8) |
| C37 | −0.0676 (2) | 0.0483 (2) | 0.75883 (16) | 0.0360 (8) |
| C38 | −0.1479 (2) | 0.0511 (2) | 0.77467 (18) | 0.0434 (9) |
| H38 | −0.1845 | 0.0120 | 0.7661 | 0.052* |
| C39 | −0.1741 (2) | 0.1100 (2) | 0.80252 (18) | 0.0462 (9) |
| H39 | −0.2275 | 0.1102 | 0.8127 | 0.055* |
| C40 | −0.1214 (2) | 0.1683 (2) | 0.81519 (18) | 0.0450 (9) |
| H40 | −0.1397 | 0.2086 | 0.8331 | 0.054* |
| C41 | −0.0410 (2) | 0.1676 (2) | 0.80142 (17) | 0.0393 (8) |
| H41 | −0.0054 | 0.2072 | 0.8109 | 0.047* |
| C42 | −0.0122 (2) | 0.10822 (18) | 0.77336 (15) | 0.0323 (7) |
| C43 | 0.0836 (2) | 0.08681 (19) | 0.92655 (15) | 0.0345 (7) |
| C44 | 0.1243 (2) | 0.02254 (19) | 0.90908 (15) | 0.0346 (7) |
| C45 | 0.0739 (2) | −0.04203 (19) | 0.89031 (16) | 0.0378 (8) |
| C46 | 0.1065 (3) | −0.1008 (2) | 0.86405 (17) | 0.0433 (9) |
| H46 | 0.1639 | −0.1016 | 0.8616 | 0.052* |
| C47 | 0.0542 (3) | −0.1577 (2) | 0.8417 (2) | 0.0555 (11) |
| H47 | 0.0760 | −0.1960 | 0.8233 | 0.067* |
| C48 | −0.0306 (3) | −0.1576 (3) | 0.8468 (2) | 0.0633 (13) |
| H48 | −0.0655 | −0.1963 | 0.8323 | 0.076* |
| C49 | −0.0636 (3) | −0.1003 (2) | 0.8731 (2) | 0.0535 (11) |
| H49 | −0.1209 | −0.1011 | 0.8758 | 0.064* |
| C50 | −0.0134 (2) | −0.0412 (2) | 0.89578 (16) | 0.0424 (9) |
| C51 | −0.0494 (2) | 0.0194 (2) | 0.92335 (16) | 0.0408 (9) |
| C52 | −0.1321 (3) | 0.0157 (2) | 0.93653 (19) | 0.0505 (10) |
| H52 | −0.1643 | −0.0258 | 0.9266 | 0.061* |
| C53 | −0.1662 (2) | 0.0706 (3) | 0.96312 (19) | 0.0524 (11) |
| H53 | −0.2208 | 0.0661 | 0.9712 | 0.063* |
| C54 | −0.1207 (2) | 0.1331 (3) | 0.97825 (18) | 0.0507 (10) |
| H54 | −0.1443 | 0.1706 | 0.9964 | 0.061* |
| C55 | −0.0392 (2) | 0.1395 (2) | 0.96614 (17) | 0.0430 (9) |
| H55 | −0.0084 | 0.1816 | 0.9762 | 0.052* |

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|---|---|---|---|---|---|
| C56 | −0.0028 (2) | 0.0833 (2) | 0.93893 (15) | 0.0379 (8) | |
| C57 | 0.4778 (2) | −0.09599 (17) | 0.87975 (15) | 0.0311 (7) | |
| C58 | 0.4046 (2) | −0.13101 (17) | 0.83829 (15) | 0.0305 (7) | |
| C59 | 0.4055 (2) | −0.20914 (17) | 0.83084 (14) | 0.0320 (7) | |
| C60 | 0.3314 (2) | −0.24949 (19) | 0.80879 (17) | 0.0412 (8) | |
| H60 | 0.2797 | −0.2260 | 0.7955 | 0.049* | |
| C61 | 0.3342 (3) | −0.3230 (2) | 0.80656 (19) | 0.0508 (10) | |
| H61 | 0.2842 | −0.3488 | 0.7931 | 0.061* | |
| C62 | 0.4101 (3) | −0.3585 (2) | 0.82407 (19) | 0.0534 (11) | |
| H62 | 0.4120 | −0.4082 | 0.8214 | 0.064* | |
| C63 | 0.4839 (3) | −0.3203 (2) | 0.84575 (19) | 0.0487 (10) | |
| H63 | 0.5352 | −0.3449 | 0.8576 | 0.058* | |
| C64 | 0.4835 (2) | −0.24541 (18) | 0.85028 (16) | 0.0367 (8) | |
| C65 | 0.5628 (2) | −0.20611 (19) | 0.87678 (16) | 0.0367 (8) | |
| C66 | 0.6421 (2) | −0.2409 (2) | 0.88592 (18) | 0.0453 (9) | |
| H66 | 0.6448 | −0.2878 | 0.8724 | 0.054* | |
| C67 | 0.7154 (3) | −0.2078 (2) | 0.91426 (19) | 0.0483 (10) | |
| H67 | 0.7673 | −0.2321 | 0.9199 | 0.058* | |
| C68 | 0.7123 (2) | −0.1384 (2) | 0.93455 (18) | 0.0441 (9) | |
| H68 | 0.7622 | −0.1167 | 0.9550 | 0.053* | |
| C69 | 0.6367 (2) | −0.10049 (19) | 0.92512 (16) | 0.0372 (8) | |
| H69 | 0.6360 | −0.0534 | 0.9384 | 0.045* | |
| C70 | 0.5598 (2) | −0.13368 (18) | 0.89503 (15) | 0.0321 (7) | |
| C71 | 0.1134 (3) | 0.1368 (4) | 0.5502 (3) | 0.100 (2) | |
| H71A | 0.0755 | 0.1011 | 0.5291 | 0.150* | |
| H71B | 0.1188 | 0.1755 | 0.5235 | 0.150* | |
| H71C | 0.0906 | 0.1547 | 0.5832 | 0.150* | |
| C72 | 0.2006 (3) | 0.1037 (3) | 0.5736 (2) | 0.0596 (12) | |
| C73 | 0.2598 (3) | 0.0972 (2) | 0.5371 (2) | 0.0513 (10) | |
| H73 | 0.2466 | 0.1145 | 0.4980 | 0.062* | |
| C74 | 0.3375 (3) | 0.0656 (2) | 0.55792 (19) | 0.0501 (10) | |
| H74 | 0.3767 | 0.0618 | 0.5330 | 0.060* | |
| C75 | 0.3582 (3) | 0.0391 (2) | 0.61574 (19) | 0.0502 (10) | |
| H75 | 0.4106 | 0.0167 | 0.6294 | 0.060* | |
| C76 | 0.3013 (3) | 0.0460 (3) | 0.6527 (2) | 0.0634 (13) | |
| H76 | 0.3150 | 0.0287 | 0.6917 | 0.076* | |
| C77 | 0.2235 (3) | 0.0787 (3) | 0.6320 (2) | 0.0722 (15) | |
| H77 | 0.1857 | 0.0842 | 0.6578 | 0.087* | |
| C78 | −0.1860 (5) | 0.0902 (4) | 0.4357 (4) | 0.087 (2) | 0.66 |
| H78A | −0.1443 | 0.0585 | 0.4248 | 0.131* | 0.66 |
| H78B | −0.1928 | 0.1314 | 0.4099 | 0.131* | 0.66 |
| H78C | −0.2397 | 0.0656 | 0.4315 | 0.131* | 0.66 |
| C79 | −0.1572 (3) | 0.1133 (3) | 0.4982 (3) | 0.0727 (19) | 0.66 |
| C80 | −0.1792 (5) | 0.0748 (4) | 0.5449 (3) | 0.080 (2) | 0.66 |
| H80 | −0.2124 | 0.0336 | 0.5364 | 0.096* | 0.66 |
| C81 | −0.1524 (6) | 0.0964 (5) | 0.6039 (4) | 0.086 (3) | 0.66 |
| H81 | −0.1681 | 0.0703 | 0.6348 | 0.103* | 0.66 |
| C82 | −0.1021 (6) | 0.1574 (5) | 0.6167 (3) | 0.082 (3) | 0.66 |

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|---|---|---|---|---|---|
| H82 | −0.0833 | 0.1721 | 0.6562 | 0.098* | 0.66 |
| C83 | −0.0800 (5) | 0.1963 (4) | 0.5703 (3) | 0.083 (2) | 0.66 |
| H83 | −0.0466 | 0.2373 | 0.5789 | 0.100* | 0.66 |
| C84 | −0.1068 (4) | 0.1750 (3) | 0.5113 (3) | 0.0769 (19) | 0.66 |
| H84 | −0.0916 | 0.2015 | 0.4805 | 0.092* | 0.66 |
| C78A | −0.1035 (9) | 0.1587 (8) | 0.4495 (6) | 0.078 (4) | 0.34 |
| H78D | −0.0889 | 0.2087 | 0.4523 | 0.118* | 0.34 |
| H78E | −0.1505 | 0.1513 | 0.4163 | 0.118* | 0.34 |
| H78F | −0.0551 | 0.1314 | 0.4433 | 0.118* | 0.34 |
| C79A | −0.1290 (7) | 0.1344 (6) | 0.5073 (7) | 0.080 (3) | 0.34 |
| C81A | −0.2097 (10) | 0.0579 (9) | 0.5603 (8) | 0.082 (3) | 0.34 |
| H81A | −0.2488 | 0.0208 | 0.5596 | 0.098* | 0.34 |
| C80A | −0.1873 (8) | 0.0791 (7) | 0.5038 (8) | 0.079 (3) | 0.34 |
| H80A | −0.2108 | 0.0567 | 0.4677 | 0.094* | 0.34 |
| C82A | −0.1790 (13) | 0.0872 (12) | 0.6100 (11) | 0.082 (3) | 0.34 |
| H82A | −0.1962 | 0.0714 | 0.6444 | 0.098* | 0.34 |
| C83A | −0.1209 (15) | 0.1416 (12) | 0.6139 (7) | 0.082 (3) | 0.34 |
| H83A | −0.0979 | 0.1629 | 0.6505 | 0.099* | 0.34 |
| C84A | −0.0965 (12) | 0.1648 (9) | 0.5594 (6) | 0.081 (2) | 0.34 |
| H84A | −0.0572 | 0.2019 | 0.5609 | 0.097* | 0.34 |
| N1 | 0.27646 (17) | 0.24607 (14) | 0.76671 (13) | 0.0330 (6) | |
| N2 | 0.37143 (17) | 0.14219 (14) | 0.79170 (13) | 0.0302 (6) | |
| N3 | 0.28561 (17) | 0.22388 (14) | 0.93075 (12) | 0.0312 (6) | |
| N4 | 0.42751 (17) | 0.12499 (14) | 0.93553 (12) | 0.0307 (6) | |
| N5 | 0.13044 (18) | 0.15645 (14) | 0.76514 (14) | 0.0337 (6) | |
| N6 | 0.18439 (17) | 0.00730 (14) | 0.76635 (13) | 0.0308 (6) | |
| N7 | 0.13358 (18) | 0.14323 (15) | 0.93093 (13) | 0.0345 (6) | |
| N8 | 0.20644 (18) | 0.03278 (15) | 0.90921 (13) | 0.0330 (6) | |
| N9 | 0.45806 (17) | −0.03173 (14) | 0.89580 (12) | 0.0301 (6) | |
| N10 | 0.34564 (17) | −0.08566 (14) | 0.81453 (13) | 0.0329 (6) | |
| O1 | 0.21502 (15) | 0.29635 (12) | 0.75199 (13) | 0.0424 (6) | |
| O2 | 0.41168 (14) | 0.07989 (11) | 0.80519 (11) | 0.0333 (5) | |
| O3 | 0.22535 (15) | 0.27495 (13) | 0.92507 (12) | 0.0399 (6) | |
| O4 | 0.34924 (14) | 0.09770 (12) | 0.91047 (11) | 0.0342 (5) | |
| O5 | 0.09813 (16) | 0.22254 (13) | 0.76779 (14) | 0.0454 (7) | |
| O6 | 0.24766 (14) | 0.05433 (12) | 0.79020 (11) | 0.0331 (5) | |
| O7 | 0.10615 (16) | 0.20776 (14) | 0.94544 (13) | 0.0445 (6) | |
| O8 | 0.25669 (15) | −0.02059 (12) | 0.89833 (11) | 0.0361 (5) | |
| O9 | 0.52088 (17) | 0.00669 (14) | 0.93202 (12) | 0.0404 (6) | |
| O10 | 0.27559 (16) | −0.11284 (13) | 0.77446 (12) | 0.0395 (6) | |
| Ni1 | 0.25135 (3) | 0.14989 (2) | 0.77620 (2) | 0.03005 (11) | |
| Ni2 | 0.24612 (3) | 0.12803 (2) | 0.92204 (2) | 0.03014 (11) | |
| Ni3 | 0.34675 (3) | 0.01380 (2) | 0.85238 (2) | 0.02978 (11) | |
| H1A | 0.149 (4) | 0.262 (3) | 0.761 (3) | 0.10 (2)* | |
| H2A | 0.166 (3) | 0.244 (3) | 0.935 (2) | 0.081 (16)* | |
| H3A | 0.488 (4) | 0.043 (3) | 0.933 (3) | 0.09 (2)* | |
| H4A | 0.233 (3) | −0.070 (3) | 0.770 (2) | 0.095 (18)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0263 (16) | 0.0267 (15) | 0.0376 (17) | −0.0007 (13) | 0.0076 (13) | 0.0027 (13) |
| C2 | 0.0271 (16) | 0.0272 (15) | 0.0329 (16) | 0.0010 (13) | 0.0088 (13) | 0.0019 (13) |
| C3 | 0.0274 (16) | 0.0301 (16) | 0.0318 (16) | −0.0026 (13) | 0.0120 (13) | −0.0014 (13) |
| C4 | 0.0296 (17) | 0.0359 (18) | 0.0379 (18) | 0.0044 (14) | 0.0095 (14) | 0.0015 (14) |
| C5 | 0.0292 (18) | 0.047 (2) | 0.0414 (19) | 0.0061 (16) | 0.0076 (15) | 0.0005 (16) |
| C6 | 0.0243 (17) | 0.055 (2) | 0.046 (2) | −0.0013 (16) | 0.0035 (15) | −0.0013 (18) |
| C7 | 0.0321 (19) | 0.045 (2) | 0.046 (2) | −0.0098 (16) | 0.0084 (15) | −0.0027 (17) |
| C8 | 0.0286 (17) | 0.0349 (17) | 0.0343 (17) | −0.0010 (14) | 0.0122 (13) | −0.0019 (14) |
| C9 | 0.0319 (17) | 0.0291 (16) | 0.0334 (16) | −0.0043 (13) | 0.0125 (13) | −0.0049 (13) |
| C10 | 0.0361 (19) | 0.0343 (18) | 0.0448 (19) | −0.0093 (15) | 0.0173 (15) | −0.0043 (15) |
| C11 | 0.049 (2) | 0.0278 (17) | 0.048 (2) | −0.0082 (16) | 0.0199 (17) | 0.0011 (15) |
| C12 | 0.048 (2) | 0.0265 (16) | 0.046 (2) | 0.0013 (15) | 0.0182 (17) | 0.0047 (15) |
| C13 | 0.0344 (18) | 0.0274 (16) | 0.0396 (18) | 0.0021 (14) | 0.0104 (14) | 0.0029 (14) |
| C14 | 0.0313 (17) | 0.0237 (15) | 0.0354 (16) | −0.0018 (13) | 0.0118 (13) | 0.0005 (13) |
| C15 | 0.0300 (17) | 0.0285 (16) | 0.0298 (15) | −0.0013 (13) | 0.0080 (13) | −0.0011 (13) |
| C16 | 0.0288 (16) | 0.0261 (15) | 0.0309 (15) | −0.0018 (13) | 0.0081 (13) | −0.0004 (12) |
| C17 | 0.0282 (16) | 0.0318 (16) | 0.0285 (15) | −0.0034 (13) | 0.0072 (12) | −0.0013 (13) |
| C18 | 0.0335 (18) | 0.0324 (17) | 0.0321 (16) | −0.0039 (14) | 0.0062 (14) | −0.0003 (14) |
| C19 | 0.0315 (18) | 0.043 (2) | 0.0338 (17) | 0.0031 (15) | 0.0052 (14) | 0.0020 (15) |
| C20 | 0.0312 (18) | 0.049 (2) | 0.0400 (19) | −0.0079 (16) | −0.0001 (15) | −0.0026 (16) |
| C21 | 0.039 (2) | 0.0372 (19) | 0.0425 (19) | −0.0116 (16) | 0.0077 (16) | −0.0027 (16) |
| C22 | 0.0322 (17) | 0.0329 (17) | 0.0312 (16) | −0.0055 (14) | 0.0095 (13) | −0.0022 (13) |
| C23 | 0.0345 (18) | 0.0299 (16) | 0.0328 (16) | −0.0010 (14) | 0.0116 (14) | −0.0016 (13) |
| C24 | 0.040 (2) | 0.0316 (17) | 0.047 (2) | −0.0064 (15) | 0.0132 (16) | −0.0014 (15) |
| C25 | 0.053 (2) | 0.0287 (17) | 0.050 (2) | −0.0040 (16) | 0.0183 (18) | −0.0005 (16) |
| C26 | 0.048 (2) | 0.0298 (17) | 0.046 (2) | 0.0042 (16) | 0.0131 (17) | 0.0056 (15) |
| C27 | 0.039 (2) | 0.0315 (17) | 0.0391 (18) | 0.0016 (15) | 0.0109 (15) | 0.0002 (14) |
| C28 | 0.0335 (17) | 0.0283 (16) | 0.0341 (17) | −0.0011 (14) | 0.0123 (14) | −0.0011 (13) |
| C29 | 0.0243 (16) | 0.0294 (16) | 0.0328 (16) | 0.0010 (13) | 0.0043 (12) | 0.0051 (13) |
| C30 | 0.0267 (16) | 0.0299 (16) | 0.0355 (17) | −0.0019 (13) | 0.0053 (13) | 0.0030 (13) |
| C31 | 0.0344 (18) | 0.0314 (17) | 0.0359 (17) | −0.0036 (14) | 0.0026 (14) | 0.0023 (14) |
| C32 | 0.037 (2) | 0.041 (2) | 0.048 (2) | −0.0034 (16) | 0.0033 (16) | −0.0064 (17) |
| C33 | 0.050 (3) | 0.040 (2) | 0.064 (3) | −0.0043 (19) | 0.001 (2) | −0.0108 (19) |
| C34 | 0.047 (2) | 0.042 (2) | 0.065 (3) | −0.0139 (19) | −0.006 (2) | −0.003 (2) |
| C35 | 0.034 (2) | 0.043 (2) | 0.060 (2) | −0.0075 (17) | −0.0004 (17) | 0.0005 (19) |
| C36 | 0.0312 (18) | 0.0355 (18) | 0.0403 (19) | −0.0055 (14) | 0.0007 (14) | 0.0057 (15) |
| C37 | 0.0289 (17) | 0.0405 (19) | 0.0374 (18) | −0.0029 (15) | 0.0040 (14) | 0.0083 (15) |
| C38 | 0.0283 (18) | 0.052 (2) | 0.049 (2) | −0.0044 (16) | 0.0051 (16) | 0.0110 (18) |
| C39 | 0.0297 (19) | 0.063 (3) | 0.048 (2) | 0.0074 (18) | 0.0115 (16) | 0.0120 (19) |
| C40 | 0.033 (2) | 0.057 (2) | 0.047 (2) | 0.0098 (18) | 0.0127 (16) | 0.0050 (18) |
| C41 | 0.0339 (19) | 0.0388 (19) | 0.046 (2) | 0.0010 (15) | 0.0088 (15) | −0.0008 (16) |
| C42 | 0.0255 (16) | 0.0349 (17) | 0.0357 (17) | 0.0006 (13) | 0.0043 (13) | 0.0063 (14) |
| C43 | 0.0300 (17) | 0.0390 (18) | 0.0344 (17) | −0.0011 (14) | 0.0059 (13) | 0.0044 (14) |
| C44 | 0.0328 (18) | 0.0368 (18) | 0.0328 (17) | −0.0041 (14) | 0.0035 (14) | 0.0078 (14) |
| C45 | 0.038 (2) | 0.0362 (18) | 0.0372 (18) | −0.0071 (15) | 0.0031 (15) | 0.0051 (15) |

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|---|---|---|---|---|---|---|
| C46 | 0.043 (2) | 0.041 (2) | 0.044 (2) | −0.0107 (17) | 0.0031 (16) | 0.0024 (16) |
| C47 | 0.063 (3) | 0.044 (2) | 0.058 (3) | −0.017 (2) | 0.008 (2) | −0.005 (2) |
| C48 | 0.056 (3) | 0.058 (3) | 0.071 (3) | −0.030 (2) | 0.001 (2) | −0.004 (2) |
| C49 | 0.043 (2) | 0.054 (3) | 0.060 (3) | −0.017 (2) | 0.0017 (19) | 0.002 (2) |
| C50 | 0.038 (2) | 0.047 (2) | 0.0387 (19) | −0.0151 (17) | 0.0003 (15) | 0.0102 (17) |
| C51 | 0.0311 (19) | 0.053 (2) | 0.0361 (18) | −0.0055 (16) | 0.0019 (14) | 0.0130 (16) |
| C52 | 0.037 (2) | 0.064 (3) | 0.049 (2) | −0.0115 (19) | 0.0057 (17) | 0.016 (2) |
| C53 | 0.030 (2) | 0.078 (3) | 0.051 (2) | 0.002 (2) | 0.0115 (17) | 0.019 (2) |
| C54 | 0.035 (2) | 0.074 (3) | 0.046 (2) | 0.005 (2) | 0.0135 (17) | 0.011 (2) |
| C55 | 0.0318 (19) | 0.054 (2) | 0.045 (2) | 0.0010 (17) | 0.0108 (16) | 0.0073 (18) |
| C56 | 0.0281 (17) | 0.050 (2) | 0.0341 (17) | −0.0037 (16) | 0.0025 (14) | 0.0097 (16) |
| C57 | 0.0320 (17) | 0.0263 (15) | 0.0364 (17) | 0.0007 (13) | 0.0102 (14) | 0.0033 (13) |
| C58 | 0.0323 (17) | 0.0262 (15) | 0.0341 (16) | 0.0016 (13) | 0.0095 (13) | 0.0031 (13) |
| C59 | 0.0381 (18) | 0.0273 (16) | 0.0303 (16) | 0.0003 (14) | 0.0061 (14) | 0.0001 (13) |
| C60 | 0.042 (2) | 0.0313 (18) | 0.048 (2) | −0.0002 (15) | 0.0036 (16) | 0.0007 (16) |
| C61 | 0.065 (3) | 0.0309 (19) | 0.050 (2) | −0.0080 (19) | −0.003 (2) | −0.0026 (17) |
| C62 | 0.076 (3) | 0.0271 (18) | 0.053 (2) | 0.0001 (19) | 0.003 (2) | −0.0054 (17) |
| C63 | 0.058 (3) | 0.0330 (19) | 0.053 (2) | 0.0136 (18) | 0.0061 (19) | 0.0004 (17) |
| C64 | 0.047 (2) | 0.0299 (17) | 0.0355 (18) | 0.0032 (15) | 0.0124 (15) | 0.0008 (14) |
| C65 | 0.0396 (19) | 0.0345 (18) | 0.0382 (18) | 0.0070 (15) | 0.0130 (15) | 0.0062 (15) |
| C66 | 0.045 (2) | 0.039 (2) | 0.054 (2) | 0.0106 (17) | 0.0135 (18) | 0.0073 (17) |
| C67 | 0.038 (2) | 0.047 (2) | 0.060 (2) | 0.0133 (18) | 0.0112 (18) | 0.0134 (19) |
| C68 | 0.0332 (19) | 0.047 (2) | 0.050 (2) | 0.0003 (16) | 0.0055 (16) | 0.0147 (18) |
| C69 | 0.0358 (19) | 0.0345 (18) | 0.0411 (19) | 0.0052 (15) | 0.0074 (15) | 0.0093 (15) |
| C70 | 0.0312 (17) | 0.0303 (16) | 0.0356 (17) | 0.0021 (14) | 0.0085 (14) | 0.0062 (14) |
| C71 | 0.055 (3) | 0.108 (5) | 0.138 (6) | 0.015 (3) | 0.025 (4) | 0.052 (4) |
| C72 | 0.047 (3) | 0.054 (3) | 0.080 (3) | 0.000 (2) | 0.019 (2) | 0.015 (2) |
| C73 | 0.055 (3) | 0.052 (2) | 0.050 (2) | −0.001 (2) | 0.0157 (19) | 0.0116 (19) |
| C74 | 0.059 (3) | 0.045 (2) | 0.053 (2) | 0.000 (2) | 0.026 (2) | −0.0001 (19) |
| C75 | 0.054 (3) | 0.045 (2) | 0.053 (2) | 0.0034 (19) | 0.014 (2) | 0.0046 (19) |
| C76 | 0.070 (3) | 0.074 (3) | 0.052 (3) | 0.018 (3) | 0.025 (2) | 0.016 (2) |
| C77 | 0.075 (3) | 0.083 (4) | 0.071 (3) | 0.017 (3) | 0.045 (3) | 0.020 (3) |
| C78 | 0.110 (6) | 0.077 (5) | 0.074 (5) | −0.002 (5) | 0.018 (5) | −0.001 (4) |
| C79 | 0.081 (4) | 0.068 (4) | 0.068 (3) | 0.006 (4) | 0.014 (3) | −0.012 (3) |
| C80 | 0.100 (5) | 0.069 (4) | 0.067 (4) | 0.005 (4) | 0.006 (4) | −0.005 (3) |
| C81 | 0.105 (5) | 0.069 (4) | 0.075 (4) | 0.007 (4) | −0.001 (4) | 0.004 (4) |
| C82 | 0.097 (5) | 0.070 (5) | 0.069 (4) | 0.009 (4) | −0.005 (4) | −0.009 (3) |
| C83 | 0.088 (4) | 0.078 (5) | 0.080 (4) | 0.007 (4) | 0.007 (4) | −0.015 (4) |
| C84 | 0.080 (4) | 0.075 (4) | 0.076 (4) | 0.010 (4) | 0.018 (4) | −0.010 (4) |
| C78A | 0.087 (8) | 0.089 (8) | 0.067 (7) | 0.002 (7) | 0.035 (6) | 0.000 (7) |
| C79A | 0.090 (5) | 0.074 (5) | 0.074 (4) | 0.010 (4) | 0.015 (4) | −0.008 (4) |
| C81A | 0.098 (6) | 0.074 (6) | 0.070 (5) | 0.002 (5) | 0.010 (5) | −0.003 (5) |
| C80A | 0.093 (6) | 0.070 (5) | 0.072 (5) | 0.001 (5) | 0.014 (5) | −0.005 (5) |
| C82A | 0.097 (6) | 0.072 (5) | 0.071 (5) | 0.007 (5) | 0.004 (5) | 0.000 (4) |
| C83A | 0.095 (6) | 0.074 (5) | 0.071 (4) | 0.006 (5) | −0.003 (5) | −0.005 (5) |
| C84A | 0.090 (5) | 0.074 (5) | 0.075 (4) | 0.008 (4) | 0.007 (4) | −0.009 (4) |
| N1 | 0.0260 (14) | 0.0272 (14) | 0.0453 (16) | 0.0056 (11) | 0.0061 (12) | 0.0058 (12) |
| N2 | 0.0292 (14) | 0.0235 (13) | 0.0386 (15) | 0.0031 (11) | 0.0087 (12) | 0.0020 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0283 (14) | 0.0289 (14) | 0.0366 (15) | 0.0044 (11) | 0.0072 (11) | 0.0010 (11) |
| N4 | 0.0267 (14) | 0.0288 (13) | 0.0366 (14) | −0.0035 (11) | 0.0064 (11) | −0.0041 (11) |
| N5 | 0.0284 (15) | 0.0259 (13) | 0.0478 (17) | 0.0024 (11) | 0.0104 (12) | 0.0030 (12) |
| N6 | 0.0275 (14) | 0.0251 (13) | 0.0394 (15) | −0.0040 (11) | 0.0060 (12) | 0.0006 (11) |
| N7 | 0.0304 (15) | 0.0345 (15) | 0.0379 (15) | −0.0016 (12) | 0.0058 (12) | 0.0002 (12) |
| N8 | 0.0307 (15) | 0.0301 (14) | 0.0389 (15) | −0.0007 (12) | 0.0084 (12) | 0.0027 (12) |
| N9 | 0.0279 (14) | 0.0247 (13) | 0.0365 (14) | −0.0019 (11) | 0.0034 (11) | 0.0023 (11) |
| N10 | 0.0294 (15) | 0.0264 (13) | 0.0415 (16) | −0.0013 (11) | 0.0039 (12) | −0.0017 (12) |
| O1 | 0.0271 (13) | 0.0255 (12) | 0.0740 (19) | 0.0064 (10) | 0.0091 (12) | 0.0141 (12) |
| O2 | 0.0295 (12) | 0.0231 (11) | 0.0480 (14) | 0.0047 (9) | 0.0098 (10) | 0.0017 (10) |
| O3 | 0.0292 (13) | 0.0282 (12) | 0.0627 (17) | 0.0058 (10) | 0.0104 (11) | 0.0020 (11) |
| O4 | 0.0255 (12) | 0.0296 (12) | 0.0474 (14) | −0.0045 (9) | 0.0072 (10) | −0.0069 (10) |
| O5 | 0.0288 (13) | 0.0255 (12) | 0.084 (2) | 0.0048 (10) | 0.0163 (13) | 0.0077 (13) |
| O6 | 0.0249 (12) | 0.0255 (11) | 0.0468 (14) | −0.0039 (9) | 0.0021 (10) | 0.0009 (10) |
| O7 | 0.0333 (14) | 0.0368 (14) | 0.0663 (18) | 0.0036 (11) | 0.0169 (12) | −0.0043 (13) |
| O8 | 0.0344 (13) | 0.0292 (12) | 0.0449 (14) | −0.0010 (10) | 0.0087 (11) | 0.0005 (10) |
| O9 | 0.0337 (14) | 0.0317 (13) | 0.0506 (15) | −0.0002 (11) | −0.0038 (11) | −0.0058 (11) |
| O10 | 0.0349 (14) | 0.0309 (12) | 0.0471 (15) | 0.0019 (11) | −0.0049 (11) | −0.0071 (11) |
| Ni1 | 0.0237 (2) | 0.0232 (2) | 0.0434 (2) | 0.00088 (16) | 0.00702 (17) | 0.00455 (17) |
| Ni2 | 0.0251 (2) | 0.0275 (2) | 0.0382 (2) | −0.00170 (16) | 0.00718 (17) | −0.00033 (17) |
| Ni3 | 0.0274 (2) | 0.0223 (2) | 0.0386 (2) | 0.00040 (16) | 0.00435 (17) | 0.00011 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.310 (4) | C55—H55 | 0.9300 |
| C1—C14 | 1.461 (4) | C57—N9 | 1.310 (4) |
| C1—C2 | 1.464 (4) | C57—C70 | 1.465 (5) |
| C2—N2 | 1.322 (4) | C57—C58 | 1.495 (5) |
| C2—C3 | 1.462 (4) | C58—N10 | 1.299 (4) |
| C3—C4 | 1.410 (5) | C58—C59 | 1.467 (4) |
| C3—C8 | 1.418 (4) | C59—C60 | 1.406 (5) |
| C4—C5 | 1.373 (5) | C59—C64 | 1.408 (5) |
| C4—H4 | 0.9300 | C60—C61 | 1.372 (5) |
| C5—C6 | 1.383 (5) | C60—H60 | 0.9300 |
| C5—H5 | 0.9300 | C61—C62 | 1.368 (6) |
| C6—C7 | 1.374 (5) | C61—H61 | 0.9300 |
| C6—H6 | 0.9300 | C62—C63 | 1.380 (6) |
| C7—C8 | 1.400 (5) | C62—H62 | 0.9300 |
| C7—H7 | 0.9300 | C63—C64 | 1.399 (5) |
| C8—C9 | 1.479 (5) | C63—H63 | 0.9300 |
| C9—C10 | 1.406 (4) | C64—C65 | 1.481 (5) |
| C9—C14 | 1.412 (5) | C65—C66 | 1.400 (5) |
| C10—C11 | 1.373 (5) | C65—C70 | 1.416 (5) |
| C10—H10 | 0.9300 | C66—C67 | 1.364 (6) |
| C11—C12 | 1.387 (5) | C66—H66 | 0.9300 |
| C11—H11 | 0.9300 | C67—C68 | 1.379 (6) |
| C12—C13 | 1.384 (5) | C67—H67 | 0.9300 |
| C12—H12 | 0.9300 | C68—C69 | 1.378 (5) |

| | | | |
|---|---|---|---|
| C13—C14 | 1.408 (4) | C68—H68 | 0.9300 |
| C13—H13 | 0.9300 | C69—C70 | 1.420 (5) |
| C15—N3 | 1.321 (4) | C69—H69 | 0.9300 |
| C15—C16 | 1.468 (4) | C71—C72 | 1.517 (7) |
| C15—C28 | 1.479 (4) | C71—H71A | 0.9600 |
| C16—N4 | 1.290 (4) | C71—H71B | 0.9600 |
| C16—C17 | 1.481 (4) | C71—H71C | 0.9600 |
| C17—C22 | 1.396 (4) | C72—C73 | 1.387 (6) |
| C17—C18 | 1.401 (5) | C72—C77 | 1.388 (7) |
| C18—C19 | 1.380 (5) | C73—C74 | 1.369 (6) |
| C18—H18 | 0.9300 | C73—H73 | 0.9300 |
| C19—C20 | 1.390 (5) | C74—C75 | 1.382 (6) |
| C19—H19 | 0.9300 | C74—H74 | 0.9300 |
| C20—C21 | 1.372 (5) | C75—C76 | 1.365 (6) |
| C20—H20 | 0.9300 | C75—H75 | 0.9300 |
| C21—C22 | 1.410 (5) | C76—C77 | 1.377 (7) |
| C21—H21 | 0.9300 | C76—H76 | 0.9300 |
| C22—C23 | 1.469 (5) | C77—H77 | 0.9300 |
| C23—C24 | 1.399 (5) | C78—C79 | 1.470 (10) |
| C23—C28 | 1.424 (5) | C78—H78A | 0.9600 |
| C24—C25 | 1.376 (5) | C78—H78B | 0.9600 |
| C24—H24 | 0.9300 | C78—H78C | 0.9600 |
| C25—C26 | 1.378 (5) | C79—C80 | 1.386 (6) |
| C25—H25 | 0.9300 | C79—C84 | 1.401 (6) |
| C26—C27 | 1.384 (5) | C80—C81 | 1.386 (7) |
| C26—H26 | 0.9300 | C80—H80 | 0.9300 |
| C27—C28 | 1.402 (5) | C81—C82 | 1.390 (7) |
| C27—H27 | 0.9300 | C81—H81 | 0.9300 |
| C29—N5 | 1.319 (4) | C82—C83 | 1.386 (7) |
| C29—C30 | 1.465 (4) | C82—H82 | 0.9300 |
| C29—C42 | 1.479 (4) | C83—C84 | 1.384 (6) |
| C30—N6 | 1.295 (4) | C83—H83 | 0.9300 |
| C30—C31 | 1.472 (5) | C84—H84 | 0.9300 |
| C31—C32 | 1.394 (5) | C78A—C79A | 1.523 (18) |
| C31—C36 | 1.399 (5) | C78A—H78D | 0.9600 |
| C32—C33 | 1.384 (5) | C78A—H78E | 0.9600 |
| C32—H32 | 0.9300 | C78A—H78F | 0.9600 |
| C33—C34 | 1.367 (6) | C79A—C84A | 1.32 (2) |
| C33—H33 | 0.9300 | C79A—C80A | 1.382 (8) |
| C34—C35 | 1.372 (6) | C81A—C82A | 1.26 (3) |
| C34—H34 | 0.9300 | C81A—C80A | 1.46 (2) |
| C35—C36 | 1.410 (5) | C81A—H81A | 0.9300 |
| C35—H35 | 0.9300 | C80A—H80A | 0.9300 |
| C36—C37 | 1.469 (5) | C82A—C83A | 1.36 (3) |
| C37—C38 | 1.403 (5) | C82A—H82A | 0.9300 |
| C37—C42 | 1.420 (5) | C83A—C84A | 1.44 (2) |
| C38—C39 | 1.375 (6) | C83A—H83A | 0.9300 |
| C38—H38 | 0.9300 | C84A—H84A | 0.9300 |

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|---|---|---|---|
| C39—C40 | 1.370 (6) | N1—O1 | 1.349 (3) |
| C39—H39 | 0.9300 | N1—Ni1 | 1.859 (3) |
| C40—C41 | 1.382 (5) | N2—O2 | 1.333 (3) |
| C40—H40 | 0.9300 | N2—Ni1 | 1.884 (3) |
| C41—C42 | 1.401 (5) | N3—O3 | 1.341 (3) |
| C41—H41 | 0.9300 | N3—Ni2 | 1.892 (3) |
| C43—N7 | 1.311 (4) | N4—O4 | 1.363 (3) |
| C43—C44 | 1.457 (5) | N5—O5 | 1.342 (3) |
| C43—C56 | 1.465 (5) | N5—Ni1 | 1.900 (3) |
| C44—N8 | 1.325 (4) | N6—O6 | 1.364 (3) |
| C44—C45 | 1.463 (5) | N7—O7 | 1.344 (4) |
| C45—C46 | 1.399 (5) | N7—Ni2 | 1.871 (3) |
| C45—C50 | 1.425 (5) | N8—O8 | 1.333 (4) |
| C46—C47 | 1.381 (5) | N8—Ni2 | 1.888 (3) |
| C46—H46 | 0.9300 | N9—O9 | 1.365 (4) |
| C47—C48 | 1.383 (6) | N9—Ni3 | 2.035 (3) |
| C47—H47 | 0.9300 | N10—O10 | 1.388 (4) |
| C48—C49 | 1.381 (7) | N10—Ni3 | 2.043 (3) |
| C48—H48 | 0.9300 | O1—H1A | 1.29 (6) |
| C49—C50 | 1.399 (5) | O2—Ni3 | 2.050 (2) |
| C49—H49 | 0.9300 | O3—H2A | 1.17 (5) |
| C50—C51 | 1.465 (6) | O4—Ni2 | 1.811 (2) |
| C51—C56 | 1.411 (5) | O4—Ni3 | 2.044 (2) |
| C51—C52 | 1.416 (5) | O5—H1A | 1.13 (6) |
| C52—C53 | 1.359 (6) | O6—Ni1 | 1.813 (2) |
| C52—H52 | 0.9300 | O6—Ni3 | 2.042 (2) |
| C53—C54 | 1.378 (6) | O7—H2A | 1.24 (6) |
| C53—H53 | 0.9300 | O8—Ni3 | 2.047 (2) |
| C54—C55 | 1.389 (5) | O9—H3A | 0.85 (6) |
| C54—H54 | 0.9300 | O10—H4A | 1.04 (6) |
| C55—C56 | 1.402 (5) | | |

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|---|---|---|---|
| N1—C1—C14 | 127.3 (3) | C60—C59—C58 | 123.0 (3) |
| N1—C1—C2 | 112.3 (3) | C64—C59—C58 | 118.0 (3) |
| C14—C1—C2 | 120.4 (3) | C61—C60—C59 | 121.1 (4) |
| N2—C2—C3 | 127.7 (3) | C61—C60—H60 | 119.5 |
| N2—C2—C1 | 111.7 (3) | C59—C60—H60 | 119.5 |
| C3—C2—C1 | 120.3 (3) | C62—C61—C60 | 120.4 (4) |
| C4—C3—C8 | 119.3 (3) | C62—C61—H61 | 119.8 |
| C4—C3—C2 | 122.9 (3) | C60—C61—H61 | 119.8 |
| C8—C3—C2 | 117.5 (3) | C61—C62—C63 | 119.8 (4) |
| C5—C4—C3 | 120.8 (3) | C61—C62—H62 | 120.1 |
| C5—C4—H4 | 119.6 | C63—C62—H62 | 120.1 |
| C3—C4—H4 | 119.6 | C62—C63—C64 | 121.7 (4) |
| C4—C5—C6 | 120.1 (3) | C62—C63—H63 | 119.2 |
| C4—C5—H5 | 120.0 | C64—C63—H63 | 119.2 |
| C6—C5—H5 | 120.0 | C63—C64—C59 | 118.2 (3) |
| C7—C6—C5 | 120.0 (3) | C63—C64—C65 | 120.5 (3) |

| | | | |
|---|---|---|---|
| C7—C6—H6 | 120.0 | C59—C64—C65 | 121.3 (3) |
| C5—C6—H6 | 120.0 | C66—C65—C70 | 118.8 (3) |
| C6—C7—C8 | 122.1 (4) | C66—C65—C64 | 120.2 (3) |
| C6—C7—H7 | 119.0 | C70—C65—C64 | 120.9 (3) |
| C8—C7—H7 | 119.0 | C67—C66—C65 | 121.6 (4) |
| C7—C8—C3 | 117.6 (3) | C67—C66—H66 | 119.2 |
| C7—C8—C9 | 121.2 (3) | C65—C66—H66 | 119.2 |
| C3—C8—C9 | 121.2 (3) | C66—C67—C68 | 119.8 (4) |
| C10—C9—C14 | 117.7 (3) | C66—C67—H67 | 120.1 |
| C10—C9—C8 | 121.0 (3) | C68—C67—H67 | 120.1 |
| C14—C9—C8 | 121.3 (3) | C69—C68—C67 | 121.3 (4) |
| C11—C10—C9 | 122.2 (3) | C69—C68—H68 | 119.3 |
| C11—C10—H10 | 118.9 | C67—C68—H68 | 119.3 |
| C9—C10—H10 | 118.9 | C68—C69—C70 | 119.7 (3) |
| C10—C11—C12 | 120.0 (3) | C68—C69—H69 | 120.1 |
| C10—C11—H11 | 120.0 | C70—C69—H69 | 120.1 |
| C12—C11—H11 | 120.0 | C65—C70—C69 | 118.7 (3) |
| C13—C12—C11 | 119.5 (3) | C65—C70—C57 | 118.0 (3) |
| C13—C12—H12 | 120.2 | C69—C70—C57 | 123.3 (3) |
| C11—C12—H12 | 120.2 | C72—C71—H71A | 109.5 |
| C12—C13—C14 | 121.1 (3) | C72—C71—H71B | 109.5 |
| C12—C13—H13 | 119.4 | H71A—C71—H71B | 109.5 |
| C14—C13—H13 | 119.4 | C72—C71—H71C | 109.5 |
| C13—C14—C9 | 119.4 (3) | H71A—C71—H71C | 109.5 |
| C13—C14—C1 | 122.9 (3) | H71B—C71—H71C | 109.5 |
| C9—C14—C1 | 117.6 (3) | C73—C72—C77 | 117.9 (4) |
| N3—C15—C16 | 118.6 (3) | C73—C72—C71 | 121.0 (5) |
| N3—C15—C28 | 124.4 (3) | C77—C72—C71 | 121.2 (5) |
| C16—C15—C28 | 117.0 (3) | C74—C73—C72 | 120.7 (4) |
| N4—C16—C15 | 126.2 (3) | C74—C73—H73 | 119.7 |
| N4—C16—C17 | 115.3 (3) | C72—C73—H73 | 119.7 |
| C15—C16—C17 | 118.5 (3) | C73—C74—C75 | 120.6 (4) |
| C22—C17—C18 | 120.3 (3) | C73—C74—H74 | 119.7 |
| C22—C17—C16 | 119.6 (3) | C75—C74—H74 | 119.7 |
| C18—C17—C16 | 120.1 (3) | C76—C75—C74 | 119.6 (4) |
| C19—C18—C17 | 120.7 (3) | C76—C75—H75 | 120.2 |
| C19—C18—H18 | 119.6 | C74—C75—H75 | 120.2 |
| C17—C18—H18 | 119.6 | C75—C76—C77 | 119.9 (4) |
| C18—C19—C20 | 119.5 (3) | C75—C76—H76 | 120.0 |
| C18—C19—H19 | 120.3 | C77—C76—H76 | 120.0 |
| C20—C19—H19 | 120.3 | C76—C77—C72 | 121.3 (4) |
| C21—C20—C19 | 120.2 (3) | C76—C77—H77 | 119.3 |
| C21—C20—H20 | 119.9 | C72—C77—H77 | 119.3 |
| C19—C20—H20 | 119.9 | C79—C78—H78A | 109.5 |
| C20—C21—C22 | 121.7 (3) | C79—C78—H78B | 109.5 |
| C20—C21—H21 | 119.2 | H78A—C78—H78B | 109.5 |
| C22—C21—H21 | 119.2 | C79—C78—H78C | 109.5 |
| C17—C22—C21 | 117.7 (3) | H78A—C78—H78C | 109.5 |

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| C17—C22—C23 | 120.3 (3) | H78B—C78—H78C | 109.5 |
| C21—C22—C23 | 122.0 (3) | C80—C79—C84 | 119.1 (5) |
| C24—C23—C28 | 117.8 (3) | C80—C79—C78 | 121.0 (5) |
| C24—C23—C22 | 121.4 (3) | C84—C79—C78 | 119.9 (5) |
| C28—C23—C22 | 120.7 (3) | C81—C80—C79 | 121.2 (5) |
| C25—C24—C23 | 122.4 (3) | C81—C80—H80 | 119.4 |
| C25—C24—H24 | 118.8 | C79—C80—H80 | 119.4 |
| C23—C24—H24 | 118.8 | C80—C81—C82 | 119.5 (5) |
| C24—C25—C26 | 119.6 (3) | C80—C81—H81 | 120.2 |
| C24—C25—H25 | 120.2 | C82—C81—H81 | 120.2 |
| C26—C25—H25 | 120.2 | C83—C82—C81 | 119.6 (5) |
| C25—C26—C27 | 119.9 (4) | C83—C82—H82 | 120.2 |
| C25—C26—H26 | 120.0 | C81—C82—H82 | 120.2 |
| C27—C26—H26 | 120.0 | C84—C83—C82 | 121.0 (5) |
| C26—C27—C28 | 121.5 (3) | C84—C83—H83 | 119.5 |
| C26—C27—H27 | 119.3 | C82—C83—H83 | 119.5 |
| C28—C27—H27 | 119.3 | C83—C84—C79 | 119.5 (5) |
| C27—C28—C23 | 118.6 (3) | C83—C84—H84 | 120.2 |
| C27—C28—C15 | 122.4 (3) | C79—C84—H84 | 120.2 |
| C23—C28—C15 | 118.9 (3) | C79A—C78A—H78D | 109.5 |
| N5—C29—C30 | 117.8 (3) | C79A—C78A—H78E | 109.5 |
| N5—C29—C42 | 125.7 (3) | H78D—C78A—H78E | 109.5 |
| C30—C29—C42 | 116.4 (3) | C79A—C78A—H78F | 109.5 |
| N6—C30—C29 | 126.8 (3) | H78D—C78A—H78F | 109.5 |
| N6—C30—C31 | 114.6 (3) | H78E—C78A—H78F | 109.5 |
| C29—C30—C31 | 118.6 (3) | C84A—C79A—C80A | 120.4 (17) |
| C32—C31—C36 | 120.4 (3) | C84A—C79A—C78A | 121.6 (11) |
| C32—C31—C30 | 120.9 (3) | C80A—C79A—C78A | 117.9 (12) |
| C36—C31—C30 | 118.7 (3) | C82A—C81A—C80A | 123.7 (16) |
| C33—C32—C31 | 120.1 (4) | C82A—C81A—H81A | 118.2 |
| C33—C32—H32 | 120.0 | C80A—C81A—H81A | 118.2 |
| C31—C32—H32 | 120.0 | C79A—C80A—C81A | 115.9 (14) |
| C34—C33—C32 | 120.1 (4) | C79A—C80A—H80A | 122.1 |
| C34—C33—H33 | 119.9 | C81A—C80A—H80A | 122.1 |
| C32—C33—H33 | 119.9 | C81A—C82A—C83A | 121 (2) |
| C33—C34—C35 | 120.7 (4) | C81A—C82A—H82A | 119.5 |
| C33—C34—H34 | 119.7 | C83A—C82A—H82A | 119.5 |
| C35—C34—H34 | 119.7 | C82A—C83A—C84A | 117.8 (17) |
| C34—C35—C36 | 121.0 (4) | C82A—C83A—H83A | 121.1 |
| C34—C35—H35 | 119.5 | C84A—C83A—H83A | 121.1 |
| C36—C35—H35 | 119.5 | C79A—C84A—C83A | 121.3 (18) |
| C31—C36—C35 | 117.8 (3) | C79A—C84A—H84A | 119.3 |
| C31—C36—C37 | 119.5 (3) | C83A—C84A—H84A | 119.3 |
| C35—C36—C37 | 122.8 (3) | C1—N1—O1 | 120.2 (3) |
| C38—C37—C42 | 118.0 (3) | C1—N1—Ni1 | 117.4 (2) |
| C38—C37—C36 | 120.8 (3) | O1—N1—Ni1 | 122.4 (2) |
| C42—C37—C36 | 121.1 (3) | C2—N2—O2 | 121.3 (3) |
| C39—C38—C37 | 121.9 (4) | C2—N2—Ni1 | 116.3 (2) |

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| C39—C38—H38 | 119.1 | O2—N2—Ni1 | 122.3 (2) |
| C37—C38—H38 | 119.1 | C15—N3—O3 | 116.8 (3) |
| C40—C39—C38 | 120.0 (4) | C15—N3—Ni2 | 126.6 (2) |
| C40—C39—H39 | 120.0 | O3—N3—Ni2 | 116.3 (2) |
| C38—C39—H39 | 120.0 | C16—N4—O4 | 119.1 (3) |
| C39—C40—C41 | 120.2 (4) | C29—N5—O5 | 116.3 (3) |
| C39—C40—H40 | 119.9 | C29—N5—Ni1 | 126.6 (2) |
| C41—C40—H40 | 119.9 | O5—N5—Ni1 | 116.3 (2) |
| C40—C41—C42 | 121.2 (4) | C30—N6—O6 | 118.6 (3) |
| C40—C41—H41 | 119.4 | C43—N7—O7 | 120.8 (3) |
| C42—C41—H41 | 119.4 | C43—N7—Ni2 | 117.0 (2) |
| C41—C42—C37 | 118.7 (3) | O7—N7—Ni2 | 122.0 (2) |
| C41—C42—C29 | 122.4 (3) | C44—N8—O8 | 121.7 (3) |
| C37—C42—C29 | 118.6 (3) | C44—N8—Ni2 | 115.9 (2) |
| N7—C43—C44 | 112.4 (3) | O8—N8—Ni2 | 122.3 (2) |
| N7—C43—C56 | 127.1 (3) | C57—N9—O9 | 117.4 (3) |
| C44—C43—C56 | 120.4 (3) | C57—N9—Ni3 | 118.8 (2) |
| N8—C44—C43 | 112.2 (3) | O9—N9—Ni3 | 122.5 (2) |
| N8—C44—C45 | 127.3 (3) | C58—N10—O10 | 117.1 (3) |
| C43—C44—C45 | 120.4 (3) | C58—N10—Ni3 | 118.1 (2) |
| C46—C45—C50 | 120.2 (3) | O10—N10—Ni3 | 123.1 (2) |
| C46—C45—C44 | 122.5 (3) | N1—O1—H1A | 101 (3) |
| C50—C45—C44 | 117.1 (3) | N2—O2—Ni3 | 111.88 (18) |
| C47—C46—C45 | 120.6 (4) | N3—O3—H2A | 103 (2) |
| C47—C46—H46 | 119.7 | N4—O4—Ni2 | 127.34 (19) |
| C45—C46—H46 | 119.7 | N4—O4—Ni3 | 116.88 (18) |
| C46—C47—C48 | 119.8 (4) | Ni2—O4—Ni3 | 115.78 (11) |
| C46—C47—H47 | 120.1 | N5—O5—H1A | 107 (3) |
| C48—C47—H47 | 120.1 | N6—O6—Ni1 | 127.55 (19) |
| C49—C48—C47 | 120.4 (4) | N6—O6—Ni3 | 116.43 (18) |
| C49—C48—H48 | 119.8 | Ni1—O6—Ni3 | 115.93 (11) |
| C47—C48—H48 | 119.8 | N7—O7—H2A | 98 (2) |
| C48—C49—C50 | 121.9 (4) | N8—O8—Ni3 | 111.97 (18) |
| C48—C49—H49 | 119.0 | N9—O9—H3A | 93 (4) |
| C50—C49—H49 | 119.0 | N10—O10—H4A | 102 (3) |
| C49—C50—C45 | 117.1 (4) | O6—Ni1—N1 | 169.58 (11) |
| C49—C50—C51 | 121.4 (4) | O6—Ni1—N2 | 87.73 (10) |
| C45—C50—C51 | 121.5 (3) | N1—Ni1—N2 | 81.94 (11) |
| C56—C51—C52 | 117.1 (4) | O6—Ni1—N5 | 91.03 (11) |
| C56—C51—C50 | 121.7 (3) | N1—Ni1—N5 | 99.21 (12) |
| C52—C51—C50 | 121.2 (4) | N2—Ni1—N5 | 176.81 (12) |
| C53—C52—C51 | 122.3 (4) | O4—Ni2—N7 | 170.22 (11) |
| C53—C52—H52 | 118.9 | O4—Ni2—N8 | 88.31 (11) |
| C51—C52—H52 | 118.9 | N7—Ni2—N8 | 81.93 (12) |
| C52—C53—C54 | 120.6 (4) | O4—Ni2—N3 | 90.94 (11) |
| C52—C53—H53 | 119.7 | N7—Ni2—N3 | 98.79 (12) |
| C54—C53—H53 | 119.7 | N8—Ni2—N3 | 177.16 (12) |
| C53—C54—C55 | 119.4 (4) | N9—Ni3—O6 | 165.53 (11) |

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| C53—C54—H54 | 120.3 | N9—Ni3—N10 | 76.02 (11) |
| C55—C54—H54 | 120.3 | O6—Ni3—N10 | 95.97 (10) |
| C54—C55—C56 | 120.9 (4) | N9—Ni3—O4 | 96.00 (10) |
| C54—C55—H55 | 119.5 | O6—Ni3—O4 | 94.37 (10) |
| C56—C55—H55 | 119.5 | N10—Ni3—O4 | 164.78 (11) |
| C55—C56—C51 | 119.8 (3) | N9—Ni3—O8 | 104.85 (10) |
| C55—C56—C43 | 123.0 (3) | O6—Ni3—O8 | 86.82 (10) |
| C51—C56—C43 | 117.3 (3) | N10—Ni3—O8 | 89.16 (10) |
| N9—C57—C70 | 128.8 (3) | O4—Ni3—O8 | 80.29 (9) |
| N9—C57—C58 | 112.0 (3) | N9—Ni3—O2 | 91.16 (10) |
| C70—C57—C58 | 119.2 (3) | O6—Ni3—O2 | 79.47 (9) |
| N10—C58—C59 | 128.4 (3) | N10—Ni3—O2 | 106.60 (10) |
| N10—C58—C57 | 112.7 (3) | O4—Ni3—O2 | 86.25 (9) |
| C59—C58—C57 | 118.8 (3) | O8—Ni3—O2 | 159.99 (9) |
| C60—C59—C64 | 118.8 (3) | | |

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| N1—C1—C2—N2 | 6.8 (4) | C50—C51—C56—C43 | −0.1 (5) |
| C14—C1—C2—N2 | −174.0 (3) | N7—C43—C56—C55 | −9.7 (6) |
| N1—C1—C2—C3 | −166.9 (3) | C44—C43—C56—C55 | 168.1 (3) |
| C14—C1—C2—C3 | 12.4 (5) | N7—C43—C56—C51 | 171.5 (3) |
| N2—C2—C3—C4 | −0.7 (5) | C44—C43—C56—C51 | −10.7 (5) |
| C1—C2—C3—C4 | 171.9 (3) | N9—C57—C58—N10 | 16.8 (4) |
| N2—C2—C3—C8 | −174.4 (3) | C70—C57—C58—N10 | −160.8 (3) |
| C1—C2—C3—C8 | −1.8 (4) | N9—C57—C58—C59 | −161.1 (3) |
| C8—C3—C4—C5 | 3.3 (5) | C70—C57—C58—C59 | 21.3 (4) |
| C2—C3—C4—C5 | −170.3 (3) | N10—C58—C59—C60 | −17.7 (6) |
| C3—C4—C5—C6 | −0.6 (5) | C57—C58—C59—C60 | 159.9 (3) |
| C4—C5—C6—C7 | −1.8 (6) | N10—C58—C59—C64 | 166.4 (3) |
| C5—C6—C7—C8 | 1.4 (6) | C57—C58—C59—C64 | −16.0 (5) |
| C6—C7—C8—C3 | 1.3 (5) | C64—C59—C60—C61 | 0.6 (6) |
| C6—C7—C8—C9 | −179.2 (3) | C58—C59—C60—C61 | −175.3 (4) |
| C4—C3—C8—C7 | −3.6 (5) | C59—C60—C61—C62 | −2.1 (6) |
| C2—C3—C8—C7 | 170.4 (3) | C60—C61—C62—C63 | 1.9 (7) |
| C4—C3—C8—C9 | 176.9 (3) | C61—C62—C63—C64 | −0.2 (7) |
| C2—C3—C8—C9 | −9.1 (4) | C62—C63—C64—C59 | −1.3 (6) |
| C7—C8—C9—C10 | 13.2 (5) | C62—C63—C64—C65 | 176.6 (4) |
| C3—C8—C9—C10 | −167.3 (3) | C60—C59—C64—C63 | 1.1 (5) |
| C7—C8—C9—C14 | −169.4 (3) | C58—C59—C64—C63 | 177.2 (3) |
| C3—C8—C9—C14 | 10.1 (5) | C60—C59—C64—C65 | −176.9 (3) |
| C14—C9—C10—C11 | 1.0 (5) | C58—C59—C64—C65 | −0.8 (5) |
| C8—C9—C10—C11 | 178.6 (3) | C63—C64—C65—C66 | 13.5 (5) |
| C9—C10—C11—C12 | −1.6 (6) | C59—C64—C65—C66 | −168.6 (3) |
| C10—C11—C12—C13 | 0.8 (5) | C63—C64—C65—C70 | −164.5 (3) |
| C11—C12—C13—C14 | 0.6 (5) | C59—C64—C65—C70 | 13.4 (5) |
| C12—C13—C14—C9 | −1.2 (5) | C70—C65—C66—C67 | 3.0 (6) |
| C12—C13—C14—C1 | −178.7 (3) | C64—C65—C66—C67 | −175.1 (4) |
| C10—C9—C14—C13 | 0.4 (5) | C65—C66—C67—C68 | −0.1 (6) |
| C8—C9—C14—C13 | −177.2 (3) | C66—C67—C68—C69 | −2.1 (6) |

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| C10—C9—C14—C1 | 178.0 (3) | C67—C68—C69—C70 | 1.3 (6) |
| C8—C9—C14—C1 | 0.5 (5) | C66—C65—C70—C69 | −3.7 (5) |
| N1—C1—C14—C13 | −14.7 (5) | C64—C65—C70—C69 | 174.3 (3) |
| C2—C1—C14—C13 | 166.2 (3) | C66—C65—C70—C57 | 174.0 (3) |
| N1—C1—C14—C9 | 167.7 (3) | C64—C65—C70—C57 | −7.9 (5) |
| C2—C1—C14—C9 | −11.4 (5) | C68—C69—C70—C65 | 1.6 (5) |
| N3—C15—C16—N4 | 26.0 (5) | C68—C69—C70—C57 | −176.0 (3) |
| C28—C15—C16—N4 | −154.2 (3) | N9—C57—C70—C65 | 173.9 (3) |
| N3—C15—C16—C17 | −153.7 (3) | C58—C57—C70—C65 | −9.0 (5) |
| C28—C15—C16—C17 | 26.0 (4) | N9—C57—C70—C69 | −8.5 (6) |
| N4—C16—C17—C22 | 166.5 (3) | C58—C57—C70—C69 | 168.6 (3) |
| C15—C16—C17—C22 | −13.8 (4) | C77—C72—C73—C74 | 1.6 (7) |
| N4—C16—C17—C18 | −14.7 (4) | C71—C72—C73—C74 | −178.3 (5) |
| C15—C16—C17—C18 | 165.1 (3) | C72—C73—C74—C75 | 0.3 (7) |
| C22—C17—C18—C19 | −1.0 (5) | C73—C74—C75—C76 | −1.4 (7) |
| C16—C17—C18—C19 | −179.9 (3) | C74—C75—C76—C77 | 0.5 (8) |
| C17—C18—C19—C20 | 1.6 (5) | C75—C76—C77—C72 | 1.5 (9) |
| C18—C19—C20—C21 | −0.4 (5) | C73—C72—C77—C76 | −2.5 (8) |
| C19—C20—C21—C22 | −1.3 (6) | C71—C72—C77—C76 | 177.3 (6) |
| C18—C17—C22—C21 | −0.6 (5) | C84—C79—C80—C81 | 0.2 (4) |
| C16—C17—C22—C21 | 178.2 (3) | C78—C79—C80—C81 | −179.8 (3) |
| C18—C17—C22—C23 | 176.3 (3) | C79—C80—C81—C82 | −0.6 (6) |
| C16—C17—C22—C23 | −4.9 (5) | C80—C81—C82—C83 | 0.7 (7) |
| C20—C21—C22—C17 | 1.8 (5) | C81—C82—C83—C84 | −0.4 (8) |
| C20—C21—C22—C23 | −175.1 (3) | C82—C83—C84—C79 | 0.1 (7) |
| C17—C22—C23—C24 | −166.6 (3) | C80—C79—C84—C83 | 0.0 (5) |
| C21—C22—C23—C24 | 10.2 (5) | C78—C79—C84—C83 | −180.0 (3) |
| C17—C22—C23—C28 | 11.0 (5) | C84A—C79A—C80A—C81A | 0.3 (6) |
| C21—C22—C23—C28 | −172.2 (3) | C78A—C79A—C80A—C81A | −179.9 (2) |
| C28—C23—C24—C25 | −1.3 (5) | C82A—C81A—C80A—C79A | 0.0 (6) |
| C22—C23—C24—C25 | 176.4 (3) | C80A—C81A—C82A—C83A | −0.5 (7) |
| C23—C24—C25—C26 | −2.0 (6) | C81A—C82A—C83A—C84A | 0.5 (8) |
| C24—C25—C26—C27 | 2.8 (6) | C80A—C79A—C84A—C83A | −0.2 (7) |
| C25—C26—C27—C28 | −0.1 (6) | C78A—C79A—C84A—C83A | 180.0 (4) |
| C26—C27—C28—C23 | −3.3 (5) | C82A—C83A—C84A—C79A | −0.2 (8) |
| C26—C27—C28—C15 | −178.9 (3) | C14—C1—N1—O1 | −1.9 (5) |
| C24—C23—C28—C27 | 3.9 (5) | C2—C1—N1—O1 | 177.3 (3) |
| C22—C23—C28—C27 | −173.8 (3) | C14—C1—N1—Ni1 | 176.6 (3) |
| C24—C23—C28—C15 | 179.6 (3) | C2—C1—N1—Ni1 | −4.2 (4) |
| C22—C23—C28—C15 | 1.9 (5) | C3—C2—N2—O2 | −9.3 (5) |
| N3—C15—C28—C27 | −24.8 (5) | C1—C2—N2—O2 | 177.6 (3) |
| C16—C15—C28—C27 | 155.5 (3) | C3—C2—N2—Ni1 | 166.7 (3) |
| N3—C15—C28—C23 | 159.6 (3) | C1—C2—N2—Ni1 | −6.4 (4) |
| C16—C15—C28—C23 | −20.1 (4) | C16—C15—N3—O3 | 173.6 (3) |
| N5—C29—C30—N6 | 28.4 (5) | C28—C15—N3—O3 | −6.2 (5) |
| C42—C29—C30—N6 | −150.6 (3) | C16—C15—N3—Ni2 | −13.4 (4) |
| N5—C29—C30—C31 | −151.3 (3) | C28—C15—N3—Ni2 | 166.8 (2) |
| C42—C29—C30—C31 | 29.7 (4) | C15—C16—N4—O4 | −4.3 (5) |

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| N6—C30—C31—C32 | −24.0 (5) | C17—C16—N4—O4 | 175.4 (3) |
| C29—C30—C31—C32 | 155.8 (3) | C30—C29—N5—O5 | 172.0 (3) |
| N6—C30—C31—C36 | 155.9 (3) | C42—C29—N5—O5 | −9.0 (5) |
| C29—C30—C31—C36 | −24.4 (5) | C30—C29—N5—Ni1 | −18.5 (4) |
| C36—C31—C32—C33 | −1.1 (6) | C42—C29—N5—Ni1 | 160.5 (3) |
| C30—C31—C32—C33 | 178.8 (4) | C29—C30—N6—O6 | −4.0 (5) |
| C31—C32—C33—C34 | −0.1 (7) | C31—C30—N6—O6 | 175.7 (3) |
| C32—C33—C34—C35 | 0.8 (7) | C44—C43—N7—O7 | 178.7 (3) |
| C33—C34—C35—C36 | −0.3 (7) | C56—C43—N7—O7 | −3.4 (5) |
| C32—C31—C36—C35 | 1.5 (5) | C44—C43—N7—Ni2 | −6.0 (4) |
| C30—C31—C36—C35 | −178.3 (3) | C56—C43—N7—Ni2 | 172.0 (3) |
| C32—C31—C36—C37 | −177.9 (3) | C43—C44—N8—O8 | 175.6 (3) |
| C30—C31—C36—C37 | 2.3 (5) | C45—C44—N8—O8 | −8.5 (5) |
| C34—C35—C36—C31 | −0.8 (6) | C43—C44—N8—Ni2 | −7.2 (4) |
| C34—C35—C36—C37 | 178.5 (4) | C45—C44—N8—Ni2 | 168.7 (3) |
| C31—C36—C37—C38 | −166.6 (3) | C70—C57—N9—O9 | −0.4 (5) |
| C35—C36—C37—C38 | 14.1 (5) | C58—C57—N9—O9 | −177.7 (3) |
| C31—C36—C37—C42 | 14.3 (5) | C70—C57—N9—Ni3 | 166.5 (3) |
| C35—C36—C37—C42 | −165.1 (3) | C58—C57—N9—Ni3 | −10.8 (4) |
| C42—C37—C38—C39 | 1.1 (5) | C59—C58—N10—O10 | −3.5 (5) |
| C36—C37—C38—C39 | −178.0 (3) | C57—C58—N10—O10 | 178.9 (3) |
| C37—C38—C39—C40 | 0.4 (6) | C59—C58—N10—Ni3 | 162.1 (3) |
| C38—C39—C40—C41 | −1.6 (6) | C57—C58—N10—Ni3 | −15.6 (4) |
| C39—C40—C41—C42 | 1.2 (6) | C2—N2—O2—Ni3 | 143.0 (3) |
| C40—C41—C42—C37 | 0.3 (5) | Ni1—N2—O2—Ni3 | −32.7 (3) |
| C40—C41—C42—C29 | −173.5 (3) | C16—N4—O4—Ni2 | −30.5 (4) |
| C38—C37—C42—C41 | −1.5 (5) | C16—N4—O4—Ni3 | 148.7 (2) |
| C36—C37—C42—C41 | 177.7 (3) | C30—N6—O6—Ni1 | −30.9 (4) |
| C38—C37—C42—C29 | 172.6 (3) | C30—N6—O6—Ni3 | 145.4 (2) |
| C36—C37—C42—C29 | −8.3 (5) | C44—N8—O8—Ni3 | 145.0 (3) |
| N5—C29—C42—C41 | −18.5 (5) | Ni2—N8—O8—Ni3 | −32.1 (3) |
| C30—C29—C42—C41 | 160.4 (3) | N6—O6—Ni1—N1 | −158.8 (6) |
| N5—C29—C42—C37 | 167.6 (3) | Ni3—O6—Ni1—N1 | 24.9 (7) |
| C30—C29—C42—C37 | −13.4 (4) | N6—O6—Ni1—N2 | −151.0 (3) |
| N7—C43—C44—N8 | 8.4 (4) | Ni3—O6—Ni1—N2 | 32.64 (14) |
| C56—C43—C44—N8 | −169.7 (3) | N6—O6—Ni1—N5 | 31.9 (3) |
| N7—C43—C44—C45 | −167.8 (3) | Ni3—O6—Ni1—N5 | −144.41 (14) |
| C56—C43—C44—C45 | 14.1 (5) | C1—N1—Ni1—O6 | 8.5 (8) |
| N8—C44—C45—C46 | −6.1 (6) | O1—N1—Ni1—O6 | −173.0 (6) |
| C43—C44—C45—C46 | 169.4 (3) | C1—N1—Ni1—N2 | 0.7 (3) |
| N8—C44—C45—C50 | 178.3 (3) | O1—N1—Ni1—N2 | 179.1 (3) |
| C43—C44—C45—C50 | −6.2 (5) | C1—N1—Ni1—N5 | 177.7 (3) |
| C50—C45—C46—C47 | 1.8 (6) | O1—N1—Ni1—N5 | −3.9 (3) |
| C44—C45—C46—C47 | −173.7 (4) | C2—N2—Ni1—O6 | −175.1 (2) |
| C45—C46—C47—C48 | −1.8 (6) | O2—N2—Ni1—O6 | 0.8 (2) |
| C46—C47—C48—C49 | 1.1 (7) | C2—N2—Ni1—N1 | 3.5 (2) |
| C47—C48—C49—C50 | −0.4 (7) | O2—N2—Ni1—N1 | 179.4 (3) |
| C48—C49—C50—C45 | 0.4 (6) | C29—N5—Ni1—O6 | −5.9 (3) |

| | | | |
|---|---|---|---|
| C48—C49—C50—C51 | 179.7 (4) | O5—N5—Ni1—O6 | 163.6 (3) |
| C46—C45—C50—C49 | −1.0 (5) | C29—N5—Ni1—N1 | 176.0 (3) |
| C44—C45—C50—C49 | 174.6 (3) | O5—N5—Ni1—N1 | −14.5 (3) |
| C46—C45—C50—C51 | 179.7 (3) | N4—O4—Ni2—N8 | −149.4 (3) |
| C44—C45—C50—C51 | −4.7 (5) | Ni3—O4—Ni2—N8 | 31.36 (14) |
| C49—C50—C51—C56 | −171.2 (4) | N4—O4—Ni2—N3 | 33.3 (3) |
| C45—C50—C51—C56 | 8.0 (5) | Ni3—O4—Ni2—N3 | −145.90 (14) |
| C49—C50—C51—C52 | 9.9 (6) | C43—N7—Ni2—N8 | 1.8 (3) |
| C45—C50—C51—C52 | −170.8 (3) | O7—N7—Ni2—N8 | 177.1 (3) |
| C56—C51—C52—C53 | −0.1 (6) | C43—N7—Ni2—N3 | 179.0 (3) |
| C50—C51—C52—C53 | 178.7 (4) | O7—N7—Ni2—N3 | −5.7 (3) |
| C51—C52—C53—C54 | 0.2 (6) | C44—N8—Ni2—O4 | −176.1 (3) |
| C52—C53—C54—C55 | −0.1 (6) | O8—N8—Ni2—O4 | 1.1 (2) |
| C53—C54—C55—C56 | −0.1 (6) | C44—N8—Ni2—N7 | 3.3 (2) |
| C54—C55—C56—C51 | 0.2 (5) | O8—N8—Ni2—N7 | −179.5 (3) |
| C54—C55—C56—C43 | −178.5 (3) | C15—N3—Ni2—O4 | −10.2 (3) |
| C52—C51—C56—C55 | −0.1 (5) | O3—N3—Ni2—O4 | 162.8 (2) |
| C50—C51—C56—C55 | −179.0 (3) | C15—N3—Ni2—N7 | 170.8 (3) |
| C52—C51—C56—C43 | 178.7 (3) | O3—N3—Ni2—N7 | −16.1 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O5 | 1.29 (6) | 1.13 (6) | 2.405 (4) | 169 (6) |
| O3—H2*A*···O7 | 1.17 (5) | 1.23 (5) | 2.402 (4) | 176 (5) |
| O9—H3*A*···N4 | 0.86 (6) | 1.82 (6) | 2.672 (4) | 175 (7) |
| O10—H4*A*···N6 | 1.04 (5) | 1.63 (5) | 2.657 (4) | 168 (4) |

**(2) Bis($\mu_2$-bis{[10-(oxidoimino)-9,10-dihydrophenanthren-9-ylidene]amino}difluoroborato)(phenanthrene-9,10-dione dioxime)trinickel(II) dichloromethane trisolvate**

*Crystal data*

$[Ni_3(C_{28}H_{16}BF_2N_4O_4)_2(C_{14}H_{10}N_2O_2)]\cdot 3CH_2Cl_2$
$M_r$ = 1456.88
Monoclinic, $P2_1/c$
$a$ = 15.6414 (8) Å
$b$ = 30.8358 (11) Å
$c$ = 14.7380 (8) Å
$\beta$ = 112.411 (6)°
$V$ = 6571.5 (6) Å$^3$
$Z$ = 4
$F(000)$ = 2968
$D_x$ = 1.473 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 25728 reflections
$\theta$ = 3.4–76.5°
$\mu$ = 1.67 mm$^{-1}$
$T$ = 100 K
Block, red
0.29 × 0.07 × 0.04 mm

*Data collection*

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 5.2940 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
$T_{min}$ = 0.303, $T_{max}$ = 1.000
25337 measured reflections
13041 independent reflections
8782 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.060
$\theta_{max}$ = 75.0°, $\theta_{min}$ = 3.4°
$h$ = −19→19
$k$ = −26→38
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.226
$S$ = 1.03
13041 reflections
896 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.108P)^2 + 8.2009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 1.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.83 e Å$^{-3}$

*Special details*

**Experimental**. CrysAlisPro. (Agilent, 2014). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. Three molecules of what appeared to be dichloromethane were found to be badly disordered. Attempts to model the disorder were unsatisfactory. The contributions to the scattering factors due to these solvent molecules were removed by use of the utility SQUEEZE (Sluis and Spek, 1990) in PLATON98 (Spek, 1998). PLATON98 was used as incorporated in WinGX (Farrugia, 1999).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3411 (3) | 0.33690 (15) | 0.7321 (4) | 0.0323 (10) |
| C2 | 0.4326 (3) | 0.33998 (16) | 0.7254 (4) | 0.0336 (11) |
| C3 | 0.4765 (4) | 0.29952 (16) | 0.7127 (4) | 0.0347 (11) |
| C4 | 0.5720 (4) | 0.29722 (18) | 0.7393 (4) | 0.0423 (12) |
| H4 | 0.6093 | 0.3220 | 0.7661 | 0.051* |
| C5 | 0.6130 (4) | 0.25876 (18) | 0.7267 (5) | 0.0499 (14) |
| H5 | 0.6781 | 0.2571 | 0.7446 | 0.060* |
| C6 | 0.5574 (4) | 0.22266 (18) | 0.6875 (5) | 0.0498 (15) |
| H6 | 0.5847 | 0.1963 | 0.6785 | 0.060* |
| C7 | 0.4637 (4) | 0.22483 (17) | 0.6619 (4) | 0.0460 (14) |
| H7 | 0.4274 | 0.1997 | 0.6361 | 0.055* |
| C8 | 0.4198 (4) | 0.26291 (15) | 0.6727 (4) | 0.0362 (11) |
| C9 | 0.3201 (4) | 0.26641 (15) | 0.6448 (4) | 0.0357 (11) |
| C10 | 0.2594 (4) | 0.23476 (16) | 0.5841 (4) | 0.0394 (12) |
| H10 | 0.2844 | 0.2106 | 0.5627 | 0.047* |
| C11 | 0.1655 (4) | 0.23823 (18) | 0.5555 (4) | 0.0438 (13) |
| H11 | 0.1267 | 0.2162 | 0.5158 | 0.053* |

| | | | | |
|---|---|---|---|---|
| C12 | 0.1264 (4) | 0.27305 (18) | 0.5831 (4) | 0.0422 (12) |
| H12 | 0.0611 | 0.2754 | 0.5620 | 0.051* |
| C13 | 0.1837 (4) | 0.30485 (16) | 0.6426 (4) | 0.0361 (11) |
| H13 | 0.1571 | 0.3291 | 0.6619 | 0.043* |
| C14 | 0.2797 (4) | 0.30177 (15) | 0.6744 (4) | 0.0336 (11) |
| C15 | 0.2126 (3) | 0.36498 (16) | 0.4672 (3) | 0.0310 (10) |
| C16 | 0.3085 (3) | 0.37760 (15) | 0.4870 (3) | 0.0295 (10) |
| C17 | 0.3700 (3) | 0.34790 (16) | 0.4634 (3) | 0.0304 (10) |
| C18 | 0.4630 (3) | 0.35767 (17) | 0.4827 (4) | 0.0352 (11) |
| H18 | 0.4869 | 0.3853 | 0.5083 | 0.042* |
| C19 | 0.5208 (4) | 0.32743 (18) | 0.4649 (4) | 0.0442 (13) |
| H19 | 0.5832 | 0.3346 | 0.4770 | 0.053* |
| C20 | 0.4864 (4) | 0.28685 (19) | 0.4294 (4) | 0.0472 (14) |
| H20 | 0.5261 | 0.2657 | 0.4196 | 0.057* |
| C21 | 0.3950 (4) | 0.27698 (18) | 0.4081 (4) | 0.0423 (12) |
| H21 | 0.3725 | 0.2491 | 0.3827 | 0.051* |
| C22 | 0.3341 (3) | 0.30700 (16) | 0.4230 (4) | 0.0330 (10) |
| C23 | 0.2352 (4) | 0.29719 (16) | 0.3911 (4) | 0.0335 (10) |
| C24 | 0.1973 (4) | 0.25910 (18) | 0.3381 (4) | 0.0423 (12) |
| H24 | 0.2378 | 0.2386 | 0.3275 | 0.051* |
| C25 | 0.1044 (4) | 0.25044 (19) | 0.3013 (4) | 0.0464 (13) |
| H25 | 0.0816 | 0.2242 | 0.2667 | 0.056* |
| C26 | 0.0436 (4) | 0.28018 (19) | 0.3149 (4) | 0.0455 (13) |
| H26 | −0.0211 | 0.2750 | 0.2874 | 0.055* |
| C27 | 0.0781 (4) | 0.31762 (18) | 0.3690 (4) | 0.0380 (11) |
| H27 | 0.0365 | 0.3376 | 0.3794 | 0.046* |
| C28 | 0.1730 (3) | 0.32636 (16) | 0.4084 (4) | 0.0341 (11) |
| C29 | 0.3296 (3) | 0.47670 (15) | 0.9399 (4) | 0.0325 (10) |
| C30 | 0.3915 (3) | 0.50074 (15) | 0.9040 (3) | 0.0316 (10) |
| C31 | 0.4137 (3) | 0.54622 (15) | 0.9300 (3) | 0.0322 (10) |
| C32 | 0.4728 (4) | 0.57048 (16) | 0.8987 (4) | 0.0386 (12) |
| H32 | 0.4988 | 0.5573 | 0.8569 | 0.046* |
| C33 | 0.4942 (4) | 0.61279 (17) | 0.9267 (4) | 0.0448 (13) |
| H33 | 0.5354 | 0.6284 | 0.9053 | 0.054* |
| C34 | 0.4558 (5) | 0.63252 (18) | 0.9862 (5) | 0.0557 (17) |
| H34 | 0.4704 | 0.6618 | 1.0061 | 0.067* |
| C35 | 0.3969 (4) | 0.60974 (17) | 1.0163 (4) | 0.0454 (14) |
| H35 | 0.3712 | 0.6239 | 1.0573 | 0.055* |
| C36 | 0.3721 (4) | 0.56675 (16) | 0.9903 (3) | 0.0340 (11) |
| C37 | 0.3088 (4) | 0.54261 (16) | 1.0242 (4) | 0.0360 (11) |
| C38 | 0.2666 (4) | 0.56390 (18) | 1.0798 (4) | 0.0418 (13) |
| H38 | 0.2772 | 0.5941 | 1.0922 | 0.050* |
| C39 | 0.2105 (4) | 0.5425 (2) | 1.1168 (4) | 0.0497 (15) |
| H39 | 0.1828 | 0.5579 | 1.1545 | 0.060* |
| C40 | 0.1938 (4) | 0.4987 (2) | 1.0998 (4) | 0.0443 (13) |
| H40 | 0.1552 | 0.4838 | 1.1261 | 0.053* |
| C41 | 0.2339 (4) | 0.47662 (17) | 1.0439 (4) | 0.0372 (11) |
| H41 | 0.2230 | 0.4464 | 1.0326 | 0.045* |

| | | | | |
|---|---|---|---|---|
| C42 | 0.2897 (4) | 0.49811 (16) | 1.0043 (3) | 0.0355 (11) |
| C43 | 0.1661 (3) | 0.49600 (19) | 0.6807 (4) | 0.0400 (12) |
| C44 | 0.2317 (3) | 0.52960 (18) | 0.6755 (4) | 0.0392 (12) |
| C45 | 0.2153 (4) | 0.5756 (2) | 0.6941 (4) | 0.0511 (16) |
| C46 | 0.2581 (4) | 0.6091 (2) | 0.6633 (5) | 0.0581 (18) |
| H46 | 0.2979 | 0.6023 | 0.6301 | 0.070* |
| C47 | 0.2434 (5) | 0.6522 (2) | 0.6804 (7) | 0.077 (3) |
| H47 | 0.2730 | 0.6749 | 0.6597 | 0.093* |
| C48 | 0.1844 (5) | 0.6615 (3) | 0.7286 (7) | 0.094 (3) |
| H48 | 0.1729 | 0.6908 | 0.7403 | 0.112* |
| C49 | 0.1427 (5) | 0.6285 (3) | 0.7595 (6) | 0.083 (3) |
| H49 | 0.1032 | 0.6356 | 0.7928 | 0.100* |
| C50 | 0.1571 (4) | 0.5845 (2) | 0.7429 (5) | 0.061 (2) |
| C51 | 0.1151 (4) | 0.5488 (3) | 0.7768 (4) | 0.062 (2) |
| C52 | 0.0734 (5) | 0.5578 (3) | 0.8439 (5) | 0.073 (2) |
| H52 | 0.0721 | 0.5866 | 0.8658 | 0.088* |
| C53 | 0.0348 (5) | 0.5250 (4) | 0.8776 (5) | 0.088 (3) |
| H53 | 0.0047 | 0.5317 | 0.9209 | 0.105* |
| C54 | 0.0385 (4) | 0.4820 (4) | 0.8502 (5) | 0.077 (3) |
| H54 | 0.0127 | 0.4596 | 0.8761 | 0.093* |
| C55 | 0.0804 (4) | 0.4722 (3) | 0.7841 (4) | 0.0604 (19) |
| H55 | 0.0838 | 0.4430 | 0.7650 | 0.072* |
| C56 | 0.1175 (4) | 0.5059 (2) | 0.7462 (4) | 0.0500 (16) |
| C57 | 0.6326 (3) | 0.48466 (16) | 0.6652 (4) | 0.0315 (10) |
| C58 | 0.5935 (3) | 0.52870 (16) | 0.6698 (3) | 0.0315 (10) |
| C59 | 0.6591 (3) | 0.56487 (15) | 0.7051 (3) | 0.0304 (10) |
| C60 | 0.6390 (4) | 0.60134 (17) | 0.7479 (4) | 0.0395 (12) |
| H60 | 0.5788 | 0.6050 | 0.7481 | 0.047* |
| C61 | 0.7056 (4) | 0.63235 (18) | 0.7902 (5) | 0.0463 (13) |
| H61 | 0.6915 | 0.6570 | 0.8207 | 0.056* |
| C62 | 0.7926 (4) | 0.62788 (17) | 0.7885 (4) | 0.0436 (13) |
| H62 | 0.8380 | 0.6496 | 0.8171 | 0.052* |
| C63 | 0.8141 (4) | 0.59185 (17) | 0.7452 (4) | 0.0363 (11) |
| H63 | 0.8743 | 0.5889 | 0.7446 | 0.044* |
| C64 | 0.7473 (3) | 0.55957 (15) | 0.7021 (3) | 0.0298 (10) |
| C65 | 0.7705 (3) | 0.52067 (16) | 0.6569 (3) | 0.0320 (10) |
| C66 | 0.8480 (3) | 0.51969 (17) | 0.6315 (4) | 0.0346 (11) |
| H66 | 0.8867 | 0.5445 | 0.6430 | 0.041* |
| C67 | 0.8690 (3) | 0.48300 (19) | 0.5900 (4) | 0.0390 (12) |
| H67 | 0.9216 | 0.4828 | 0.5728 | 0.047* |
| C68 | 0.8134 (4) | 0.44667 (18) | 0.5735 (4) | 0.0409 (12) |
| H68 | 0.8281 | 0.4215 | 0.5450 | 0.049* |
| C69 | 0.7366 (3) | 0.44671 (18) | 0.5982 (4) | 0.0389 (12) |
| H69 | 0.6988 | 0.4216 | 0.5867 | 0.047* |
| C70 | 0.7146 (3) | 0.48316 (16) | 0.6398 (4) | 0.0332 (11) |
| N1 | 0.3219 (3) | 0.36493 (12) | 0.7882 (3) | 0.0321 (9) |
| N2 | 0.4789 (3) | 0.37504 (13) | 0.7289 (3) | 0.0339 (9) |
| N3 | 0.1712 (3) | 0.39220 (13) | 0.5053 (3) | 0.0316 (9) |

| | | | | |
|---|---|---|---|---|
| N4 | 0.3296 (3) | 0.41530 (13) | 0.5315 (3) | 0.0290 (8) |
| N5 | 0.3158 (3) | 0.43671 (13) | 0.9063 (3) | 0.0337 (9) |
| N6 | 0.4215 (3) | 0.47684 (11) | 0.8493 (3) | 0.0288 (8) |
| N7 | 0.1558 (3) | 0.46191 (15) | 0.6258 (3) | 0.0364 (10) |
| N8 | 0.3047 (3) | 0.52333 (14) | 0.6565 (3) | 0.0359 (9) |
| N9 | 0.5880 (3) | 0.45401 (13) | 0.6849 (3) | 0.0346 (9) |
| N10 | 0.5047 (3) | 0.52610 (13) | 0.6498 (3) | 0.0378 (10) |
| O1 | 0.2406 (3) | 0.35856 (11) | 0.8007 (3) | 0.0397 (8) |
| O2 | 0.4437 (2) | 0.41270 (10) | 0.7481 (3) | 0.0329 (7) |
| O3 | 0.0833 (2) | 0.38339 (12) | 0.4931 (3) | 0.0436 (9) |
| O4 | 0.4102 (2) | 0.43359 (11) | 0.5495 (2) | 0.0319 (7) |
| O5 | 0.2580 (3) | 0.41112 (11) | 0.9310 (3) | 0.0422 (9) |
| O6 | 0.4795 (2) | 0.49203 (10) | 0.8119 (3) | 0.0324 (7) |
| O7 | 0.0898 (3) | 0.43277 (13) | 0.6260 (3) | 0.0448 (9) |
| O8 | 0.3220 (2) | 0.48291 (11) | 0.6323 (3) | 0.0347 (8) |
| O9 | 0.6191 (2) | 0.41229 (11) | 0.6839 (3) | 0.0373 (8) |
| H1A | 0.582 (4) | 0.3945 (14) | 0.694 (5) | 0.056* |
| O10 | 0.4608 (3) | 0.56409 (12) | 0.6526 (3) | 0.0463 (9) |
| H2A | 0.395 (5) | 0.5572 (5) | 0.654 (5) | 0.069* |
| Ni1 | 0.37718 (6) | 0.41976 (2) | 0.82564 (6) | 0.0306 (2) |
| Ni2 | 0.23963 (5) | 0.44031 (3) | 0.57163 (6) | 0.0301 (2) |
| Ni3 | 0.45817 (5) | 0.46682 (2) | 0.67739 (6) | 0.0277 (2) |
| F1 | 0.3252 (3) | 0.34124 (11) | 0.9649 (3) | 0.0556 (9) |
| F2 | 0.1678 (3) | 0.35125 (12) | 0.9084 (3) | 0.0601 (10) |
| F3 | −0.0369 (2) | 0.39118 (12) | 0.5394 (3) | 0.0613 (10) |
| F4 | 0.0009 (2) | 0.44772 (11) | 0.4612 (3) | 0.0506 (8) |
| B1 | 0.2493 (5) | 0.3650 (2) | 0.9034 (6) | 0.0486 (16) |
| B2 | 0.0335 (4) | 0.4143 (2) | 0.5275 (6) | 0.0437 (15) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.044 (3) | 0.021 (2) | 0.029 (2) | 0.0022 (19) | 0.011 (2) | 0.0065 (19) |
| C2 | 0.042 (3) | 0.026 (2) | 0.030 (3) | 0.002 (2) | 0.011 (2) | 0.004 (2) |
| C3 | 0.052 (3) | 0.023 (2) | 0.028 (2) | 0.003 (2) | 0.014 (2) | 0.000 (2) |
| C4 | 0.051 (3) | 0.030 (3) | 0.042 (3) | 0.005 (2) | 0.013 (2) | −0.002 (2) |
| C5 | 0.058 (3) | 0.035 (3) | 0.052 (4) | 0.010 (3) | 0.015 (3) | −0.004 (3) |
| C6 | 0.064 (4) | 0.029 (3) | 0.055 (4) | 0.017 (3) | 0.022 (3) | −0.001 (3) |
| C7 | 0.068 (4) | 0.024 (3) | 0.038 (3) | 0.001 (2) | 0.012 (3) | −0.002 (2) |
| C8 | 0.061 (3) | 0.016 (2) | 0.029 (3) | 0.001 (2) | 0.015 (2) | 0.0017 (19) |
| C9 | 0.058 (3) | 0.020 (2) | 0.028 (2) | −0.002 (2) | 0.014 (2) | 0.006 (2) |
| C10 | 0.065 (3) | 0.019 (2) | 0.032 (3) | −0.006 (2) | 0.016 (2) | 0.002 (2) |
| C11 | 0.059 (3) | 0.033 (3) | 0.035 (3) | −0.016 (2) | 0.014 (2) | 0.001 (2) |
| C12 | 0.054 (3) | 0.036 (3) | 0.036 (3) | −0.010 (2) | 0.015 (2) | 0.002 (2) |
| C13 | 0.049 (3) | 0.028 (3) | 0.031 (3) | −0.005 (2) | 0.015 (2) | 0.003 (2) |
| C14 | 0.049 (3) | 0.023 (2) | 0.024 (2) | −0.006 (2) | 0.010 (2) | 0.0060 (19) |
| C15 | 0.036 (2) | 0.032 (3) | 0.023 (2) | 0.0051 (19) | 0.0079 (18) | 0.006 (2) |
| C16 | 0.041 (2) | 0.026 (2) | 0.025 (2) | 0.0059 (19) | 0.0159 (19) | 0.0028 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.041 (2) | 0.029 (2) | 0.022 (2) | 0.0046 (19) | 0.0133 (19) | 0.0010 (19) |
| C18 | 0.039 (2) | 0.034 (3) | 0.032 (3) | 0.001 (2) | 0.013 (2) | −0.002 (2) |
| C19 | 0.041 (3) | 0.041 (3) | 0.049 (3) | 0.006 (2) | 0.016 (2) | −0.007 (3) |
| C20 | 0.050 (3) | 0.041 (3) | 0.050 (3) | 0.011 (2) | 0.018 (3) | −0.010 (3) |
| C21 | 0.048 (3) | 0.033 (3) | 0.044 (3) | 0.001 (2) | 0.015 (2) | −0.010 (2) |
| C22 | 0.045 (3) | 0.030 (3) | 0.025 (2) | 0.002 (2) | 0.015 (2) | −0.002 (2) |
| C23 | 0.048 (3) | 0.029 (3) | 0.026 (2) | 0.000 (2) | 0.016 (2) | 0.003 (2) |
| C24 | 0.054 (3) | 0.038 (3) | 0.040 (3) | −0.005 (2) | 0.023 (3) | −0.009 (2) |
| C25 | 0.061 (3) | 0.042 (3) | 0.038 (3) | −0.013 (3) | 0.021 (3) | −0.014 (3) |
| C26 | 0.050 (3) | 0.049 (3) | 0.033 (3) | −0.011 (3) | 0.012 (2) | −0.005 (3) |
| C27 | 0.043 (3) | 0.037 (3) | 0.033 (3) | 0.002 (2) | 0.013 (2) | 0.004 (2) |
| C28 | 0.042 (3) | 0.029 (2) | 0.028 (2) | 0.002 (2) | 0.010 (2) | 0.008 (2) |
| C29 | 0.045 (3) | 0.023 (2) | 0.026 (2) | 0.0069 (19) | 0.011 (2) | 0.0031 (19) |
| C30 | 0.042 (2) | 0.024 (2) | 0.025 (2) | 0.0043 (19) | 0.0094 (19) | 0.0014 (19) |
| C31 | 0.048 (3) | 0.021 (2) | 0.021 (2) | 0.0047 (19) | 0.0066 (19) | 0.0026 (19) |
| C32 | 0.058 (3) | 0.025 (2) | 0.030 (3) | 0.006 (2) | 0.014 (2) | −0.001 (2) |
| C33 | 0.072 (4) | 0.023 (3) | 0.039 (3) | −0.004 (2) | 0.021 (3) | −0.001 (2) |
| C34 | 0.095 (5) | 0.020 (3) | 0.051 (4) | −0.003 (3) | 0.027 (3) | −0.009 (3) |
| C35 | 0.075 (4) | 0.028 (3) | 0.033 (3) | 0.006 (3) | 0.020 (3) | −0.006 (2) |
| C36 | 0.050 (3) | 0.024 (2) | 0.023 (2) | 0.003 (2) | 0.009 (2) | −0.0012 (19) |
| C37 | 0.045 (3) | 0.032 (3) | 0.021 (2) | 0.009 (2) | 0.002 (2) | 0.001 (2) |
| C38 | 0.053 (3) | 0.038 (3) | 0.028 (3) | 0.009 (2) | 0.008 (2) | −0.009 (2) |
| C39 | 0.065 (4) | 0.054 (4) | 0.030 (3) | 0.014 (3) | 0.018 (3) | −0.008 (3) |
| C40 | 0.054 (3) | 0.054 (4) | 0.023 (2) | 0.011 (3) | 0.011 (2) | 0.004 (2) |
| C41 | 0.046 (3) | 0.031 (3) | 0.033 (3) | 0.004 (2) | 0.013 (2) | 0.004 (2) |
| C42 | 0.052 (3) | 0.028 (3) | 0.019 (2) | 0.010 (2) | 0.006 (2) | 0.0008 (19) |
| C43 | 0.032 (2) | 0.056 (3) | 0.026 (2) | 0.014 (2) | 0.0044 (19) | −0.007 (2) |
| C44 | 0.032 (2) | 0.046 (3) | 0.031 (3) | 0.011 (2) | 0.003 (2) | −0.010 (2) |
| C45 | 0.036 (3) | 0.057 (4) | 0.045 (3) | 0.017 (3) | −0.002 (2) | −0.021 (3) |
| C46 | 0.043 (3) | 0.039 (3) | 0.074 (5) | 0.008 (2) | 0.002 (3) | −0.024 (3) |
| C47 | 0.052 (4) | 0.056 (4) | 0.103 (6) | 0.009 (3) | 0.006 (4) | −0.036 (4) |
| C48 | 0.054 (4) | 0.070 (5) | 0.123 (8) | 0.019 (4) | −0.005 (4) | −0.062 (5) |
| C49 | 0.053 (4) | 0.093 (6) | 0.082 (6) | 0.024 (4) | 0.001 (4) | −0.048 (5) |
| C50 | 0.037 (3) | 0.080 (5) | 0.048 (4) | 0.018 (3) | −0.003 (3) | −0.034 (4) |
| C51 | 0.043 (3) | 0.104 (6) | 0.028 (3) | 0.023 (3) | 0.002 (2) | −0.024 (3) |
| C52 | 0.045 (3) | 0.129 (7) | 0.036 (3) | 0.022 (4) | 0.005 (3) | −0.028 (4) |
| C53 | 0.041 (3) | 0.186 (11) | 0.031 (3) | 0.028 (5) | 0.007 (3) | −0.022 (5) |
| C54 | 0.045 (3) | 0.155 (9) | 0.028 (3) | 0.007 (4) | 0.009 (3) | −0.001 (4) |
| C55 | 0.037 (3) | 0.115 (6) | 0.025 (3) | 0.006 (3) | 0.007 (2) | −0.010 (3) |
| C56 | 0.031 (2) | 0.087 (5) | 0.027 (3) | 0.013 (3) | 0.006 (2) | −0.012 (3) |
| C57 | 0.034 (2) | 0.031 (3) | 0.027 (2) | 0.0035 (19) | 0.0096 (19) | −0.003 (2) |
| C58 | 0.037 (2) | 0.034 (3) | 0.026 (2) | 0.000 (2) | 0.0141 (19) | −0.002 (2) |
| C59 | 0.041 (2) | 0.027 (2) | 0.025 (2) | 0.0019 (19) | 0.0137 (19) | 0.0026 (19) |
| C60 | 0.054 (3) | 0.032 (3) | 0.037 (3) | −0.002 (2) | 0.023 (2) | 0.001 (2) |
| C61 | 0.065 (4) | 0.031 (3) | 0.048 (3) | 0.000 (3) | 0.028 (3) | −0.007 (3) |
| C62 | 0.061 (3) | 0.027 (3) | 0.042 (3) | −0.012 (2) | 0.018 (3) | −0.004 (2) |
| C63 | 0.044 (3) | 0.034 (3) | 0.030 (3) | −0.004 (2) | 0.012 (2) | 0.005 (2) |
| C64 | 0.041 (2) | 0.028 (2) | 0.018 (2) | 0.0001 (19) | 0.0091 (18) | 0.0051 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C65 | 0.041 (2) | 0.031 (3) | 0.022 (2) | 0.001 (2) | 0.0104 (19) | 0.0010 (19) |
| C66 | 0.037 (2) | 0.037 (3) | 0.028 (2) | 0.000 (2) | 0.0108 (19) | 0.006 (2) |
| C67 | 0.033 (2) | 0.052 (3) | 0.031 (3) | 0.009 (2) | 0.011 (2) | 0.005 (2) |
| C68 | 0.044 (3) | 0.042 (3) | 0.038 (3) | 0.002 (2) | 0.017 (2) | −0.011 (2) |
| C69 | 0.039 (3) | 0.041 (3) | 0.036 (3) | −0.004 (2) | 0.013 (2) | −0.009 (2) |
| C70 | 0.032 (2) | 0.034 (3) | 0.030 (2) | −0.0023 (19) | 0.0083 (19) | −0.003 (2) |
| N1 | 0.042 (2) | 0.0176 (18) | 0.039 (2) | −0.0029 (16) | 0.0183 (18) | 0.0038 (17) |
| N2 | 0.047 (2) | 0.020 (2) | 0.034 (2) | 0.0032 (17) | 0.0156 (18) | −0.0009 (17) |
| N3 | 0.0329 (19) | 0.029 (2) | 0.032 (2) | −0.0009 (16) | 0.0119 (17) | 0.0026 (17) |
| N4 | 0.0354 (19) | 0.027 (2) | 0.026 (2) | 0.0023 (16) | 0.0130 (16) | 0.0018 (16) |
| N5 | 0.053 (2) | 0.0196 (19) | 0.032 (2) | 0.0056 (17) | 0.0206 (19) | 0.0067 (17) |
| N6 | 0.038 (2) | 0.0146 (17) | 0.032 (2) | −0.0032 (15) | 0.0109 (16) | 0.0013 (16) |
| N7 | 0.034 (2) | 0.046 (3) | 0.029 (2) | 0.0027 (18) | 0.0125 (17) | 0.0015 (19) |
| N8 | 0.038 (2) | 0.032 (2) | 0.033 (2) | 0.0069 (17) | 0.0086 (17) | −0.0043 (18) |
| N9 | 0.042 (2) | 0.027 (2) | 0.036 (2) | −0.0039 (17) | 0.0156 (18) | −0.0092 (18) |
| N10 | 0.052 (2) | 0.025 (2) | 0.040 (2) | 0.0038 (18) | 0.021 (2) | −0.0010 (19) |
| O1 | 0.049 (2) | 0.0295 (18) | 0.046 (2) | −0.0043 (15) | 0.0243 (17) | −0.0047 (16) |
| O2 | 0.055 (2) | 0.0144 (15) | 0.0378 (19) | 0.0011 (13) | 0.0274 (16) | 0.0017 (14) |
| O3 | 0.0344 (18) | 0.039 (2) | 0.058 (2) | −0.0016 (15) | 0.0185 (17) | −0.0068 (19) |
| O4 | 0.0332 (16) | 0.0310 (17) | 0.0326 (18) | −0.0019 (13) | 0.0137 (14) | −0.0042 (15) |
| O5 | 0.064 (2) | 0.0268 (18) | 0.047 (2) | −0.0021 (16) | 0.034 (2) | 0.0006 (17) |
| O6 | 0.0429 (18) | 0.0201 (15) | 0.0347 (18) | −0.0032 (13) | 0.0155 (15) | −0.0033 (14) |
| O7 | 0.043 (2) | 0.054 (2) | 0.043 (2) | −0.0077 (17) | 0.0235 (17) | −0.0037 (19) |
| O8 | 0.0345 (16) | 0.0273 (17) | 0.041 (2) | 0.0049 (13) | 0.0123 (15) | −0.0044 (15) |
| O9 | 0.0384 (18) | 0.0263 (17) | 0.048 (2) | 0.0018 (14) | 0.0167 (16) | −0.0074 (16) |
| O10 | 0.057 (2) | 0.0255 (18) | 0.059 (3) | 0.0003 (16) | 0.025 (2) | 0.0035 (18) |
| Ni1 | 0.0451 (5) | 0.0169 (4) | 0.0317 (4) | 0.0006 (3) | 0.0168 (4) | 0.0009 (3) |
| Ni2 | 0.0342 (4) | 0.0274 (4) | 0.0293 (4) | 0.0031 (3) | 0.0127 (3) | −0.0014 (3) |
| Ni3 | 0.0348 (4) | 0.0182 (4) | 0.0311 (4) | 0.0013 (3) | 0.0137 (3) | 0.0008 (3) |
| F1 | 0.071 (2) | 0.0393 (18) | 0.058 (2) | 0.0011 (16) | 0.0272 (18) | 0.0146 (16) |
| F2 | 0.072 (2) | 0.048 (2) | 0.072 (3) | −0.0111 (17) | 0.041 (2) | −0.0011 (19) |
| F3 | 0.053 (2) | 0.056 (2) | 0.083 (3) | −0.0035 (16) | 0.0350 (19) | −0.004 (2) |
| F4 | 0.0507 (18) | 0.0436 (19) | 0.049 (2) | 0.0051 (15) | 0.0097 (15) | −0.0025 (16) |
| B1 | 0.061 (4) | 0.037 (4) | 0.051 (4) | −0.002 (3) | 0.025 (3) | −0.001 (3) |
| B2 | 0.045 (3) | 0.035 (3) | 0.059 (4) | −0.005 (3) | 0.028 (3) | −0.003 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.307 (6) | C44—C45 | 1.485 (8) |
| C1—C2 | 1.475 (7) | C45—C50 | 1.385 (9) |
| C1—C14 | 1.482 (7) | C45—C46 | 1.399 (10) |
| C2—N2 | 1.291 (6) | C46—C47 | 1.388 (9) |
| C2—C3 | 1.470 (7) | C46—H46 | 0.9500 |
| C3—C4 | 1.394 (7) | C47—C48 | 1.392 (12) |
| C3—C8 | 1.418 (7) | C47—H47 | 0.9500 |
| C4—C5 | 1.394 (7) | C48—C49 | 1.375 (14) |
| C4—H4 | 0.9500 | C48—H48 | 0.9500 |
| C5—C6 | 1.396 (9) | C49—C50 | 1.413 (10) |

| | | | |
|---|---|---|---|
| C5—H5 | 0.9500 | C49—H49 | 0.9500 |
| C6—C7 | 1.367 (8) | C50—C51 | 1.464 (11) |
| C6—H6 | 0.9500 | C51—C52 | 1.403 (9) |
| C7—C8 | 1.400 (7) | C51—C56 | 1.405 (10) |
| C7—H7 | 0.9500 | C52—C53 | 1.364 (13) |
| C8—C9 | 1.458 (8) | C52—H52 | 0.9500 |
| C9—C14 | 1.410 (7) | C53—C54 | 1.395 (13) |
| C9—C10 | 1.417 (7) | C53—H53 | 0.9500 |
| C10—C11 | 1.369 (8) | C54—C55 | 1.399 (9) |
| C10—H10 | 0.9500 | C54—H54 | 0.9500 |
| C11—C12 | 1.372 (8) | C55—C56 | 1.404 (10) |
| C11—H11 | 0.9500 | C55—H55 | 0.9500 |
| C12—C13 | 1.391 (7) | C57—N9 | 1.273 (6) |
| C12—H12 | 0.9500 | C57—C70 | 1.466 (7) |
| C13—C14 | 1.395 (7) | C57—C58 | 1.502 (7) |
| C13—H13 | 0.9500 | C58—N10 | 1.308 (6) |
| C15—N3 | 1.309 (6) | C58—C59 | 1.470 (7) |
| C15—C28 | 1.464 (7) | C59—C60 | 1.383 (7) |
| C15—C16 | 1.467 (7) | C59—C64 | 1.407 (7) |
| C16—N4 | 1.314 (6) | C60—C61 | 1.376 (8) |
| C16—C17 | 1.464 (6) | C60—H60 | 0.9500 |
| C17—C18 | 1.404 (7) | C61—C62 | 1.377 (8) |
| C17—C22 | 1.416 (7) | C61—H61 | 0.9500 |
| C18—C19 | 1.391 (7) | C62—C63 | 1.385 (8) |
| C18—H18 | 0.9500 | C62—H62 | 0.9500 |
| C19—C20 | 1.384 (8) | C63—C64 | 1.407 (7) |
| C19—H19 | 0.9500 | C63—H63 | 0.9500 |
| C20—C21 | 1.376 (8) | C64—C65 | 1.483 (7) |
| C20—H20 | 0.9500 | C65—C66 | 1.398 (7) |
| C21—C22 | 1.404 (7) | C65—C70 | 1.414 (7) |
| C21—H21 | 0.9500 | C66—C67 | 1.384 (7) |
| C22—C23 | 1.465 (7) | C66—H66 | 0.9500 |
| C23—C24 | 1.410 (7) | C67—C68 | 1.381 (8) |
| C23—C28 | 1.418 (7) | C67—H67 | 0.9500 |
| C24—C25 | 1.370 (8) | C68—C69 | 1.382 (7) |
| C24—H24 | 0.9500 | C68—H68 | 0.9500 |
| C25—C26 | 1.389 (8) | C69—C70 | 1.385 (7) |
| C25—H25 | 0.9500 | C69—H69 | 0.9500 |
| C26—C27 | 1.390 (8) | N1—O1 | 1.367 (5) |
| C26—H26 | 0.9500 | N1—Ni1 | 1.883 (4) |
| C27—C28 | 1.399 (7) | N2—O2 | 1.360 (5) |
| C27—H27 | 0.9500 | N3—O3 | 1.346 (5) |
| C29—N5 | 1.315 (6) | N3—Ni2 | 1.872 (4) |
| C29—C30 | 1.469 (7) | N4—O4 | 1.312 (5) |
| C29—C42 | 1.476 (7) | N4—Ni2 | 1.887 (4) |
| C30—N6 | 1.304 (6) | N5—O5 | 1.350 (5) |
| C30—C31 | 1.460 (7) | N5—Ni1 | 1.865 (4) |
| C31—C32 | 1.398 (8) | N6—O6 | 1.314 (5) |

| | | | |
|---|---|---|---|
| C31—C36 | 1.432 (7) | N6—Ni1 | 1.875 (4) |
| C32—C33 | 1.371 (7) | N7—O7 | 1.370 (6) |
| C32—H32 | 0.9500 | N7—Ni2 | 1.897 (4) |
| C33—C34 | 1.379 (8) | N8—O8 | 1.352 (5) |
| C33—H33 | 0.9500 | N9—O9 | 1.378 (5) |
| C34—C35 | 1.361 (9) | N9—Ni3 | 2.029 (4) |
| C34—H34 | 0.9500 | N10—O10 | 1.367 (5) |
| C35—C36 | 1.393 (7) | N10—Ni3 | 2.064 (4) |
| C35—H35 | 0.9500 | O1—B1 | 1.480 (8) |
| C36—C37 | 1.470 (8) | O2—Ni1 | 1.829 (3) |
| C37—C38 | 1.397 (7) | O2—Ni3 | 2.025 (3) |
| C37—C42 | 1.411 (7) | O3—B2 | 1.440 (7) |
| C38—C39 | 1.368 (9) | O4—Ni3 | 2.022 (3) |
| C38—H38 | 0.9500 | O5—B1 | 1.471 (8) |
| C39—C40 | 1.379 (9) | O6—Ni3 | 2.036 (3) |
| C39—H39 | 0.9500 | O7—B2 | 1.493 (8) |
| C40—C41 | 1.390 (8) | O8—Ni2 | 1.819 (3) |
| C40—H40 | 0.9500 | O8—Ni3 | 2.036 (3) |
| C41—C42 | 1.389 (8) | O9—H1A | 0.85 (7) |
| C41—H41 | 0.9500 | O10—H2A | 1.06 (7) |
| C43—N7 | 1.298 (7) | F1—B1 | 1.395 (8) |
| C43—C56 | 1.471 (7) | F2—B1 | 1.372 (8) |
| C43—C44 | 1.481 (8) | F3—B2 | 1.378 (7) |
| C44—N8 | 1.290 (7) | F4—B2 | 1.377 (8) |

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| N1—C1—C2 | 117.6 (4) | C48—C49—H49 | 119.1 |
| N1—C1—C14 | 126.3 (5) | C50—C49—H49 | 119.1 |
| C2—C1—C14 | 116.2 (4) | C45—C50—C49 | 117.4 (8) |
| N2—C2—C3 | 115.7 (5) | C45—C50—C51 | 119.8 (6) |
| N2—C2—C1 | 126.5 (4) | C49—C50—C51 | 122.8 (7) |
| C3—C2—C1 | 117.8 (4) | C52—C51—C56 | 119.2 (8) |
| C4—C3—C8 | 120.7 (5) | C52—C51—C50 | 118.9 (7) |
| C4—C3—C2 | 120.7 (5) | C56—C51—C50 | 121.9 (6) |
| C8—C3—C2 | 118.7 (5) | C53—C52—C51 | 120.0 (8) |
| C3—C4—C5 | 120.3 (5) | C53—C52—H52 | 120.0 |
| C3—C4—H4 | 119.9 | C51—C52—H52 | 120.0 |
| C5—C4—H4 | 119.9 | C52—C53—C54 | 121.7 (7) |
| C4—C5—C6 | 119.2 (6) | C52—C53—H53 | 119.1 |
| C4—C5—H5 | 120.4 | C54—C53—H53 | 119.1 |
| C6—C5—H5 | 120.4 | C53—C54—C55 | 119.2 (9) |
| C7—C6—C5 | 120.6 (5) | C53—C54—H54 | 120.4 |
| C7—C6—H6 | 119.7 | C55—C54—H54 | 120.4 |
| C5—C6—H6 | 119.7 | C54—C55—C56 | 119.5 (8) |
| C6—C7—C8 | 122.0 (5) | C54—C55—H55 | 120.2 |
| C6—C7—H7 | 119.0 | C56—C55—H55 | 120.2 |
| C8—C7—H7 | 119.0 | C55—C56—C51 | 120.2 (6) |
| C7—C8—C3 | 117.3 (5) | C55—C56—C43 | 120.3 (6) |
| C7—C8—C9 | 123.3 (5) | C51—C56—C43 | 119.3 (6) |

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| C3—C8—C9 | 119.4 (4) | N9—C57—C70 | 130.1 (5) |
| C14—C9—C10 | 117.2 (5) | N9—C57—C58 | 113.1 (4) |
| C14—C9—C8 | 121.8 (4) | C70—C57—C58 | 116.8 (4) |
| C10—C9—C8 | 121.0 (5) | N10—C58—C59 | 131.6 (4) |
| C11—C10—C9 | 121.5 (5) | N10—C58—C57 | 110.5 (4) |
| C11—C10—H10 | 119.3 | C59—C58—C57 | 117.4 (4) |
| C9—C10—H10 | 119.3 | C60—C59—C64 | 120.4 (5) |
| C10—C11—C12 | 121.1 (5) | C60—C59—C58 | 121.9 (4) |
| C10—C11—H11 | 119.4 | C64—C59—C58 | 117.5 (4) |
| C12—C11—H11 | 119.4 | C61—C60—C59 | 120.5 (5) |
| C11—C12—C13 | 119.0 (5) | C61—C60—H60 | 119.8 |
| C11—C12—H12 | 120.5 | C59—C60—H60 | 119.8 |
| C13—C12—H12 | 120.5 | C60—C61—C62 | 120.3 (5) |
| C12—C13—C14 | 121.1 (5) | C60—C61—H61 | 119.8 |
| C12—C13—H13 | 119.5 | C62—C61—H61 | 119.8 |
| C14—C13—H13 | 119.5 | C61—C62—C63 | 120.3 (5) |
| C13—C14—C9 | 120.0 (5) | C61—C62—H62 | 119.9 |
| C13—C14—C1 | 121.5 (5) | C63—C62—H62 | 119.9 |
| C9—C14—C1 | 118.3 (5) | C62—C63—C64 | 120.4 (5) |
| N3—C15—C28 | 127.5 (5) | C62—C63—H63 | 119.8 |
| N3—C15—C16 | 112.3 (4) | C64—C63—H63 | 119.8 |
| C28—C15—C16 | 120.1 (4) | C59—C64—C63 | 118.1 (5) |
| N4—C16—C17 | 127.5 (4) | C59—C64—C65 | 121.3 (4) |
| N4—C16—C15 | 112.2 (4) | C63—C64—C65 | 120.6 (4) |
| C17—C16—C15 | 120.2 (4) | C66—C65—C70 | 118.4 (5) |
| C18—C17—C22 | 119.4 (4) | C66—C65—C64 | 121.5 (4) |
| C18—C17—C16 | 122.8 (5) | C70—C65—C64 | 120.0 (4) |
| C22—C17—C16 | 117.7 (4) | C67—C66—C65 | 120.8 (5) |
| C19—C18—C17 | 121.0 (5) | C67—C66—H66 | 119.6 |
| C19—C18—H18 | 119.5 | C65—C66—H66 | 119.6 |
| C17—C18—H18 | 119.5 | C68—C67—C66 | 120.1 (5) |
| C20—C19—C18 | 119.4 (5) | C68—C67—H67 | 119.9 |
| C20—C19—H19 | 120.3 | C66—C67—H67 | 119.9 |
| C18—C19—H19 | 120.3 | C67—C68—C69 | 120.3 (5) |
| C21—C20—C19 | 120.4 (5) | C67—C68—H68 | 119.9 |
| C21—C20—H20 | 119.8 | C69—C68—H68 | 119.9 |
| C19—C20—H20 | 119.8 | C68—C69—C70 | 120.4 (5) |
| C20—C21—C22 | 121.8 (5) | C68—C69—H69 | 119.8 |
| C20—C21—H21 | 119.1 | C70—C69—H69 | 119.8 |
| C22—C21—H21 | 119.1 | C69—C70—C65 | 120.0 (5) |
| C21—C22—C17 | 117.9 (5) | C69—C70—C57 | 121.9 (4) |
| C21—C22—C23 | 120.6 (5) | C65—C70—C57 | 118.1 (4) |
| C17—C22—C23 | 121.3 (4) | C1—N1—O1 | 116.1 (4) |
| C24—C23—C28 | 117.1 (5) | C1—N1—Ni1 | 126.1 (3) |
| C24—C23—C22 | 121.3 (5) | O1—N1—Ni1 | 115.8 (3) |
| C28—C23—C22 | 121.6 (5) | C2—N2—O2 | 117.3 (4) |
| C25—C24—C23 | 122.7 (5) | C15—N3—O3 | 117.4 (4) |
| C25—C24—H24 | 118.6 | C15—N3—Ni2 | 117.0 (3) |

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| C23—C24—H24 | 118.6 | O3—N3—Ni2 | 125.6 (3) |
| C24—C25—C26 | 119.7 (5) | O4—N4—C16 | 121.4 (4) |
| C24—C25—H25 | 120.2 | O4—N4—Ni2 | 122.3 (3) |
| C26—C25—H25 | 120.2 | C16—N4—Ni2 | 116.2 (3) |
| C25—C26—C27 | 119.6 (5) | C29—N5—O5 | 118.5 (4) |
| C25—C26—H26 | 120.2 | C29—N5—Ni1 | 116.9 (4) |
| C27—C26—H26 | 120.2 | O5—N5—Ni1 | 124.6 (3) |
| C26—C27—C28 | 121.1 (5) | C30—N6—O6 | 121.7 (4) |
| C26—C27—H27 | 119.5 | C30—N6—Ni1 | 116.8 (3) |
| C28—C27—H27 | 119.5 | O6—N6—Ni1 | 121.5 (3) |
| C27—C28—C23 | 119.7 (5) | C43—N7—O7 | 116.4 (4) |
| C27—C28—C15 | 123.0 (5) | C43—N7—Ni2 | 127.2 (4) |
| C23—C28—C15 | 117.3 (4) | O7—N7—Ni2 | 114.4 (3) |
| N5—C29—C30 | 112.0 (4) | C44—N8—O8 | 118.6 (4) |
| N5—C29—C42 | 127.8 (5) | C57—N9—O9 | 117.6 (4) |
| C30—C29—C42 | 120.3 (4) | C57—N9—Ni3 | 117.9 (3) |
| N6—C30—C31 | 126.9 (5) | O9—N9—Ni3 | 122.1 (3) |
| N6—C30—C29 | 112.3 (4) | C58—N10—O10 | 116.3 (4) |
| C31—C30—C29 | 120.9 (4) | C58—N10—Ni3 | 115.7 (3) |
| C32—C31—C36 | 118.8 (4) | O10—N10—Ni3 | 122.3 (3) |
| C32—C31—C30 | 123.2 (5) | N1—O1—B1 | 113.0 (4) |
| C36—C31—C30 | 118.0 (5) | N2—O2—Ni1 | 127.1 (3) |
| C33—C32—C31 | 121.8 (5) | N2—O2—Ni3 | 117.6 (3) |
| C33—C32—H32 | 119.1 | Ni1—O2—Ni3 | 115.17 (16) |
| C31—C32—H32 | 119.1 | N3—O3—B2 | 118.8 (4) |
| C32—C33—C34 | 119.7 (6) | N4—O4—Ni3 | 113.1 (3) |
| C32—C33—H33 | 120.1 | N5—O5—B1 | 119.5 (4) |
| C34—C33—H33 | 120.1 | N6—O6—Ni3 | 112.9 (3) |
| C35—C34—C33 | 119.5 (5) | N7—O7—B2 | 114.4 (4) |
| C35—C34—H34 | 120.2 | N8—O8—Ni2 | 128.3 (3) |
| C33—C34—H34 | 120.2 | N8—O8—Ni3 | 115.4 (3) |
| C34—C35—C36 | 123.6 (5) | Ni2—O8—Ni3 | 116.21 (17) |
| C34—C35—H35 | 118.2 | N9—O9—H1A | 109.5 |
| C36—C35—H35 | 118.2 | N10—O10—H2A | 109.5 |
| C35—C36—C31 | 116.6 (5) | O2—Ni1—N5 | 170.30 (16) |
| C35—C36—C37 | 122.7 (5) | O2—Ni1—N6 | 88.27 (16) |
| C31—C36—C37 | 120.7 (4) | N5—Ni1—N6 | 82.07 (18) |
| C38—C37—C42 | 118.0 (5) | O2—Ni1—N1 | 90.96 (16) |
| C38—C37—C36 | 119.4 (5) | N5—Ni1—N1 | 98.53 (18) |
| C42—C37—C36 | 122.6 (5) | N6—Ni1—N1 | 173.25 (18) |
| C39—C38—C37 | 121.8 (5) | O8—Ni2—N3 | 170.42 (16) |
| C39—C38—H38 | 119.1 | O8—Ni2—N4 | 88.60 (16) |
| C37—C38—H38 | 119.1 | N3—Ni2—N4 | 81.88 (17) |
| C38—C39—C40 | 120.3 (5) | O8—Ni2—N7 | 90.78 (17) |
| C38—C39—H39 | 119.8 | N3—Ni2—N7 | 98.56 (19) |
| C40—C39—H39 | 119.8 | N4—Ni2—N7 | 173.36 (18) |
| C39—C40—C41 | 119.4 (6) | O4—Ni3—O2 | 89.28 (14) |
| C39—C40—H40 | 120.3 | O4—Ni3—N9 | 87.74 (15) |

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| C41—C40—H40 | 120.3 | O2—Ni3—N9 | 96.72 (16) |
| C42—C41—C40 | 120.9 (5) | O4—Ni3—O6 | 165.12 (14) |
| C42—C41—H41 | 119.6 | O2—Ni3—O6 | 79.77 (13) |
| C40—C41—H41 | 119.6 | N9—Ni3—O6 | 103.43 (16) |
| C41—C42—C37 | 119.6 (5) | O4—Ni3—O8 | 81.29 (14) |
| C41—C42—C29 | 123.0 (5) | O2—Ni3—O8 | 93.48 (15) |
| C37—C42—C29 | 117.4 (5) | N9—Ni3—O8 | 164.91 (17) |
| N7—C43—C56 | 127.1 (6) | O6—Ni3—O8 | 89.28 (14) |
| N7—C43—C44 | 117.3 (5) | O4—Ni3—N10 | 107.36 (16) |
| C56—C43—C44 | 115.5 (5) | O2—Ni3—N10 | 161.43 (17) |
| N8—C44—C43 | 126.5 (5) | N9—Ni3—N10 | 76.28 (17) |
| N8—C44—C45 | 114.4 (5) | O6—Ni3—N10 | 85.12 (16) |
| C43—C44—C45 | 119.1 (5) | O8—Ni3—N10 | 97.08 (16) |
| C50—C45—C46 | 120.8 (6) | F2—B1—F1 | 112.4 (5) |
| C50—C45—C44 | 118.7 (7) | F2—B1—O5 | 105.9 (5) |
| C46—C45—C44 | 120.5 (5) | F1—B1—O5 | 111.2 (5) |
| C47—C46—C45 | 121.0 (7) | F2—B1—O1 | 106.8 (5) |
| C47—C46—H46 | 119.5 | F1—B1—O1 | 108.5 (5) |
| C45—C46—H46 | 119.5 | O5—B1—O1 | 112.0 (5) |
| C46—C47—C48 | 118.5 (9) | F4—B2—F3 | 112.3 (5) |
| C46—C47—H47 | 120.7 | F4—B2—O3 | 110.4 (5) |
| C48—C47—H47 | 120.7 | F3—B2—O3 | 105.4 (5) |
| C49—C48—C47 | 120.5 (7) | F4—B2—O7 | 109.1 (5) |
| C49—C48—H48 | 119.7 | F3—B2—O7 | 106.1 (5) |
| C47—C48—H48 | 119.7 | O3—B2—O7 | 113.4 (5) |
| C48—C49—C50 | 121.7 (8) | | |

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| N1—C1—C2—N2 | −33.6 (7) | C54—C55—C56—C43 | 176.8 (5) |
| C14—C1—C2—N2 | 146.8 (5) | C52—C51—C56—C55 | −1.5 (8) |
| N1—C1—C2—C3 | 146.9 (5) | C50—C51—C56—C55 | 176.8 (5) |
| C14—C1—C2—C3 | −32.8 (6) | C52—C51—C56—C43 | −176.3 (5) |
| N2—C2—C3—C4 | 22.9 (7) | C50—C51—C56—C43 | 2.0 (8) |
| C1—C2—C3—C4 | −157.5 (5) | N7—C43—C56—C55 | 24.5 (8) |
| N2—C2—C3—C8 | −157.1 (5) | C44—C43—C56—C55 | −157.4 (5) |
| C1—C2—C3—C8 | 22.6 (7) | N7—C43—C56—C51 | −160.7 (5) |
| C8—C3—C4—C5 | 0.1 (8) | C44—C43—C56—C51 | 17.4 (7) |
| C2—C3—C4—C5 | −179.8 (5) | N9—C57—C58—N10 | −28.2 (6) |
| C3—C4—C5—C6 | −0.2 (9) | C70—C57—C58—N10 | 152.2 (4) |
| C4—C5—C6—C7 | −0.2 (10) | N9—C57—C58—C59 | 145.3 (4) |
| C5—C6—C7—C8 | 0.7 (10) | C70—C57—C58—C59 | −34.4 (6) |
| C6—C7—C8—C3 | −0.7 (8) | N10—C58—C59—C60 | 17.3 (8) |
| C6—C7—C8—C9 | 179.0 (5) | C57—C58—C59—C60 | −154.5 (5) |
| C4—C3—C8—C7 | 0.3 (8) | N10—C58—C59—C64 | −168.3 (5) |
| C2—C3—C8—C7 | −179.7 (5) | C57—C58—C59—C64 | 19.9 (6) |
| C4—C3—C8—C9 | −179.5 (5) | C64—C59—C60—C61 | −1.7 (8) |
| C2—C3—C8—C9 | 0.5 (7) | C58—C59—C60—C61 | 172.6 (5) |
| C7—C8—C9—C14 | 166.8 (5) | C59—C60—C61—C62 | 1.4 (9) |
| C3—C8—C9—C14 | −13.4 (7) | C60—C61—C62—C63 | −0.8 (9) |

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| C7—C8—C9—C10 | −15.0 (8) | C61—C62—C63—C64 | 0.3 (8) |
| C3—C8—C9—C10 | 164.8 (5) | C60—C59—C64—C63 | 1.2 (7) |
| C14—C9—C10—C11 | −0.2 (7) | C58—C59—C64—C63 | −173.3 (4) |
| C8—C9—C10—C11 | −178.5 (5) | C60—C59—C64—C65 | 179.8 (4) |
| C9—C10—C11—C12 | 1.3 (8) | C58—C59—C64—C65 | 5.3 (6) |
| C10—C11—C12—C13 | −1.1 (8) | C62—C63—C64—C59 | −0.6 (7) |
| C11—C12—C13—C14 | −0.1 (8) | C62—C63—C64—C65 | −179.2 (5) |
| C12—C13—C14—C9 | 1.2 (7) | C59—C64—C65—C66 | 164.0 (5) |
| C12—C13—C14—C1 | 175.8 (5) | C63—C64—C65—C66 | −17.5 (7) |
| C10—C9—C14—C13 | −1.0 (7) | C59—C64—C65—C70 | −17.0 (7) |
| C8—C9—C14—C13 | 177.2 (5) | C63—C64—C65—C70 | 161.6 (5) |
| C10—C9—C14—C1 | −175.8 (4) | C70—C65—C66—C67 | 0.5 (7) |
| C8—C9—C14—C1 | 2.5 (7) | C64—C65—C66—C67 | 179.6 (4) |
| N1—C1—C14—C13 | 26.0 (7) | C65—C66—C67—C68 | −0.3 (8) |
| C2—C1—C14—C13 | −154.4 (5) | C66—C67—C68—C69 | 0.0 (8) |
| N1—C1—C14—C9 | −159.3 (5) | C67—C68—C69—C70 | 0.0 (8) |
| C2—C1—C14—C9 | 20.3 (6) | C68—C69—C70—C65 | 0.2 (8) |
| N3—C15—C16—N4 | −5.2 (6) | C68—C69—C70—C57 | 178.7 (5) |
| C28—C15—C16—N4 | 173.2 (4) | C66—C65—C70—C69 | −0.5 (7) |
| N3—C15—C16—C17 | 170.7 (4) | C64—C65—C70—C69 | −179.5 (4) |
| C28—C15—C16—C17 | −10.9 (7) | C66—C65—C70—C57 | −179.1 (4) |
| N4—C16—C17—C18 | −3.1 (8) | C64—C65—C70—C57 | 1.9 (7) |
| C15—C16—C17—C18 | −178.4 (4) | N9—C57—C70—C69 | 24.8 (8) |
| N4—C16—C17—C22 | 174.2 (5) | C58—C57—C70—C69 | −155.6 (5) |
| C15—C16—C17—C22 | −1.0 (7) | N9—C57—C70—C65 | −156.6 (5) |
| C22—C17—C18—C19 | −1.5 (8) | C58—C57—C70—C65 | 23.0 (6) |
| C16—C17—C18—C19 | 175.9 (5) | C2—C1—N1—O1 | −173.7 (4) |
| C17—C18—C19—C20 | −1.3 (9) | C14—C1—N1—O1 | 6.0 (7) |
| C18—C19—C20—C21 | 2.5 (9) | C2—C1—N1—Ni1 | 23.2 (6) |
| C19—C20—C21—C22 | −1.1 (9) | C14—C1—N1—Ni1 | −157.2 (4) |
| C20—C21—C22—C17 | −1.7 (8) | C3—C2—N2—O2 | −175.1 (4) |
| C20—C21—C22—C23 | 174.2 (5) | C1—C2—N2—O2 | 5.3 (7) |
| C18—C17—C22—C21 | 2.9 (7) | C28—C15—N3—O3 | 2.9 (7) |
| C16—C17—C22—C21 | −174.6 (5) | C16—C15—N3—O3 | −178.9 (4) |
| C18—C17—C22—C23 | −172.9 (4) | C28—C15—N3—Ni2 | −176.9 (4) |
| C16—C17—C22—C23 | 9.6 (7) | C16—C15—N3—Ni2 | 1.4 (5) |
| C21—C22—C23—C24 | −5.0 (8) | C17—C16—N4—O4 | 9.2 (7) |
| C17—C22—C23—C24 | 170.7 (5) | C15—C16—N4—O4 | −175.3 (4) |
| C21—C22—C23—C28 | 177.8 (5) | C17—C16—N4—Ni2 | −168.8 (4) |
| C17—C22—C23—C28 | −6.6 (7) | C15—C16—N4—Ni2 | 6.8 (5) |
| C28—C23—C24—C25 | 2.0 (8) | C30—C29—N5—O5 | −178.1 (4) |
| C22—C23—C24—C25 | −175.3 (5) | C42—C29—N5—O5 | 0.8 (8) |
| C23—C24—C25—C26 | 0.8 (9) | C30—C29—N5—Ni1 | 1.0 (5) |
| C24—C25—C26—C27 | −2.5 (9) | C42—C29—N5—Ni1 | 179.9 (4) |
| C25—C26—C27—C28 | 1.4 (8) | C31—C30—N6—O6 | 1.7 (7) |
| C26—C27—C28—C23 | 1.5 (8) | C29—C30—N6—O6 | −178.3 (4) |
| C26—C27—C28—C15 | −178.9 (5) | C31—C30—N6—Ni1 | −178.0 (4) |
| C24—C23—C28—C27 | −3.1 (7) | C29—C30—N6—Ni1 | 2.0 (5) |

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| C22—C23—C28—C27 | 174.2 (5) | C56—C43—N7—O7 | 2.8 (8) |
| C24—C23—C28—C15 | 177.3 (5) | C44—C43—N7—O7 | −175.3 (4) |
| C22—C23—C28—C15 | −5.4 (7) | C56—C43—N7—Ni2 | −160.1 (4) |
| N3—C15—C28—C27 | 12.4 (8) | C44—C43—N7—Ni2 | 21.8 (7) |
| C16—C15—C28—C27 | −165.7 (5) | C43—C44—N8—O8 | 4.6 (8) |
| N3—C15—C28—C23 | −168.0 (5) | C45—C44—N8—O8 | −175.8 (4) |
| C16—C15—C28—C23 | 13.9 (7) | C70—C57—N9—O9 | 0.4 (8) |
| N5—C29—C30—N6 | −1.9 (6) | C58—C57—N9—O9 | −179.2 (4) |
| C42—C29—C30—N6 | 179.1 (4) | C70—C57—N9—Ni3 | −162.4 (4) |
| N5—C29—C30—C31 | 178.1 (4) | C58—C57—N9—Ni3 | 18.0 (5) |
| C42—C29—C30—C31 | −0.9 (7) | C59—C58—N10—O10 | 7.1 (8) |
| N6—C30—C31—C32 | −0.6 (8) | C57—C58—N10—O10 | 179.3 (4) |
| C29—C30—C31—C32 | 179.4 (5) | C59—C58—N10—Ni3 | −147.0 (4) |
| N6—C30—C31—C36 | 179.1 (5) | C57—C58—N10—Ni3 | 25.2 (5) |
| C29—C30—C31—C36 | −0.9 (7) | C1—N1—O1—B1 | 137.4 (5) |
| C36—C31—C32—C33 | 2.2 (8) | Ni1—N1—O1—B1 | −57.6 (5) |
| C30—C31—C32—C33 | −178.1 (5) | C2—N2—O2—Ni1 | 32.8 (6) |
| C31—C32—C33—C34 | −1.0 (9) | C2—N2—O2—Ni3 | −142.9 (4) |
| C32—C33—C34—C35 | −0.1 (10) | C15—N3—O3—B2 | −175.3 (5) |
| C33—C34—C35—C36 | 0.0 (10) | Ni2—N3—O3—B2 | 4.4 (7) |
| C34—C35—C36—C31 | 1.2 (8) | C16—N4—O4—Ni3 | −145.0 (4) |
| C34—C35—C36—C37 | 179.5 (6) | Ni2—N4—O4—Ni3 | 32.9 (4) |
| C32—C31—C36—C35 | −2.2 (7) | C29—N5—O5—B1 | −173.4 (5) |
| C30—C31—C36—C35 | 178.1 (5) | Ni1—N5—O5—B1 | 7.6 (7) |
| C32—C31—C36—C37 | 179.4 (4) | C30—N6—O6—Ni3 | −146.0 (4) |
| C30—C31—C36—C37 | −0.3 (7) | Ni1—N6—O6—Ni3 | 33.6 (4) |
| C35—C36—C37—C38 | 4.1 (7) | C43—N7—O7—B2 | 139.1 (5) |
| C31—C36—C37—C38 | −177.6 (4) | Ni2—N7—O7—B2 | −55.7 (5) |
| C35—C36—C37—C42 | −174.7 (5) | C44—N8—O8—Ni2 | 29.2 (6) |
| C31—C36—C37—C42 | 3.6 (7) | C44—N8—O8—Ni3 | −146.7 (4) |
| C42—C37—C38—C39 | 1.9 (8) | N2—O2—Ni1—N6 | 152.7 (4) |
| C36—C37—C38—C39 | −177.0 (5) | Ni3—O2—Ni1—N6 | −31.5 (2) |
| C37—C38—C39—C40 | −0.1 (9) | N2—O2—Ni1—N1 | −34.0 (4) |
| C38—C39—C40—C41 | −0.6 (8) | Ni3—O2—Ni1—N1 | 141.8 (2) |
| C39—C40—C41—C42 | −0.6 (8) | C29—N5—Ni1—N6 | 0.0 (4) |
| C40—C41—C42—C37 | 2.4 (8) | O5—N5—Ni1—N6 | 179.0 (4) |
| C40—C41—C42—C29 | −176.4 (5) | C29—N5—Ni1—N1 | −173.2 (4) |
| C38—C37—C42—C41 | −3.0 (7) | O5—N5—Ni1—N1 | 5.8 (4) |
| C36—C37—C42—C41 | 175.8 (4) | C30—N6—Ni1—O2 | 177.9 (4) |
| C38—C37—C42—C29 | 175.9 (4) | O6—N6—Ni1—O2 | −1.7 (3) |
| C36—C37—C42—C29 | −5.2 (7) | C30—N6—Ni1—N5 | −1.2 (4) |
| N5—C29—C42—C41 | 4.0 (8) | O6—N6—Ni1—N5 | 179.1 (4) |
| C30—C29—C42—C41 | −177.2 (4) | C1—N1—Ni1—O2 | 4.2 (4) |
| N5—C29—C42—C37 | −174.9 (5) | O1—N1—Ni1—O2 | −159.1 (3) |
| C30—C29—C42—C37 | 3.9 (7) | C1—N1—Ni1—N5 | −177.8 (4) |
| N7—C43—C44—N8 | −29.8 (8) | O1—N1—Ni1—N5 | 19.0 (4) |
| C56—C43—C44—N8 | 151.8 (5) | N8—O8—Ni2—N4 | 157.2 (4) |
| N7—C43—C44—C45 | 150.5 (5) | Ni3—O8—Ni2—N4 | −27.0 (2) |

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| C56—C43—C44—C45 | −27.8 (7) | N8—O8—Ni2—N7 | −29.5 (4) |
| N8—C44—C45—C50 | −161.0 (5) | Ni3—O8—Ni2—N7 | 146.4 (2) |
| C43—C44—C45—C50 | 18.7 (7) | C15—N3—Ni2—N4 | 1.7 (4) |
| N8—C44—C45—C46 | 18.7 (8) | O3—N3—Ni2—N4 | −178.0 (4) |
| C43—C44—C45—C46 | −161.6 (5) | C15—N3—Ni2—N7 | −171.6 (4) |
| C50—C45—C46—C47 | −0.2 (9) | O3—N3—Ni2—N7 | 8.7 (4) |
| C44—C45—C46—C47 | −179.9 (6) | O4—N4—Ni2—O8 | −3.9 (3) |
| C45—C46—C47—C48 | −0.4 (11) | C16—N4—Ni2—O8 | 174.1 (4) |
| C46—C47—C48—C49 | 0.8 (12) | O4—N4—Ni2—N3 | 177.1 (4) |
| C47—C48—C49—C50 | −0.6 (12) | C16—N4—Ni2—N3 | −4.9 (3) |
| C46—C45—C50—C49 | 0.4 (9) | C43—N7—Ni2—O8 | 2.3 (5) |
| C44—C45—C50—C49 | −179.9 (5) | O7—N7—Ni2—O8 | −161.0 (3) |
| C46—C45—C50—C51 | −178.3 (5) | C43—N7—Ni2—N3 | −179.8 (5) |
| C44—C45—C50—C51 | 1.4 (8) | O7—N7—Ni2—N3 | 16.9 (4) |
| C48—C49—C50—C45 | 0.0 (10) | N5—O5—B1—F2 | −161.0 (5) |
| C48—C49—C50—C51 | 178.7 (7) | N5—O5—B1—F1 | 76.6 (7) |
| C45—C50—C51—C52 | 166.2 (5) | N5—O5—B1—O1 | −45.0 (7) |
| C49—C50—C51—C52 | −12.4 (9) | N1—O1—B1—F2 | −170.9 (4) |
| C45—C50—C51—C56 | −12.1 (8) | N1—O1—B1—F1 | −49.6 (6) |
| C49—C50—C51—C56 | 169.3 (6) | N1—O1—B1—O5 | 73.6 (6) |
| C56—C51—C52—C53 | −0.8 (9) | N3—O3—B2—F4 | 80.1 (6) |
| C50—C51—C52—C53 | −179.1 (6) | N3—O3—B2—F3 | −158.4 (5) |
| C51—C52—C53—C54 | 2.5 (10) | N3—O3—B2—O7 | −42.7 (7) |
| C52—C53—C54—C55 | −1.9 (10) | N7—O7—B2—F4 | −50.1 (6) |
| C53—C54—C55—C56 | −0.4 (9) | N7—O7—B2—F3 | −171.4 (4) |
| C54—C55—C56—C51 | 2.1 (8) | N7—O7—B2—O3 | 73.4 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O9—H1*A*···N2 | 0.85 | 1.96 | 2.771 (6) | 158 |
| O10—H2*A*···N8 | 1.06 | 1.77 | 2.765 (6) | 155 |