Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Diiodido-2$\kappa^2 I$-bis(4-methylpyridine-1$\kappa N$)-$\mu$-{2,2′-[1,3-propanediylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4 O,N,N',O'$:2$\kappa^2 O,O'$}nickel(II)zinc(II)

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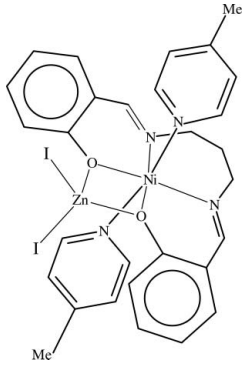
Received 24 August 2007; accepted 3 September 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.014 Å; $R$ factor = 0.033; $wR$ factor = 0.075; data-to-parameter ratio = 10.6.

The title compound, $[ZnI_2Ni(C_{17}H_{16}N_2O_2)(C_6H_7N)_2]$, is a heterodinuclear zinc–nickel complex. The $Ni^{II}$ ion is in a distorted octahedral coordination environment formed by two O and two N atoms from a chelating salpd$^{2-}$ ligand [salpd$^{2-}$= *N*,*N*′-bis(salicylidene)-1,3-propanediamine, $C_{17}H_{16}N_2O_2$] in the equatorial plane and two N atoms of two methylpyridine ligands ($C_6H_7N$) in the axial positions. The coordination around the $Zn^{II}$ ion is distorted tetrahedral, with two bridging O atoms of the chelating salpd$^{2-}$ ligand and two I atoms. The average Zn—O and Zn—I distances are 1.986 (5) and 2.5327 (11) Å, respectively. The crystal structure is stabilized by weak C—H···N and C—H···I hydrogen bonds.

## Related literature

For general background, see: Bertini *et al.* (1994); Barandika *et al.* (1999). For related literature, see: Tatar *et al.* (1999); Atakol, Tatar *et al.* (1999); Atakol, Arıcı *et al.* (1999); Svoboda *et al.* (2001); Arıcı *et al.* (2001, 2006); Arıcı & Aksu (2002); Tatar (2002); Tatar, Atakol & Arıcı (2002); Tatar, Atakol & Ülkü (2002); Colon *et al.* (2004); Metalobos *et al.* (2004); Atakol *et al.* (2006); Yu *et al.* (2007).




## Experimental

### Crystal data

$[ZnI_2Ni(C_{17}H_{16}N_2O_2)(C_6H_7N)_2]$
$M_r$ = 844.45
Monoclinic, *Cc*
*a* = 9.3523 (11) Å
*b* = 19.615 (3) Å
*c* = 17.4933 (10) Å
$\beta$ = 105.390 (12)°
*V* = 3094.0 (6) Å$^3$
*Z* = 4
Mo *K*$\alpha$ radiation
$\mu$ = 3.41 mm$^{-1}$
*T* = 293 (2) K
0.2 × 0.2 × 0.2 mm

### Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: $\psi$ scan North *et al.* (1968)
$T_{min}$ = 0.506, $T_{max}$ = 0.511
7375 measured reflections
3745 independent reflections
2491 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.052
3 standard reflections
frequency: 120 min
intensity decay: 2%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.075
*S* = 1.01
3745 reflections
352 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: 0.00 (2)

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10*B*···I1$^{i}$ | 0.97 | 3.03 | 3.981 (10) | 166 |
| C22—H22···N2 | 0.93 | 2.61 | 3.078 (10) | 111 |
| C28—H28···N2 | 0.93 | 2.51 | 3.086 (15) | 120 |

Symmetry code: (i) $x+\frac{1}{2}, y-\frac{1}{2}, z$.

**Table 2**
Comparision of some crystallographic properties of corresponding dinuclear complexes.

$M_c$ is the central metal ion, $M_t$ is the terminal metal ion and *R* is the ion bonded to the terminal metal ion.

| Compound $[M_tR_2M_c]$ | Space group | $M_c\cdots M_t$ (Å) | $M_t$—*R* (Å) |
|---|---|---|---|
| (I) | Monoclinic *Cc* | 3.0634 (13) | 2.5320 (11)–2.5333 (10) |
| (II) | Monoclinic *Cc* | 3.0738 (19) | 2.3412 (18)–2.3628 (16) |
| (III) | Monoclinic *Cc* | 3.0695 (11) | 2.5303 (9)–2.5424 (9) |
| (IV) | Monoclinic $P2_1/c$ | 3.0757 (6) | 2.208 (1)–2.208 (1) |
| (V) | Monoclinik $P2_1/n$ | 3.0800 (9) | 2.3309 (9)–2.3508 (10) |
| (VI) | Monoclinic $P2_1$ | Not given | 2.216 (4)–2.200 (4) |
| (VII) | Orthorhombic $P2_12_12_1$ | 3.0917 (15) | 2.3356 (16)–2.3634 (15) |
| (VIII) | Orthorhombic $P2_12_12_1$ | 3.161 (1) | 2.2163 (14)–2.2054 (14) |
| (IX) | Orthorhombic $P2_12_12_1$ | 3.1464 (16) | 2.5373 (14)–2.5527 (14) |
| (*X*) | Triclinic $P\overline{1}$ | 3.5301 (8) | 2.3430 (10)–2.325 (2) |
| (XI) | Triclinic $P\overline{1}$ | 3.4859 (7) | 2.320 (2)–2.324 (2) |

Notes: (II) $[ZnBr_2Ni(salpd^{2-})(DMF)_2]$ (Arıcı *et al.*, 2001); (III) $[ZnI_2Ni(salpd^{2-})(DMF)]$ (Tatar, 2002); (IV) $[ZnCl_2Cu(salpd^{2-})]$ (Tatar *et al.*, 1999); (V) $[ZnBr_2Cu(LDMH_2)$-(piperidine)] (Svoboda *et al.*, 2001); (VI) $[ZnCl_2Zn(salpd^{2-})(MeOH)]$ (Atakol, Tatar *et al.*, 1999); (VII) $[ZnBr_2Ni(salpd^{2-})(DMF)]$ (Tatar, Atakol & Arıcı, 2002); (VIII) $[ZnCl_2Zn(salpd^{2-})(DMF)]$ (Tatar, Atakol & Ülkü, 2002); (IX) $[ZnI_2Zn(salpd^{2-})(DMF)]$ (Arıcı & Aksu, 2002); (X) $[HgCl_2Cu(salpd^{2-})]$ (Atakol, Arıcı *et al.*, 1999); (XI) $[HgCl_2Ni(salpd^{2-})]$ (Arıcı *et al.*, 2006). salpd$^{2-}$ = *N*,*N*′-bis(salicylidene)-1,3-propanediamine ($C_{17}H_{16}N_2O_2$), $LDMH_2$ = *N*,*N*′-bis(salicylidene)-2,2′-dimethyl-1,3-propanediamine ($C_{19}H_{22}N_2O_2$), DMF = dimethylformamide ($C_3H_7NO$), piperidine ($C_5H_{11}N$), methylpyridine ($C_6H_7N$).

 doi:10.1107/S1600536807043061  

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Partial support of this work by Hacettepe University Scientific Research Department (project No. 00.01.602.003) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2490).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2489-m2490 [ **doi:10.1107/S1600536807043061** ]

# Diiodido-2$\kappa^2 I$-bis(4-methylpyridine-1$\kappa N$)-$\mu$-{2,2'-[1,3-propanediylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4 O,N,N',O'$:2$\kappa^2 O,O'$}nickel(II)zinc(II)

**L. Tatar Yildirim, O. Atakol and G. Kavak**

## Comment

Zinc$^{II}$ ion is the first in a row of essential rare elements for living beings. It has been recognized to be an activator for more than 120 hydrolytic enzymes. Nickel, which exists extremely in living organism, has allergic and cancerogen effects on skin and organism (Bertini *et al.*, 1994). Oxygen-bridged polynuclear complexes of transition series are of interest because of their magnetic properties (Barandika *et al.*, 1999; Atakol *et al.*, 2006) and their structures (Colon *et al.*, 2004; Metalobos *et al.*, 2004; Yu *et al.*, 2007). Dinuclear metal complexes on Schiff-base ligands have been the subject on considerable interest in our laboratory, *e.g.* [$ZnCl_2Cu(salpd^{2-})$] (Tatar *et al.*, 1999); [$ZnCl_2Zn(salpd^{2-})(MeOH)$] (Atakol, Tatar *et al.*, 1999); [$HgCl_2Cu(salpd^{2-})$] (Atakol, Arıcı *et al.*, 1999); [$ZnBr_2Cu(LDMH_2)$(piperidine)] (Svoboda *et al.*, 2001); [$ZnBr_2Ni(salpd^{2-})(dmf)_2$] (Arıcı *et al.*, 2001); [$ZnI_2Ni(salpd^{2-})(dmf)$] (Tatar, 2002); [$ZnBr_2Ni(salpd^{2-})(dmf)$] (Tatar, Atakol & Arıcı, 2002); [$ZnCl_2Zn(salpd^{2-})(dmf)$] (Tatar, Atakol & Ülkü, 2002); [$ZnI_2Zn(salpd^{2-})(dmf)$] (Arıcı & Aksu, 2002); [$HgCl_2Ni(salpd^{2-})$] (Arıcı *et al.*, 2006). We describe here the structure of a new heteronuclear dimeric complex, [$ZnI_2Ni(salpd^{2-})$(methyl pyridine)$_2$]. Where $salpd^{2-}$= *N*,*N*'-bis(salicylidene)-1,3-propanediamine ($C_{17}H_{16}N_2O_2$), $LDMH_2$ = *N*,*N*'-bis(salicylidene)-2,2'-dimethyl-1, 3-propanediamine ($C_{19}H_{22}N_2O_2$), dmf = dimethylformamide ($C_3H_7NO$), piperidine ($C_5H_{11}N$), methyl pyridine ($C_6H_7N$).

In the title complex (Fig. 1), the Ni$^{II}$ ion is in a distorted octahedral coordination environment, formed by two O and N atoms from chelating $salpd^{2-}$ ligand in the equatorial plane [Ni—O1= 2.038 (5), Ni—O2= 2.029 (5), Ni—N1= 2.016 (7) and 2.021 (6) Å] and two N atoms of two symmetry-related methyl pyridine ligands in the axial positions [Ni—N3=2.177 (6) and Ni—N4= 2.214 (7) Å]. The bond angles around the Ni atom range between 79.52 (19) and 100.1 (3)°. The distance of atom Ni from the O1/O2/N1/N2 mean plane is 0.0050 (10) Å. The equatorial plane (O1/O2/N1/N2) is almost perpendicular of the (N3/Ni/N4) plane, dihedral angle between them is 89 (2)°.

The coordination around the Zn$^{II}$ ion is distorted tetrahedral, with two bridging O atoms of the chelating $salpd^{2-}$ ligand [Zn—O1=1.985 (5) and Zn—O2=1.987 (5) Å] and two iodine atoms. The bond angles around the Zn atom range between 81.9 (2) and 116.49 (16)°. The planes Zn/O1/Ni/O2 and I1/Zn/I2 are almast perpendicular each other, dihedral angle between these two plane is 88.06 (13)°.

The six-membered chelate ring (Ni, N1, C8, C9, C10, N2) adopts a boat conformation, indicated by the endocyclic torsion angles and by the deviations of *para*-positioned boat atoms Ni 0.0552 (10)Å and C9 0.713 (11)Å from the mean plane through N1, N2, C8 and C10. The crystal structure is stabilized by weak hydrogen bonds (Table 1). The moecule has an intermolecular hydrogen bonding set involving the two molecules: [C10—H10B···I1$^{i}$] (symmetry code: (i) $x$ + 1/2, $y$ −

1/2, *z*). The molecule also has two intramolecular hydrogen bonds between the N atoms and the phenyl hydrogen atoms: [C22—H22···N2] and [C28—H28···N2].

A comparison of the space group, $M_c\cdots M_t$ and $M_t$—$R$ distances are given in Table 2 for the similar oxygen-bridged dinuclear complexes reported previously. Where $M_c$ (Cu, Zn, Ni) central metal ion, $M_t$ (Zn, Hg) terminal metal ion and $R$ (Cl, Br, I) is the ion which bonded to terminal metal ion. The distances from the Zn ion to I ions are longer than the distances from Zn and Hg ions to Cl and Br ions as given in the table 2.

### Experimental

Ammonia solution (30 ml) was added to a solution of bis(*N*,*N*'-salicylidene)-1,3-propanediamine (0.565 g, 2 mmol) in hot ethanol (75 ml) and mixture heated to boiling. A solution of $NiCl_2{\cdot}2H_2O$ (0.475 g, 2 mmol) in hot water (30 ml) was then added and the resulting mixture set aside. After 2 h, the light-green nickel complex was filtered off and dried at 413 K for 4 h. This complex (0.338 g, 1 mmol) was dissolved in hot dioxane (80 ml). 4-methylpyridine (0.7 ml) was added to this solution followed by $ZnI_2$ (0.320 g, 1 mmol) in hot methanol (10 ml). This resulting mixture was set aside for 4 d and the light-pink crystals which formed were filtered off and dried in air.

### Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x$ = 1.5 for methyl H, and $x$ = 1.2 for all other H atoms.

### Figures

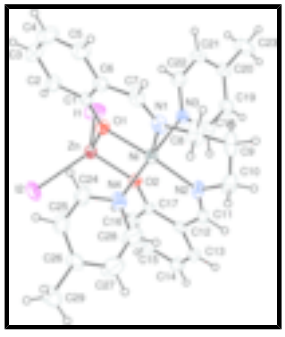

Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

### Diiodido-2κ2I-bis(4-methylpyridine-1κ*N*)-μ-{2,2'-[1,3-propanediylbis (nitrilomethylidyne)]diphenolato-1κ4*O*,*N*,*N*',*O*':2κ2*O*,*O*'}nickel(II)zinc(II)

*Crystal data*

| | |
|---|---|
| $[ZnI_2Ni(C_{17}H_{16}N_2O_2)(C_6H_7N)_2]$ | $F_{000}$ = 1648 |
| $M_r$ = 844.45 | $D_x$ = 1.813 Mg m$^{-3}$ |
| Monoclinic, *Cc* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: C -2yc | Cell parameters from 25 reflections |

| | |
|---|---|
| $a$ = 9.3523 (11) Å | θ = 10.8–18.2º |
| $b$ = 19.615 (3) Å | μ = 3.41 $mm^{-1}$ |
| $c$ = 17.4933 (10) Å | $T$ = 293 (2) K |
| β = 105.390 (12)º | Prism, light pink |
| $V$ = 3094.0 (6) $Å^3$ | 0.2 × 0.2 × 0.2 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius TurboCAD-4 diffractometer | $\theta_{max}$ = 28.0º |
| non–profiled ω scans | $\theta_{min}$ = 3.0º |
| Absorption correction: ψ scan North *et al.* (1968) | $h$ = −12→11 |
| $T_{min}$ = 0.506, $T_{max}$ = 0.511 | $k$ = −25→25 |
| 7375 measured reflections | $l$ = 0→23 |
| 3745 independent reflections | 3 standard reflections |
| 2491 reflections with $I > 2\sigma(I)$ | every 120 min |
| $R_{int}$ = 0.052 | intensity decay: 2% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: geomt |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.033 | $w = 1/[\sigma^2(F_o^2) + (0.0323P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.075 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.48 e $Å^{-3}$ |
| 3745 reflections | $\Delta\rho_{min}$ = −0.49 e $Å^{-3}$ |
| 352 parameters | Extinction correction: none |
| 2 restraints | Absolute structure: Flack (1983), no Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.00 (2) |
| Secondary atom site location: difference Fourier map | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| I1 | 0.73246 (8) | 0.54913 (3) | 0.50165 (4) | 0.0737 (2) |
| I2 | 0.45922 (6) | 0.38306 (5) | 0.39646 (4) | 0.0825 (3) |
| N3 | 1.1124 (6) | 0.4104 (3) | 0.5796 (4) | 0.0402 (15) |
| N4 | 0.8329 (7) | 0.2347 (4) | 0.4816 (5) | 0.0523 (17) |
| C17 | 0.9014 (7) | 0.3837 (4) | 0.3684 (4) | 0.0339 (15) |
| C6 | 0.8512 (8) | 0.3134 (4) | 0.6975 (5) | 0.0448 (19) |
| C1 | 0.7703 (8) | 0.3564 (4) | 0.6384 (5) | 0.0418 (18) |
| N1 | 1.0419 (7) | 0.2727 (4) | 0.6372 (4) | 0.0497 (17) |
| C16 | 0.8181 (8) | 0.4269 (5) | 0.3089 (5) | 0.046 (2) |
| H16 | 0.7415 | 0.4525 | 0.3191 | 0.055* |
| N2 | 1.1280 (7) | 0.2918 (3) | 0.4796 (5) | 0.0469 (16) |
| C10 | 1.2571 (10) | 0.2511 (5) | 0.5233 (6) | 0.066 (3) |
| H10A | 1.3434 | 0.2653 | 0.5064 | 0.079* |
| H10B | 1.2385 | 0.2036 | 0.5089 | 0.079* |
| C15 | 0.8466 (10) | 0.4322 (5) | 0.2361 (5) | 0.054 (2) |
| H15 | 0.7889 | 0.4612 | 0.1981 | 0.065* |
| C12 | 1.0187 (8) | 0.3464 (4) | 0.3498 (5) | 0.0416 (18) |
| C2 | 0.6478 (9) | 0.3922 (5) | 0.6507 (5) | 0.050 (2) |
| H2 | 0.5916 | 0.4202 | 0.6112 | 0.06* |
| C7 | 0.9816 (8) | 0.2741 (4) | 0.6944 (5) | 0.047 (2) |
| H7 | 1.0249 | 0.2474 | 0.7384 | 0.057* |
| C8 | 1.1750 (9) | 0.2272 (5) | 0.6478 (7) | 0.072 (3) |
| H8A | 1.1435 | 0.1833 | 0.6238 | 0.087* |
| H8B | 1.2192 | 0.22 | 0.704 | 0.087* |
| C14 | 0.9603 (10) | 0.3952 (5) | 0.2184 (5) | 0.059 (2) |
| H14 | 0.9782 | 0.3984 | 0.1687 | 0.071* |
| C13 | 1.0462 (9) | 0.3532 (5) | 0.2763 (5) | 0.050 (2) |
| H13 | 1.1242 | 0.329 | 0.2656 | 0.061* |
| C11 | 1.1229 (8) | 0.3050 (4) | 0.4076 (6) | 0.050 (2) |
| H11 | 1.1977 | 0.2851 | 0.3892 | 0.059* |
| C5 | 0.8103 (11) | 0.3083 (5) | 0.7696 (5) | 0.060 (2) |
| H5 | 0.8647 | 0.2802 | 0.8097 | 0.072* |
| C21 | 1.2878 (9) | 0.4929 (5) | 0.5621 (5) | 0.055 (2) |
| H21 | 1.3415 | 0.5107 | 0.5289 | 0.066* |
| C24 | 0.7084 (11) | 0.2176 (5) | 0.4993 (8) | 0.075 (3) |
| H24 | 0.6758 | 0.2456 | 0.5342 | 0.09* |
| C20 | 1.3033 (9) | 0.5210 (5) | 0.6369 (5) | 0.050 (2) |
| C9 | 1.2916 (9) | 0.2572 (6) | 0.6106 (7) | 0.074 (3) |
| H9A | 1.3042 | 0.3051 | 0.6246 | 0.089* |
| H9B | 1.3855 | 0.2347 | 0.6336 | 0.089* |
| C22 | 1.1943 (8) | 0.4396 (4) | 0.5373 (5) | 0.0465 (19) |
| H22 | 1.1871 | 0.4223 | 0.487 | 0.056* |
| C19 | 1.2176 (9) | 0.4922 (5) | 0.6806 (5) | 0.054 (2) |
| H19 | 1.2203 | 0.51 | 0.7302 | 0.065* |
| C3 | 0.6112 (11) | 0.3852 (5) | 0.7228 (6) | 0.065 (3) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.5304 | 0.409 | 0.7308 | 0.079* |
| C18 | 1.1265 (9) | 0.4369 (5) | 0.6519 (5) | 0.054 (2) |
| H18 | 1.0731 | 0.4174 | 0.6842 | 0.065* |
| C26 | 0.6544 (10) | 0.1222 (5) | 0.4138 (5) | 0.054 (2) |
| C23 | 1.4028 (13) | 0.5818 (7) | 0.6642 (7) | 0.088 (4) |
| H23A | 1.3432 | 0.6214 | 0.6655 | 0.132* |
| H23B | 1.4627 | 0.5894 | 0.6282 | 0.132* |
| H23C | 1.4657 | 0.5732 | 0.7163 | 0.132* |
| C4 | 0.6915 (13) | 0.3442 (6) | 0.7816 (6) | 0.073 (3) |
| H4 | 0.6663 | 0.3405 | 0.8294 | 0.088* |
| C27 | 0.7775 (14) | 0.1392 (7) | 0.3926 (8) | 0.102 (3) |
| H27 | 0.8074 | 0.1129 | 0.3554 | 0.123* |
| C25 | 0.6249 (11) | 0.1618 (6) | 0.4700 (7) | 0.075 (3) |
| H25 | 0.5447 | 0.1509 | 0.4897 | 0.091* |
| C28 | 0.8598 (14) | 0.1951 (7) | 0.4255 (8) | 0.109 (5) |
| H28 | 0.9412 | 0.2061 | 0.4069 | 0.131* |
| C29 | 0.5603 (11) | 0.0619 (5) | 0.3769 (7) | 0.075 (3) |
| H29A | 0.4888 | 0.0524 | 0.406 | 0.112* |
| H29B | 0.6226 | 0.0228 | 0.3784 | 0.112* |
| H29C | 0.5097 | 0.0723 | 0.3228 | 0.112* |
| Zn | 0.71340 (8) | 0.42196 (4) | 0.47615 (5) | 0.0380 (2) |
| Ni | 0.97304 (9) | 0.32289 (5) | 0.53338 (6) | 0.0385 (2) |
| O2 | 0.8738 (5) | 0.3799 (3) | 0.4371 (3) | 0.0403 (12) |
| O1 | 0.8033 (5) | 0.3648 (3) | 0.5702 (3) | 0.0394 (12) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I1 | 0.1176 (5) | 0.0392 (3) | 0.0708 (4) | 0.0039 (4) | 0.0364 (4) | −0.0027 (3) |
| I2 | 0.0421 (3) | 0.1351 (7) | 0.0646 (4) | −0.0282 (4) | 0.0040 (3) | −0.0020 (4) |
| N3 | 0.034 (3) | 0.036 (4) | 0.050 (4) | 0.003 (3) | 0.011 (3) | 0.000 (3) |
| N4 | 0.046 (4) | 0.043 (4) | 0.069 (5) | −0.007 (3) | 0.015 (3) | −0.002 (4) |
| C17 | 0.033 (3) | 0.034 (4) | 0.039 (4) | −0.007 (3) | 0.015 (3) | −0.006 (3) |
| C6 | 0.048 (4) | 0.041 (5) | 0.044 (5) | −0.006 (4) | 0.010 (4) | 0.003 (4) |
| C1 | 0.036 (4) | 0.039 (4) | 0.053 (5) | −0.012 (3) | 0.016 (4) | −0.013 (4) |
| N1 | 0.045 (3) | 0.043 (4) | 0.058 (4) | 0.000 (3) | 0.008 (3) | 0.013 (3) |
| C16 | 0.038 (4) | 0.057 (5) | 0.041 (5) | −0.008 (4) | 0.007 (3) | −0.009 (4) |
| N2 | 0.034 (3) | 0.037 (4) | 0.074 (5) | 0.005 (3) | 0.021 (3) | 0.003 (3) |
| C10 | 0.057 (5) | 0.052 (6) | 0.094 (8) | 0.016 (5) | 0.029 (5) | 0.010 (5) |
| C15 | 0.051 (5) | 0.062 (6) | 0.045 (5) | −0.015 (4) | 0.006 (4) | 0.004 (4) |
| C12 | 0.040 (4) | 0.043 (5) | 0.042 (4) | −0.013 (4) | 0.010 (3) | −0.016 (4) |
| C2 | 0.047 (4) | 0.051 (6) | 0.053 (5) | 0.001 (4) | 0.016 (4) | 0.008 (4) |
| C7 | 0.044 (4) | 0.041 (5) | 0.055 (5) | −0.004 (4) | 0.010 (4) | 0.016 (4) |
| C8 | 0.056 (6) | 0.061 (6) | 0.102 (8) | 0.017 (5) | 0.025 (5) | 0.049 (6) |
| C14 | 0.058 (5) | 0.079 (7) | 0.045 (5) | −0.018 (5) | 0.023 (4) | −0.011 (5) |
| C13 | 0.043 (4) | 0.061 (6) | 0.051 (5) | −0.011 (4) | 0.019 (4) | −0.023 (4) |
| C11 | 0.033 (4) | 0.046 (5) | 0.074 (6) | −0.011 (3) | 0.022 (4) | −0.020 (5) |
| C5 | 0.073 (6) | 0.061 (6) | 0.048 (5) | −0.005 (5) | 0.017 (4) | 0.010 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 0.049 (5) | 0.060 (6) | 0.058 (6) | −0.014 (4) | 0.020 (4) | 0.002 (5) |
| C24 | 0.064 (6) | 0.056 (6) | 0.120 (9) | −0.015 (5) | 0.049 (6) | −0.020 (7) |
| C20 | 0.045 (4) | 0.051 (5) | 0.049 (5) | −0.009 (4) | 0.002 (4) | −0.006 (4) |
| C9 | 0.038 (4) | 0.066 (7) | 0.116 (9) | 0.020 (4) | 0.015 (5) | 0.033 (6) |
| C22 | 0.053 (5) | 0.040 (5) | 0.045 (4) | −0.006 (4) | 0.011 (4) | 0.002 (4) |
| C19 | 0.055 (5) | 0.063 (6) | 0.043 (5) | −0.007 (4) | 0.009 (4) | −0.014 (4) |
| C3 | 0.080 (6) | 0.062 (7) | 0.068 (6) | 0.008 (5) | 0.042 (5) | 0.003 (5) |
| C18 | 0.048 (4) | 0.062 (6) | 0.053 (5) | −0.009 (4) | 0.017 (4) | 0.001 (4) |
| C26 | 0.060 (5) | 0.040 (5) | 0.061 (5) | −0.021 (4) | 0.016 (4) | −0.004 (4) |
| C23 | 0.088 (7) | 0.089 (9) | 0.079 (8) | −0.046 (7) | 0.010 (6) | −0.027 (7) |
| C4 | 0.099 (8) | 0.077 (8) | 0.055 (6) | −0.010 (6) | 0.039 (6) | 0.008 (5) |
| C27 | 0.104 | 0.113 (11) | 0.111 | −0.057 (7) | 0.065 (5) | −0.058 (8) |
| C25 | 0.059 (5) | 0.068 (7) | 0.111 (9) | −0.024 (5) | 0.041 (6) | −0.027 (6) |
| C28 | 0.117 (9) | 0.108 (10) | 0.134 (11) | −0.074 (8) | 0.089 (9) | −0.071 (9) |
| C29 | 0.072 (6) | 0.061 (7) | 0.083 (7) | −0.021 (5) | 0.005 (5) | 0.005 (5) |
| Zn | 0.0342 (4) | 0.0389 (5) | 0.0400 (5) | 0.0034 (4) | 0.0084 (4) | 0.0014 (4) |
| Ni | 0.0336 (4) | 0.0344 (5) | 0.0477 (6) | 0.0013 (4) | 0.0108 (4) | 0.0022 (4) |
| O2 | 0.037 (2) | 0.047 (3) | 0.039 (3) | 0.007 (2) | 0.011 (2) | 0.001 (2) |
| O1 | 0.040 (3) | 0.046 (3) | 0.034 (3) | 0.001 (2) | 0.013 (2) | 0.008 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| I1—Zn | 2.5320 (11) | C13—H13 | 0.93 |
| I2—Zn | 2.5333 (10) | C11—H11 | 0.93 |
| N3—C22 | 1.328 (10) | C5—C4 | 1.377 (15) |
| N3—C18 | 1.341 (11) | C5—H5 | 0.93 |
| N3—Ni | 2.177 (6) | C21—C22 | 1.358 (11) |
| N4—C24 | 1.325 (11) | C21—C20 | 1.392 (12) |
| N4—C28 | 1.326 (12) | C21—H21 | 0.93 |
| N4—Ni | 2.214 (7) | C24—C25 | 1.363 (13) |
| C17—O2 | 1.296 (9) | C24—H24 | 0.93 |
| C17—C16 | 1.406 (11) | C20—C19 | 1.368 (13) |
| C17—C12 | 1.426 (10) | C20—C23 | 1.509 (13) |
| C6—C1 | 1.392 (11) | C9—H9A | 0.97 |
| C6—C5 | 1.416 (12) | C9—H9B | 0.97 |
| C6—C7 | 1.456 (11) | C22—H22 | 0.93 |
| C1—O1 | 1.319 (9) | C19—C18 | 1.389 (12) |
| C1—C2 | 1.408 (11) | C19—H19 | 0.93 |
| N1—C7 | 1.272 (10) | C3—C4 | 1.363 (15) |
| N1—C8 | 1.503 (11) | C3—H3 | 0.93 |
| N1—Ni | 2.016 (7) | C18—H18 | 0.93 |
| C16—C15 | 1.372 (12) | C26—C25 | 1.339 (14) |
| C16—H16 | 0.93 | C26—C27 | 1.341 (13) |
| N2—C11 | 1.274 (11) | C26—C29 | 1.513 (12) |
| N2—C10 | 1.479 (11) | C23—H23A | 0.96 |
| N2—Ni | 2.021 (6) | C23—H23B | 0.96 |
| C10—C9 | 1.480 (16) | C23—H23C | 0.96 |
| C10—H10A | 0.97 | C4—H4 | 0.93 |
| C10—H10B | 0.97 | C27—C28 | 1.376 (15) |

| | | | |
|---|---|---|---|
| C15—C14 | 1.390 (13) | C27—H27 | 0.93 |
| C15—H15 | 0.93 | C25—H25 | 0.93 |
| C12—C13 | 1.383 (11) | C28—H28 | 0.93 |
| C12—C11 | 1.452 (13) | C29—H29A | 0.96 |
| C2—C3 | 1.398 (12) | C29—H29B | 0.96 |
| C2—H2 | 0.93 | C29—H29C | 0.96 |
| C7—H7 | 0.93 | Zn—O1 | 1.985 (5) |
| C8—C9 | 1.528 (13) | Zn—O2 | 1.987 (5) |
| C8—H8A | 0.97 | Zn—Ni | 3.0634 (12) |
| C8—H8B | 0.97 | Ni—O2 | 2.029 (5) |
| C14—C13 | 1.385 (14) | Ni—O1 | 2.038 (5) |
| C14—H14 | 0.93 | | |
| C22—N3—C18 | 115.6 (7) | N3—C22—H22 | 117.5 |
| C22—N3—Ni | 120.7 (5) | C21—C22—H22 | 117.5 |
| C18—N3—Ni | 123.7 (5) | C20—C19—C18 | 121.1 (8) |
| C24—N4—C28 | 112.1 (8) | C20—C19—H19 | 119.5 |
| C24—N4—Ni | 124.3 (7) | C18—C19—H19 | 119.5 |
| C28—N4—Ni | 123.5 (6) | C4—C3—C2 | 121.4 (9) |
| O2—C17—C16 | 120.9 (7) | C4—C3—H3 | 119.3 |
| O2—C17—C12 | 122.4 (7) | C2—C3—H3 | 119.3 |
| C16—C17—C12 | 116.7 (7) | N3—C18—C19 | 122.7 (8) |
| C1—C6—C5 | 118.8 (8) | N3—C18—H18 | 118.6 |
| C1—C6—C7 | 126.1 (7) | C19—C18—H18 | 118.6 |
| C5—C6—C7 | 115.0 (8) | C25—C26—C27 | 114.7 (9) |
| O1—C1—C6 | 122.4 (7) | C25—C26—C29 | 123.9 (8) |
| O1—C1—C2 | 118.1 (7) | C27—C26—C29 | 121.4 (9) |
| C6—C1—C2 | 119.5 (7) | C20—C23—H23A | 109.5 |
| C7—N1—C8 | 116.2 (7) | C20—C23—H23B | 109.5 |
| C7—N1—Ni | 126.6 (6) | H23A—C23—H23B | 109.5 |
| C8—N1—Ni | 117.2 (6) | C20—C23—H23C | 109.5 |
| C15—C16—C17 | 121.8 (8) | H23A—C23—H23C | 109.5 |
| C15—C16—H16 | 119.1 | H23B—C23—H23C | 109.5 |
| C17—C16—H16 | 119.1 | C3—C4—C5 | 119.4 (9) |
| C11—N2—C10 | 115.6 (7) | C3—C4—H4 | 120.3 |
| C11—N2—Ni | 123.7 (6) | C5—C4—H4 | 120.3 |
| C10—N2—Ni | 120.7 (6) | C26—C27—C28 | 120.5 (10) |
| N2—C10—C9 | 114.5 (8) | C26—C27—H27 | 119.7 |
| N2—C10—H10A | 108.6 | C28—C27—H27 | 119.7 |
| C9—C10—H10A | 108.6 | C26—C25—C24 | 122.2 (9) |
| N2—C10—H10B | 108.6 | C26—C25—H25 | 118.9 |
| C9—C10—H10B | 108.6 | C24—C25—H25 | 118.9 |
| H10A—C10—H10B | 107.6 | N4—C28—C27 | 125.5 (9) |
| C16—C15—C14 | 121.0 (9) | N4—C28—H28 | 117.2 |
| C16—C15—H15 | 119.5 | C27—C28—H28 | 117.2 |
| C14—C15—H15 | 119.5 | C26—C29—H29A | 109.5 |
| C13—C12—C17 | 120.5 (8) | C26—C29—H29B | 109.5 |
| C13—C12—C11 | 116.4 (7) | H29A—C29—H29B | 109.5 |
| C17—C12—C11 | 122.9 (7) | C26—C29—H29C | 109.5 |
| C3—C2—C1 | 119.5 (8) | H29A—C29—H29C | 109.5 |

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| C3—C2—H2 | 120.2 | H29B—C29—H29C | 109.5 |
| C1—C2—H2 | 120.2 | O1—Zn—O2 | 81.9 (2) |
| N1—C7—C6 | 126.2 (8) | O1—Zn—I1 | 114.59 (15) |
| N1—C7—H7 | 116.9 | O2—Zn—I1 | 116.48 (16) |
| C6—C7—H7 | 116.9 | O1—Zn—I2 | 114.53 (15) |
| N1—C8—C9 | 112.4 (7) | O2—Zn—I2 | 111.69 (15) |
| N1—C8—H8A | 109.1 | I1—Zn—I2 | 113.93 (4) |
| C9—C8—H8A | 109.1 | O1—Zn—Ni | 41.06 (13) |
| N1—C8—H8B | 109.1 | O2—Zn—Ni | 40.81 (15) |
| C9—C8—H8B | 109.1 | I1—Zn—Ni | 123.69 (4) |
| H8A—C8—H8B | 107.9 | I2—Zn—Ni | 122.37 (4) |
| C13—C14—C15 | 118.5 (8) | N1—Ni—N2 | 100.1 (3) |
| C13—C14—H14 | 120.7 | N1—Ni—O2 | 169.6 (2) |
| C15—C14—H14 | 120.7 | N2—Ni—O2 | 90.3 (2) |
| C12—C13—C14 | 121.5 (8) | N1—Ni—O1 | 90.1 (2) |
| C12—C13—H13 | 119.3 | N2—Ni—O1 | 169.8 (3) |
| C14—C13—H13 | 119.3 | O2—Ni—O1 | 79.52 (19) |
| N2—C11—C12 | 130.1 (7) | N1—Ni—N3 | 91.9 (3) |
| N2—C11—H11 | 115 | N2—Ni—N3 | 88.8 (2) |
| C12—C11—H11 | 115 | O2—Ni—N3 | 88.3 (2) |
| C4—C5—C6 | 121.3 (9) | O1—Ni—N3 | 90.3 (2) |
| C4—C5—H5 | 119.4 | N1—Ni—N4 | 90.0 (3) |
| C6—C5—H5 | 119.4 | N2—Ni—N4 | 89.6 (3) |
| C22—C21—C20 | 120.2 (8) | O2—Ni—N4 | 90.0 (3) |
| C22—C21—H21 | 119.9 | O1—Ni—N4 | 91.0 (2) |
| C20—C21—H21 | 119.9 | N3—Ni—N4 | 177.7 (3) |
| N4—C24—C25 | 124.5 (9) | N1—Ni—Zn | 129.8 (2) |
| N4—C24—H24 | 117.8 | N2—Ni—Zn | 130.1 (2) |
| C25—C24—H24 | 117.8 | O2—Ni—Zn | 39.77 (14) |
| C19—C20—C21 | 115.5 (8) | O1—Ni—Zn | 39.77 (13) |
| C19—C20—C23 | 123.6 (8) | N3—Ni—Zn | 88.04 (16) |
| C21—C20—C23 | 120.8 (8) | N4—Ni—Zn | 91.72 (18) |
| C10—C9—C8 | 115.1 (9) | C17—O2—Zn | 130.5 (5) |
| C10—C9—H9A | 108.5 | C17—O2—Ni | 130.0 (5) |
| C8—C9—H9A | 108.5 | Zn—O2—Ni | 99.4 (2) |
| C10—C9—H9B | 108.5 | C1—O1—Zn | 132.2 (5) |
| C8—C9—H9B | 108.5 | C1—O1—Ni | 128.6 (5) |
| H9A—C9—H9B | 107.5 | Zn—O1—Ni | 99.2 (2) |
| N3—C22—C21 | 124.9 (8) | | |
| C5—C6—C1—O1 | 178.7 (7) | C18—N3—Ni—O2 | 126.5 (6) |
| C7—C6—C1—O1 | 1.7 (13) | C22—N3—Ni—O1 | −135.4 (6) |
| C5—C6—C1—C2 | −1.8 (12) | C18—N3—Ni—O1 | 47.0 (6) |
| C7—C6—C1—C2 | −178.8 (7) | C22—N3—Ni—N4 | −12 (6) |
| O2—C17—C16—C15 | 179.3 (7) | C18—N3—Ni—N4 | 171 (6) |
| C12—C17—C16—C15 | 0.9 (11) | C22—N3—Ni—Zn | −95.7 (5) |
| C11—N2—C10—C9 | 158.8 (8) | C18—N3—Ni—Zn | 86.7 (6) |
| Ni—N2—C10—C9 | −21.2 (11) | C24—N4—Ni—N1 | 72.8 (9) |
| C17—C16—C15—C14 | −0.3 (13) | C28—N4—Ni—N1 | −111.3 (10) |
| O2—C17—C12—C13 | −178.6 (7) | C24—N4—Ni—N2 | 172.9 (9) |

| | | | |
|---|---|---|---|
| C16—C17—C12—C13 | −0.2 (10) | C28—N4—Ni—N2 | −11.2 (10) |
| O2—C17—C12—C11 | −4.5 (11) | C24—N4—Ni—O2 | −96.8 (9) |
| C16—C17—C12—C11 | 173.9 (7) | C28—N4—Ni—O2 | 79.2 (10) |
| O1—C1—C2—C3 | −179.1 (8) | C24—N4—Ni—O1 | −17.3 (9) |
| C6—C1—C2—C3 | 1.5 (12) | C28—N4—Ni—O1 | 158.7 (10) |
| C8—N1—C7—C6 | −179.2 (8) | C24—N4—Ni—N3 | −141 (6) |
| Ni—N1—C7—C6 | −1.3 (12) | C28—N4—Ni—N3 | 35 (6) |
| C1—C6—C7—N1 | −0.2 (14) | C24—N4—Ni—Zn | −57.0 (9) |
| C5—C6—C7—N1 | −177.2 (9) | C28—N4—Ni—Zn | 118.9 (10) |
| C7—N1—C8—C9 | −144.4 (9) | O1—Zn—Ni—N1 | −1.9 (3) |
| Ni—N1—C8—C9 | 37.5 (11) | O2—Zn—Ni—N1 | −179.4 (4) |
| C16—C15—C14—C13 | −0.9 (13) | I1—Zn—Ni—N1 | 87.9 (3) |
| C17—C12—C13—C14 | −1.0 (12) | I2—Zn—Ni—N1 | −93.1 (3) |
| C11—C12—C13—C14 | −175.5 (8) | O1—Zn—Ni—N2 | −179.5 (3) |
| C15—C14—C13—C12 | 1.6 (13) | O2—Zn—Ni—N2 | 3.0 (3) |
| C10—N2—C11—C12 | −175.9 (8) | I1—Zn—Ni—N2 | −89.7 (3) |
| Ni—N2—C11—C12 | 4.2 (12) | I2—Zn—Ni—N2 | 89.3 (3) |
| C13—C12—C11—N2 | 177.6 (8) | O1—Zn—Ni—O2 | 177.5 (3) |
| C17—C12—C11—N2 | 3.3 (13) | I1—Zn—Ni—O2 | −92.8 (2) |
| C1—C6—C5—C4 | 1.0 (14) | I2—Zn—Ni—O2 | 86.3 (2) |
| C7—C6—C5—C4 | 178.3 (9) | O2—Zn—Ni—O1 | −177.5 (3) |
| C28—N4—C24—C25 | 6.4 (18) | I1—Zn—Ni—O1 | 89.8 (2) |
| Ni—N4—C24—C25 | −177.2 (10) | I2—Zn—Ni—O1 | −91.2 (2) |
| C22—C21—C20—C19 | −1.2 (13) | O1—Zn—Ni—N3 | −92.8 (3) |
| C22—C21—C20—C23 | −177.9 (10) | O2—Zn—Ni—N3 | 89.8 (3) |
| N2—C10—C9—C8 | 66.8 (11) | I1—Zn—Ni—N3 | −2.99 (17) |
| N1—C8—C9—C10 | −77.1 (12) | I2—Zn—Ni—N3 | 176.05 (17) |
| C18—N3—C22—C21 | −0.2 (12) | O1—Zn—Ni—N4 | 89.6 (3) |
| Ni—N3—C22—C21 | −177.9 (7) | O2—Zn—Ni—N4 | −87.9 (3) |
| C20—C21—C22—N3 | 0.0 (13) | I1—Zn—Ni—N4 | 179.3 (2) |
| C21—C20—C19—C18 | 2.5 (13) | I2—Zn—Ni—N4 | −1.6 (2) |
| C23—C20—C19—C18 | 179.1 (10) | C16—C17—O2—Zn | 5.2 (10) |
| C1—C2—C3—C4 | −0.2 (15) | C12—C17—O2—Zn | −176.5 (5) |
| C22—N3—C18—C19 | 1.5 (12) | C16—C17—O2—Ni | 179.8 (5) |
| Ni—N3—C18—C19 | 179.2 (7) | C12—C17—O2—Ni | −1.9 (10) |
| C20—C19—C18—N3 | −2.8 (14) | O1—Zn—O2—C17 | 174.1 (6) |
| C2—C3—C4—C5 | −0.7 (17) | I1—Zn—O2—C17 | −72.4 (6) |
| C6—C5—C4—C3 | 0.3 (16) | I2—Zn—O2—C17 | 60.9 (6) |
| C25—C26—C27—C28 | −3(2) | Ni—Zn—O2—C17 | 175.8 (7) |
| C29—C26—C27—C28 | 178.5 (14) | O1—Zn—O2—Ni | −1.7 (2) |
| C27—C26—C25—C24 | 4.1 (18) | I1—Zn—O2—Ni | 111.79 (17) |
| C29—C26—C25—C24 | −176.9 (11) | I2—Zn—O2—Ni | −114.90 (16) |
| N4—C24—C25—C26 | −7(2) | N1—Ni—O2—C17 | −173.1 (12) |
| C24—N4—C28—C27 | −5(2) | N2—Ni—O2—C17 | 6.5 (6) |
| Ni—N4—C28—C27 | 178.8 (13) | O1—Ni—O2—C17 | −174.2 (6) |
| C26—C27—C28—N4 | 3(3) | N3—Ni—O2—C17 | 95.2 (6) |
| C7—N1—Ni—N2 | −179.6 (7) | N4—Ni—O2—C17 | −83.1 (6) |
| C8—N1—Ni—N2 | −1.7 (7) | Zn—Ni—O2—C17 | −175.8 (7) |
| C7—N1—Ni—O2 | 0.0 (19) | N1—Ni—O2—Zn | 2.7 (15) |

| | | | |
|---|---|---|---|
| C8—N1—Ni—O2 | 177.9 (12) | N2—Ni—O2—Zn | −177.7 (3) |
| C7—N1—Ni—O1 | 1.0 (7) | O1—Ni—O2—Zn | 1.6 (2) |
| C8—N1—Ni—O1 | 179.0 (6) | N3—Ni—O2—Zn | −88.9 (2) |
| C7—N1—Ni—N3 | 91.3 (7) | N4—Ni—O2—Zn | 92.7 (3) |
| C8—N1—Ni—N3 | −90.8 (6) | C6—C1—O1—Zn | −179.2 (5) |
| C7—N1—Ni—N4 | −90.0 (7) | C2—C1—O1—Zn | 1.4 (10) |
| C8—N1—Ni—N4 | 87.9 (6) | C6—C1—O1—Ni | −1.7 (10) |
| C7—N1—Ni—Zn | 2.2 (8) | C2—C1—O1—Ni | 178.8 (5) |
| C8—N1—Ni—Zn | −179.8 (5) | O2—Zn—O1—C1 | 179.7 (6) |
| C11—N2—Ni—N1 | 172.7 (7) | I1—Zn—O1—C1 | 64.2 (6) |
| C10—N2—Ni—N1 | −7.2 (7) | I2—Zn—O1—C1 | −70.2 (6) |
| C11—N2—Ni—O2 | −7.2 (7) | Ni—Zn—O1—C1 | 178.0 (7) |
| C10—N2—Ni—O2 | 172.9 (6) | O2—Zn—O1—Ni | 1.7 (2) |
| C11—N2—Ni—O1 | −11.0 (19) | I1—Zn—O1—Ni | −113.79 (16) |
| C10—N2—Ni—O1 | 169.1 (12) | I2—Zn—O1—Ni | 111.85 (16) |
| C11—N2—Ni—N3 | −95.5 (7) | N1—Ni—O1—C1 | 0.5 (6) |
| C10—N2—Ni—N3 | 84.5 (6) | N2—Ni—O1—C1 | −175.9 (13) |
| C11—N2—Ni—N4 | 82.8 (7) | O2—Ni—O1—C1 | −179.7 (6) |
| C10—N2—Ni—N4 | −97.2 (6) | N3—Ni—O1—C1 | −91.5 (6) |
| C11—N2—Ni—Zn | −9.1 (8) | N4—Ni—O1—C1 | 90.5 (6) |
| C10—N2—Ni—Zn | 170.9 (5) | Zn—Ni—O1—C1 | −178.1 (7) |
| C22—N3—Ni—N1 | 134.5 (6) | N1—Ni—O1—Zn | 178.5 (3) |
| C18—N3—Ni—N1 | −43.1 (7) | N2—Ni—O1—Zn | 2.2 (15) |
| C22—N3—Ni—N2 | 34.4 (6) | O2—Ni—O1—Zn | −1.6 (2) |
| C18—N3—Ni—N2 | −143.1 (7) | N3—Ni—O1—Zn | 86.6 (2) |
| C22—N3—Ni—O2 | −55.9 (6) | N4—Ni—O1—Zn | −91.4 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10B···I1$^{i}$ | 0.97 | 3.03 | 3.981 (10) | 166 |
| C22—H22···N2 | 0.93 | 2.61 | 3.078 (10) | 111 |
| C28—H28···N2 | 0.93 | 2.51 | 3.086 (15) | 120 |

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

***Table 2***

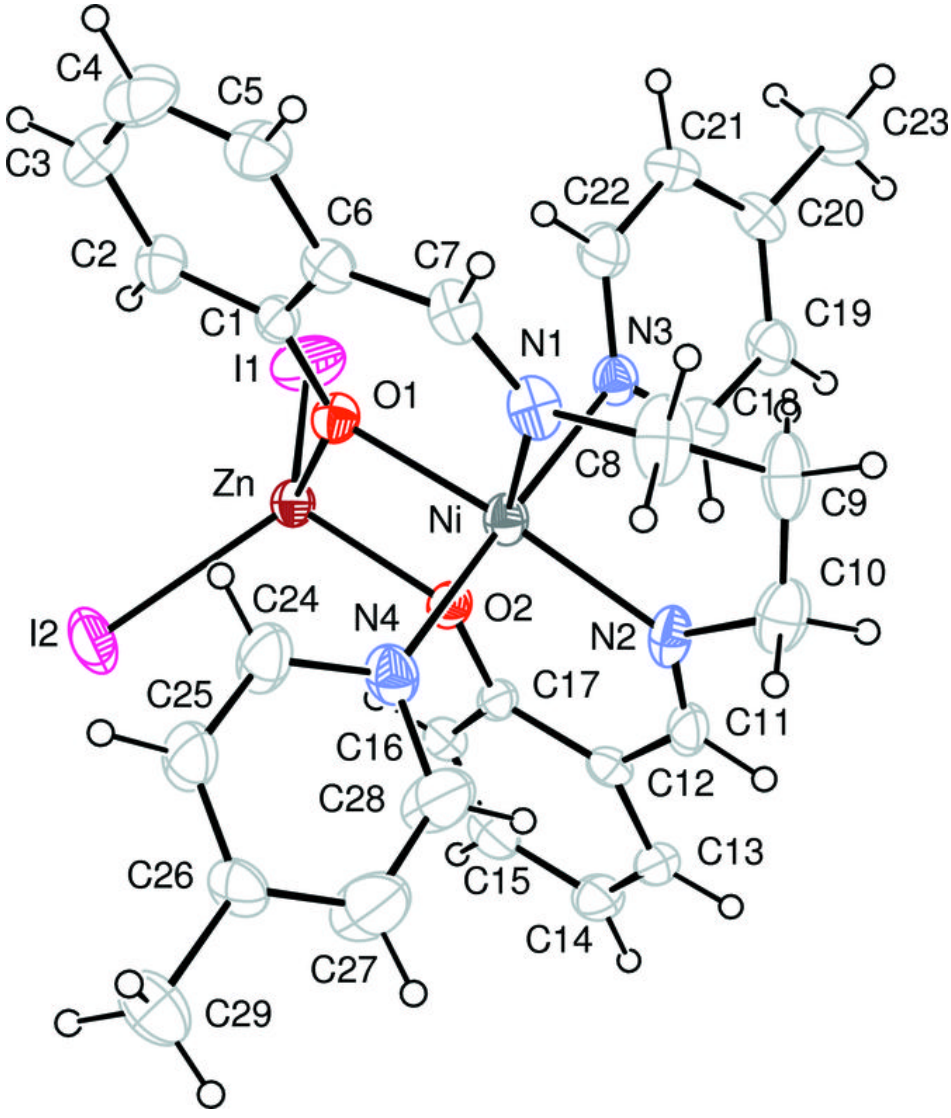
*Table 2. Comparision of the some crystallographic properties of corresponding dinuclear complexes.*

| Compound [$M_tR_2M_c$] | Space Group | $M_c\cdots M_t$ (Å) | $M_t$-$R$ (Å) |
|---|---|---|---|
| (I) | Monoclinic *Cc* | 3.0634 (13) | 2.5320 (11)–2.5333 (10) |
| (II) | Monoclinic *Cc* | 3.0738 (19) | 2.3412 (18)–2.3628 (16) |
| (III) | Monoclinic *Cc* | 3.0695 (11) | 2.5303 (9)–2.5424 (9) |
| (IV) | Monoclinic $P2_1/c$ | 3.0757 (6) | 2.208 (1)–2.208 (1) |
| (V) | Monoclinik $P2_1/n$ | 3.0800 (9) | 2.3309 (9)–2.3508 (10) |
| (VI) | Monoclinic $P2_1$ | not_given | 2.216 (4)–2.200 (4) |
| (VII) | Orthorhombic $P2_12_12_1$ | 3.0917 (15) | 2.3356 (16)–2.3634 (15) |
| (VIII) | Orthorhombic $P2_12_12_1$ | 3.161 (1) | 2.2163 (14)–2.2054 (14) |
| (IX) | Orthorhombic $P2_12_12_1$ | 3.1464 (16) | 2.5373 (14)–2.5527 (14) |

| | | | |
|---|---|---|---|
| (*X*) | Triclinic P-1 | 3.5301 (8) | 2.3430 (10)–2.325 (2) |
| (XI) | Triclinic P-1 | 3.4859 (7) | 2.320 (2)–2.324 (2) |

Notes: (II) $[ZnBr_2Ni(salpd^{2-})(DMF)_2]$ (Arıcı *et al.*, 2001); (III) $[ZnI_2Ni(salpd^{2-})(DMF)]$ (Tatar, 2002); (IV) $[ZnCl_2Cu(salpd^{2-})]$ (Tatar *et al.*, 1999); (V) $[ZnBr_2Cu(LDMH_2)(piperidine)]$ (Svoboda *et al.*, 2001); (VI) $[ZnCl_2Zn(salpd^{2-})(MeOH)]$ (Atakol, Tatar *et al.*, 1999); (VII) $[ZnBr_2Ni(salpd^{2-})(DMF)]$ (Tatar, Atakol, Arıcı, 2002); (VIII) $[ZnCl_2Zn(salpd^{2-})(DMF)]$ (Tatar, Atakol, Ülkü, 2002); (IX) $[ZnI_2Zn(salpd^{2-})(DMF)]$ (Arıcı & Aksu, 2002); (*X*) $[HgCl_2Cu(salpd^{2-})]$ (Atakol, Arıcı *et al.*, 1999); (XI) $[HgCl_2Ni(salpd^{2-})]$ Arıcı *et al.*, 2006). $salpd^{2-}$ = *N*,*N*'-bis(salicylidene)-1,3-propanediamine ($C_{17}H_{16}N_2O_2$), $LDMH_2$ = *N*,*N*'-bis(salicylidene)-2,2'-dimethyl-1, 3-propanediamine ($C_{19}H_{22}N_2O_2$), DMF = dimethylformamide ($C_3H_7NO$), piperidine ($C_5H_{11}N$), methylpyridine ($C_6H_7N$).

**Fig. 1**


C4
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C28
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