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# $\mu$-Acetato-$\kappa^2O$:$O'$-[7,23-dibenzyl-15,31-dichloro-3,7,11,19,23,27-hexaazatricyclo[27.3.1.1$^{13,17}$]tetratriconta-1(32),2,11,13,15,17(34),18,27,29(33),30-decaene-33,34-diolato-$\kappa^{10}N^4,N^5,N^6,O^1,O^2$:$N^1,N^2,N^3,O^1,O^2$]dinickel(II) perchlorate acetonitrile disolvate

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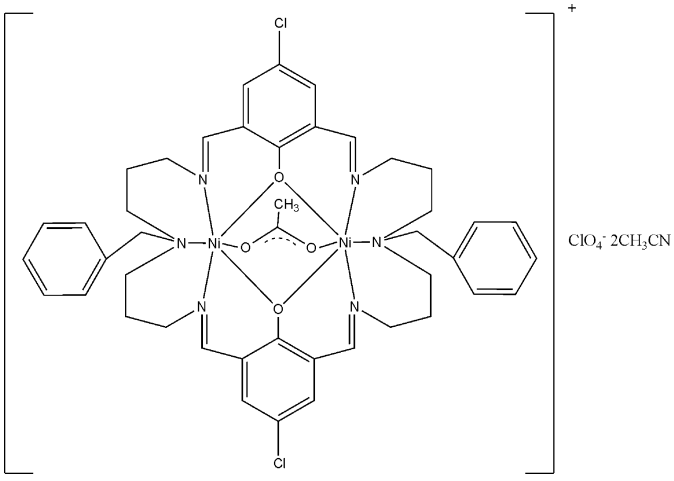
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.060; $wR$ factor = 0.158; data-to-parameter ratio = 16.2.

The title complex, $[Ni_2(C_{42}H_{46}Cl_2N_6O_2)(C_2H_3O_2)]ClO_4\cdot 2CH_3CN$, was synthesized by condensation of 2,6-diformyl-4-chlorophenol with *N*,*N*-bis(aminopropyl)benzylamine in the presence of Ni$^{II}$ ions. The ligand is a 28-membered macrocycle with two identical pendant arms. The coordination geometries of the Ni atoms are both octahedral. The two Ni atoms are bridged by two phenolate O atoms of the macrocyclic ligand and one acetate ligand, with an Ni···Ni distance of 3.147 (4) Å.

## Related literature

For related literature, see: Gou & Fenton (1994); Luo *et al.* (2002); Turonek *et al.* (1995); Zeng *et al.* (1998).




## Experimental

### Crystal data

$[Ni_2(C_{42}H_{46}Cl_2N_6O_2)(C_2H_3O_2)]ClO_4\cdot 2C_2H_3N$
$M_r$ = 1095.77
Monoclinic, $P2_1/n$
$a$ = 16.7957 (14) Å
$b$ = 17.2146 (15) Å
$c$ = 18.0209 (15) Å
$\beta$ = 99.305 (2)°
$V$ = 5141.8 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.95 mm$^{-1}$
$T$ = 273 (2) K
0.32 × 0.26 × 0.24 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.7, $T_{max}$ = 0.8
29289 measured reflections
10096 independent reflections
7248 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.158
$S$ = 1.08
10096 reflections
623 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.98 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2351).

## References

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# supplementary materials

*Acta Cryst.* (2008). E**64**, m18 [ **doi:10.1107/S1600536807061399** ]

# $\mu$-Acetato-$\kappa^2O$:$O'$-[7,23-dibenzyl-15,31-dichloro-3,7,11,19,23,27-hexaazatricyclo[27.3.1.1$^{13,17}$]tetratriconta-1(32),2,11,13,15,17(34),18,27,29(33),30-decaene-33,34-diolato-$\kappa^{10}N^4,N^5,N^6,O^1,O^2$:$N^1,N^2,N^3,O^1,O^2$]dinickel(II) perchlorate acetonitrile disolvate

**J. Kong, H. Zhou and Z.-Q. Pan**

## Comment

Pendant-arm marocyclic complexes have attracted much interest in recent decades. Because there is a concept that, by having pendant arm attached at appropriate positions on the macrocyclic framework, an "opened cryptand" would result, leading to modified complexation property over the corresponding clathrochelates or simple macrocyclic precursors (Zeng *et al.*, 1998). Transition metal complexes with pendant-arm ligands, usually synthesized by cyclocondensation of 2,6-diformyl-4- chlorophenol and diamine the stepwise template reaction, have been studies extensively (Luo *et al.*, 2002, Zeng *et al.*, 1998). However, the dinuclear nickel complex of this ligand(I) has not been published. Here, we report the synthesis and crystal structure of the complex.

The crystal structure is composed of complex cations, perchlorate anions and solvent acetonitrile molecules. Neither the perchlorate ion nor the acetonitrile molecules participate in coordination of the Ni atoms. The complex cation is extremely twisted owing to the flexility of macrocyclic ligand as well as the requirement of Ni coordination with donor atoms. The structure of (I) is shown in Fig. 1. The coordination geometry of Ni1 is similar to that of $Ni_2$. The coordination polyhedron around $Ni_1$ is a distorted octahedron, whose equatorial plane is formed by one imine $N_6$, one tertiary $N_5$, two phenolate $O_1$ and $O_2$ with the mean deviation of 0.0541 (4) Å. The axial positions are occupied by $N_4$ and $O_3$, respectively. the band length of $Ni_1$—O is fall in the range 2.033 (3)–2.082 (3) Å, but the two $Ni_1$—*N*(imine) bonds[2.081 (4) and 2.092 (3) Å, respectively] are shorter significantly than the $Ni_1$—N(tertiary) [2.201 (3) Å]. The Ni···Ni separation is 3.147 (4) Å. The two benzyl groups attached to $N_2$ and $N_5$ respectively are *cis* to each other.

## Experimental

2,6-diformyl-4-chlorophenol was prepared by a modification of the literature method (Gou & Fenton, 1994). *N*,*N*-bis(aminopropyl)- benzylamine prepared by literature method of (Turonek *et al.*, 1995). The title complex was synthesized by the following procedure: 0.5 mmol *N*,*N*-bis(aminopropyl)-benzylamine in 15 ml of absolute methanol was added dropwise to a methanol solution (30 ml) containing 0.5 mmol 2,6-diformyl-4-methylphenol and 0.5 mmol $Ni(OAc)_2.H_2O$. After stirring the mixture for 10 h at room temperature, a green solution formed. A methanol solution (10 ml) containing $Ni(ClO_4)_2.4H_2O$(0.5 mmol) was added dropwise. A yellow-green solution was produced after stirring at room temperature for 4 h. Green needle-shaped crystals suitable for X-ray diffraction were obtained by slow evaporation from acetonitrile over three days.

### Refinement

All H atoms for C—H distances were placed in calculated positions in the range 0.93–0.97 Å, and included in the refinement in the riding-model approximation, with $U_{iso}$(H) = 1.2–1.5 $U_{eq}$(C).

### Figures

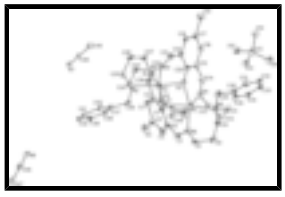

Fig. 1. A view of the title complex, showing the labeling of the non-H atoms and 30% probability ellipsoids. H atoms have been omitted.

### μ-Acetato-κ$^2$*O*:*O*'-[7,23-dibenzyl-15,31-dichloro- 3,7,11,19,23,27-hexaazatricyclo[27.3.1.1$^{13,17}$]tetratriconta-1(32),2,11,13,15,17 (34),18,27,29 (33),30- decaene-33,34-diolato-κ$^{10}$*N*$^4$,*N*$^5$,*N*$^6$,*O*$^1$, *O*$^2$:*N*$^1$,*N*$^2$,*N*$^3$,*O*$^1$,*O*$^2$] dinickel perchlorate acetonitrile disolvate

*Crystal data*

| | |
|---|---|
| $[Ni_2(C_{42}H_{46}Cl_2N_6O_2)(C_2H_3O_2)]ClO_4{\cdot}2C_2H_3N$ | $F_{000}$ = 2280 |
| $M_r$ = 1095.77 | $D_x$ = 1.415 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 5427 reflections |
| $a$ = 16.7957 (14) Å | θ = 2.2–26.0º |
| $b$ = 17.2146 (15) Å | μ = 0.95 mm$^{-1}$ |
| $c$ = 18.0209 (15) Å | $T$ = 273 (2) K |
| β = 99.305 (2)º | Needle, green |
| $V$ = 5141.8 (8) Å$^3$ | 0.32 × 0.26 × 0.24 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 10096 independent reflections |
| Radiation source: sealed tube | 7248 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.041 |
| $T$ = 273(2) K | $\theta_{max}$ = 26.0º |
| phi and ω scans | $\theta_{min}$ = 2.2º |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h$ = −16→20 |
| $T_{min}$ = 0.7, $T_{max}$ = 0.8 | $k$ = −19→21 |
| 29289 measured reflections | $l$ = −22→22 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.061$ | H-atom parameters constrained |
| $wR(F^2) = 0.158$ | $w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 1.990P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 10096 reflections | $\Delta\rho_{max} = 0.81$ e Å$^{-3}$ |
| 623 parameters | $\Delta\rho_{min} = -0.98$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

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

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5447 (2) | 0.4856 (2) | 0.3737 (2) | 0.0384 (8) |
| C2 | 0.6266 (3) | 0.5068 (2) | 0.3850 (2) | 0.0433 (9) |
| C3 | 0.6790 (3) | 0.4856 (3) | 0.4510 (2) | 0.0504 (11) |
| H3 | 0.7328 | 0.5010 | 0.4588 | 0.060* |
| C4 | 0.6471 (3) | 0.4392 (2) | 0.5066 (2) | 0.0437 (9) |
| C5 | 0.5708 (3) | 0.4157 (2) | 0.4929 (2) | 0.0466 (10) |
| H5 | 0.5513 | 0.3851 | 0.5285 | 0.056* |
| C6 | 0.5182 (3) | 0.4354 (2) | 0.4263 (2) | 0.0414 (9) |
| C7 | 0.4348 (3) | 0.4073 (2) | 0.4149 (2) | 0.0441 (10) |
| H7 | 0.4104 | 0.3986 | 0.4570 | 0.053* |
| C8 | 0.3076 (2) | 0.3736 (3) | 0.3447 (2) | 0.0441 (10) |
| H8A | 0.2761 | 0.4198 | 0.3293 | 0.053* |
| H8B | 0.2976 | 0.3597 | 0.3945 | 0.053* |
| C9 | 0.2760 (3) | 0.3071 (3) | 0.2904 (3) | 0.0587 (12) |
| H9A | 0.2184 | 0.3020 | 0.2897 | 0.070* |
| H9B | 0.3011 | 0.2590 | 0.3100 | 0.070* |
| C10 | 0.2912 (3) | 0.3175 (3) | 0.2086 (2) | 0.0449 (10) |
| H10A | 0.2648 | 0.2748 | 0.1792 | 0.054* |

| | | | | |
|---|---|---|---|---|
| H10B | 0.2643 | 0.3648 | 0.1891 | 0.054* |
| C11 | 0.4153 (3) | 0.2448 (2) | 0.2070 (3) | 0.0480 (10) |
| H11A | 0.4513 | 0.2384 | 0.1704 | 0.058* |
| H11B | 0.3749 | 0.2041 | 0.1982 | 0.058* |
| C12 | 0.4646 (3) | 0.2343 (3) | 0.2870 (3) | 0.0528 (11) |
| H12A | 0.4307 | 0.2494 | 0.3233 | 0.063* |
| H12B | 0.4769 | 0.1796 | 0.2946 | 0.063* |
| C13 | 0.5404 (3) | 0.2781 (3) | 0.3032 (3) | 0.0536 (11) |
| H13A | 0.5496 | 0.2934 | 0.3556 | 0.064* |
| H13B | 0.5847 | 0.2449 | 0.2947 | 0.064* |
| C14 | 0.5897 (3) | 0.3469 (3) | 0.2101 (3) | 0.0495 (10) |
| H14 | 0.6267 | 0.3062 | 0.2151 | 0.059* |
| C15 | 0.5962 (3) | 0.4036 (2) | 0.1500 (2) | 0.0457 (10) |
| C16 | 0.6554 (3) | 0.3915 (3) | 0.1043 (2) | 0.0472 (10) |
| H16 | 0.6873 | 0.3472 | 0.1118 | 0.057* |
| C17 | 0.6677 (3) | 0.4424 (3) | 0.0493 (2) | 0.0490 (11) |
| C18 | 0.6236 (3) | 0.5072 (3) | 0.0399 (2) | 0.0471 (10) |
| H18 | 0.6330 | 0.5419 | 0.0028 | 0.056* |
| C19 | 0.5643 (3) | 0.5255 (2) | 0.0825 (2) | 0.0440 (10) |
| C20 | 0.5473 (2) | 0.4692 (3) | 0.1378 (2) | 0.0427 (9) |
| C21 | 0.5214 (3) | 0.5981 (3) | 0.0724 (3) | 0.0547 (12) |
| H21 | 0.5127 | 0.6200 | 0.0246 | 0.066* |
| C22 | 0.4451 (3) | 0.7055 (3) | 0.1046 (3) | 0.0513 (11) |
| H22A | 0.3897 | 0.6932 | 0.1094 | 0.062* |
| H22B | 0.4457 | 0.7186 | 0.0524 | 0.062* |
| C23 | 0.4703 (3) | 0.7769 (3) | 0.1520 (2) | 0.0480 (10) |
| H23A | 0.4356 | 0.8200 | 0.1334 | 0.058* |
| H23B | 0.5251 | 0.7907 | 0.1467 | 0.058* |
| C24 | 0.4660 (3) | 0.7642 (2) | 0.2374 (2) | 0.0438 (9) |
| H24A | 0.4738 | 0.8141 | 0.2623 | 0.053* |
| H24B | 0.4119 | 0.7468 | 0.2413 | 0.053* |
| C25 | 0.6092 (3) | 0.7352 (3) | 0.2870 (2) | 0.0491 (11) |
| H25A | 0.6374 | 0.7196 | 0.3360 | 0.059* |
| H25B | 0.6077 | 0.7915 | 0.2866 | 0.059* |
| C26 | 0.6611 (3) | 0.7089 (3) | 0.2275 (2) | 0.0527 (12) |
| H26A | 0.6321 | 0.7218 | 0.1780 | 0.063* |
| H26B | 0.7107 | 0.7388 | 0.2350 | 0.063* |
| C27 | 0.6823 (3) | 0.6259 (3) | 0.2279 (3) | 0.0508 (11) |
| H27A | 0.7379 | 0.6194 | 0.2519 | 0.061* |
| H27B | 0.6779 | 0.6077 | 0.1765 | 0.061* |
| C28 | 0.6636 (3) | 0.5506 (3) | 0.3313 (2) | 0.0467 (10) |
| H28 | 0.7187 | 0.5596 | 0.3441 | 0.056* |
| C29 | 0.3746 (3) | 0.3459 (3) | 0.1126 (2) | 0.0484 (10) |
| H29A | 0.3524 | 0.3979 | 0.1061 | 0.058* |
| H29B | 0.4303 | 0.3487 | 0.1046 | 0.058* |
| C30 | 0.3289 (3) | 0.2947 (3) | 0.0519 (2) | 0.0500 (11) |
| C31 | 0.3671 (3) | 0.2357 (3) | 0.0197 (3) | 0.0542 (11) |
| H31 | 0.4209 | 0.2244 | 0.0374 | 0.065* |
| C32 | 0.3247 (3) | 0.1931 (3) | −0.0397 (3) | 0.0491 (10) |

| | | | | |
|---|---|---|---|---|
| H32 | 0.3497 | 0.1515 | −0.0594 | 0.059* |
| C33 | 0.2477 (3) | 0.2114 (2) | −0.0690 (3) | 0.0462 (10) |
| H33 | 0.2216 | 0.1849 | −0.1110 | 0.055* |
| C34 | 0.2073 (3) | 0.2696 (2) | −0.0366 (2) | 0.0432 (9) |
| H34 | 0.1534 | 0.2805 | −0.0546 | 0.052* |
| C35 | 0.2489 (3) | 0.3106 (3) | 0.0226 (3) | 0.0552 (12) |
| H35 | 0.2227 | 0.3504 | 0.0439 | 0.066* |
| C36 | 0.5011 (3) | 0.6952 (3) | 0.3556 (2) | 0.0460 (10) |
| H36A | 0.5317 | 0.6517 | 0.3795 | 0.055* |
| H36B | 0.4446 | 0.6803 | 0.3479 | 0.055* |
| C37 | 0.5120 (3) | 0.7639 (3) | 0.4106 (3) | 0.0527 (11) |
| C38 | 0.4489 (3) | 0.8212 (3) | 0.4079 (3) | 0.0478 (10) |
| H38 | 0.4029 | 0.8176 | 0.3716 | 0.057* |
| C39 | 0.4566 (3) | 0.8796 (3) | 0.4576 (2) | 0.0455 (10) |
| H39 | 0.4172 | 0.9180 | 0.4536 | 0.055* |
| C40 | 0.5231 (2) | 0.8839 (2) | 0.5158 (2) | 0.0428 (10) |
| H40 | 0.5266 | 0.9232 | 0.5516 | 0.051* |
| C41 | 0.5814 (3) | 0.8304 (2) | 0.5188 (2) | 0.0431 (10) |
| H41 | 0.6255 | 0.8334 | 0.5573 | 0.052* |
| C42 | 0.5786 (3) | 0.7691 (3) | 0.4654 (2) | 0.0463 (10) |
| H42 | 0.6207 | 0.7337 | 0.4677 | 0.056* |
| C43 | 0.3289 (2) | 0.5568 (2) | 0.2186 (2) | 0.0410 (9) |
| C44 | 0.2420 (3) | 0.5854 (3) | 0.2063 (2) | 0.0459 (10) |
| H44A | 0.2380 | 0.6304 | 0.2370 | 0.069* |
| H44B | 0.2075 | 0.5452 | 0.2200 | 0.069* |
| H44C | 0.2258 | 0.5986 | 0.1544 | 0.069* |
| C46 | 0.5706 (3) | 1.0022 (3) | 0.8446 (3) | 0.0529 (11) |
| C48 | 0.6614 (3) | 0.9861 (3) | 0.2799 (2) | 0.0444 (10) |
| C111 | 0.5752 (3) | 0.9916 (3) | 0.9238 (3) | 0.0587 (12) |
| H7A | 0.5754 | 0.9404 | 0.9343 | 0.088* |
| H7B | 0.6210 | 1.0134 | 0.9477 | 0.088* |
| H7C | 0.5325 | 1.0142 | 0.9393 | 0.088* |
| C112 | 0.6952 (3) | 0.9316 (3) | 0.2343 (2) | 0.0481 (10) |
| H8C | 0.6900 | 0.8833 | 0.2521 | 0.072* |
| H8D | 0.6693 | 0.9345 | 0.1865 | 0.072* |
| H8E | 0.7478 | 0.9424 | 0.2356 | 0.072* |
| Cl1 | 0.70869 (8) | 0.41975 (7) | 0.58362 (7) | 0.0568 (3) |
| Cl2 | 0.73998 (8) | 0.42420 (7) | −0.00057 (7) | 0.0620 (3) |
| Cl3 | 0.64598 (7) | 0.15587 (6) | 0.06422 (6) | 0.0473 (3) |
| N1 | 0.6295 (2) | 0.5785 (2) | 0.2680 (2) | 0.0492 (9) |
| N2 | 0.5251 (2) | 0.7073 (2) | 0.2805 (2) | 0.0444 (8) |
| N3 | 0.4957 (2) | 0.6330 (2) | 0.1232 (2) | 0.0467 (9) |
| N4 | 0.5390 (2) | 0.3470 (2) | 0.25636 (19) | 0.0436 (8) |
| N5 | 0.3744 (2) | 0.3212 (2) | 0.1943 (2) | 0.0457 (8) |
| N6 | 0.3943 (2) | 0.3941 (2) | 0.3504 (2) | 0.0432 (8) |
| N7 | 0.6331 (2) | 1.0322 (2) | 0.3179 (2) | 0.0484 (9) |
| N8 | 0.5666 (2) | 1.0108 (2) | 0.7794 (2) | 0.0506 (9) |
| Ni1 | 0.43937 (3) | 0.42058 (3) | 0.25238 (3) | 0.03695 (14) |
| Ni2 | 0.50518 (3) | 0.58905 (3) | 0.23164 (3) | 0.03986 (15) |

| | | | | |
|---|---|---|---|---|
| O1 | 0.49362 (17) | 0.51229 (16) | 0.31702 (15) | 0.0408 (6) |
| O2 | 0.48682 (16) | 0.48320 (16) | 0.17442 (15) | 0.0418 (6) |
| O3 | 0.33703 (18) | 0.48490 (17) | 0.22122 (18) | 0.0493 (7) |
| O4 | 0.38232 (19) | 0.60574 (17) | 0.22422 (17) | 0.0496 (7) |
| O11 | 0.64001 (18) | 0.06817 (17) | 0.08605 (17) | 0.0492 (7) |
| O12 | 0.70489 (18) | 0.19800 (17) | 0.11967 (17) | 0.0481 (7) |
| O13 | 0.56391 (17) | 0.19927 (16) | 0.06237 (16) | 0.0445 (7) |
| O14 | 0.68326 (18) | 0.16370 (17) | −0.00305 (16) | 0.0476 (7) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.043 (2) | 0.0327 (19) | 0.039 (2) | 0.0000 (16) | 0.0061 (17) | 0.0031 (16) |
| C2 | 0.050 (2) | 0.037 (2) | 0.043 (2) | 0.0014 (18) | 0.0087 (19) | 0.0033 (17) |
| C3 | 0.055 (3) | 0.053 (3) | 0.040 (2) | 0.005 (2) | 0.000 (2) | −0.0005 (19) |
| C4 | 0.043 (2) | 0.040 (2) | 0.049 (2) | 0.0114 (17) | 0.0092 (18) | 0.0056 (18) |
| C5 | 0.061 (3) | 0.041 (2) | 0.038 (2) | 0.0020 (19) | 0.0070 (19) | −0.0003 (17) |
| C6 | 0.054 (3) | 0.037 (2) | 0.034 (2) | 0.0032 (18) | 0.0107 (18) | 0.0008 (16) |
| C7 | 0.051 (3) | 0.035 (2) | 0.048 (2) | −0.0010 (18) | 0.013 (2) | 0.0031 (17) |
| C8 | 0.039 (2) | 0.058 (3) | 0.040 (2) | −0.0178 (19) | 0.0186 (18) | 0.0039 (18) |
| C9 | 0.059 (3) | 0.057 (3) | 0.061 (3) | −0.020 (2) | 0.012 (2) | 0.002 (2) |
| C10 | 0.052 (3) | 0.042 (2) | 0.038 (2) | −0.0114 (19) | −0.0018 (18) | −0.0038 (17) |
| C11 | 0.039 (2) | 0.041 (2) | 0.060 (3) | −0.0062 (18) | −0.002 (2) | 0.007 (2) |
| C12 | 0.048 (3) | 0.055 (3) | 0.052 (3) | 0.011 (2) | −0.004 (2) | 0.016 (2) |
| C13 | 0.055 (3) | 0.050 (3) | 0.053 (3) | 0.010 (2) | 0.002 (2) | 0.007 (2) |
| C14 | 0.045 (2) | 0.050 (2) | 0.051 (2) | 0.0066 (19) | 0.000 (2) | −0.003 (2) |
| C15 | 0.051 (3) | 0.042 (2) | 0.043 (2) | −0.0012 (18) | 0.0052 (19) | −0.0095 (17) |
| C16 | 0.047 (2) | 0.042 (2) | 0.055 (3) | −0.0082 (18) | 0.014 (2) | −0.0110 (19) |
| C17 | 0.055 (3) | 0.047 (2) | 0.044 (2) | −0.018 (2) | 0.008 (2) | −0.0114 (19) |
| C18 | 0.053 (3) | 0.044 (2) | 0.044 (2) | −0.021 (2) | 0.010 (2) | −0.0078 (18) |
| C19 | 0.050 (3) | 0.046 (2) | 0.035 (2) | −0.0175 (19) | 0.0041 (18) | −0.0001 (17) |
| C20 | 0.038 (2) | 0.051 (2) | 0.039 (2) | −0.0065 (18) | 0.0061 (17) | 0.0036 (18) |
| C21 | 0.060 (3) | 0.059 (3) | 0.043 (2) | −0.005 (2) | 0.002 (2) | 0.011 (2) |
| C22 | 0.043 (2) | 0.058 (3) | 0.050 (2) | 0.004 (2) | −0.001 (2) | 0.012 (2) |
| C23 | 0.046 (2) | 0.051 (2) | 0.047 (2) | −0.0090 (19) | 0.0079 (19) | 0.0175 (19) |
| C24 | 0.048 (2) | 0.043 (2) | 0.042 (2) | 0.0093 (18) | 0.0145 (19) | 0.0119 (18) |
| C25 | 0.060 (3) | 0.047 (2) | 0.043 (2) | −0.014 (2) | 0.017 (2) | −0.0071 (19) |
| C26 | 0.058 (3) | 0.059 (3) | 0.044 (2) | −0.021 (2) | 0.018 (2) | 0.015 (2) |
| C27 | 0.054 (3) | 0.052 (3) | 0.049 (2) | −0.020 (2) | 0.015 (2) | 0.006 (2) |
| C28 | 0.039 (2) | 0.055 (3) | 0.045 (2) | −0.0066 (19) | 0.0055 (18) | 0.004 (2) |
| C29 | 0.045 (2) | 0.049 (2) | 0.044 (2) | −0.0147 (19) | −0.0133 (19) | 0.0090 (19) |
| C30 | 0.053 (3) | 0.051 (3) | 0.042 (2) | −0.014 (2) | −0.007 (2) | −0.0004 (19) |
| C31 | 0.044 (3) | 0.058 (3) | 0.059 (3) | −0.004 (2) | 0.007 (2) | 0.000 (2) |
| C32 | 0.041 (2) | 0.043 (2) | 0.064 (3) | 0.0026 (18) | 0.011 (2) | −0.003 (2) |
| C33 | 0.040 (2) | 0.044 (2) | 0.052 (2) | −0.0163 (18) | −0.0002 (19) | −0.0088 (19) |
| C34 | 0.038 (2) | 0.046 (2) | 0.042 (2) | −0.0115 (17) | −0.0052 (17) | −0.0014 (18) |
| C35 | 0.049 (3) | 0.047 (3) | 0.063 (3) | −0.011 (2) | −0.013 (2) | −0.007 (2) |
| C36 | 0.040 (2) | 0.050 (2) | 0.049 (2) | −0.0181 (19) | 0.0121 (19) | 0.0007 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C37 | 0.044 (3) | 0.048 (2) | 0.067 (3) | −0.011 (2) | 0.014 (2) | 0.001 (2) |
| C38 | 0.042 (2) | 0.051 (2) | 0.053 (2) | −0.0150 (19) | 0.014 (2) | −0.013 (2) |
| C39 | 0.047 (2) | 0.042 (2) | 0.049 (2) | 0.0074 (18) | 0.0093 (19) | −0.0139 (18) |
| C40 | 0.042 (2) | 0.049 (2) | 0.041 (2) | −0.0155 (19) | 0.0162 (18) | −0.0165 (18) |
| C41 | 0.044 (2) | 0.044 (2) | 0.042 (2) | −0.0215 (18) | 0.0106 (18) | −0.0119 (17) |
| C42 | 0.050 (3) | 0.043 (2) | 0.046 (2) | −0.0134 (19) | 0.0082 (19) | −0.0047 (18) |
| C43 | 0.040 (2) | 0.039 (2) | 0.044 (2) | 0.0084 (17) | 0.0056 (17) | 0.0072 (17) |
| C44 | 0.043 (2) | 0.056 (3) | 0.038 (2) | 0.0119 (19) | 0.0066 (18) | 0.0082 (18) |
| C46 | 0.040 (2) | 0.047 (3) | 0.072 (3) | −0.0084 (19) | 0.011 (2) | −0.005 (2) |
| C48 | 0.047 (2) | 0.047 (2) | 0.043 (2) | −0.0166 (18) | 0.0157 (19) | −0.0142 (18) |
| C111 | 0.053 (3) | 0.048 (3) | 0.069 (3) | −0.014 (2) | −0.008 (2) | −0.009 (2) |
| C112 | 0.049 (2) | 0.045 (2) | 0.049 (2) | 0.0059 (19) | 0.004 (2) | 0.0067 (19) |
| Cl1 | 0.0675 (8) | 0.0461 (6) | 0.0541 (6) | 0.0129 (5) | 0.0015 (5) | −0.0038 (5) |
| Cl2 | 0.0666 (8) | 0.0560 (7) | 0.0645 (7) | 0.0165 (6) | 0.0137 (6) | 0.0127 (6) |
| Cl3 | 0.0482 (6) | 0.0417 (5) | 0.0497 (6) | 0.0084 (4) | 0.0013 (4) | 0.0062 (4) |
| N1 | 0.0360 (19) | 0.061 (2) | 0.051 (2) | −0.0126 (16) | 0.0080 (16) | 0.0057 (17) |
| N2 | 0.0396 (19) | 0.0402 (18) | 0.054 (2) | −0.0043 (15) | 0.0079 (16) | 0.0092 (15) |
| N3 | 0.0375 (19) | 0.049 (2) | 0.051 (2) | −0.0089 (15) | −0.0018 (16) | 0.0133 (17) |
| N4 | 0.048 (2) | 0.0424 (19) | 0.0374 (18) | 0.0069 (15) | −0.0029 (16) | 0.0008 (14) |
| N5 | 0.045 (2) | 0.0403 (19) | 0.048 (2) | −0.0078 (15) | −0.0030 (16) | 0.0002 (15) |
| N6 | 0.045 (2) | 0.0385 (18) | 0.047 (2) | −0.0050 (15) | 0.0108 (16) | 0.0077 (15) |
| N7 | 0.047 (2) | 0.050 (2) | 0.049 (2) | −0.0150 (16) | 0.0102 (17) | −0.0119 (17) |
| N8 | 0.045 (2) | 0.053 (2) | 0.057 (2) | −0.0151 (17) | 0.0171 (18) | 0.0003 (18) |
| Ni1 | 0.0350 (3) | 0.0339 (3) | 0.0409 (3) | −0.00144 (19) | 0.0027 (2) | 0.0042 (2) |
| Ni2 | 0.0403 (3) | 0.0377 (3) | 0.0403 (3) | −0.0052 (2) | 0.0027 (2) | 0.0072 (2) |
| O1 | 0.0424 (15) | 0.0386 (14) | 0.0391 (15) | −0.0069 (12) | −0.0002 (12) | 0.0029 (11) |
| O2 | 0.0382 (15) | 0.0452 (16) | 0.0422 (15) | −0.0033 (12) | 0.0071 (12) | 0.0042 (12) |
| O3 | 0.0396 (16) | 0.0440 (17) | 0.0633 (19) | −0.0017 (13) | 0.0055 (14) | 0.0025 (14) |
| O4 | 0.0487 (18) | 0.0436 (17) | 0.0556 (18) | 0.0033 (14) | 0.0056 (14) | 0.0090 (14) |
| O11 | 0.0451 (17) | 0.0441 (16) | 0.0544 (18) | −0.0075 (13) | −0.0042 (14) | 0.0017 (13) |
| O12 | 0.0498 (18) | 0.0424 (16) | 0.0535 (18) | −0.0031 (13) | 0.0120 (14) | 0.0082 (13) |
| O13 | 0.0435 (16) | 0.0440 (16) | 0.0451 (15) | −0.0043 (12) | 0.0047 (13) | 0.0107 (13) |
| O14 | 0.0449 (17) | 0.0519 (17) | 0.0470 (16) | −0.0004 (13) | 0.0102 (13) | 0.0050 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.306 (5) | C27—N1 | 1.478 (5) |
| C1—C2 | 1.405 (6) | C27—H27A | 0.9700 |
| C1—C6 | 1.407 (5) | C27—H27B | 0.9700 |
| C2—C3 | 1.408 (6) | C28—N1 | 1.285 (6) |
| C2—C28 | 1.445 (6) | C28—H28 | 0.9300 |
| C3—C4 | 1.450 (6) | C29—C30 | 1.514 (6) |
| C3—H3 | 0.9300 | C29—N5 | 1.533 (5) |
| C4—C5 | 1.328 (6) | C29—H29A | 0.9700 |
| C4—Cl1 | 1.626 (4) | C29—H29B | 0.9700 |
| C5—C6 | 1.413 (6) | C30—C31 | 1.378 (7) |
| C5—H5 | 0.9300 | C30—C35 | 1.389 (6) |
| C6—C7 | 1.465 (6) | C31—C32 | 1.394 (7) |
| C7—N6 | 1.270 (6) | C31—H31 | 0.9300 |

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|---|---|---|---|
| C7—H7 | 0.9300 | C32—C33 | 1.353 (6) |
| C8—N6 | 1.484 (5) | C32—H32 | 0.9300 |
| C8—C9 | 1.543 (6) | C33—C34 | 1.390 (6) |
| C8—H8A | 0.9700 | C33—H33 | 0.9300 |
| C8—H8B | 0.9700 | C34—C35 | 1.372 (6) |
| C9—C10 | 1.546 (6) | C34—H34 | 0.9300 |
| C9—H9A | 0.9700 | C35—H35 | 0.9300 |
| C9—H9B | 0.9700 | C36—N2 | 1.488 (5) |
| C10—N5 | 1.462 (6) | C36—C37 | 1.534 (6) |
| C10—H10A | 0.9700 | C36—H36A | 0.9700 |
| C10—H10B | 0.9700 | C36—H36B | 0.9700 |
| C11—N5 | 1.485 (5) | C37—C42 | 1.369 (6) |
| C11—C12 | 1.553 (6) | C37—C38 | 1.444 (7) |
| C11—H11A | 0.9700 | C38—C39 | 1.338 (6) |
| C11—H11B | 0.9700 | C38—H38 | 0.9300 |
| C12—C13 | 1.468 (7) | C39—C40 | 1.406 (6) |
| C12—H12A | 0.9700 | C39—H39 | 0.9300 |
| C12—H12B | 0.9700 | C40—C41 | 1.338 (6) |
| C13—N4 | 1.452 (6) | C40—H40 | 0.9300 |
| C13—H13A | 0.9700 | C41—C42 | 1.423 (6) |
| C13—H13B | 0.9700 | C41—H41 | 0.9300 |
| C14—N4 | 1.283 (6) | C42—H42 | 0.9300 |
| C14—C15 | 1.476 (6) | C43—O4 | 1.224 (5) |
| C14—H14 | 0.9300 | C43—O3 | 1.245 (5) |
| C15—C20 | 1.394 (6) | C43—C44 | 1.521 (6) |
| C15—C16 | 1.405 (6) | C44—H44A | 0.9600 |
| C16—C17 | 1.363 (6) | C44—H44B | 0.9600 |
| C16—H16 | 0.9300 | C44—H44C | 0.9600 |
| C17—C18 | 1.335 (7) | C46—N8 | 1.175 (6) |
| C17—Cl2 | 1.652 (5) | C46—C111 | 1.430 (7) |
| C18—C19 | 1.388 (6) | C48—N7 | 1.195 (5) |
| C18—H18 | 0.9300 | C48—C112 | 1.424 (6) |
| C19—C21 | 1.440 (7) | C111—H7A | 0.8999 |
| C19—C20 | 1.450 (6) | C111—H7B | 0.8999 |
| C20—O2 | 1.320 (5) | C111—H7C | 0.9001 |
| C21—N3 | 1.230 (6) | C112—H8C | 0.9000 |
| C21—H21 | 0.9300 | C112—H8D | 0.9000 |
| C22—N3 | 1.517 (6) | C112—H8E | 0.9000 |
| C22—C23 | 1.518 (7) | Cl3—O14 | 1.458 (3) |
| C22—H22A | 0.9700 | Cl3—O12 | 1.478 (3) |
| C22—H22B | 0.9700 | Cl3—O13 | 1.564 (3) |
| C23—C24 | 1.566 (6) | Cl3—O11 | 1.567 (3) |
| C23—H23A | 0.9700 | N1—Ni2 | 2.092 (4) |
| C23—H23B | 0.9700 | N2—Ni2 | 2.222 (4) |
| C24—N2 | 1.515 (5) | N3—Ni2 | 2.078 (4) |
| C24—H24A | 0.9700 | N4—Ni1 | 2.091 (4) |
| C24—H24B | 0.9700 | N5—Ni1 | 2.200 (3) |
| C25—N2 | 1.479 (6) | N6—Ni1 | 2.082 (3) |
| C25—C26 | 1.556 (6) | Ni1—O2 | 2.033 (3) |

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|---|---|---|---|
| C25—H25A | 0.9700 | Ni1—O3 | 2.046 (3) |
| C25—H25B | 0.9700 | Ni1—O1 | 2.082 (3) |
| C26—C27 | 1.471 (7) | Ni2—O1 | 2.061 (3) |
| C26—H26A | 0.9700 | Ni2—O4 | 2.066 (3) |
| C26—H26B | 0.9700 | Ni2—O2 | 2.092 (3) |
| O1—C1—C2 | 121.8 (3) | C30—C31—H31 | 120.1 |
| O1—C1—C6 | 120.2 (4) | C32—C31—H31 | 120.1 |
| C2—C1—C6 | 118.0 (4) | C33—C32—C31 | 121.0 (4) |
| C1—C2—C3 | 121.3 (4) | C33—C32—H32 | 119.5 |
| C1—C2—C28 | 123.7 (4) | C31—C32—H32 | 119.5 |
| C3—C2—C28 | 115.0 (4) | C32—C33—C34 | 120.2 (4) |
| C2—C3—C4 | 118.4 (4) | C32—C33—H33 | 119.9 |
| C2—C3—H3 | 120.8 | C34—C33—H33 | 119.9 |
| C4—C3—H3 | 120.8 | C35—C34—C33 | 118.4 (4) |
| C5—C4—C3 | 119.5 (4) | C35—C34—H34 | 120.8 |
| C5—C4—Cl1 | 123.9 (4) | C33—C34—H34 | 120.8 |
| C3—C4—Cl1 | 116.6 (3) | C34—C35—C30 | 122.3 (5) |
| C4—C5—C6 | 122.5 (4) | C34—C35—H35 | 118.9 |
| C4—C5—H5 | 118.7 | C30—C35—H35 | 118.9 |
| C6—C5—H5 | 118.7 | N2—C36—C37 | 117.3 (3) |
| C1—C6—C5 | 119.8 (4) | N2—C36—H36A | 108.0 |
| C1—C6—C7 | 120.6 (4) | C37—C36—H36A | 108.0 |
| C5—C6—C7 | 119.5 (4) | N2—C36—H36B | 108.0 |
| N6—C7—C6 | 123.1 (4) | C37—C36—H36B | 108.0 |
| N6—C7—H7 | 118.5 | H36A—C36—H36B | 107.2 |
| C6—C7—H7 | 118.5 | C42—C37—C38 | 119.2 (4) |
| N6—C8—C9 | 117.0 (4) | C42—C37—C36 | 121.0 (4) |
| N6—C8—H8A | 108.1 | C38—C37—C36 | 119.6 (4) |
| C9—C8—H8A | 108.1 | C39—C38—C37 | 120.0 (4) |
| N6—C8—H8B | 108.1 | C39—C38—H38 | 120.0 |
| C9—C8—H8B | 108.1 | C37—C38—H38 | 120.0 |
| H8A—C8—H8B | 107.3 | C38—C39—C40 | 121.2 (4) |
| C8—C9—C10 | 115.2 (4) | C38—C39—H39 | 119.4 |
| C8—C9—H9A | 108.5 | C40—C39—H39 | 119.4 |
| C10—C9—H9A | 108.5 | C41—C40—C39 | 118.8 (4) |
| C8—C9—H9B | 108.5 | C41—C40—H40 | 120.6 |
| C10—C9—H9B | 108.5 | C39—C40—H40 | 120.6 |
| H9A—C9—H9B | 107.5 | C40—C41—C42 | 122.6 (4) |
| N5—C10—C9 | 118.8 (4) | C40—C41—H41 | 118.7 |
| N5—C10—H10A | 107.6 | C42—C41—H41 | 118.7 |
| C9—C10—H10A | 107.6 | C37—C42—C41 | 118.1 (4) |
| N5—C10—H10B | 107.6 | C37—C42—H42 | 121.0 |
| C9—C10—H10B | 107.6 | C41—C42—H42 | 121.0 |
| H10A—C10—H10B | 107.0 | O4—C43—O3 | 127.4 (4) |
| N5—C11—C12 | 114.1 (4) | O4—C43—C44 | 117.5 (4) |
| N5—C11—H11A | 108.7 | O3—C43—C44 | 115.1 (4) |
| C12—C11—H11A | 108.7 | C43—C44—H44A | 109.5 |
| N5—C11—H11B | 108.7 | C43—C44—H44B | 109.5 |
| C12—C11—H11B | 108.7 | H44A—C44—H44B | 109.5 |

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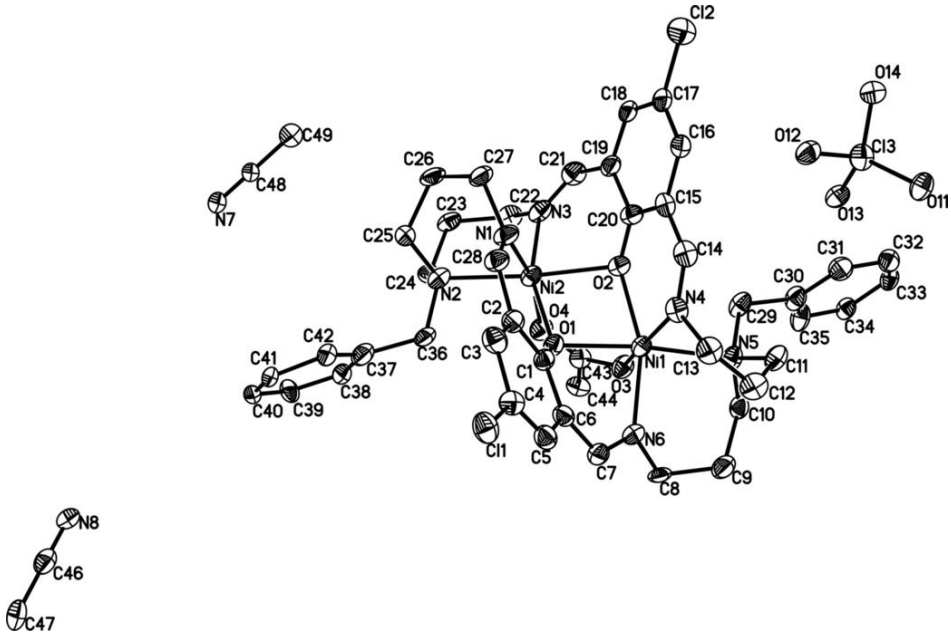
|---|---|---|---|
| H11A—C11—H11B | 107.6 | C43—C44—H44C | 109.5 |
| C13—C12—C11 | 116.1 (4) | H44A—C44—H44C | 109.5 |
| C13—C12—H12A | 108.3 | H44B—C44—H44C | 109.5 |
| C11—C12—H12A | 108.3 | N8—C46—C111 | 179.8 (6) |
| C13—C12—H12B | 108.3 | N7—C48—C112 | 179.6 (5) |
| C11—C12—H12B | 108.3 | C46—C111—H7A | 109.5 |
| H12A—C12—H12B | 107.4 | C46—C111—H7B | 109.2 |
| N4—C13—C12 | 111.8 (4) | H7A—C111—H7B | 109.5 |
| N4—C13—H13A | 109.3 | C46—C111—H7C | 109.7 |
| C12—C13—H13A | 109.3 | H7A—C111—H7C | 109.5 |
| N4—C13—H13B | 109.3 | H7B—C111—H7C | 109.5 |
| C12—C13—H13B | 109.3 | C48—C112—H8C | 109.4 |
| H13A—C13—H13B | 107.9 | C48—C112—H8D | 109.8 |
| N4—C14—C15 | 127.7 (4) | H8C—C112—H8D | 109.5 |
| N4—C14—H14 | 116.2 | C48—C112—H8E | 109.2 |
| C15—C14—H14 | 116.2 | H8C—C112—H8E | 109.5 |
| C20—C15—C16 | 118.8 (4) | H8D—C112—H8E | 109.5 |
| C20—C15—C14 | 122.7 (4) | O14—Cl3—O12 | 100.74 (18) |
| C16—C15—C14 | 118.5 (4) | O14—Cl3—O13 | 115.71 (17) |
| C17—C16—C15 | 122.5 (4) | O12—Cl3—O13 | 105.76 (17) |
| C17—C16—H16 | 118.8 | O14—Cl3—O11 | 110.56 (18) |
| C15—C16—H16 | 118.8 | O12—Cl3—O11 | 111.48 (17) |
| C18—C17—C16 | 118.8 (4) | O13—Cl3—O11 | 111.93 (16) |
| C18—C17—Cl2 | 122.1 (4) | C28—N1—C27 | 115.1 (4) |
| C16—C17—Cl2 | 119.0 (4) | C28—N1—Ni2 | 126.2 (3) |
| C17—C18—C19 | 123.6 (4) | C27—N1—Ni2 | 116.5 (3) |
| C17—C18—H18 | 118.2 | C25—N2—C36 | 111.6 (3) |
| C19—C18—H18 | 118.2 | C25—N2—C24 | 111.6 (3) |
| C18—C19—C21 | 121.1 (4) | C36—N2—C24 | 107.8 (3) |
| C18—C19—C20 | 117.8 (4) | C25—N2—Ni2 | 114.2 (3) |
| C21—C19—C20 | 121.1 (4) | C36—N2—Ni2 | 100.8 (2) |
| O2—C20—C15 | 123.4 (4) | C24—N2—Ni2 | 110.1 (3) |
| O2—C20—C19 | 118.3 (4) | C21—N3—C22 | 119.3 (4) |
| C15—C20—C19 | 118.3 (4) | C21—N3—Ni2 | 122.6 (3) |
| N3—C21—C19 | 124.0 (4) | C22—N3—Ni2 | 117.5 (3) |
| N3—C21—H21 | 118.0 | C14—N4—C13 | 115.2 (4) |
| C19—C21—H21 | 118.0 | C14—N4—Ni1 | 126.1 (3) |
| N3—C22—C23 | 116.5 (4) | C13—N4—Ni1 | 116.9 (3) |
| N3—C22—H22A | 108.2 | C10—N5—C11 | 111.5 (3) |
| C23—C22—H22A | 108.2 | C10—N5—C29 | 109.4 (3) |
| N3—C22—H22B | 108.2 | C11—N5—C29 | 108.6 (4) |
| C23—C22—H22B | 108.2 | C10—N5—Ni1 | 111.4 (3) |
| H22A—C22—H22B | 107.3 | C11—N5—Ni1 | 115.7 (3) |
| C22—C23—C24 | 112.7 (3) | C29—N5—Ni1 | 99.4 (2) |
| C22—C23—H23A | 109.1 | C7—N6—C8 | 118.7 (3) |
| C24—C23—H23A | 109.1 | C7—N6—Ni1 | 121.6 (3) |
| C22—C23—H23B | 109.1 | C8—N6—Ni1 | 118.7 (3) |
| C24—C23—H23B | 109.1 | O2—Ni1—O3 | 85.94 (12) |
| H23A—C23—H23B | 107.8 | O2—Ni1—N6 | 159.97 (13) |

| | | | |
|---|---|---|---|
| N2—C24—C23 | 117.7 (3) | O3—Ni1—N6 | 86.93 (13) |
| N2—C24—H24A | 107.9 | O2—Ni1—O1 | 78.44 (11) |
| C23—C24—H24A | 107.9 | O3—Ni1—O1 | 90.88 (12) |
| N2—C24—H24B | 107.9 | N6—Ni1—O1 | 82.98 (12) |
| C23—C24—H24B | 107.9 | O2—Ni1—N4 | 86.79 (13) |
| H24A—C24—H24B | 107.2 | O3—Ni1—N4 | 165.88 (13) |
| N2—C25—C26 | 119.0 (4) | N6—Ni1—N4 | 103.73 (14) |
| N2—C25—H25A | 107.6 | O1—Ni1—N4 | 99.49 (13) |
| C26—C25—H25A | 107.6 | O2—Ni1—N5 | 107.66 (12) |
| N2—C25—H25B | 107.6 | O3—Ni1—N5 | 87.70 (13) |
| C26—C25—H25B | 107.6 | N6—Ni1—N5 | 90.71 (14) |
| H25A—C25—H25B | 107.0 | O1—Ni1—N5 | 173.61 (12) |
| C27—C26—C25 | 116.2 (3) | N4—Ni1—N5 | 83.00 (14) |
| C27—C26—H26A | 108.2 | O1—Ni2—O4 | 85.63 (11) |
| C25—C26—H26A | 108.2 | O1—Ni2—N3 | 159.00 (13) |
| C27—C26—H26B | 108.2 | O4—Ni2—N3 | 87.96 (13) |
| C25—C26—H26B | 108.2 | O1—Ni2—O2 | 77.61 (11) |
| H26A—C26—H26B | 107.4 | O4—Ni2—O2 | 91.33 (12) |
| C26—C27—N1 | 112.0 (4) | N3—Ni2—O2 | 82.58 (13) |
| C26—C27—H27A | 109.2 | O1—Ni2—N1 | 85.41 (13) |
| N1—C27—H27A | 109.2 | O4—Ni2—N1 | 165.40 (14) |
| C26—C27—H27B | 109.2 | N3—Ni2—N1 | 104.32 (14) |
| N1—C27—H27B | 109.2 | O2—Ni2—N1 | 97.98 (14) |
| H27A—C27—H27B | 107.9 | O1—Ni2—N2 | 108.53 (12) |
| N1—C28—C2 | 127.7 (4) | O4—Ni2—N2 | 89.01 (13) |
| N1—C28—H28 | 116.1 | N3—Ni2—N2 | 91.31 (14) |
| C2—C28—H28 | 116.1 | O2—Ni2—N2 | 173.86 (12) |
| C30—C29—N5 | 117.0 (3) | N1—Ni2—N2 | 82.94 (14) |
| C30—C29—H29A | 108.1 | C1—O1—Ni2 | 132.8 (2) |
| N5—C29—H29A | 108.1 | C1—O1—Ni1 | 110.1 (2) |
| C30—C29—H29B | 108.1 | Ni2—O1—Ni1 | 98.86 (11) |
| N5—C29—H29B | 108.1 | C20—O2—Ni1 | 132.0 (3) |
| H29A—C29—H29B | 107.3 | C20—O2—Ni2 | 109.9 (2) |
| C31—C30—C35 | 118.2 (4) | Ni1—O2—Ni2 | 99.45 (12) |
| C31—C30—C29 | 121.1 (4) | C43—O3—Ni1 | 129.1 (3) |
| C35—C30—C29 | 120.4 (4) | C43—O4—Ni2 | 128.4 (3) |
| C30—C31—C32 | 119.8 (4) | | |

**Fig. 1**


Cl2
O14
C18
C17
C16
O12
Cl3
C49
C26
C27
C21
C19
C48
C15
O13
O11
N7
C22
N3
C20
C23
N1
C25
C14
C31
C32
C28
O2
C30
C33
C24
N2
Ni2
N4
C2
O4
C29
C34
C42
O1
C35
C41
C36
C3
N5
C37
Ni1
C13
C11
C1
C43
O3
C38
C12
C40
C39
C4
C44
C10
C6
N6
Cl1
C5
C7
C9
C8
N8
C46
C47