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# [5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]nickel(II)–toluene–dichloromethane (3/2/4): a mixed solvate

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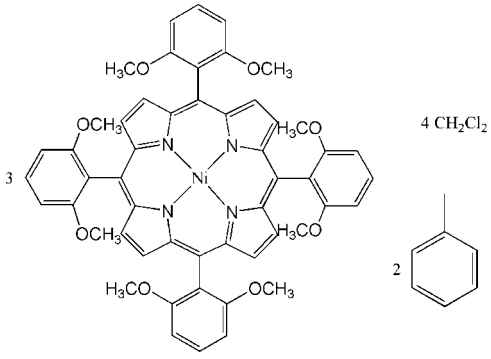
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.048; $wR$ factor = 0.117; data-to-parameter ratio = 14.4.

The crystal structure, electronic spectroscopy, and $^1$H NMR data for the title compound, $[Ni(C_{52}H_{44}N_4O_8)]\cdot0.67C_7H_8\cdot1.33CH_2Cl_2$, are reported. The compound was prepared by the reaction of nickel(II) acetate with the ligand in refluxing glacial acetic acid. The asymmetric unit consists of 1.5 nickel porphyrins, two dichloromethane molecules and one toluene molecule. One of the nickel–porphyrinate molecules is located on an inversion center and is planar in the solid state, while the other assumes a saddle-shaped geometry. In both cases, the nickel ion is four-coordinate.

## Related literature

For details of the synthesis, see: Tsuchida *et al.* (1990). For related examples of *ortho*-substituted porphyrins, see: Bhyrappa *et al.* (1997). For related literature, see: Allen (2002); Arciero & Hooper (1997); Arciero *et al.* (1993); Igarashi *et al.* (1997); Kadish *et al.* (2002); Rothemund & Menotti (1948).




## Experimental

### Crystal data

$[Ni(C_{52}H_{44}N_4O_8)]\cdot0.67C_7H_8\cdot1.33CH_2Cl_2$
$M_r$ = 1086.26
Monoclinic, $P2_1/n$
$a$ = 16.8286 (10) Å
$b$ = 26.1041 (15) Å
$c$ = 17.6845 (10) Å
$\beta$ = 92.813 (1)°
$V$ = 7759.4 (8) Å$^3$
$Z$ = 6
Mo $K\alpha$ radiation
$\mu$ = 0.57 mm$^{-1}$
$T$ = 100 (2) K
0.35 × 0.35 × 0.35 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS* in *SAINT-Plus*; Bruker, 2003)
$T_{min}$ = 0.583, $T_{max}$ = 0.818
72528 measured reflections
15859 independent reflections
13340 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.117
$S$ = 1.07
15859 reflections
1100 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.07 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We thank Brian Gilmartin at the Pennsylvania State University for technical assistance in collecting NMR data. The SMART APEX diffractometer was funded by NSF grant 0087210, by Ohio Board of Regents grant CAP-491, and by YSU. This material is based upon work supported by the National Science Foundation under grant No. 0525440.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2051).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2824 [ **doi:10.1107/S1600536807051872** ]

# [5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]nickel(II)-toluene-dichloromethane (3/2/4):a mixed solvate

**D. Conrad, J. DeCoskey, C. Yeisley, M. Zeller, A. D. Hunter and E. P. Zovinka**

## Comment

The chemistry of the enzyme hydroxylamine oxidoreductase (HAO) from nitrosomonas europaea has been of interest for a number of years (Arciero & Hooper, 1997). The X-ray crystal structure of HAO shows a complex trimer with each subunit containing seven c-type heme units in addition to a novel heme at the active site, heme P460 (Igarashi *et al.*, 1997). The 5-coordinate heme P460 active site appears to have originated from a five-coordinate c-type heme from one subunit that has been modified with a covalent crosslink to a tyrosine residue from the adjacent subunit (Arciero & Hooper, 1997; Igarashi *et al.*, 1997; Arciero *et al.*, 1993). The C3 ring carbon of the tyrosine is linked to the 5 *meso* position of the heme, so that the oxygen of the tyrosine is "*ortho*" to the porphyrin *meso* carbon (Igarashi *et al.*, 1997; Arciero *et al.*, 1993). In order to explore the chemistry of synthetic models of heme P460, we have begun a systematic examination of *ortho* substituted porphyrins, beginning with tetra(2',6'-dimethoxyphenyl)porphyrin, ($H_2$T-2',6'-DMP)P. The molecule has oxygen substituents in the *ortho* position and serves as the non reactive control to compare with the more redox active ligand, tetra(2',6'-dihydroxyphenyl)porphyrin. Future work will focus on synthesizing and studying the more reactive metal ligand complexes with the biologically important iron ion.

The characterized metalloporphyrin is stable to both air and moisture in both the solid and solution environments. Following purification, different solvent systems including toluene, were examined in order to determine the best system. X-ray quality crystals were obtained by layering a dichloromethane solution of the metalloporphyrin with pentane. The asymmetric unit consists of 1.5 nickel porphyrins, 2 dichloromethanes, and one toluene molecule. The toluene molecule was carried over from the test solutions. One of the Ni[T(2',6'-DMP)P] molecules is located on an inversion center and is planar in the solid state (Figure 1) while the other assumes a saddle-shaped geometry (Figure 2). In both cases the nickel ion are 1.9474 (19)Å and 1.9554 (19)Å while they range between 1.9198 (19)Å and 1.9319 (19)Å for the ruffled complex. Non-planar nickel porphyrins are commonly known to exist because the small nickel ion favors a short metal-nitrogen bond distance leading to porphyrin conformational flexibility (Kadish *et al.*, 2002). The coordination geometry is unexceptional and similar to other nickel porphyrin systems, average Ni—N bond distance of 1.920 Å listed in the Cambridge Crystallographic Database (Allen, 2002).

## Experimental

All of the starting materials were purchased from Aldrich and used without further purification. The ligand, 5,10,15,20-tetra-(2',6'-dimethoxyphenyl)porphyrin, [($H_2$T-2',6'-DMP)P] was synthesized following literature methods (Tsuchida *et al.*, 1990). The porphyrin ligand, ($H_2$T-2',6'-DMP)P, (17.0 mg, $2.0\times10^{-5}$ mol) was dissolved in glacial acetic acid (20 ml). Nickel acetate (0.50 mg, $2.0\times10^{-4}$ mol) was added after all of the ligand dissolved and then heated to reflux at 391 K (118 °C) for half an hour (Rothemund, 1948). Upon cooling, the solvent was removed through rotary evaporation. The resulting red crystals were dissolved in dichloromethane and the solution was chromatographed on a dry alumina column with dichloromethane as the eluent. (60% Yield); Rf (Alumina, DCM) 0.95; I·*R*·(KBr): 1587, 1471, 1431, 1348, 1250 [$\mu_{as}$ (C—O—C)],

1110, and 1002 [μ (C—H)] $cm^{-1}$; $\lambda_{max}$(DCM): 413, 526, and 557 nm; ε: 1.2×105, 7.8×103, and 2.2×103 $cm^{-1}M^{-1.1}$HNMR ($CDCl_3$): 3.5(–OMe), 6.9–7.5(aromatic), and 8.6(pyrrole) p.p.m..

### Refinement

Methyl and methylene chloride H atoms were placed in calculated positions with C—H = 0.98 and 0.99 Å, respectively. All other H atoms were located in difference density Fourier maps. H atoms were refined with $U_{iso}$(H) = 1.2 $U_{eq}$ or 1.5 $U_{eq}$ ($C_{Me}$ only) of the respective carrier atoms.

### Figures

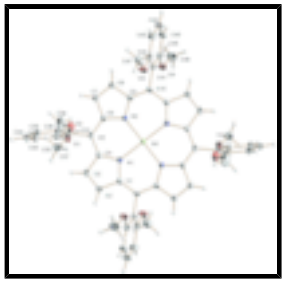

Fig. 1. Ellipsoid (50% probability) plot of planar Ni[T(2',6'-DMP)P]

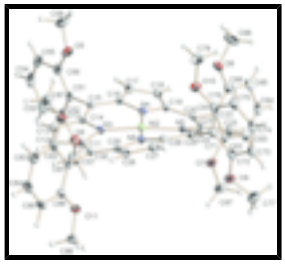

Fig. 2. : Ellispoid (50% probability) plot of saddle-shaped Ni[T(2',6'-DMP)P]

### [5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]nickel(II)–toluene– dichloromethane (3/2/4)

*Crystal data*

| | |
|---|---|
| $[Ni(C_{52}H_{44}N_4O_8)]\cdot 0.67C_7H_8\cdot 1.33CH_2Cl_2$ | $F_{000}$ = 3392 |
| $M_r$ = 1086.26 | $D_x$ = 1.395 Mg $m^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 9043 reflections |
| $a$ = 16.8286 (10) Å | θ = 2.3–32.0º |
| $b$ = 26.1041 (15) Å | μ = 0.57 $mm^{-1}$ |
| $c$ = 17.6845 (10) Å | $T$ = 100 (2) K |
| β = 92.813 (1)º | Octagonal column, red |
| $V$ = 7759.4 (8) $Å^3$ | 0.35 × 0.35 × 0.35 mm |
| $Z$ = 6 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 15859 independent reflections |
| Radiation source: fine-focus sealed tube | 13340 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.036$ |
| $T = 100(2)$ K | $\theta_{max} = 26.4^{o}$ |
| ω scans | $\theta_{min} = 1.4^{o}$ |
| Absorption correction: multi-scan (SADABS in SAINT-Plus; Bruker, 2003) | $h = -21 \rightarrow 21$ |
| $T_{min} = 0.583$, $T_{max} = 0.818$ | $k = 0 \rightarrow 32$ |
| 72528 measured reflections | $l = 0 \rightarrow 22$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.117$ | $w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 10.5281P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.07$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 15859 reflections | $\Delta\rho_{max} = 1.07$ e Å$^{-3}$ |
| 1100 parameters | $\Delta\rho_{min} = -0.59$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. Hydrogen atoms of the solvent molecules and methyl hydrogen atoms were placed in calculated positions and were refined with an isotropic displacement parameter 1.2 (methylene, aromatic) or 1.5 (methyl) times that of the adjacent carbon atom. Methyl hydrogen atoms were allowed to rotate to best fit the experimental electron density. All other hydrogen atoms were located in the difference Fourier map and were refined with an isotropic displacement parameter 1.2 times that of the adjacent carbon atom.

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| Ni2 | 0.596867 (17) | 0.241274 (11) | 0.612644 (16) | 0.01220 (8) |
| N4 | 0.68062 (11) | 0.28069 (8) | 0.57001 (11) | 0.0142 (4) |
| N3 | 0.53415 (11) | 0.24643 (7) | 0.51849 (11) | 0.0141 (4) |
| O7 | 0.89977 (10) | 0.18742 (7) | 0.63691 (10) | 0.0237 (4) |
| N6 | 0.50932 (11) | 0.20910 (7) | 0.65961 (11) | 0.0141 (4) |
| N5 | 0.66332 (11) | 0.22972 (7) | 0.70310 (11) | 0.0137 (4) |
| O8 | 0.84678 (11) | 0.35033 (7) | 0.72834 (11) | 0.0262 (4) |
| O11 | 0.40439 (10) | 0.09919 (7) | 0.48806 (11) | 0.0236 (4) |
| O6 | 0.69411 (11) | 0.25715 (7) | 0.33494 (10) | 0.0251 (4) |
| O10 | 0.49128 (11) | 0.27889 (7) | 0.86637 (10) | 0.0265 (4) |
| C19 | 0.75781 (14) | 0.28722 (9) | 0.59886 (13) | 0.0151 (5) |
| O12 | 0.27877 (11) | 0.25079 (7) | 0.55419 (12) | 0.0273 (4) |
| C61 | 0.87726 (14) | 0.26963 (10) | 0.68284 (13) | 0.0171 (5) |
| O9 | 0.60155 (12) | 0.11457 (7) | 0.87314 (10) | 0.0267 (4) |
| C21 | 0.74458 (14) | 0.23685 (9) | 0.71209 (13) | 0.0149 (5) |
| C16 | 0.67716 (14) | 0.30818 (9) | 0.50290 (13) | 0.0158 (5) |
| C20 | 0.79052 (13) | 0.26313 (9) | 0.66264 (13) | 0.0148 (5) |
| C11 | 0.46349 (14) | 0.22146 (9) | 0.49961 (13) | 0.0159 (5) |
| C81 | 0.33861 (14) | 0.17382 (10) | 0.52166 (13) | 0.0179 (5) |
| C76 | 0.50707 (15) | 0.23676 (10) | 0.90949 (14) | 0.0206 (5) |
| O5 | 0.56918 (13) | 0.40381 (7) | 0.42029 (12) | 0.0332 (5) |
| C51 | 0.62966 (14) | 0.33097 (10) | 0.37358 (14) | 0.0196 (5) |
| C63 | 1.01218 (15) | 0.23661 (11) | 0.69016 (14) | 0.0227 (5) |
| H63 | 1.0486 (18) | 0.2099 (12) | 0.6846 (17) | 0.027* |
| C14 | 0.55155 (14) | 0.27339 (9) | 0.45416 (13) | 0.0161 (5) |
| C25 | 0.56294 (14) | 0.20379 (9) | 0.79141 (13) | 0.0170 (5) |
| C71 | 0.54430 (14) | 0.19650 (10) | 0.87226 (13) | 0.0183 (5) |
| C26 | 0.50200 (14) | 0.20021 (9) | 0.73618 (13) | 0.0163 (5) |
| C24 | 0.64059 (14) | 0.21387 (9) | 0.77339 (13) | 0.0161 (5) |
| C66 | 0.90475 (15) | 0.31501 (10) | 0.71644 (14) | 0.0204 (5) |
| C27 | 0.42455 (15) | 0.18019 (10) | 0.74965 (15) | 0.0199 (5) |
| H27 | 0.4072 (17) | 0.1712 (11) | 0.7960 (17) | 0.024* |
| C29 | 0.43799 (14) | 0.19333 (9) | 0.62593 (14) | 0.0159 (5) |
| C18 | 0.80039 (15) | 0.32123 (10) | 0.55187 (14) | 0.0180 (5) |
| H18 | 0.8524 (18) | 0.3318 (11) | 0.5610 (16) | 0.022* |
| C13 | 0.49232 (15) | 0.26431 (10) | 0.39483 (14) | 0.0198 (5) |
| H13 | 0.4931 (17) | 0.2790 (11) | 0.3487 (17) | 0.024* |
| C82 | 0.26848 (15) | 0.20226 (10) | 0.52574 (15) | 0.0218 (5) |
| C12 | 0.43876 (15) | 0.23178 (10) | 0.42224 (14) | 0.0199 (5) |
| H12 | 0.3946 (18) | 0.2196 (11) | 0.3989 (17) | 0.024* |
| C15 | 0.61727 (14) | 0.30463 (9) | 0.44733 (13) | 0.0163 (5) |
| C86 | 0.33303 (15) | 0.12423 (10) | 0.49208 (14) | 0.0206 (5) |
| C30 | 0.41679 (14) | 0.19564 (9) | 0.54936 (13) | 0.0153 (5) |
| C28 | 0.38597 (15) | 0.17516 (9) | 0.68174 (14) | 0.0186 (5) |
| H28 | 0.3333 (18) | 0.1630 (11) | 0.6689 (16) | 0.022* |
| C23 | 0.70803 (15) | 0.20973 (10) | 0.82528 (14) | 0.0193 (5) |
| H23 | 0.7059 (17) | 0.2007 (11) | 0.8756 (17) | 0.023* |
| C64 | 1.03728 (16) | 0.28227 (12) | 0.72230 (15) | 0.0255 (6) |
| H64 | 1.0896 (19) | 0.2870 (12) | 0.7353 (17) | 0.031* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.75053 (15) | 0.33476 (10) | 0.49350 (14) | 0.0192 (5) |
| H17 | 0.7602 (17) | 0.3581 (11) | 0.4515 (17) | 0.023* |
| C88 | 0.40178 (17) | 0.04627 (10) | 0.46742 (16) | 0.0260 (6) |
| H88A | 0.3704 | 0.0273 | 0.5034 | 0.039* |
| H88B | 0.4560 | 0.0325 | 0.4684 | 0.039* |
| H88C | 0.3772 | 0.0427 | 0.4163 | 0.039* |
| C62 | 0.93145 (14) | 0.23035 (10) | 0.66991 (13) | 0.0178 (5) |
| C74 | 0.51001 (15) | 0.18744 (11) | 1.02360 (15) | 0.0241 (6) |
| H74 | 0.4990 (18) | 0.1845 (12) | 1.0741 (18) | 0.029* |
| C73 | 0.54676 (16) | 0.14733 (11) | 0.98899 (15) | 0.0242 (6) |
| H73 | 0.5597 (18) | 0.1172 (12) | 1.0135 (18) | 0.029* |
| C22 | 0.77252 (15) | 0.22230 (10) | 0.78716 (14) | 0.0179 (5) |
| H22 | 0.8257 (18) | 0.2238 (11) | 0.8041 (16) | 0.022* |
| C72 | 0.56433 (15) | 0.15206 (10) | 0.91275 (14) | 0.0210 (5) |
| C52 | 0.67073 (15) | 0.30599 (11) | 0.31744 (14) | 0.0221 (5) |
| C56 | 0.60523 (16) | 0.38164 (11) | 0.36116 (16) | 0.0259 (6) |
| C75 | 0.48903 (15) | 0.23228 (11) | 0.98583 (15) | 0.0238 (6) |
| H75 | 0.4628 (18) | 0.2612 (12) | 1.0097 (17) | 0.029* |
| C85 | 0.26012 (16) | 0.10302 (11) | 0.46886 (17) | 0.0272 (6) |
| H85 | 0.2583 (18) | 0.0686 (13) | 0.4495 (18) | 0.033* |
| C65 | 0.98518 (16) | 0.32191 (11) | 0.73549 (14) | 0.0241 (6) |
| H65 | 1.0034 (18) | 0.3505 (12) | 0.7589 (17) | 0.029* |
| C67 | 0.95131 (17) | 0.14461 (11) | 0.62543 (17) | 0.0291 (6) |
| H67A | 0.9947 | 0.1552 | 0.5938 | 0.044* |
| H67B | 0.9209 | 0.1169 | 0.6001 | 0.044* |
| H67C | 0.9735 | 0.1325 | 0.6745 | 0.044* |
| C78 | 0.4623 (2) | 0.32409 (12) | 0.90185 (17) | 0.0370 (7) |
| H78A | 0.4090 | 0.3176 | 0.9195 | 0.055* |
| H78B | 0.4600 | 0.3523 | 0.8653 | 0.055* |
| H78C | 0.4982 | 0.3333 | 0.9450 | 0.055* |
| C54 | 0.65872 (17) | 0.38009 (13) | 0.23798 (17) | 0.0339 (7) |
| H54 | 0.6695 (19) | 0.3962 (13) | 0.190 (2) | 0.041* |
| C87 | 0.20951 (17) | 0.28180 (11) | 0.55885 (17) | 0.0297 (6) |
| H87A | 0.1831 | 0.2851 | 0.5084 | 0.045* |
| H87B | 0.2248 | 0.3158 | 0.5780 | 0.045* |
| H87C | 0.1730 | 0.2658 | 0.5933 | 0.045* |
| C53 | 0.68507 (16) | 0.33037 (13) | 0.24927 (15) | 0.0293 (6) |
| H53 | 0.7141 (19) | 0.3126 (12) | 0.2121 (19) | 0.035* |
| C83 | 0.19512 (16) | 0.18168 (12) | 0.50232 (17) | 0.0283 (6) |
| H83 | 0.1481 (19) | 0.2020 (12) | 0.5056 (18) | 0.034* |
| C84 | 0.19222 (17) | 0.13226 (12) | 0.47404 (18) | 0.0315 (7) |
| H84 | 0.142 (2) | 0.1179 (13) | 0.4588 (18) | 0.038* |
| C57 | 0.75223 (17) | 0.23331 (12) | 0.28985 (17) | 0.0331 (7) |
| H57A | 0.7305 | 0.2296 | 0.2377 | 0.050* |
| H57B | 0.7657 | 0.1994 | 0.3107 | 0.050* |
| H57C | 0.8002 | 0.2546 | 0.2903 | 0.050* |
| C55 | 0.61919 (18) | 0.40616 (13) | 0.29261 (18) | 0.0340 (7) |
| H55 | 0.601 (2) | 0.4378 (14) | 0.2860 (19) | 0.041* |
| C77 | 0.6456 (2) | 0.07702 (13) | 0.91679 (19) | 0.0421 (8) |

| | | | | |
|---|---|---|---|---|
| H77A | 0.6825 | 0.0942 | 0.9531 | 0.063* |
| H77B | 0.6757 | 0.0555 | 0.8830 | 0.063* |
| H77C | 0.6087 | 0.0556 | 0.9442 | 0.063* |
| C58 | 0.5607 (2) | 0.45806 (12) | 0.4196 (2) | 0.0420 (8) |
| H58A | 0.6127 | 0.4740 | 0.4131 | 0.063* |
| H58B | 0.5399 | 0.4694 | 0.4676 | 0.063* |
| H58C | 0.5238 | 0.4682 | 0.3777 | 0.063* |
| C68 | 0.8687 (2) | 0.39563 (13) | 0.7681 (2) | 0.0446 (9) |
| H68A | 0.8940 | 0.3866 | 0.8174 | 0.067* |
| H68B | 0.8212 | 0.4164 | 0.7756 | 0.067* |
| H68C | 0.9062 | 0.4153 | 0.7388 | 0.067* |
| Ni1 | 1.0000 | 0.0000 | 0.5000 | 0.01166 (9) |
| O1 | 0.77710 (10) | 0.14246 (7) | 0.45736 (10) | 0.0232 (4) |
| N2 | 0.95487 (11) | 0.02206 (7) | 0.40132 (11) | 0.0135 (4) |
| N1 | 0.89857 (11) | 0.01353 (7) | 0.54459 (11) | 0.0133 (4) |
| O3 | 1.11481 (11) | 0.10768 (7) | 0.28228 (10) | 0.0251 (4) |
| O4 | 1.09479 (11) | −0.06494 (7) | 0.22073 (10) | 0.0247 (4) |
| O2 | 0.70622 (11) | −0.01526 (7) | 0.35264 (12) | 0.0299 (4) |
| C4 | 0.82942 (14) | 0.03238 (9) | 0.50919 (13) | 0.0146 (5) |
| C31 | 0.73783 (14) | 0.06384 (9) | 0.40707 (13) | 0.0155 (5) |
| C5 | 0.81837 (14) | 0.04401 (9) | 0.43304 (13) | 0.0147 (5) |
| C6 | 0.87830 (14) | 0.03886 (9) | 0.38304 (13) | 0.0155 (5) |
| C2 | 0.79852 (14) | 0.02140 (9) | 0.62966 (14) | 0.0175 (5) |
| H2 | 0.7739 (16) | 0.0204 (11) | 0.6768 (16) | 0.021* |
| C9 | 0.99282 (14) | 0.02552 (9) | 0.33387 (13) | 0.0152 (5) |
| C41 | 1.10539 (14) | 0.02204 (9) | 0.24785 (13) | 0.0162 (5) |
| C10 | 1.07108 (14) | 0.01279 (9) | 0.32309 (13) | 0.0146 (5) |
| C1 | 0.87928 (14) | 0.00641 (9) | 0.61884 (13) | 0.0153 (5) |
| C3 | 0.76809 (15) | 0.03784 (9) | 0.56207 (14) | 0.0173 (5) |
| H3 | 0.7178 (17) | 0.0510 (11) | 0.5498 (16) | 0.021* |
| C7 | 0.86906 (15) | 0.05238 (10) | 0.30469 (14) | 0.0185 (5) |
| H7 | 0.8211 (18) | 0.0655 (11) | 0.2842 (16) | 0.022* |
| C32 | 0.71661 (15) | 0.11368 (10) | 0.42606 (14) | 0.0196 (5) |
| C8 | 0.93984 (15) | 0.04450 (9) | 0.27425 (14) | 0.0179 (5) |
| H8 | 0.9556 (16) | 0.0515 (11) | 0.2239 (17) | 0.022* |
| C46 | 1.11854 (15) | −0.01760 (10) | 0.19747 (14) | 0.0197 (5) |
| C36 | 0.68011 (15) | 0.03202 (10) | 0.37257 (15) | 0.0214 (5) |
| C34 | 0.58228 (16) | 0.09765 (11) | 0.38401 (15) | 0.0256 (6) |
| H34 | 0.5295 (19) | 0.1092 (12) | 0.3801 (17) | 0.031* |
| C33 | 0.63846 (16) | 0.13127 (11) | 0.41439 (15) | 0.0232 (6) |
| H33 | 0.6255 (18) | 0.1634 (12) | 0.4278 (17) | 0.028* |
| C42 | 1.12752 (15) | 0.07169 (10) | 0.22874 (14) | 0.0202 (5) |
| C35 | 0.60150 (16) | 0.04870 (11) | 0.36158 (16) | 0.0253 (6) |
| H35 | 0.5617 (19) | 0.0263 (12) | 0.3412 (17) | 0.030* |
| C37 | 0.75520 (18) | 0.18772 (11) | 0.49739 (16) | 0.0293 (6) |
| H37A | 0.7317 | 0.2127 | 0.4615 | 0.044* |
| H37B | 0.8026 | 0.2025 | 0.5233 | 0.044* |
| H37C | 0.7163 | 0.1788 | 0.5347 | 0.044* |
| C44 | 1.17342 (18) | 0.04142 (12) | 0.11123 (16) | 0.0307 (7) |

| | | | | |
|---|---|---|---|---|
| H44 | 1.1991 (19) | 0.0461 (12) | 0.0677 (19) | 0.037* |
| C43 | 1.16141 (17) | 0.08176 (12) | 0.15954 (16) | 0.0279 (6) |
| H43 | 1.1753 (19) | 0.1135 (13) | 0.1495 (18) | 0.034* |
| C47 | 1.13464 (18) | 0.15975 (10) | 0.26538 (18) | 0.0309 (6) |
| H47A | 1.1915 | 0.1621 | 0.2562 | 0.046* |
| H47B | 1.1225 | 0.1817 | 0.3083 | 0.046* |
| H47C | 1.1035 | 0.1710 | 0.2201 | 0.046* |
| C45 | 1.15278 (17) | −0.00822 (12) | 0.12861 (15) | 0.0269 (6) |
| H45 | 1.1582 (18) | −0.0353 (12) | 0.0956 (18) | 0.032* |
| C48 | 1.1157 (2) | −0.10829 (11) | 0.17662 (18) | 0.0379 (7) |
| H48A | 1.0897 | −0.1057 | 0.1260 | 0.057* |
| H48B | 1.0983 | −0.1397 | 0.2012 | 0.057* |
| H48C | 1.1736 | −0.1092 | 0.1724 | 0.057* |
| C38 | 0.6501 (2) | −0.04850 (12) | 0.3142 (2) | 0.0472 (9) |
| H38A | 0.6095 | −0.0588 | 0.3489 | 0.071* |
| H38B | 0.6777 | −0.0790 | 0.2964 | 0.071* |
| H38C | 0.6248 | −0.0305 | 0.2708 | 0.071* |
| Cl1 | 0.56586 (5) | 0.08927 (3) | 0.59577 (5) | 0.03955 (19) |
| Cl2 | 0.60288 (5) | 0.02551 (3) | 0.72804 (5) | 0.0425 (2) |
| C98 | 0.6032 (3) | 0.08763 (13) | 0.6895 (2) | 0.0544 (10) |
| H98A | 0.5708 | 0.1104 | 0.7204 | 0.065* |
| H98B | 0.6584 | 0.1009 | 0.6920 | 0.065* |
| Cl3 | 0.91634 (7) | 0.16930 (4) | 0.17449 (6) | 0.0580 (3) |
| Cl4 | 0.87511 (8) | 0.10083 (4) | 0.04958 (6) | 0.0727 (4) |
| C99 | 0.9249 (2) | 0.15800 (14) | 0.0773 (2) | 0.0499 (9) |
| H99A | 0.9818 | 0.1553 | 0.0661 | 0.060* |
| H99B | 0.9017 | 0.1871 | 0.0480 | 0.060* |
| C94 | 0.4412 (4) | 1.0101 (3) | 0.8930 (3) | 0.106 (2) |
| H94 | 0.4951 | 1.0199 | 0.9028 | 0.127* |
| C91 | 0.3222 (2) | 0.89776 (14) | 0.8166 (2) | 0.0481 (9) |
| H91A | 0.2679 | 0.8882 | 0.8287 | 0.072* |
| H91B | 0.3595 | 0.8717 | 0.8366 | 0.072* |
| H91C | 0.3256 | 0.9001 | 0.7616 | 0.072* |
| C95 | 0.3817 (4) | 1.0449 (3) | 0.9115 (4) | 0.0999 (19) |
| H95 | 0.3947 | 1.0779 | 0.9312 | 0.120* |
| C92 | 0.3420 (2) | 0.94673 (17) | 0.8504 (2) | 0.0513 (9) |
| C97 | 0.2852 (3) | 0.98259 (17) | 0.8662 (3) | 0.0628 (11) |
| H97 | 0.2308 | 0.9753 | 0.8538 | 0.075* |
| C93 | 0.4256 (3) | 0.96124 (19) | 0.8604 (2) | 0.0669 (13) |
| H93 | 0.4672 | 0.9392 | 0.8459 | 0.080* |
| C96 | 0.3056 (3) | 1.0300 (2) | 0.9004 (3) | 0.0848 (17) |
| H96 | 0.2644 | 1.0519 | 0.9159 | 0.102* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni2 | 0.01087 (14) | 0.01424 (15) | 0.01158 (14) | −0.00010 (11) | 0.00142 (11) | −0.00092 (11) |
| N4 | 0.0120 (9) | 0.0166 (10) | 0.0141 (9) | 0.0004 (8) | 0.0022 (7) | −0.0026 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0135 (10) | 0.0170 (10) | 0.0118 (9) | 0.0001 (8) | 0.0018 (7) | −0.0009 (8) |
| O7 | 0.0203 (9) | 0.0212 (9) | 0.0297 (10) | 0.0046 (7) | 0.0021 (8) | −0.0025 (8) |
| N6 | 0.0130 (10) | 0.0151 (10) | 0.0143 (9) | 0.0000 (8) | 0.0024 (7) | −0.0007 (8) |
| N5 | 0.0136 (10) | 0.0153 (10) | 0.0124 (9) | 0.0014 (8) | 0.0014 (7) | −0.0021 (8) |
| O8 | 0.0208 (9) | 0.0256 (10) | 0.0322 (10) | −0.0015 (8) | −0.0008 (8) | −0.0126 (8) |
| O11 | 0.0191 (9) | 0.0173 (9) | 0.0343 (10) | 0.0004 (7) | −0.0004 (8) | −0.0054 (8) |
| O6 | 0.0246 (10) | 0.0296 (10) | 0.0218 (9) | −0.0030 (8) | 0.0085 (8) | −0.0020 (8) |
| O10 | 0.0332 (11) | 0.0270 (10) | 0.0200 (9) | 0.0077 (8) | 0.0081 (8) | −0.0013 (8) |
| C19 | 0.0133 (11) | 0.0165 (12) | 0.0157 (11) | 0.0008 (9) | 0.0025 (9) | −0.0046 (9) |
| O12 | 0.0174 (9) | 0.0235 (10) | 0.0407 (11) | 0.0047 (7) | −0.0021 (8) | −0.0096 (8) |
| C61 | 0.0148 (12) | 0.0239 (13) | 0.0126 (11) | −0.0034 (10) | 0.0006 (9) | 0.0011 (9) |
| O9 | 0.0343 (11) | 0.0226 (10) | 0.0235 (10) | 0.0024 (8) | 0.0045 (8) | −0.0002 (8) |
| C21 | 0.0146 (11) | 0.0131 (11) | 0.0172 (11) | 0.0024 (9) | 0.0008 (9) | −0.0024 (9) |
| C16 | 0.0175 (12) | 0.0148 (11) | 0.0152 (11) | 0.0020 (9) | 0.0025 (9) | −0.0016 (9) |
| C20 | 0.0124 (11) | 0.0168 (12) | 0.0153 (11) | 0.0003 (9) | 0.0018 (9) | −0.0071 (9) |
| C11 | 0.0152 (12) | 0.0162 (11) | 0.0162 (11) | 0.0021 (9) | 0.0008 (9) | −0.0022 (9) |
| C81 | 0.0180 (12) | 0.0202 (12) | 0.0156 (11) | −0.0020 (10) | 0.0002 (9) | 0.0015 (9) |
| C76 | 0.0166 (12) | 0.0269 (14) | 0.0183 (12) | −0.0017 (10) | 0.0020 (9) | −0.0008 (10) |
| O5 | 0.0423 (12) | 0.0232 (10) | 0.0338 (11) | 0.0084 (9) | 0.0006 (9) | 0.0043 (9) |
| C51 | 0.0150 (12) | 0.0253 (13) | 0.0181 (12) | −0.0054 (10) | −0.0030 (9) | 0.0042 (10) |
| C63 | 0.0172 (13) | 0.0335 (15) | 0.0176 (12) | 0.0049 (11) | 0.0025 (10) | 0.0067 (11) |
| C14 | 0.0164 (12) | 0.0162 (12) | 0.0156 (11) | 0.0047 (9) | 0.0021 (9) | −0.0010 (9) |
| C25 | 0.0192 (12) | 0.0161 (12) | 0.0162 (12) | −0.0006 (9) | 0.0043 (9) | −0.0011 (9) |
| C71 | 0.0146 (12) | 0.0262 (13) | 0.0143 (11) | −0.0030 (10) | 0.0019 (9) | −0.0011 (10) |
| C26 | 0.0170 (12) | 0.0171 (12) | 0.0153 (11) | 0.0021 (9) | 0.0059 (9) | −0.0027 (9) |
| C24 | 0.0182 (12) | 0.0143 (11) | 0.0162 (11) | 0.0006 (9) | 0.0028 (9) | −0.0024 (9) |
| C66 | 0.0181 (12) | 0.0269 (14) | 0.0162 (12) | −0.0009 (10) | 0.0020 (9) | −0.0004 (10) |
| C27 | 0.0181 (12) | 0.0228 (13) | 0.0194 (12) | −0.0008 (10) | 0.0067 (10) | 0.0004 (10) |
| C29 | 0.0135 (11) | 0.0134 (11) | 0.0209 (12) | 0.0017 (9) | 0.0017 (9) | −0.0020 (9) |
| C18 | 0.0146 (12) | 0.0199 (12) | 0.0195 (12) | −0.0034 (10) | 0.0023 (9) | −0.0008 (10) |
| C13 | 0.0187 (13) | 0.0261 (14) | 0.0147 (12) | 0.0003 (10) | 0.0002 (9) | 0.0011 (10) |
| C82 | 0.0182 (13) | 0.0249 (13) | 0.0222 (13) | 0.0000 (10) | −0.0011 (10) | −0.0018 (11) |
| C12 | 0.0168 (12) | 0.0239 (13) | 0.0188 (12) | −0.0017 (10) | −0.0017 (10) | −0.0029 (10) |
| C15 | 0.0168 (12) | 0.0151 (12) | 0.0173 (11) | 0.0022 (9) | 0.0036 (9) | 0.0007 (9) |
| C86 | 0.0173 (12) | 0.0220 (13) | 0.0225 (13) | 0.0003 (10) | 0.0013 (10) | −0.0002 (10) |
| C30 | 0.0127 (11) | 0.0144 (11) | 0.0190 (12) | 0.0028 (9) | 0.0016 (9) | −0.0023 (9) |
| C28 | 0.0139 (12) | 0.0183 (12) | 0.0239 (13) | −0.0020 (10) | 0.0034 (10) | −0.0013 (10) |
| C23 | 0.0219 (13) | 0.0215 (13) | 0.0147 (12) | −0.0003 (10) | 0.0011 (10) | 0.0002 (10) |
| C64 | 0.0132 (12) | 0.0460 (17) | 0.0170 (12) | −0.0039 (12) | −0.0016 (10) | 0.0052 (12) |
| C17 | 0.0200 (13) | 0.0186 (12) | 0.0191 (12) | −0.0016 (10) | 0.0032 (10) | 0.0012 (10) |
| C88 | 0.0296 (15) | 0.0183 (13) | 0.0302 (15) | 0.0010 (11) | 0.0010 (11) | −0.0022 (11) |
| C62 | 0.0177 (12) | 0.0238 (13) | 0.0120 (11) | 0.0002 (10) | 0.0015 (9) | 0.0036 (9) |
| C74 | 0.0193 (13) | 0.0395 (16) | 0.0138 (12) | −0.0079 (11) | 0.0044 (10) | −0.0003 (11) |
| C73 | 0.0219 (13) | 0.0306 (15) | 0.0200 (13) | −0.0075 (11) | −0.0004 (10) | 0.0043 (11) |
| C22 | 0.0158 (12) | 0.0213 (13) | 0.0164 (12) | −0.0002 (10) | −0.0020 (9) | −0.0018 (10) |
| C72 | 0.0188 (12) | 0.0257 (13) | 0.0188 (12) | −0.0037 (10) | 0.0026 (10) | −0.0017 (10) |
| C52 | 0.0152 (12) | 0.0321 (15) | 0.0189 (12) | −0.0079 (11) | −0.0009 (10) | 0.0012 (11) |
| C56 | 0.0214 (13) | 0.0276 (14) | 0.0283 (14) | −0.0041 (11) | −0.0038 (11) | 0.0060 (11) |
| C75 | 0.0186 (13) | 0.0345 (15) | 0.0186 (13) | −0.0022 (11) | 0.0052 (10) | −0.0039 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C85 | 0.0243 (14) | 0.0227 (14) | 0.0340 (15) | −0.0044 (11) | −0.0037 (11) | −0.0059 (12) |
| C65 | 0.0213 (13) | 0.0351 (16) | 0.0157 (12) | −0.0094 (12) | 0.0004 (10) | −0.0030 (11) |
| C67 | 0.0319 (15) | 0.0229 (14) | 0.0332 (15) | 0.0069 (12) | 0.0094 (12) | 0.0014 (12) |
| C78 | 0.0453 (19) | 0.0361 (17) | 0.0300 (16) | 0.0179 (14) | 0.0072 (13) | −0.0049 (13) |
| C54 | 0.0255 (15) | 0.052 (2) | 0.0240 (14) | −0.0140 (14) | −0.0038 (12) | 0.0179 (14) |
| C87 | 0.0256 (15) | 0.0316 (15) | 0.0322 (15) | 0.0098 (12) | 0.0027 (12) | −0.0062 (12) |
| C53 | 0.0199 (13) | 0.0488 (18) | 0.0192 (13) | −0.0125 (13) | 0.0020 (11) | 0.0027 (13) |
| C83 | 0.0143 (13) | 0.0337 (16) | 0.0366 (16) | 0.0020 (11) | −0.0010 (11) | −0.0028 (13) |
| C84 | 0.0183 (14) | 0.0358 (16) | 0.0396 (17) | −0.0065 (12) | −0.0060 (12) | −0.0048 (13) |
| C57 | 0.0249 (15) | 0.0431 (18) | 0.0323 (16) | −0.0026 (13) | 0.0115 (12) | −0.0084 (13) |
| C55 | 0.0299 (16) | 0.0340 (17) | 0.0369 (17) | −0.0071 (13) | −0.0091 (13) | 0.0173 (14) |
| C77 | 0.054 (2) | 0.0326 (17) | 0.0401 (18) | 0.0138 (15) | 0.0014 (15) | 0.0043 (14) |
| C58 | 0.0438 (19) | 0.0247 (16) | 0.057 (2) | 0.0080 (14) | −0.0073 (16) | 0.0017 (15) |
| C68 | 0.0324 (17) | 0.0385 (19) | 0.063 (2) | −0.0021 (14) | 0.0007 (15) | −0.0281 (17) |
| Ni1 | 0.0108 (2) | 0.0125 (2) | 0.0118 (2) | 0.00122 (15) | 0.00184 (15) | 0.00077 (16) |
| O1 | 0.0208 (9) | 0.0195 (9) | 0.0291 (10) | 0.0050 (7) | −0.0023 (7) | −0.0079 (8) |
| N2 | 0.0127 (9) | 0.0137 (10) | 0.0141 (9) | 0.0009 (7) | 0.0017 (7) | 0.0006 (8) |
| N1 | 0.0124 (9) | 0.0140 (9) | 0.0136 (9) | 0.0000 (7) | 0.0013 (7) | 0.0001 (8) |
| O3 | 0.0336 (11) | 0.0161 (9) | 0.0264 (10) | −0.0035 (8) | 0.0112 (8) | 0.0021 (7) |
| O4 | 0.0330 (11) | 0.0187 (9) | 0.0231 (9) | 0.0005 (8) | 0.0099 (8) | −0.0028 (7) |
| O2 | 0.0236 (10) | 0.0205 (10) | 0.0448 (12) | −0.0026 (8) | −0.0075 (9) | −0.0047 (9) |
| C4 | 0.0132 (11) | 0.0110 (11) | 0.0195 (12) | −0.0014 (9) | 0.0009 (9) | −0.0002 (9) |
| C31 | 0.0123 (11) | 0.0197 (12) | 0.0146 (11) | 0.0027 (9) | 0.0022 (9) | 0.0041 (9) |
| C5 | 0.0131 (11) | 0.0132 (11) | 0.0177 (11) | −0.0006 (9) | −0.0017 (9) | −0.0023 (9) |
| C6 | 0.0142 (11) | 0.0143 (11) | 0.0182 (12) | 0.0003 (9) | 0.0011 (9) | −0.0005 (9) |
| C2 | 0.0156 (12) | 0.0188 (12) | 0.0184 (12) | 0.0006 (9) | 0.0043 (9) | −0.0001 (10) |
| C9 | 0.0182 (12) | 0.0105 (11) | 0.0170 (11) | −0.0002 (9) | 0.0011 (9) | 0.0000 (9) |
| C41 | 0.0130 (11) | 0.0212 (12) | 0.0145 (11) | 0.0010 (9) | 0.0019 (9) | 0.0034 (9) |
| C10 | 0.0178 (12) | 0.0114 (11) | 0.0151 (11) | −0.0014 (9) | 0.0051 (9) | −0.0001 (9) |
| C1 | 0.0150 (11) | 0.0127 (11) | 0.0184 (12) | −0.0011 (9) | 0.0026 (9) | −0.0001 (9) |
| C3 | 0.0137 (12) | 0.0178 (12) | 0.0206 (12) | 0.0007 (9) | 0.0010 (9) | −0.0017 (10) |
| C7 | 0.0192 (13) | 0.0204 (12) | 0.0158 (12) | 0.0032 (10) | −0.0001 (10) | 0.0014 (10) |
| C32 | 0.0194 (13) | 0.0243 (13) | 0.0153 (12) | 0.0026 (10) | 0.0024 (9) | 0.0017 (10) |
| C8 | 0.0201 (12) | 0.0193 (12) | 0.0145 (12) | 0.0016 (10) | 0.0016 (9) | 0.0018 (10) |
| C46 | 0.0181 (12) | 0.0232 (13) | 0.0181 (12) | 0.0015 (10) | 0.0020 (10) | 0.0014 (10) |
| C36 | 0.0185 (13) | 0.0224 (13) | 0.0233 (13) | −0.0005 (10) | 0.0015 (10) | 0.0048 (10) |
| C34 | 0.0144 (13) | 0.0388 (16) | 0.0237 (13) | 0.0073 (11) | 0.0030 (10) | 0.0109 (12) |
| C33 | 0.0202 (13) | 0.0274 (14) | 0.0221 (13) | 0.0092 (11) | 0.0037 (10) | 0.0026 (11) |
| C42 | 0.0173 (12) | 0.0224 (13) | 0.0214 (13) | 0.0015 (10) | 0.0047 (10) | 0.0018 (10) |
| C35 | 0.0164 (13) | 0.0325 (15) | 0.0265 (14) | −0.0054 (11) | −0.0038 (10) | 0.0063 (12) |
| C37 | 0.0347 (16) | 0.0242 (14) | 0.0287 (15) | 0.0070 (12) | −0.0010 (12) | −0.0091 (12) |
| C44 | 0.0314 (16) | 0.0424 (18) | 0.0194 (13) | −0.0033 (13) | 0.0125 (12) | 0.0044 (12) |
| C43 | 0.0325 (15) | 0.0277 (15) | 0.0241 (14) | −0.0049 (12) | 0.0070 (11) | 0.0082 (12) |
| C47 | 0.0353 (16) | 0.0157 (13) | 0.0425 (17) | −0.0041 (11) | 0.0096 (13) | 0.0025 (12) |
| C45 | 0.0284 (15) | 0.0330 (16) | 0.0200 (13) | −0.0007 (12) | 0.0079 (11) | −0.0046 (12) |
| C48 | 0.056 (2) | 0.0216 (15) | 0.0380 (17) | 0.0058 (14) | 0.0166 (15) | −0.0060 (13) |
| C38 | 0.0360 (18) | 0.0269 (16) | 0.077 (3) | −0.0056 (14) | −0.0147 (17) | −0.0142 (17) |
| Cl1 | 0.0371 (4) | 0.0414 (4) | 0.0392 (4) | 0.0162 (3) | −0.0074 (3) | −0.0107 (3) |
| Cl2 | 0.0602 (5) | 0.0289 (4) | 0.0393 (4) | 0.0004 (4) | 0.0128 (4) | −0.0051 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C98 | 0.097 (3) | 0.0266 (17) | 0.0376 (19) | 0.0003 (18) | −0.0127 (19) | −0.0066 (14) |
| Cl3 | 0.0790 (7) | 0.0395 (5) | 0.0535 (5) | −0.0142 (5) | −0.0165 (5) | 0.0081 (4) |
| Cl4 | 0.1128 (10) | 0.0517 (6) | 0.0563 (6) | −0.0378 (6) | 0.0321 (6) | −0.0142 (5) |
| C99 | 0.053 (2) | 0.0367 (19) | 0.061 (2) | −0.0149 (16) | 0.0108 (18) | 0.0124 (17) |
| C94 | 0.075 (4) | 0.157 (6) | 0.082 (4) | −0.053 (4) | −0.017 (3) | 0.012 (4) |
| C91 | 0.046 (2) | 0.057 (2) | 0.0427 (19) | 0.0159 (17) | 0.0148 (16) | 0.0271 (17) |
| C95 | 0.082 (4) | 0.103 (5) | 0.114 (5) | −0.009 (4) | −0.002 (4) | −0.028 (4) |
| C92 | 0.048 (2) | 0.067 (3) | 0.0395 (19) | 0.0072 (19) | 0.0044 (16) | 0.0194 (18) |
| C97 | 0.050 (2) | 0.066 (3) | 0.073 (3) | −0.002 (2) | 0.008 (2) | −0.013 (2) |
| C93 | 0.063 (3) | 0.084 (3) | 0.051 (2) | −0.023 (2) | −0.018 (2) | 0.018 (2) |
| C96 | 0.058 (3) | 0.089 (4) | 0.107 (4) | 0.002 (3) | −0.006 (3) | −0.061 (3) |

*Geometric parameters (Å, °)*

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|---|---|---|---|
| Ni2—N6 | 1.9198 (19) | C53—H53 | 0.96 (3) |
| Ni2—N4 | 1.928 (2) | C83—C84 | 1.383 (4) |
| Ni2—N5 | 1.9300 (19) | C83—H83 | 0.96 (3) |
| Ni2—N3 | 1.9319 (19) | C84—H84 | 0.95 (3) |
| N4—C19 | 1.383 (3) | C57—H57A | 0.9800 |
| N4—C16 | 1.386 (3) | C57—H57B | 0.9800 |
| N3—C14 | 1.381 (3) | C57—H57C | 0.9800 |
| N3—C11 | 1.383 (3) | C55—H55 | 0.89 (4) |
| O7—C62 | 1.360 (3) | C77—H77A | 0.9800 |
| O7—C67 | 1.435 (3) | C77—H77B | 0.9800 |
| N6—C29 | 1.377 (3) | C77—H77C | 0.9800 |
| N6—C26 | 1.385 (3) | C58—H58A | 0.9800 |
| N5—C21 | 1.381 (3) | C58—H58B | 0.9800 |
| N5—C24 | 1.382 (3) | C58—H58C | 0.9800 |
| O8—C66 | 1.366 (3) | C68—H68A | 0.9800 |
| O8—C68 | 1.415 (3) | C68—H68B | 0.9800 |
| O11—C86 | 1.372 (3) | C68—H68C | 0.9800 |
| O11—C88 | 1.429 (3) | Ni1—N1 | 1.9474 (19) |
| O6—C52 | 1.365 (3) | Ni1—N1$^{i}$ | 1.9474 (19) |
| O6—C57 | 1.434 (3) | Ni1—N2 | 1.9554 (19) |
| O10—C76 | 1.357 (3) | Ni1—N2$^{i}$ | 1.9554 (19) |
| O10—C78 | 1.433 (3) | O1—C32 | 1.361 (3) |
| C19—C20 | 1.382 (3) | O1—C37 | 1.435 (3) |
| C19—C18 | 1.432 (3) | N2—C9 | 1.383 (3) |
| O12—C82 | 1.371 (3) | N2—C6 | 1.384 (3) |
| O12—C87 | 1.425 (3) | N1—C1 | 1.381 (3) |
| C61—C66 | 1.394 (4) | N1—C4 | 1.384 (3) |
| C61—C62 | 1.399 (3) | O3—C42 | 1.358 (3) |
| C61—C20 | 1.495 (3) | O3—C47 | 1.435 (3) |
| O9—C72 | 1.373 (3) | O4—C46 | 1.368 (3) |
| O9—C77 | 1.432 (4) | O4—C48 | 1.428 (3) |
| C21—C20 | 1.378 (3) | O2—C36 | 1.362 (3) |
| C21—C22 | 1.437 (3) | O2—C38 | 1.430 (3) |
| C16—C15 | 1.376 (3) | C4—C5 | 1.384 (3) |
| C16—C17 | 1.433 (3) | C4—C3 | 1.433 (3) |

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|---|---|---|---|
| C11—C30 | 1.383 (3) | C31—C32 | 1.395 (3) |
| C11—C12 | 1.436 (3) | C31—C36 | 1.396 (4) |
| C81—C86 | 1.398 (4) | C31—C5 | 1.502 (3) |
| C81—C82 | 1.399 (4) | C5—C6 | 1.380 (3) |
| C81—C30 | 1.494 (3) | C6—C7 | 1.431 (3) |
| C76—C75 | 1.403 (3) | C2—C3 | 1.347 (3) |
| C76—C71 | 1.404 (4) | C2—C1 | 1.436 (3) |
| O5—C56 | 1.363 (3) | C2—H2 | 0.95 (3) |
| O5—C58 | 1.423 (4) | C9—C10 | 1.381 (3) |
| C51—C52 | 1.399 (4) | C9—C8 | 1.435 (3) |
| C51—C56 | 1.399 (4) | C41—C46 | 1.390 (4) |
| C51—C15 | 1.498 (3) | C41—C42 | 1.395 (3) |
| C63—C64 | 1.378 (4) | C41—C10 | 1.496 (3) |
| C63—C62 | 1.398 (4) | C10—C1$^{i}$ | 1.385 (3) |
| C63—H63 | 0.94 (3) | C1—C10$^{i}$ | 1.385 (3) |
| C14—C15 | 1.384 (3) | C3—H3 | 0.93 (3) |
| C14—C13 | 1.431 (3) | C7—C8 | 1.347 (3) |
| C25—C26 | 1.384 (3) | C7—H7 | 0.93 (3) |
| C25—C24 | 1.385 (3) | C32—C33 | 1.399 (4) |
| C25—C71 | 1.491 (3) | C8—H8 | 0.96 (3) |
| C71—C72 | 1.396 (4) | C46—C45 | 1.394 (4) |
| C26—C27 | 1.435 (3) | C36—C35 | 1.397 (4) |
| C24—C23 | 1.428 (3) | C34—C33 | 1.379 (4) |
| C66—C65 | 1.390 (4) | C34—C35 | 1.381 (4) |
| C27—C28 | 1.343 (4) | C34—H34 | 0.94 (3) |
| C27—H27 | 0.91 (3) | C33—H33 | 0.90 (3) |
| C29—C30 | 1.385 (3) | C42—C43 | 1.400 (4) |
| C29—C28 | 1.432 (3) | C35—H35 | 0.95 (3) |
| C18—C17 | 1.345 (4) | C37—H37A | 0.9800 |
| C18—H18 | 0.92 (3) | C37—H37B | 0.9800 |
| C13—C12 | 1.346 (4) | C37—H37C | 0.9800 |
| C13—H13 | 0.90 (3) | C44—C43 | 1.377 (4) |
| C82—C83 | 1.391 (4) | C44—C45 | 1.380 (4) |
| C12—H12 | 0.89 (3) | C44—H44 | 0.91 (3) |
| C86—C85 | 1.390 (4) | C43—H43 | 0.88 (3) |
| C28—H28 | 0.96 (3) | C47—H47A | 0.9800 |
| C23—C22 | 1.346 (4) | C47—H47B | 0.9800 |
| C23—H23 | 0.92 (3) | C47—H47C | 0.9800 |
| C64—C65 | 1.384 (4) | C45—H45 | 0.92 (3) |
| C64—H64 | 0.91 (3) | C48—H48A | 0.9800 |
| C17—H17 | 0.98 (3) | C48—H48B | 0.9800 |
| C88—H88A | 0.9800 | C48—H48C | 0.9800 |
| C88—H88B | 0.9800 | C38—H38A | 0.9800 |
| C88—H88C | 0.9800 | C38—H38B | 0.9800 |
| C74—C73 | 1.375 (4) | C38—H38C | 0.9800 |
| C74—C75 | 1.385 (4) | Cl1—C98 | 1.745 (4) |
| C74—H74 | 0.92 (3) | Cl2—C98 | 1.759 (4) |
| C73—C72 | 1.400 (4) | C98—H98A | 0.9900 |

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|---|---|---|---|
| C73—H73 | 0.92 (3) | C98—H98B | 0.9900 |
| C22—H22 | 0.93 (3) | Cl3—C99 | 1.757 (4) |
| C52—C53 | 1.395 (4) | Cl4—C99 | 1.769 (4) |
| C56—C55 | 1.401 (4) | C99—H99A | 0.9900 |
| C75—H75 | 0.98 (3) | C99—H99B | 0.9900 |
| C85—C84 | 1.381 (4) | C94—C95 | 1.403 (9) |
| C85—H85 | 0.96 (3) | C94—C93 | 1.420 (8) |
| C65—H65 | 0.90 (3) | C94—H94 | 0.9500 |
| C67—H67A | 0.9800 | C91—C92 | 1.444 (6) |
| C67—H67B | 0.9800 | C91—H91A | 0.9800 |
| C67—H67C | 0.9800 | C91—H91B | 0.9800 |
| C78—H78A | 0.9800 | C91—H91C | 0.9800 |
| C78—H78B | 0.9800 | C95—C96 | 1.343 (7) |
| C78—H78C | 0.9800 | C95—H95 | 0.9500 |
| C54—C55 | 1.379 (5) | C92—C97 | 1.377 (6) |
| C54—C53 | 1.383 (5) | C92—C93 | 1.458 (6) |
| C54—H54 | 0.97 (3) | C97—C96 | 1.412 (6) |
| C87—H87A | 0.9800 | C97—H97 | 0.9500 |
| C87—H87B | 0.9800 | C93—H93 | 0.9500 |
| C87—H87C | 0.9800 | C96—H96 | 0.9500 |
| N6—Ni2—N4 | 173.60 (8) | C84—C83—H83 | 121.6 (19) |
| N6—Ni2—N5 | 89.93 (8) | C82—C83—H83 | 119.5 (19) |
| N4—Ni2—N5 | 90.14 (8) | C85—C84—C83 | 121.7 (3) |
| N6—Ni2—N3 | 90.28 (8) | C85—C84—H84 | 119 (2) |
| N4—Ni2—N3 | 90.27 (8) | C83—C84—H84 | 119 (2) |
| N5—Ni2—N3 | 174.32 (8) | O6—C57—H57A | 109.5 |
| C19—N4—C16 | 104.56 (19) | O6—C57—H57B | 109.5 |
| C19—N4—Ni2 | 127.81 (16) | H57A—C57—H57B | 109.5 |
| C16—N4—Ni2 | 127.62 (16) | O6—C57—H57C | 109.5 |
| C14—N3—C11 | 104.83 (19) | H57A—C57—H57C | 109.5 |
| C14—N3—Ni2 | 128.06 (16) | H57B—C57—H57C | 109.5 |
| C11—N3—Ni2 | 127.04 (16) | C54—C55—C56 | 119.2 (3) |
| C62—O7—C67 | 118.4 (2) | C54—C55—H55 | 123 (2) |
| C29—N6—C26 | 104.79 (19) | C56—C55—H55 | 118 (2) |
| C29—N6—Ni2 | 127.95 (16) | O9—C77—H77A | 109.5 |
| C26—N6—Ni2 | 127.10 (16) | O9—C77—H77B | 109.5 |
| C21—N5—C24 | 104.65 (19) | H77A—C77—H77B | 109.5 |
| C21—N5—Ni2 | 127.19 (16) | O9—C77—H77C | 109.5 |
| C24—N5—Ni2 | 128.14 (16) | H77A—C77—H77C | 109.5 |
| C66—O8—C68 | 118.0 (2) | H77B—C77—H77C | 109.5 |
| C86—O11—C88 | 117.2 (2) | O5—C58—H58A | 109.5 |
| C52—O6—C57 | 118.4 (2) | O5—C58—H58B | 109.5 |
| C76—O10—C78 | 118.9 (2) | H58A—C58—H58B | 109.5 |
| C20—C19—N4 | 125.1 (2) | O5—C58—H58C | 109.5 |
| C20—C19—C18 | 124.4 (2) | H58A—C58—H58C | 109.5 |
| N4—C19—C18 | 110.5 (2) | H58B—C58—H58C | 109.5 |
| C82—O12—C87 | 117.2 (2) | O8—C68—H68A | 109.5 |
| C66—C61—C62 | 119.2 (2) | O8—C68—H68B | 109.5 |
| C66—C61—C20 | 119.9 (2) | H68A—C68—H68B | 109.5 |

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| C62—C61—C20 | 121.0 (2) | O8—C68—H68C | 109.5 |
| C72—O9—C77 | 116.8 (2) | H68A—C68—H68C | 109.5 |
| C20—C21—N5 | 125.2 (2) | H68B—C68—H68C | 109.5 |
| C20—C21—C22 | 123.3 (2) | N1—Ni1—N1$^{i}$ | 180.0 |
| N5—C21—C22 | 110.4 (2) | N1—Ni1—N2 | 89.90 (8) |
| C15—C16—N4 | 125.1 (2) | N1$^{i}$—Ni1—N2 | 90.10 (8) |
| C15—C16—C17 | 123.7 (2) | N1—Ni1—N2$^{i}$ | 90.10 (8) |
| N4—C16—C17 | 110.5 (2) | N1$^{i}$—Ni1—N2$^{i}$ | 89.90 (8) |
| C21—C20—C19 | 122.1 (2) | N2—Ni1—N2$^{i}$ | 180.00 (12) |
| C21—C20—C61 | 118.4 (2) | C32—O1—C37 | 116.8 (2) |
| C19—C20—C61 | 119.2 (2) | C9—N2—C6 | 104.00 (19) |
| N3—C11—C30 | 125.8 (2) | C9—N2—Ni1 | 127.83 (16) |
| N3—C11—C12 | 110.3 (2) | C6—N2—Ni1 | 128.16 (16) |
| C30—C11—C12 | 123.4 (2) | C1—N1—C4 | 104.26 (19) |
| C86—C81—C82 | 118.0 (2) | C1—N1—Ni1 | 127.76 (16) |
| C86—C81—C30 | 121.2 (2) | C4—N1—Ni1 | 127.98 (16) |
| C82—C81—C30 | 120.8 (2) | C42—O3—C47 | 117.6 (2) |
| O10—C76—C75 | 124.2 (2) | C46—O4—C48 | 117.9 (2) |
| O10—C76—C71 | 115.0 (2) | C36—O2—C38 | 117.3 (2) |
| C75—C76—C71 | 120.8 (2) | C5—C4—N1 | 126.0 (2) |
| C56—O5—C58 | 117.6 (2) | C5—C4—C3 | 123.1 (2) |
| C52—C51—C56 | 118.7 (2) | N1—C4—C3 | 110.9 (2) |
| C52—C51—C15 | 119.9 (2) | C32—C31—C36 | 118.7 (2) |
| C56—C51—C15 | 121.2 (2) | C32—C31—C5 | 119.1 (2) |
| C64—C63—C62 | 118.8 (3) | C36—C31—C5 | 121.8 (2) |
| C64—C63—H63 | 119.8 (19) | C6—C5—C4 | 122.3 (2) |
| C62—C63—H63 | 121.3 (19) | C6—C5—C31 | 121.0 (2) |
| N3—C14—C15 | 125.1 (2) | C4—C5—C31 | 116.7 (2) |
| N3—C14—C13 | 110.6 (2) | C5—C6—N2 | 125.6 (2) |
| C15—C14—C13 | 124.4 (2) | C5—C6—C7 | 123.2 (2) |
| C26—C25—C24 | 121.7 (2) | N2—C6—C7 | 111.1 (2) |
| C26—C25—C71 | 119.0 (2) | C3—C2—C1 | 106.8 (2) |
| C24—C25—C71 | 119.3 (2) | C3—C2—H2 | 128.7 (17) |
| C72—C71—C76 | 118.9 (2) | C1—C2—H2 | 124.4 (17) |
| C72—C71—C25 | 122.8 (2) | C10—C9—N2 | 126.0 (2) |
| C76—C71—C25 | 118.3 (2) | C10—C9—C8 | 123.0 (2) |
| C25—C26—N6 | 125.5 (2) | N2—C9—C8 | 111.1 (2) |
| C25—C26—C27 | 123.7 (2) | C46—C41—C42 | 118.9 (2) |
| N6—C26—C27 | 110.4 (2) | C46—C41—C10 | 122.0 (2) |
| N5—C24—C25 | 124.7 (2) | C42—C41—C10 | 119.0 (2) |
| N5—C24—C23 | 110.8 (2) | C9—C10—C1$^{i}$ | 122.0 (2) |
| C25—C24—C23 | 124.5 (2) | C9—C10—C41 | 119.8 (2) |
| O8—C66—C65 | 124.7 (2) | C1$^{i}$—C10—C41 | 118.2 (2) |
| O8—C66—C61 | 114.5 (2) | N1—C1—C10$^{i}$ | 126.3 (2) |
| C65—C66—C61 | 120.8 (2) | N1—C1—C2 | 111.0 (2) |
| C28—C27—C26 | 106.9 (2) | C10$^{i}$—C1—C2 | 122.7 (2) |
| C28—C27—H27 | 127.9 (18) | C2—C3—C4 | 107.0 (2) |

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| C26—C27—H27 | 125.2 (18) | C2—C3—H3 | 128.8 (17) |
| N6—C29—C30 | 126.0 (2) | C4—C3—H3 | 124.1 (17) |
| N6—C29—C28 | 110.5 (2) | C8—C7—C6 | 107.0 (2) |
| C30—C29—C28 | 123.5 (2) | C8—C7—H7 | 131.7 (18) |
| C17—C18—C19 | 107.3 (2) | C6—C7—H7 | 121.1 (18) |
| C17—C18—H18 | 127.3 (18) | O1—C32—C31 | 114.7 (2) |
| C19—C18—H18 | 125.4 (18) | O1—C32—C33 | 123.9 (2) |
| C12—C13—C14 | 107.2 (2) | C31—C32—C33 | 121.4 (2) |
| C12—C13—H13 | 129.3 (19) | C7—C8—C9 | 106.8 (2) |
| C14—C13—H13 | 123.5 (19) | C7—C8—H8 | 129.3 (17) |
| O12—C82—C83 | 124.1 (2) | C9—C8—H8 | 123.9 (17) |
| O12—C82—C81 | 114.7 (2) | O4—C46—C41 | 114.9 (2) |
| C83—C82—C81 | 121.2 (2) | O4—C46—C45 | 124.1 (2) |
| C13—C12—C11 | 107.1 (2) | C41—C46—C45 | 121.0 (2) |
| C13—C12—H12 | 128.1 (19) | O2—C36—C31 | 115.2 (2) |
| C11—C12—H12 | 124.8 (19) | O2—C36—C35 | 124.2 (2) |
| C16—C15—C14 | 122.5 (2) | C31—C36—C35 | 120.6 (2) |
| C16—C15—C51 | 117.6 (2) | C33—C34—C35 | 122.3 (2) |
| C14—C15—C51 | 119.5 (2) | C33—C34—H34 | 117.0 (19) |
| O11—C86—C85 | 123.9 (2) | C35—C34—H34 | 120.6 (19) |
| O11—C86—C81 | 114.7 (2) | C34—C33—C32 | 118.0 (3) |
| C85—C86—C81 | 121.5 (2) | C34—C33—H33 | 121.6 (19) |
| C11—C30—C29 | 121.1 (2) | C32—C33—H33 | 120 (2) |
| C11—C30—C81 | 119.7 (2) | O3—C42—C41 | 114.9 (2) |
| C29—C30—C81 | 119.0 (2) | O3—C42—C43 | 124.3 (2) |
| C27—C28—C29 | 107.4 (2) | C41—C42—C43 | 120.8 (2) |
| C27—C28—H28 | 130.2 (17) | C34—C35—C36 | 118.8 (3) |
| C29—C28—H28 | 122.4 (17) | C34—C35—H35 | 120.6 (19) |
| C22—C23—C24 | 107.1 (2) | C36—C35—H35 | 120.5 (19) |
| C22—C23—H23 | 128.0 (18) | O1—C37—H37A | 109.5 |
| C24—C23—H23 | 124.8 (18) | O1—C37—H37B | 109.5 |
| C63—C64—C65 | 122.2 (2) | H37A—C37—H37B | 109.5 |
| C63—C64—H64 | 120 (2) | O1—C37—H37C | 109.5 |
| C65—C64—H64 | 118 (2) | H37A—C37—H37C | 109.5 |
| C18—C17—C16 | 107.0 (2) | H37B—C37—H37C | 109.5 |
| C18—C17—H17 | 128.6 (17) | C43—C44—C45 | 122.2 (3) |
| C16—C17—H17 | 124.4 (17) | C43—C44—H44 | 121 (2) |
| O11—C88—H88A | 109.5 | C45—C44—H44 | 117 (2) |
| O11—C88—H88B | 109.5 | C44—C43—C42 | 118.5 (3) |
| H88A—C88—H88B | 109.5 | C44—C43—H43 | 123 (2) |
| O11—C88—H88C | 109.5 | C42—C43—H43 | 118 (2) |
| H88A—C88—H88C | 109.5 | O3—C47—H47A | 109.5 |
| H88B—C88—H88C | 109.5 | O3—C47—H47B | 109.5 |
| O7—C62—C63 | 124.2 (2) | H47A—C47—H47B | 109.5 |
| O7—C62—C61 | 115.4 (2) | O3—C47—H47C | 109.5 |
| C63—C62—C61 | 120.4 (2) | H47A—C47—H47C | 109.5 |
| C73—C74—C75 | 122.6 (2) | H47B—C47—H47C | 109.5 |
| C73—C74—H74 | 118.9 (19) | C44—C45—C46 | 118.6 (3) |
| C75—C74—H74 | 118.5 (19) | C44—C45—H45 | 123 (2) |

| | | | |
|---|---|---|---|
| C74—C73—C72 | 118.8 (3) | C46—C45—H45 | 118 (2) |
| C74—C73—H73 | 122.9 (19) | O4—C48—H48A | 109.5 |
| C72—C73—H73 | 118 (2) | O4—C48—H48B | 109.5 |
| C23—C22—C21 | 107.0 (2) | H48A—C48—H48B | 109.5 |
| C23—C22—H22 | 129.5 (18) | O4—C48—H48C | 109.5 |
| C21—C22—H22 | 123.5 (18) | H48A—C48—H48C | 109.5 |
| O9—C72—C71 | 115.8 (2) | H48B—C48—H48C | 109.5 |
| O9—C72—C73 | 123.5 (2) | O2—C38—H38A | 109.5 |
| C71—C72—C73 | 120.7 (2) | O2—C38—H38B | 109.5 |
| O6—C52—C53 | 124.2 (3) | H38A—C38—H38B | 109.5 |
| O6—C52—C51 | 114.9 (2) | O2—C38—H38C | 109.5 |
| C53—C52—C51 | 120.9 (3) | H38A—C38—H38C | 109.5 |
| O5—C56—C51 | 114.8 (2) | H38B—C38—H38C | 109.5 |
| O5—C56—C55 | 124.7 (3) | Cl1—C98—Cl2 | 112.50 (19) |
| C51—C56—C55 | 120.5 (3) | Cl1—C98—H98A | 109.1 |
| C74—C75—C76 | 118.2 (3) | Cl2—C98—H98A | 109.1 |
| C74—C75—H75 | 123.5 (18) | Cl1—C98—H98B | 109.1 |
| C76—C75—H75 | 118.3 (18) | Cl2—C98—H98B | 109.1 |
| C84—C85—C86 | 118.8 (3) | H98A—C98—H98B | 107.8 |
| C84—C85—H85 | 121.9 (19) | Cl3—C99—Cl4 | 110.61 (18) |
| C86—C85—H85 | 119.3 (19) | Cl3—C99—H99A | 109.5 |
| C64—C65—C66 | 118.7 (3) | Cl4—C99—H99A | 109.5 |
| C64—C65—H65 | 120 (2) | Cl3—C99—H99B | 109.5 |
| C66—C65—H65 | 122 (2) | Cl4—C99—H99B | 109.5 |
| O7—C67—H67A | 109.5 | H99A—C99—H99B | 108.1 |
| O7—C67—H67B | 109.5 | C95—C94—C93 | 123.8 (5) |
| H67A—C67—H67B | 109.5 | C95—C94—H94 | 118.1 |
| O7—C67—H67C | 109.5 | C93—C94—H94 | 118.1 |
| H67A—C67—H67C | 109.5 | C92—C91—H91A | 109.5 |
| H67B—C67—H67C | 109.5 | C92—C91—H91B | 109.5 |
| O10—C78—H78A | 109.5 | H91A—C91—H91B | 109.5 |
| O10—C78—H78B | 109.5 | C92—C91—H91C | 109.5 |
| H78A—C78—H78B | 109.5 | H91A—C91—H91C | 109.5 |
| O10—C78—H78C | 109.5 | H91B—C91—H91C | 109.5 |
| H78A—C78—H78C | 109.5 | C96—C95—C94 | 117.7 (6) |
| H78B—C78—H78C | 109.5 | C96—C95—H95 | 121.2 |
| C55—C54—C53 | 121.6 (3) | C94—C95—H95 | 121.2 |
| C55—C54—H54 | 121 (2) | C97—C92—C91 | 122.4 (4) |
| C53—C54—H54 | 117 (2) | C97—C92—C93 | 118.3 (4) |
| O12—C87—H87A | 109.5 | C91—C92—C93 | 118.8 (4) |
| O12—C87—H87B | 109.5 | C92—C97—C96 | 121.7 (4) |
| H87A—C87—H87B | 109.5 | C92—C97—H97 | 119.2 |
| O12—C87—H87C | 109.5 | C96—C97—H97 | 119.2 |
| H87A—C87—H87C | 109.5 | C94—C93—C92 | 116.1 (5) |
| H87B—C87—H87C | 109.5 | C94—C93—H93 | 121.9 |
| C54—C53—C52 | 119.0 (3) | C92—C93—H93 | 121.9 |
| C54—C53—H53 | 122 (2) | C95—C96—C97 | 121.8 (5) |
| C52—C53—H53 | 119 (2) | C95—C96—H96 | 119.1 |
| C84—C83—C82 | 118.9 (3) | C97—C96—H96 | 119.1 |

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

**Fig. 1**

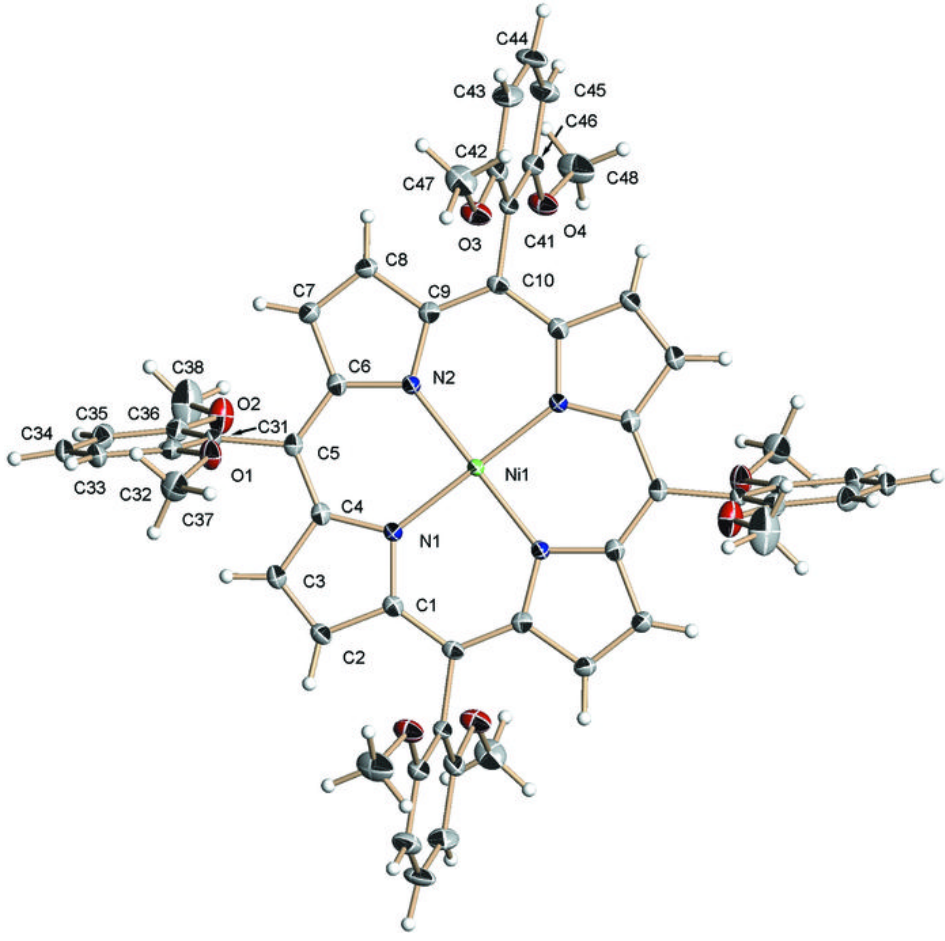
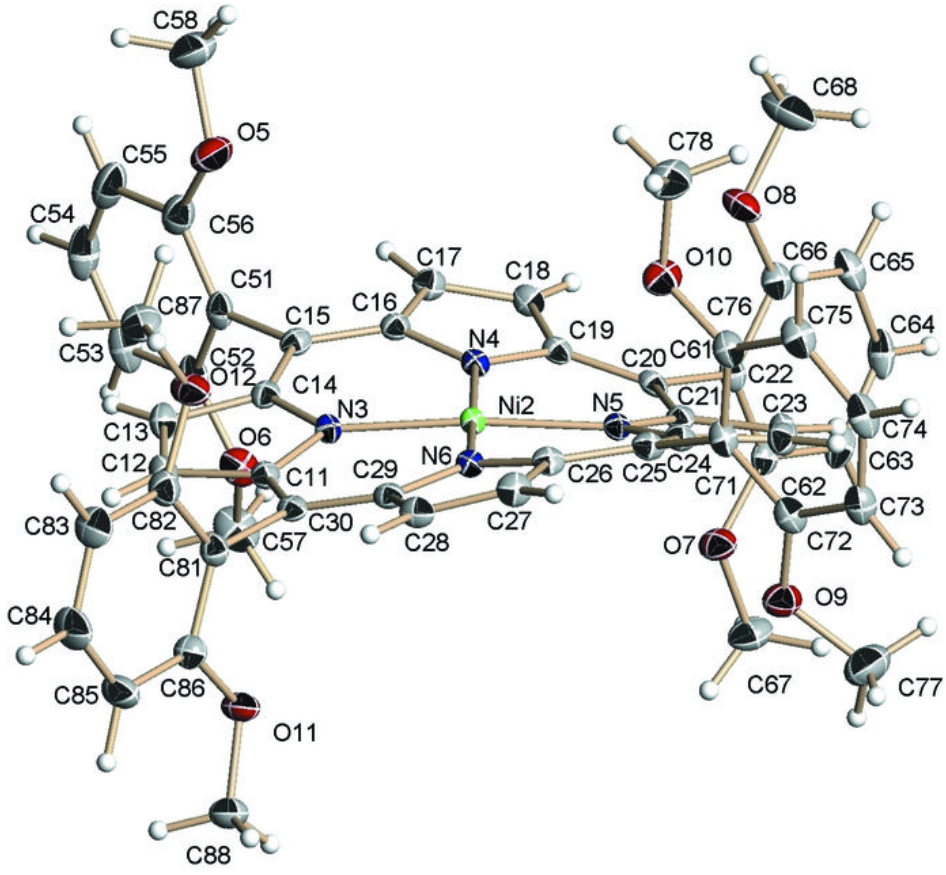


**Fig. 2**


C58
O5
C55
C54
C56
C51
C87
C53
C52
O12
C14
N3
C13
O6
C12
C11
C29
N6
C26
C25
C24
C71
C62
C73
C72
O7
O9
C67
C77
C83
C82
C30
C57
C28
C27
C81
C84
C85
C86
O11
C88
C68
C78
O8
O10
C66
C65
C17
C18
C16
C15
N4
C19
C20
C61
C76
C75
C64
C22
C21
C23
C74
Ni2
N5
C63