

Table 2. Selected geometric parameters (\AA , $^\circ$) for (6)

Co1—C5	1.808 (2)	Mn1—C4	1.861 (2)
Co1—C6	1.813 (2)	Mn1—C10	2.050 (2)
Co1—C7	1.822 (2)	Mn1—C9	2.107 (2)
Co1—C9	1.941 (2)	O8—C11	1.196 (2)
Co1—C10	1.970 (2)	O9—C11	1.331 (3)
Co1—Mn1	2.5468 (4)	O9—C12	1.456 (3)
Mn1—C1	1.814 (2)	C8—C9	1.494 (3)
Mn1—C3	1.838 (2)	C9—C10	1.328 (3)
Mn1—C2	1.844 (2)	C10—C11	1.474 (3)
C9—Co1—C10	39.68 (8)	C8—C9—Mn1	135.5 (2)
C9—Co1—Mn1	53.98 (6)	Co1—C9—Mn1	77.84 (7)
C10—Co1—Mn1	52.10 (5)	C9—C10—C11	133.3 (2)
C10—Mn1—C9	37.22 (7)	C9—C10—Co1	68.99 (12)
C10—Mn1—Co1	49.32 (5)	C11—C10—Co1	136.20 (14)
C9—Mn1—Co1	48.17 (5)	C9—C10—Mn1	73.73 (12)
C11—O9—C12	115.9 (2)	C11—C10—Mn1	137.82 (14)
C10—C9—C8	138.1 (2)	Co1—C10—Mn1	78.59 (7)
C10—C9—Co1	71.34 (11)	O8—C11—O9	124.5 (2)
C8—C9—Co1	136.5 (2)	O8—C11—C10	123.7 (2)
C10—C9—Mn1	69.05 (11)	O9—C11—C10	111.8 (2)

Methyl H-atom positions for both (5) and (6) were calculated ($C-H = 0.96$ and 0.97\AA , respectively) after the location of at least one H atom from the electron-density map. Three of the four methyl groups have disordered H-atom positions and their occupancies were fixed at 0.5. All H atoms were treated with a riding model and the U_{iso} value was defined as $1.5U_{eq}(C)$.

For both compounds, data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structures: *SHELXTL* (Siemens, 1995); program(s) used to refine structures: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1210). Services for accessing these data are described at the back of the journal.

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[[μ -Bis(salicylidene)-1,3-propanediaminato]-bis(4-methylpyridine)nickel(II)] dichloro-zinc(II)†

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Abstract

The title compound, $[\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)(\text{C}_6\text{H}_7\text{N})_2\text{-}\{\text{ZnCl}_2\}]$, is a heteronuclear dimeric complex. The Ni atom has an irregular octahedral environment involving two O atoms and two N atoms from the bis(salicylidene)-1,3-propanediaminate ligand in the equatorial plane, and two N atoms from the two 4-methylpyridine groups in the apical positions. The Ni—O—Zn, O—Zn—O, Zn—O—Ni and O—Ni—O angles in the bridged plane are $99.58(9)$, $80.59(8)$, $100.57(9)$ and $79.26(8)^\circ$, respectively. The Ni···Zn distance is $3.0896(9) \text{\AA}$.

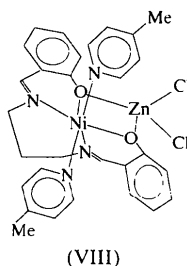
Comment

Dinuclear homo- or heterometal complexes with double oxygen bridges have subnormal magnetic moments due to super-exchange interactions between the bridged metal ions. The magnetic interactions depend on the immediate environment of the bridge, as well as on the ligand arrangement about the metal ions. Structural details of doubly oxygen-bridged homonuclear dimeric copper(II) complexes have been reported previously (Kato *et al.*, 1964; Barclay & Hoskins, 1965; Butcher & Sinn, 1976; Kato & Muto, 1988). Dinuclear and trinuclear homo- or heterometal complexes based on Schiff base

† Systematic name: dichloro- $2\kappa^2\text{Cl}$ -bis(4-methylpyridine- $1\kappa\text{N}$)- μ - $\{2,2'$ -[1,3-propanediylbis(nitrilomethylidene)]diphenolato}- $1\kappa^4\text{O},\text{N},\text{N}',\text{O}'$: $2\kappa^2\text{O},\text{O}'$ -nickel(II)zinc(II).

ligands have been the subject of considerable interest in our laboratories and we have reported the structures of [Cu₂(C₁₁H₁₀ClNO₂)₂] (Tahir *et al.*, 1996), [Cu₂(C₁₄H₁₁NO₂)₂] (Ülkü, Ercan, Atakol, Ercan & Gencer, 1997), Ni₃{(SALPD)(CH₃CO₂)[(CH₃)₂SO]}₂ (Ülkü, Tahir *et al.*, 1997), Cd{Ni(SALPD)(CH₃CO₂)[(CH₃)₂CHNO]}₂ (Ülkü, Ercan, Atakol & Dinçer, 1997), [Cu₂(C₁₂H₁₃NO₂)₂] (Atakol *et al.*, 1997), [Cu₂(C₁₂H₁₃NO₂)₂] (Atakol *et al.*, 1997), [Cu₂(C₁₂H₁₃NO₂)₂] (Ülkü *et al.*, 1998), Ni₂{Cu(SALPD)(NO₂)[(CH₃)₂CHNO]}₂·2[(CH₃)₂CHNO] (Tahir *et al.*, 1998), Mn{Ni(SALPD)(CH₃CO₂)[(CH₃)₂CHNO]}₂ (Ercan & Atakol, 1998), Cd{Cu(SALPD)(CH₃CO₂)₂·C₄H₈O₂} (Ercan, Ülkü *et al.*, 1998), Cu₃{(SALPD)(CH₃CO₂)₂·C₄H₈O₂} [Atakol *et al.*, 1999; SALPD²⁻ is *N,N'*-bis(salicylidene)-1,3-propanediaminate], [Cu{Zn(C₂₃H₂₁I₂N₃O₂)}] (Ercan, Arıcı, Akay *et al.*, 1999), [Ni{Zn(C₃₁H₃₄I₂N₄O₂)}] (Arıcı *et al.*, 1999) and [Cu{Zn(C₁₇H₁₆I₂N₂O₂)}] (Ercan, Arıcı, Ülkü *et al.*, 1999). The magnetic properties are currently under investigation.

We describe here a new heteronuclear dimeric complex, [Ni(SALPD)(C₆H₇N)₂{ZnCl₂}], (VIII), the structure determination of which was undertaken in order to permit a comparison of its bridging environment with those of similar dimeric systems.



The coordination around the Ni^{II} ion in the heterodimeric complex is an irregular octahedron involving two bridging O atoms and two N atoms from the SALPD²⁻ ligand in the equatorial plane (Fig. 1). In the axial positions of this irregular octahedron, there is an N atom from each of the two 4-methylpyridine groups, *i.e.* N3 and N4. The distortion of the regular pyramids is revealed by the bond angles between the apical and equatorial donor atoms (Table 1). The value of this distortion (represented by τ) is 0.014 for the Ni^{II} ion. τ [$(\beta - \alpha)/60^\circ$; α and β are the two largest angles around the central atom] is equal to 0 in a regular square pyramid (Addison *et al.*, 1984; Uhlenbrock *et al.*, 1996). The coordination plane composed of atoms N1, N2, O1 and O2, and the bridging plane composed of atoms Ni, O1, Zn and O2 have a dihedral angle of $0.44(9)^\circ$ between them. The Ni—O1—Zn and O1—Ni—O2 bridging angles are $99.58(9)$ and $79.26(8)^\circ$, respectively. This dihedral angle, as well as the bridging angle, influences the magnetic properties of the systems. The Ni···Zn distance [$3.0896(9)$ Å] is long

for a direct interaction. The Ni—O1—Zn—O2 bridging plane is approximately planar. The Ni atom is located $-0.0025(5)$ Å from the coordination best plane.

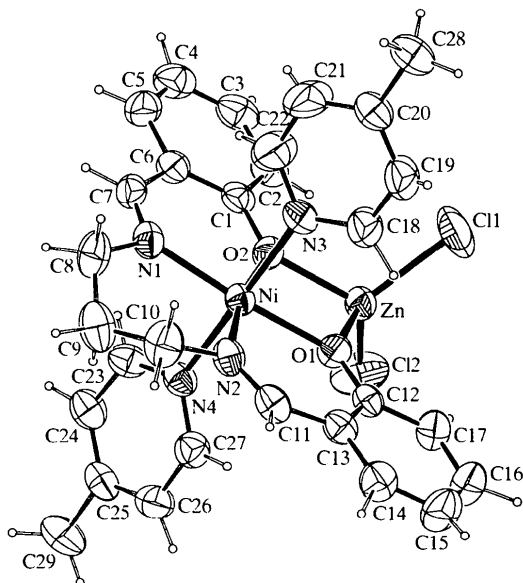


Fig. 1. PLATON (Spek, 1998) drawing of (VIII) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small circles of arbitrary radii.

The six-membered chelate ring composed of atoms Ni, N1, C8, C9, C10 and N2 has a boat conformation. The distances of two *para*-positioned boat atoms, Ni and C9, from their respective planes are $0.061(5)$ and $0.532(4)$ Å. The coordination plane makes dihedral angles of $87.44(8)$ and $89.10(6)^\circ$ with the N3 and N4 4-methylpyridine groups, respectively. A comparison of the dihedral angle (κ) between the bridging plane and the coordination plane around the Ni atom, along with related distance ranges and the bridging angle (φ), are given in Table 2 for eight dimeric metal complexes studied recently in this laboratory. The bond lengths and angles of the eight structures within the ligands show usual values.

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 the mixture heated to boiling. A solution of NiCl₂·2H₂O (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 ZnCl₂ (0.136 g, 1 mmol) in hot methanol (10 ml). The resulting mixture was set aside for 4 d

and the light-brown crystals which formed were filtered off and dried in air. Because the structure has 4-methylpyridine groups, crystals decay after 3–4 d in air. If a big crystal is chosen, the undecayed part is bigger than the decayed part. On the other hand, crystals could not be cut because they were fragile.

Crystal data

[NiZnCl₂(C₁₇H₁₆N₂O₂)
(C₆H₇N)₂]

$M_r = 661.55$

Monoclinic

Cc

$a = 9.069$ (5) Å

$b = 19.378$ (6) Å

$c = 16.964$ (7) Å

$\beta = 105.15$ (5)°

$V = 2878$ (2) Å³

$Z = 4$

$D_x = 1.527$ Mg m⁻³

D_m not measured

Data collection

Enraf–Nonius CAD-4
diffractometer

$\omega/2\theta$ scans

Absorption correction:

empirical *via* ψ scans

(Fair, 1990)

$T_{\min} = 0.678$, $T_{\max} = 0.748$

5629 measured reflections

2836 independent reflections

(plus 2793 Friedel-related
reflections)

Refinement

Refinement on F^2

$R(F) = 0.029$

$wR(F^2) = 0.076$

$S = 1.11$

5629 reflections

413 parameters

H-atom parameters

constrained

$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2$
 $+ 1.0395P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25

reflections

$\theta = 2.41$ – 10.31 °

$\mu = 1.71$ mm⁻¹

$T = 301$ (2) K

Prism

$0.98 \times 0.17 \times 0.17$ mm

Light brown

5473 reflections with
 $I > 2\sigma(I)$

$\theta_{\max} = 26$ °

$h = -11 \rightarrow 11$

$k = -23 \rightarrow 0$

$l = -20 \rightarrow 20$

3 standard reflections

frequency: 120 min

intensity decay: 1.6%

$\Delta\rho_{\max} = 0.47$ e Å⁻³

$\Delta\rho_{\min} = -0.65$ e Å⁻³

Extinction correction:

SHELXL97

Extinction coefficient:

0.0023 (2)

Scattering factors from *Inter-*

national Tables for X-ray

Crystallography (Vol. IV)

Absolute structure:

Flack (1983)

Flack parameter = 0.016 (9)

Table 1. Selected geometric parameters (Å, °)

Ni···Zn	3.0896 (9)	O2—Ni	2.022 (2)
Cl1—Zn	2.2110 (16)	N1—Ni	2.033 (3)
Cl2—Zn	2.2081 (12)	N2—Ni	2.033 (2)
O1—Zn	2.009 (2)	N3—Ni	2.209 (2)
O1—Ni	2.037 (2)	N4—Ni	2.179 (2)
O2—Zn	1.994 (2)		
Zn—O1—Ni	99.58 (9)	O1—Ni—N4	89.88 (9)
C1—O2—Zn	129.99 (18)	O2—Ni—N3	90.62 (10)
C1—O2—Ni	128.95 (18)	N1—Ni—N3	90.61 (10)
Zn—O2—Ni	100.57 (9)	N2—Ni—N3	89.73 (10)
O2—Ni—N1	90.92 (9)	O1—Ni—N3	90.52 (9)
O2—Ni—N2	169.38 (9)	N4—Ni—N3	179.16 (10)
N1—Ni—N2	99.69 (10)	O2—Zn—O1	80.59 (8)

O2—Ni—O1	79.26 (8)	O2—Zn—Cl2	116.05 (7)
N1—Ni—O1	170.13 (9)	O1—Zn—Cl2	114.81 (7)
N2—Ni—O1	90.12 (9)	O2—Zn—Cl1	112.11 (8)
O2—Ni—N4	88.73 (10)	O1—Zn—Cl1	112.24 (8)
N1—Ni—N4	88.87 (10)	Cl2—Zn—Cl1	116.07 (6)
N2—Ni—N4	91.01 (10)		

Table 2. Structural data (Å), bridging angles and dihedral angles (φ and κ , °) for eight homo- and hetero-dinuclear metal complexes

Complex	$M(\text{Cu},\text{Ni})$ — O_{bridge}	$M(\text{Cu},\text{Ni})$ ··· $M(\text{Cu},\text{Zn})$	φ	κ
(I)	1.941 (5)–1.950 (4)	2.994 (2)	100.6 (2)	5 (1)
(II)	1.930 (1)–1.982 (9)	3.073 (2)	103.5 (4)	11.3 (8)
(III)	1.885 (3)–1.976 (3)	3.021 (2)	102.8 (1)	2.9 (9)– 8.0 (3)
(IV)	1.938 (3)–1.955 (3)	3.047 (6)	103.4 (1)	12.7 (2)
(V)	1.973 (3)–1.974 (2)	3.1013 (7)	102.5 (1)–102.7 (1)	11.4 (4)
(VI)	2.030 (3)–2.039 (2)	3.0753 (7)	98.8 (1)–99.7 (1)	3.5 (9)
(VII)	1.939 (5)–1.949 (5)	3.0933 (7)	103.1 (2)–103.3 (2)	1.9 (3)
(VIII)	2.021 (2)–2.039 (2)	3.0896 (9)	100.63 (9)–102.63 (9)	0.44 (9)

Notes: (I) is [Cu₂(C₁₁H₁₀ClNO₂)₂] (Tahir *et al.*, 1996); (II) is [Cu₂(C₁₄H₁₁NO₂)₂] (Ülkü, Ercan, Atakol, Ercan & Gencer, 1997); (III) is [Cu₂(C₁₂H₁₃NO₂)₂] (Atakol *et al.*, 1997); (IV) is [Cu₂(C₁₂H₁₃NO₂)₂] (Ülkü *et al.*, 1998); (V) is [Cu{Zn(C₂₃H₂₁I₂N₃O₂)}] (Ercan, Arıcı, Akay *et al.*, 1999); (VI) is [Ni{Zn(C₃₁H₃₄I₂N₄O₂)}] (Arici *et al.*, 1999); (VII) is [Cu{Zn(C₁₇H₁₆I₂N₂O₂)}] (Ercan, Arıcı, Ülkü *et al.*, 1999); (VIII) is [NiZnCl₂(C₁₇H₁₆N₂O₂)(C₆H₇N)₂] (the title compound).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1993). Cell refinement: *CAD-4 EXPRESS*. Data reduction: *X-RED* (Stoe & Cie, 1996). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Software used to prepare material for publication: *SHELXL93*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1264). Services for accessing these data are described at the back of the journal.

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A three-dimensional framework formed from cadmium(II) cyanide and 1-methylimidazole

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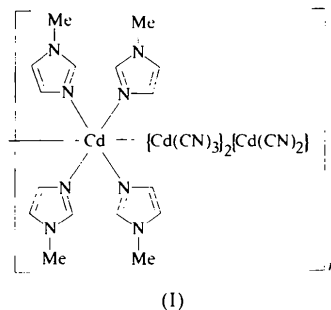
Abstract

The three-dimensional structure of octacyanotetrakis(1-methylimidazole-*N*³)tetracadmium(II) clathrate, [Cd₄(CN)₈(C₄H₆N₂)₄], contains three kinds of Cd atoms, *i.e.* tetrahedral Cd1 and octahedral Cd2 and Cd3 in a 2:1:1 ratio; atoms Cd2 and Cd3 lie on inversion centres. The Cd1 and Cd2 centres are coordinated by four and six cyano groups, respectively. The Cd3 centre is coordinated by two cyano groups and four 1-methylimidazole ligands. The three-dimensional framework provides hexagonal channels which are occupied by 1-methylimidazole ligands coordinated to the Cd3 centre.

Comment

The synthesis and characterization of polymeric multi-dimensional frameworks is of great current interest be-

cause they may be useful as catalysts, molecular sieves, optical materials *etc* (Haushalter & Mundi, 1992). As a strategy for designing infinite frameworks using cyanometallate complex hosts, Iwamoto and co-workers (Iwamoto, 1991) have employed various complementary ligands for stabilizing multi-dimensional structures. They have obtained various types of polymeric structures, such as one-dimensional chains, two-dimensional layers and three-dimensional networks (Iwamoto, 1996). Recently, Kim (1996) has studied imidazole as a complementary ligand for designing novel multi-dimensional frameworks and reported the variations of ligating behaviour of the imidazole and host topology in the resulting multi-dimensional structures. As an extension of that study, we have introduced 1-methylimidazole as a complementary ligand. We report here the novel structure of octacyanotetrakis(1-methylimidazole-*N*³)tetracadmium(II) clathrate, [Cd₄(CN)₈(C₄H₆N₂)₄], (I).



As shown in Figs. 1 and 2, the structure of (I) has cyanide bridges between the three kinds of Cd atoms, *i.e.* tetrahedral Cd1 and octahedral Cd2 and Cd3 in a 2:1:1 ratio. Cd1 is tetrahedrally coordinated by four cyano groups, Cd2 is octahedrally coordinated by six cyano groups, and Cd3 is octahedrally coordinated by two cyano groups and four 1-methylimidazole ligands. The tetrahedral Cd1 centre is linked to three octahedral Cd2 and one octahedral Cd3 *via* cyanide bridging ligands, the octahedral Cd2 centre is linked to six tetrahedral Cd1 centres *via* cyanide bridging ligands, and the octahedral Cd3 centre is linked to two tetrahedral Cd1 centres *via* cyanide bridging ligands and is also coordinated by four 1-methylimidazole ligands. The Cd—C and Cd—N bond lengths and angles (Table 1) are similar to those reported previously (Kim, 1996). The geometry of the 1-methylimidazole ligand is as expected.

As shown in Fig. 2, the three-dimensional host framework contains channels running in the *b* direction. These elongated hexagonal channels are occupied by the 1-methylimidazole ligands coordinated to the Cd3 centre. In this crystal structure, the 1-methylimidazole ligand appears to play two roles in building up the host framework; one is to block a coordination site of the Cd atom and the other is to occupy the channel space.