

N	0.3344 (4)	0.1491 (8)	0.5808 (8)	0.035 (1)
C1	0.2440 (4)	0.1641 (9)	0.5308 (9)	0.039 (2)
C2	0.2233 (5)	0.157 (1)	0.3794 (9)	0.044 (2)
C3	0.1358 (5)	0.166 (1)	0.340 (1)	0.065 (3)
C4	0.0735 (6)	0.185 (2)	0.448 (1)	0.100 (5)
C5	0.0978 (8)	0.196 (3)	0.597 (2)	0.144 (8)
C6	0.1834 (6)	0.183 (2)	0.642 (1)	0.095 (4)
C7	0.165 (1)	0.154 (3)	0.073 (2)	0.098 (6)
HO3	0.398 (6)	0.002 (11)	1.063 (10)	0.04 (3)
HO4	0.458 (4)	0.346 (8)	1.175 (7)	0.01 (2)

Table 2. Selected bond lengths (Å) and angles (°)

As—O1	1.647 (5)	C1—C6	1.36 (1)
As—O2	1.658 (4)	C1—C2	1.36 (1)
As—O4	1.700 (5)	C2—C3	1.39 (1)
As—O3	1.705 (6)	C3—C4	1.36 (2)
O5—C3	1.36 (1)	C4—C5	1.36 (2)
O5—C7	1.40 (2)	C5—C6	1.38 (2)
N—C1	1.463 (9)		
O1—As—O2	115.4 (2)	C2—C1—N	120.4 (6)
O1—As—O4	106.1 (3)	C1—C2—C3	117.5 (7)
O2—As—O4	110.3 (3)	C4—C3—O5	114.0 (7)
O1—As—O3	108.4 (3)	C4—C3—C2	121.4 (8)
O2—As—O3	109.8 (2)	O5—C3—C2	124.6 (8)
O4—As—O3	106.4 (3)	C3—C4—C5	118.8 (9)
C3—O5—C7	118.7 (9)	C4—C5—C6	122.2 (10)
C6—C1—C2	122.9 (7)	C1—C6—C5	117.2 (9)
C6—C1—N	116.7 (7)		

Table 3. Hydrogen-bonding geometry (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
N—H1N...O1	1.096 (6)	1.696 (5)	2.723 (8)	153.9 (4)
N—H2N...O1 <sup>i</sup>	0.84 (9)	1.88 (9)	2.712 (8)	173 (8)
N—H3N...O2 <sup>ii</sup>	0.82 (8)	2.08 (8)	2.864 (9)	160 (7)
O3—HO3...O2 <sup>iii</sup>	0.64 (8)	1.98 (8)	2.621 (7)	172 (10)
O4—HO4...O2 <sup>iv</sup>	0.67 (6)	2.00 (6)	2.632 (7)	157 (7)

Symmetry codes: (i)  $x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (ii)  $1 - x, \frac{1}{2} - y, z - \frac{1}{2}$ ; (iii)  $1 - x, -y, 2 - z$ ; (iv)  $1 - x, \frac{1}{2} - y, \frac{1}{2} + z$ .

Data were corrected for Lorentz-polarization effects. The structure was solved by direct methods and refined by full-matrix least-squares methods.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS86*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DU1130). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## Supramolecular Structure of a Cadmium–Silver Complex Forming a Two-Dimensional Network Embracing One-Dimensional Chains in a Layered Crystal Structure

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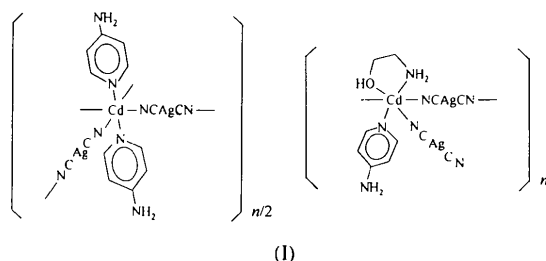
### Abstract

The polymeric coordination compound, poly[*trans*-bis(4-aminopyridine)cadmium(II)-bis[ $\mu$ -dicyanoargentato(I)-*N:N'*]] – *catena*-poly[(2-aminoethanol-*N,O*)-(4-aminopyridine)[dicyanoargentato(I)-*N*]cadmium(II)- $\mu$ -[dicyanoargentato(I)-*N:N'*]] (1/2), {[Cd(4-ampy)<sub>2</sub> – { $\mu$ -Ag(CN)<sub>2</sub>}<sub>2</sub>]}<sub>2</sub> · [Cd(meas)(4-ampy){Ag(CN)<sub>2</sub>}<sub>2</sub>]{ $\mu$ -Ag(CN)<sub>2</sub>}<sub>2</sub>]<sub>n</sub> (4-ampy = 4-aminopyridine, C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>; mea = 2-aminoethanol, C<sub>2</sub>H<sub>7</sub>NO) has a supramolecular structure composed of a two-dimensional network of Cd–NCAgCN–Cd spans, where each Cd is ligated by two 4-ampy ligands in *trans* positions, embracing one-dimensional chains of (–Cd–NCAgCN–)<sub>n</sub>. In these chains each Cd is monodentately ligated by an –NCAgCN ‘branch’ and a 4-ampy ligand, and bidentately chelated by mea. The network is stacked along the *b* axis to give a layered crystal structure, in which each monodentate –NCAgCN branch protruding from the chain penetrates through the mesh to form a hydrogen bond with the OH group of the mea ligand in the crystallographically equivalent chain in the adjacent layer.

### Comment

Dicyanoargentate(I) linking other coordination centres such as Cd<sup>II</sup>, Cu<sup>I</sup> and Zn<sup>II</sup> has provided a variety of self-assembled multidimensional structures: a three-dimensional textile interwoven by the two-dimensional networks of *trans*-[Cd(NH<sub>3</sub>)<sub>2</sub>{Ag(CN)<sub>2</sub>}<sub>2</sub>]<sub>n</sub> (Soma & Iwamoto, 1995); a two-dimensional layer clathrate stacked by the doubly interwoven net-

work of  $trans$ -[Cd(4-mepy)<sub>2</sub>{Ag(CN)<sub>2</sub>]<sub>2</sub>]<sub>n</sub> accommodating 4-mepy guests in the meshes of the network (4-mepy = 4-methylpyridine) (Soma & Iwamoto, 1994); a doubly interpenetrating three-dimensional lattice of  $trans$ -[Cd(4,4'-bpy)<sub>2</sub>{Ag(CN)<sub>2</sub>]<sub>2</sub>]<sub>n</sub> and a triply interpenetrating three-dimensional lattice of [Cd(pyrz){Ag<sub>2</sub>(CN)<sub>3</sub>}{Ag(CN)<sub>2</sub>}]<sub>n</sub> (4,4'-bpy = 4,4'-bipyridine, pyrz = pyrazine) (Soma, Yuge & Iwamoto, 1994); positively charged one-dimensional chains in {[Zn(en)<sub>2</sub>{Ag(CN)<sub>2</sub>][Ag(CN)<sub>2</sub>]}<sub>n</sub> (en = 1,2-diaminoethane) (Kappenstein, Ouli, Guerin, Černák & Chomič, 1988) and {[Cu(2,2'-bpy)<sub>2</sub>{Ag(CN)<sub>2</sub>][Ag(CN)<sub>2</sub>]}<sub>n</sub> (2,2'-bpy = 2,2'-bipyridine) (Černák, Gérard & Chomič, 1993); a triply interpenetrating negatively charged three-dimensional lattice in [Rb[Cd{Ag(CN)<sub>2</sub>]<sub>3</sub>]}<sub>n</sub> (Hoskins, Robson & Scarlett, 1994). The present polymeric coordination complex, (I), appends an unprecedented supramolecular structure to this array.



As shown in Figs. 2 and 3, the present compound  $\{[Cd(4-ampy)_2\{\mu-Ag(CN)_2\}_2] \cdot [Cd(mea)(4-ampy)\{Ag(CN)_2\}\{\mu-Ag(CN)_2\}_2]\}_n$  (4-ampy = 4-aminopyridine; mea = 2-aminoethanol) is composed of a two-dimensional network of  $[Cd(4-ampy)_2\{\mu-Ag(CN)_2\}_2]$ <sub>n</sub> and one-dimensional chains of  $[Cd(mea)(4-ampy)-$

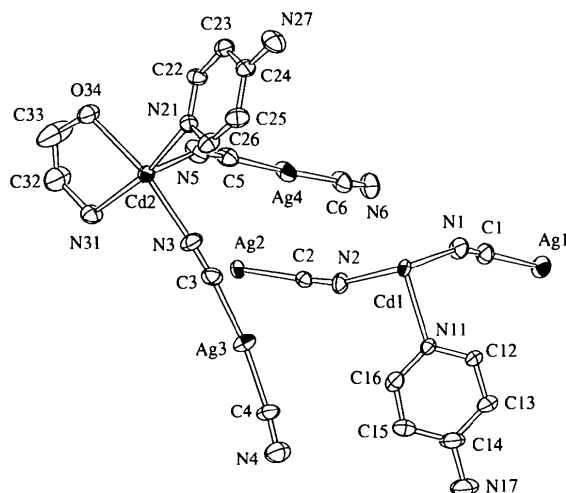


Fig. 1. View of the asymmetric unit showing the atomic labelling scheme. Displacement ellipsoids are plotted at the 30% probability level.

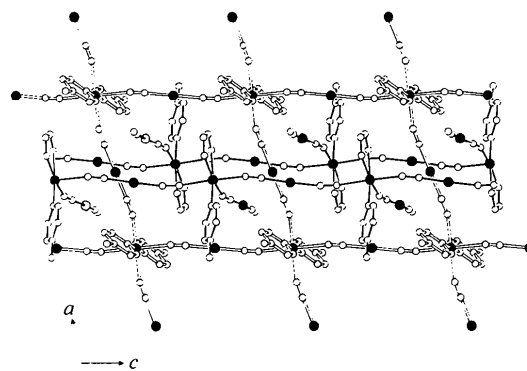


Fig. 2. View of the two-dimensional layer along with the branched one-dimensional chains. Cd and Ag are shown as shaded circles. O, N and C atoms are shown as smaller open circles. The two-dimensional network is drawn with open bonds and the branched one-dimensional chains with solid bonds.

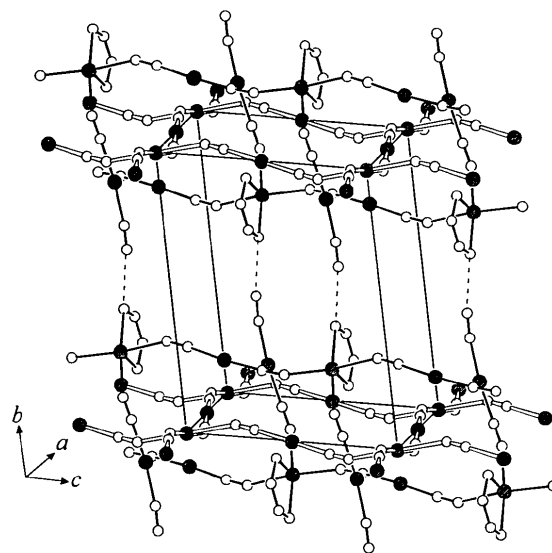


Fig. 3. Packing diagram of the complexes. Hydrogen bonds are shown with broken lines. All of the 4-ampy ligands have been omitted for clarity.

$\{Ag(CN)_2\}\{\mu-Ag(CN)_2\}_n$  running above and beneath the network.

The two-dimensional network with the rhombus mesh of the  $-(NCAgCN)-$  edge spanning the  $trans$ -[Cd(4-ampy)<sub>2</sub>]<sup>2+</sup> cations extends along the  $ac$  plane with a slight puckering due to the bending angles of 158(1)° at N1 and 158.6(9)° at N2. The Cd atoms at the origin and equivalent positions are spanned by the  $-(NCAgCN)-$  edges along the  $a$  and  $c$  axes, respectively, so that the span lengths correspond to the  $a$  and  $c$  dimensions of the unit cell [10.882(4) and 10.824(2) Å]; the acute angle of the rhombus is  $\sim 75^\circ$ . No significant differences are observed in the Cd1—N1 and Cd—N2 distances in the network [2.363(9) and 2.360(9) Å, re-

spectively], but the octahedron is axially compressed with a Cd1—N11 distance of 2.284 (9) Å.

The one-dimensional chain of (–Cd–NCAgCN–)<sub>n</sub> extends along the *c* axis at *x* ≈ 0.35 with bending angles of 153 (1)° at N5 and 163 (1)° at N6; the span length corresponds to the *c* dimension as well as one of the mesh spans in the two-dimensional network. The Cd is coordinated by two monodentate ligands, 4-ampy and –NCAgCN, and one chelating mea from the out-of-axial directions. The octahedral coordination is considerably distorted: the Cd—N and Cd—O distances range from 2.280 (7) (N21) to 2.44 (1) Å (O34) and the angles from 85.8 (3) to 97.5 (4)°. As for the chelation of mea to Cd in supramolecular structures, a previous example is [Cd(mea)(dahxn){Ni(CN)<sub>4</sub>}] (dahxn = 1,6-diaminohexane) (Yuge, Nishikiori & Iwamoto, 1996).

The two-dimensional network embracing the one-dimensional chains is stacked along the *b* axis to form a layered structure. From each of the chains running at both sides of the network, monodentate –NCAgCN branches protrude to either side through the mesh. The unligated N-end of the monodentate –NCAgCN branch, N4, is hydrogen-bonded at a distance of 2.75 (1) Å to O34 of a mea ligand which is chelated to a Cd atom in the crystallographically equivalent chain of the adjacent layer. The NH<sub>2</sub> groups of 4-ampy, both in the network and the chain, do not appear to participate in any hydrogen bonding.

The Ag···Ag distances between the chain and the network [Ag2···Ag4 3.0465 (8) Å] and between the chains [Ag3···Ag4 3.196 (1) Å] are slightly longer than those in silver metal (2.89 Å; Calvert, 1995), although such short distances are not unusual in crystal structures involving two-coordinate Ag atoms: 3.081 (3) Å in {[Cd(4-mepy)<sub>2</sub>{Ag(CN)<sub>2</sub>}<sub>2</sub>}.4-mepy}<sub>n</sub> (Soma & Iwamoto, 1994), 2.9879 (9) Å in {[Cd(4-mepy)<sub>4</sub>{Ag<sub>2</sub>(CN)<sub>3</sub>}][Ag(CN)<sub>2</sub>]}<sub>n</sub> (Soma & Iwamoto, 1994), 3.144 (1) Å in [Cd(pyrz){Ag<sub>2</sub>(CN)<sub>3</sub>}{Ag(CN)<sub>2</sub>}]<sub>n</sub> (Soma, Yuge & Iwamoto, 1994) and 3.196 (3) Å in [Cd(NH<sub>3</sub>)<sub>2</sub>{Ag(CN)<sub>2</sub>}<sub>2</sub>]<sub>n</sub> (Soma & Iwamoto, 1995).

The monodentate behaviour of [Ag(CN)<sub>2</sub>]<sup>–</sup> as a ligand has been observed for the discrete complexes [Cr(en)<sub>2</sub>{Ag(CN)<sub>2</sub>}<sub>2</sub>]ClO<sub>4</sub> (Sakaguchi, Tomioka & Yoneda, 1985) and [SnCl{Ag(CN)<sub>2</sub>}Ph<sub>3</sub>][N(PPh<sub>3</sub>)<sub>2</sub>] (Carcelli, Ferrari, Pelizza, Pelizza, Predieri & Solinas, 1992). To our knowledge, the present structure is the first example not only of a two-dimensional network embracing one-dimensional chains but also of the coexistence of bridging and monodentate dicyanoargentate(I) in a well defined supramolecular structure.

## Experimental

To an aqueous solution containing 1.14 g (5 mmol) of CdCl<sub>2</sub>·2.5H<sub>2</sub>O and 1.99 g (10 mmol) of KAg(CN)<sub>2</sub>, appropriate amounts of citric acid and 2-aminoethanol were added to

adjust the pH to 10 in a final volume of 200 cm<sup>3</sup>, followed by addition of 0.47 g (5 mmol) of 4-ampy. After the solution was allowed to stand in a refrigerator at 278 K for several weeks, colourless needle-like crystals of the title compound were obtained.

## Crystal data

[Ag<sub>2</sub>Cd(CN)<sub>4</sub>(C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>)<sub>2</sub>].-  
2[Ag<sub>2</sub>Cd(CN)<sub>4</sub>(C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>)-  
(C<sub>2</sub>H<sub>7</sub>NO)]

*M<sub>r</sub>* = 897.64

Triclinic

*P* $\bar{1}$

*a* = 10.882 (3) Å

*b* = 13.295 (4) Å

*c* = 10.824 (2) Å

α = 104.89 (2)°

β = 104.95 (2)°

γ = 68.68 (2)°

*V* = 1386.2 (6) Å<sup>3</sup>

*Z* = 1

*D<sub>x</sub>* = 2.15 Mg m<sup>–3</sup>

*D<sub>m</sub>* = 2.15 (1) Mg m<sup>–3</sup>

*D<sub>m</sub>* measured by flotation in  
mesitylene–bromoforn

Mo *K*α radiation

λ = 0.71069 Å

Cell parameters from 25

reflections

θ = 17.38–19.51°

μ = 3.228 mm<sup>–1</sup>

*T* = 293 K

Needle

0.25 × 0.10 × 0.08 mm

Colourless

## Data collection

Rigaku AFC-5S diffractometer

ω/2θ scans

Absorption correction:

ψ scans (North, Phillips

& Mathews, 1968)

*T<sub>min</sub>* = 0.608, *T<sub>max</sub>* =

0.999

8660 measured reflections

6502 independent reflections

4025 observed reflections

[*F* > 4σ(*F*)]

*R<sub>int</sub>* = 0.0043

θ<sub>max</sub> = 19.51°

*h* = 0 → 15

*k* = –19 → 19

*l* = –15 → 15

3 standard reflections

monitored every 150

reflections

intensity decay: none

## Refinement

Refinement on *F*

*R* = 0.0568

*wR* = 0.0476

*S* = 1.546

4025 reflections

317 parameters

H-atom parameters not

refined

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*) + 0.0001*F<sub>o</sub>*<sup>2</sup>]

(Δ/σ)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 1.02 e Å<sup>–3</sup>

Δρ<sub>min</sub> = –1.09 e Å<sup>–3</sup>

Extinction correction:

*SHELX76* (Sheldrick, 1976)

Extinction coefficient:

0.00119 (6)

Atomic scattering factors

from *SHELX76*

(Sheldrick, 1976) for C,

H, N; *International Tables*

for *X-ray Crystallography*

(1974, Vol. IV Table

2.2B) for Ag, Cd

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

	$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>U<sub>eq</sub></i>
Cd1	0	0	0	0.0334 (4)
Cd2	0.36360 (8)	0.21764 (6)	–0.34838 (7)	0.0399 (3)
Ag1	0	0	1/2	0.0595 (7)

Ag2	1/2	0	0	0.0518 (6)
Ag3	0.34616 (10)	-0.16797 (8)	-0.28340 (10)	0.0635 (5)
Ag4	0.34605 (10)	0.22103 (8)	0.14386 (8)	0.0620 (5)
N1	0.0049 (10)	0.0436 (8)	0.2267 (8)	0.056 (5)
C1	0.0051 (11)	0.0312 (9)	0.3246 (10)	0.051 (5)
N2	0.2329 (8)	-0.0335 (7)	0.0273 (9)	0.049 (4)
C2	0.3292 (9)	-0.0242 (8)	0.0187 (9)	0.039 (4)
N3	0.3171 (10)	0.0624 (8)	-0.3506 (9)	0.060 (5)
C3	0.3225 (11)	-0.0175 (9)	-0.3246 (11)	0.052 (5)
N4	0.3990 (11)	-0.4185 (9)	-0.2730 (12)	0.082 (6)
C4	0.3790 (13)	-0.3274 (10)	-0.2685 (12)	0.061 (6)
N5	0.3664 (10)	0.2685 (8)	-0.1250 (8)	0.065 (5)
C5	0.3612 (11)	0.2546 (9)	-0.0275 (11)	0.054 (5)
N6	0.3399 (10)	0.1878 (9)	0.4235 (9)	0.065 (5)
C6	0.3346 (12)	0.1976 (10)	0.3205 (11)	0.058 (6)
N11	0.0398 (8)	-0.1790 (7)	0.0095 (7)	0.039 (4)
C12	-0.0213 (10)	-0.2079 (8)	0.0815 (10)	0.043 (5)
C13	0.0170 (13)	-0.3128 (10)	0.1045 (12)	0.064 (6)
C14	0.1234 (14)	-0.3946 (9)	0.0482 (13)	0.071 (7)
C15	0.1852 (12)	-0.3658 (9)	-0.0314 (11)	0.058 (6)
C16	0.1400 (11)	-0.2593 (9)	-0.0466 (9)	0.049 (5)
N17	0.1652 (14)	-0.5009 (9)	0.0691 (13)	0.116 (8)
N21	0.1478 (8)	0.3323 (7)	-0.3776 (8)	0.044 (4)
C22	0.1059 (11)	0.4387 (9)	-0.3236 (10)	0.048 (5)
C23	-0.0263 (11)	0.5058 (9)	-0.3389 (10)	0.051 (5)
C24	-0.1264 (12)	0.4586 (10)	-0.4166 (11)	0.056 (6)
C25	-0.0831 (12)	0.3450 (10)	-0.4744 (12)	0.064 (6)
C26	0.0531 (12)	0.2875 (10)	-0.4525 (11)	0.057 (6)
N27	-0.2615 (10)	0.5189 (9)	-0.4378 (10)	0.077 (6)
N31	0.5930 (8)	0.1277 (7)	-0.3271 (9)	0.056 (4)
C32	0.6660 (13)	0.2072 (13)	-0.3039 (18)	0.102 (9)
C33	0.6070 (13)	0.3102 (14)	-0.315 (2)	0.155 (14)
O34	0.4674 (7)	0.3560 (6)	-0.3319 (8)	0.063 (4)

Table 2. Selected bond lengths (Å) and angles (°)

Cd1—N1	2.363 (9)	N6—C6	1.14 (2)
Cd1—N2	2.360 (9)	N11—C12	1.34 (2)
Cd1—N11	2.284 (9)	N11—C16	1.36 (1)
Cd2—N3	2.290 (12)	C12—C13	1.37 (2)
Cd2—N5	2.332 (9)	C13—C14	1.41 (2)
Cd2—N6'	2.359 (10)	C14—C15	1.41 (2)
Cd2—N21	2.280 (7)	C14—N17	1.38 (2)
Cd2—N31	2.322 (8)	C15—C16	1.36 (2)
Cd2—O34	2.435 (10)	N21—C22	1.34 (1)
Ag1—C1	2.063 (13)	N21—C26	1.36 (2)
Ag2—C2	2.064 (12)	C22—C23	1.38 (1)
Ag3—C3	2.072 (13)	C23—C24	1.43 (2)
Ag3—C4	2.059 (13)	C24—C25	1.43 (2)
Ag4—C5	2.075 (13)	C24—N27	1.39 (2)
Ag4—C6	2.056 (13)	C25—C26	1.39 (2)
N1—C1	1.11 (2)	N27—C24	1.39 (1)
N2—C2	1.13 (2)	N31—C32	1.48 (2)
N3—C3	1.15 (2)	C32—C33	1.31 (2)
N4—C4	1.14 (2)	C33—O34	1.40 (2)
N5—C5	1.14 (2)		
N1—Cd1—N2	92.5 (3)	Ag4—C5—N5	176.1 (11)
N1—Cd1—N11	88.4 (3)	Cd2 <sup>ii</sup> —N6—C6	163.0 (11)
N2—Cd1—N11	89.8 (3)	Ag4—C6—N6	172.8 (12)
N3—Cd2—N5	90.1 (4)	Cd1—N11—C12	122.3 (6)
N3—Cd2—N6'	93.8 (4)	Cd1—N11—C16	119.6 (9)
N3—Cd2—N21	97.5 (4)	C12—N11—C16	117.7 (10)
N3—Cd2—N31	93.2 (4)	N11—C12—C13	122.6 (10)
N3—Cd2—O34	166.5 (3)	C12—C13—C14	118.9 (14)
N5—Cd2—N21	87.8 (3)	C13—C14—C15	118.9 (12)
N5—Cd2—N6'	172.8 (3)	C13—C14—N17	120.8 (15)
N5—Cd2—N31	94.6 (3)	C15—C14—N17	120.4 (12)
N5—Cd2—O34	88.7 (4)	C14—C15—C16	117.3 (10)
N21—Cd2—N6'	85.8 (3)	N11—C16—C15	124.6 (13)
N21—Cd2—N31	169.1 (4)	Cd2—N21—C22	125.8 (7)
N21—Cd2—O34	95.9 (3)	Cd2—N21—C26	116.9 (6)
N31—Cd2—N6'	91.2 (3)	C22—N21—C26	117.3 (8)
N31—Cd2—O34	73.5 (3)	N21—C22—C23	124.8 (10)
O34—Cd2—N6'	88.8 (4)	C22—C23—C24	118.0 (10)
C3—Ag3—C4	171.5 (5)	C23—C24—C25	117.7 (10)
C5—Ag4—C6	175.9 (5)	C23—C24—N27	122.5 (10)

Cd1—N1—C1	157.7 (10)	C25—C24—N27	119.8 (11)
Ag1—C1—N1	176.2 (11)	C24—C25—C26	118.3 (12)
Cd1—N2—C2	158.6 (9)	N21—C26—C25	123.8 (10)
Ag2—C2—N2	177.2 (9)	Cd2—N31—C32	110.4 (7)
Cd2—N3—C3	161.5 (8)	N31—C32—C33	123.6 (12)
Ag3—C3—N3	175.5 (10)	C32—C33—O34	121.0 (17)
Ag3—C4—N4	173.1 (12)	Cd2—O34—C33	110.8 (10)
Cd2—N5—C5	153.4 (10)		

Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $x, y, 1 + z$ .

Table 3. Contact distances (Å)

Ag2...Ag4	3.0465 (8)	N4...O34 <sup>ii</sup>	2.75 (1)
Ag3...Ag4 <sup>i</sup>	3.196 (1)		

Symmetry codes: (i)  $1 - x, -y, -z$ ; (ii)  $x, y - 1, z$ .

All non-H atoms were refined anisotropically. All H atoms, fixed at calculated positions with an isotropic displacement parameter  $U_{iso} = 6.0 \text{ \AA}^2$ , were included in  $F_c$  calculations.

Data collection: *MSCIAFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSCIAFC Diffractometer Control Software*. Data reduction: *SHELX76* (Sheldrick, 1976). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELX76*. Molecular graphics: *ORTEPII* (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1315). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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