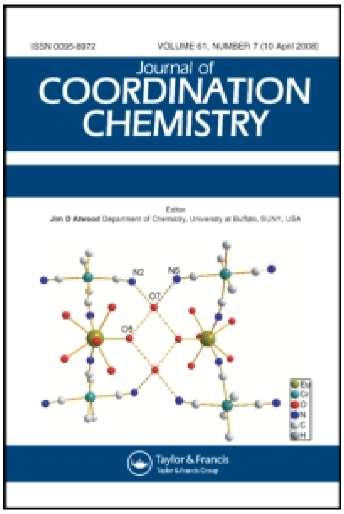

Journal of Coordination Chemistry
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713455674

NEW THREE DIMENSIONAL $[Cd(CN)_2]_n$ FRAMEWORK FORMED WITH CADMIUM CYANIDE AND $Cd(CN)_2\cdot$(18-CROWN-6): CRYSTAL STRUCTURE OF $[Cd(CN)_2]\cdot 1/2[Cd(CN)_2$ (18-CROWN-6)$]\cdot 3/2EtOH$

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To cite this Article Kim, Jaheon and Kim, Kimoon(1996) 'NEW THREE DIMENSIONAL $[Cd(CN)_2]_n$ FRAMEWORK FORMED WITH CADMIUM CYANIDE AND $Cd(CN)_2\cdot$(18-CROWN-6): CRYSTAL STRUCTURE OF $[Cd(CN)_2]\cdot 1/2[Cd(CN)_2$ (18-CROWN-6)$]\cdot 3/2EtOH$ ', Journal of Coordination Chemistry, 37: 1, 7 — 15
To link to this Article: DOI: 10.1080/00958979608023536
URL: http://dx.doi.org/10.1080/00958979608023536

J. Coord. Chem., 1996, Vol 37, pp. 7–15
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NEW THREE DIMENSIONAL $[Cd(CN)_2]_n$ FRAMEWORK FORMED WITH CADMIUM CYANIDE AND $Cd(CN)_2\cdot$(18-CROWN-6): CRYSTAL STRUCTURE OF $[Cd(CN)_2]\cdot 1/2[Cd(CN)_2\cdot$(18-CROWN-6)]$\cdot$3/2EtOH[†]

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(Received March 16, 1995; in final form August 23, 1995)

The cadmium complex $Cd(CN)_2\cdot$(18-crown-6) (**1**) was synthesized and its structure was determined by X-ray crystallography. The cadmium ion in **1** has a hexagonal bipyramidal geometry containing six equatorial oxygen atoms from the crown ether and two axial CN ligands. The NC-Cd-CN 'rod' is perfectly linear with an end-to-end distance of 6.509 (12) Å. When **1** was allowed to diffuse into a cadmium cyanide solution, the infinite coordination complex $[Cd(CN)_2]\cdot 1/2[(Cd(CN)_2\cdot$(18-crown-6)]$\cdot$3/2EtOH (**2**) was obtained in which the cadmium macrocycle **1** was trapped in a 10-faced-cage formed by the $[Cd(CN)_2]$n framework. The terminal nitrogen atoms of **1** bind two Cd centers across the cage. The trapped $Cd(CN)_2\cdot$(18-crown-6) has a significantly bent NC-Cd-CN unit and the crown ether ligand disordered over two orientations. The $[Cd(CN)_2]_n$ framework viewed down the c axis shows two types of channels, one octagonal and one tetragonal, which are filled with $Cd(CN)_2\cdot$(18-crown-6) and ethanol molecules, respectively. Crystallographic data of **1**: trigonal, space group $R\bar{3}$ (hexagonal axis), a = 11.757 (1), c = 12.105 (1) Å, V = 1449.1 (2) Å^3, Z = 3, R = 0.0566, R_w = 0.0674 for 827 unique reflections ($I > 3\sigma(I)$). Crystallographic data of **2**: orthorhombic, *Pbcn*, a = 16.632 (1), b = 17.391 (3), c = 15.685 (2) Å, V = 4536.8 (9) Å^3, Z = 8. R = 0.0486, R_w = 0.0492 for 929 unique reflections ($I > 3\sigma(I)$).

KEYWORDS: cadmium, cyanide, framework, 18-crown-6, X-ray structures

INTRODUCTION

Recent studies showed that cadmium cyanide forms inclusion complexes with various organic molecules.[1-5] The inorganic host $Cd(CN)_2$ adopts a variety of 3D frameworks with large channels or cavities to accommodate the guest molecules: for example, the $[Cd(CN)_2]_n$ frameworks include small hydrocarbon molecules in an adamatane-like cavity[1] or alcohols in the linear channels.[2-4] The structure of the $[Cd(CN)_2]_n$ framework appears to be very sensitive to the nature of the guest molecules as small changes in the guest molecule often lead to totally different

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[†] Dedicated to Professor T. Iwamoto on the occasion of his 60th birthday.

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$[Cd(CN)_2]_n$ frameworks.[4] Such flexibility of the $[Cd(CN)_2]_n$ framework stems mainly from the fact that cadmium metal ions can adopt various coordination numbers and coordination geometries. One may see that the guest molecules serve as 'templates' around which the $[Cd(CN)_2]_n$ frameworks grow. In these inclusion compounds there are only weak interactions such as van der Waals interaction or hydrogen bonding between the host cadmium cyanide and the guest molecules. Nevertheless, such weak interactions are important in maintaining the clathrate structures as the $[Cd(CN)_2]_n$ frameworks collapse upon loss of the guest molecules.

When cadmium cyanide is crystallized in the presence of strongly coordinating organic molecules such as pyridine, bipyridine and pyrazine, it forms infinite coordination complexes with new types of 2-D or 3-D $[Cd(CN)_2]_n$ frameworks, which include the organic molecules coordinated to the metal centers.[6-8] For instance, $Cd(CN)_2 \cdot py$ (py = pyridine)[6,7] has a 3-D $[Cd(CN)_2]_n$ framework similar to that of the Hofmann-Td type inclusion compound[9] whereas $Cd(CN)_2 \cdot pz$ (pz = pyrazine) contains square-grid $[Cd(CN)_2]_n$ sheet linked by pyrazine bridges.[8] In the structure of $Cd(CN)_2 \cdot 1/2(4,4'\text{-bipy})$ (bipy = bipyridine)[7] a bipyridine molecule resides in a cavity of the 3-D $[Cd(CN)_2]_n$ framework while forming a bridge between two cadmium centers across the cavity. In these cases the organic molecules may be considered as 'coordinating templates' to generate new 2-D or 3-D $[Cd(CN)_2]_n$ frameworks.

Recently, we determined the crystal structure of $Cd(CN)_2 \cdot$(18-crown-6) in which the cadmium ion is coordinated by six oxygen atoms of the macrocycle and by two axial cyanide ligands to form a linear NC-Cd-CN 'rod'. It occurred to us that $Cd(CN)_2 \cdot$(18-crown-6) may be used as a coordinating 'template' to build up a new 3-D $[Cd(CN)_2]_n$ framework when cadmium cyanide is crystallized in the presence of the cadmium macrocycle. In this paper we report the structures of $Cd(CN)_2 \cdot$(18-crown-6) and $[Cd(CN)_2] \cdot 1/2[Cd(CN)_2 \cdot (18\text{-crown-6})] \cdot 3/2EtOH$ in which the coordination compound $Cd(CN)_2 \cdot$(18-crown-6) is trapped in a cage formed in the new 3-D $[Cd(CN)_2]_n$ framework. The cage is the largest among those in the known $[Cd(CN)_2]_n$ frameworks.

EXPERIMENTAL

Syntheses

$Cd(CN)_2 \cdot$(18-crown-6), (1)

To 4 mmol of $Cd(CN)_2$ aqueous solution (10 cm^3) was added 18-crown-6 ($C_{12}H_{24}O_6$, 0.119 g, 0.45 mmol). After 2 h stirring, the white precipitate was filtered, washed with water and acetone and dried in air (0.167 g, 86%). Recrystallization from methanol yielded colorless rectangular crystals suitable for X-ray analysis. *Anal.* Calcd.: (%) C, 39.21; H, 5.65; N, 6.53. Found: C, 38.45; H, 5.85; N, 6.23.

$[Cd(CN)_2] \cdot 1/2(Cd(CN)_2 \cdot (18\text{-crown-6})] \cdot 3/2EtOH$ (2)

An ethanol solution of **1** was layered over a saturated cadmium cyanide aqueous solution in a diffusion tube. After a week colorless crystals of **2** were obtained from the diffusion tube. The compound was characterized by single crystal X-ray crystallography.

X-ray Crystal Structure Determination of **1** *and* **2**

A crystal of **1** on the tip of a glass fiber or that of **2** in a sealed capillary with mother liquor was mounted on an Enraf-Nonius CAD4 diffractometer before the intensity data were collected with Mo Kα radiation at room temperature. Cell parameters and an orientation matrix for data collection were obtained from least squares refinement, using the setting angles of 25 reflections in the range of $15.6° < 2\theta < 25.4°$ for **1** and $20.8° < 2\theta < 31.6°$ for **2**. The crystallographic data and additional details of data collection and refinement are summarized in Table 1. The intensities of 3 standard reflections, recorded every 3 h of X-ray exposure, showed no systematic changes. The intensity data were corrected for Lorentz and polarization effect. The structures were solved by Patterson methods and subsequent difference Fourier methods (SHELXS-86). No absorption or extinction corrections were applied. All nonhydrogen atoms of **1** were refined anisotropically. The positions of hydrogen atoms of **1** idealized (d(C-H) = 0.95 Å) with isotropic thermal parameters of 1.3 times those of bonded carbon atoms were included in the calculation of structure factors as fixed contributions. The discrimination of C and N of the

Table 1 Crystallographic data for **1** and **2**

compound	**1**	**2**
formula	$Cd(CN)_2 \cdot C_{12}H_{24}O_6$	$Cd_{2.5}C_{14}H_{21}N_5O_{4.5}$
f.w.	428.76	612.38
crystal system	trigonal	orthorhombic
space group	$R\bar{3}$ (No. 148)	*Pbcn* (No. 60)
a, Å	11.757(1)	16.632(1)
b, Å	11.757(1)	17.391(3)
c, Å	12.105(1)	15.685(2)
vol, $Å^3$	1449.1(2)	4536(9)
Z	3	8
temp, °C	23	
d(calcd), g/cm^3	1.474	1.793
λ(Mo-Kα), Å	0.71073	
monochromator	graphite	
linear abs. coeff., cm^{-1}	11.3	23.0
crystal size, mm	0.35 x 0.25 x 0.15	0.35 x 0.25 x 0.15
take-off angle, deg	2,0	
scan mode	ω/2θ	ω/2θ
ω-san width, deg	0.75 + 0.35 tan θ	1.0 + 0.35 tan θ
2θ limits, deg	60	44
weighting scheme	$w = 4(F_o)^2/[\sigma(F_o)^2]^2$	
No. of data collected	2005	2152
No. of unique data	920	2124
No. of unique data with $I > 3\sigma(I)$	827	929
No. of variables	37	202
R	0.0566	0.0486
Rw	0.0674	0.0492
G.O.F.	0.864	1.268

$R = \Sigma\|F_o| - |F_c\|/\Sigma|F_o|$. $Rw = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$; $w = 4F_o^2/\sigma^2(F_o^2)$; $\sigma(F_o^2) = [\sigma(I) + (p \cdot F_o^2)^2]^{1/2}$.

Table 2 Fractional atomic coordinates and equivalent thermal parameters for **1**

Atom	*x*	*y*	*z*	B_{eq}(Å^2)
Cd	0.0	0.0	0.0	3.78(1)
O	0.2213(3)	0.2439(3)	-0.0138(3)	4.18(8)
N	0.0	0.0	-0.2689(7)	5.3(1)
C	0.0	0.0	-0.1754(7)	3.6(1)
C(1)	0.2085(6)	0.3454(5)	0.0356(6)	5.2(1)
C(2)	0.3436(5)	0.2520(5)	0.0124(6)	5.0(1)
H(1)	0.285	0.428	0.021	6.9
H(2)	0.196	0.332	0.113	6.9
H(3)	0.352	0.251	0.093	6.7
H(4)	0.414	0.332	-0.014	6.7

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\mathbf{a}_j$ Hydrogen atoms were refined isotropically.

cyanides between Cd(2) and Cd(3) in **2** was not possible on the basis of the present X-ray data; therefore, each atom was represented by 'CN' and assigned as a half N and a half C. The macrocyclic ligand in **2** was disordered to take two orientations each with a half site occupancy factor; the thermal factors for the carbon and oxygen atoms in the macrocycle were refined isotropically. Hydrogen atoms in the macrocycle were not included in the refinement. Nonhydrogen atoms except for those of the disordered the 18-crown-6 ligand and solvent molecules were refined anisotropically for **2**. The final cycles of refinement converged to the residuals given in Table 1. All the calculations except for the heavy atom methods were carried out with the Enraf-Nonius MolEN program package. Positional and equivalent isotropic thermal parameters of **1** and **2** are listed in Tables 2 and 3, respectively.

RESULTS AND DISCUSSION

Structure of Cd(CN)$_2$·(18-crown-6) (1)

The compound **1** is isostructural to CdCl$_2$·(18-crown-6)[10] (Fig. 1). The selected bond distances and angles are given in Table 4. The molecule has $\bar{3}$ symmetry with

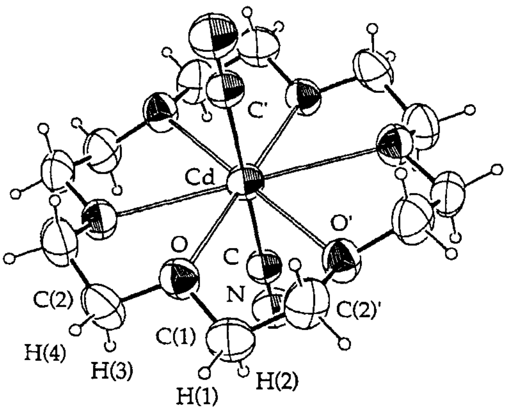

Figure 1 Molecular structure of **1** with atomic labels

Table 3 Fractional atomic coordinates and equivalent thermal parameters for **2**

Atom	*x*	*y*	*z*	B_{eq}(Å^2)
Cd(1)	0.000	0.0475(2)	0.250	5.05(7)
Cd(2)	0.1198(1)	0.3544(1)	0.5622(1)	5.35(5)
Cd(3)	0.2921(1)	0.1229(1)	0.3999(1)	4.76(4)
CN(1)	0.338(1)	-0.035(1)	0.503(2)	5.9(6)
CN(2)	0.422(1)	0.167(1)	0.437(1)	5.0(5)
CN(3)	0.338(1)	0.150(1)	0.196(1)	6.4(6)
CN(4)	0.230(1)	0.216(1)	0.470(1)	6.3(7)
CN(5)	0.188(1)	0.259(1)	0.505(1)	6.5(7)
CN(6)	0.487(1)	0.165(1)	0.440(1)	5.2(6)
CN(7)	0.319(1)	0.141(1)	0.266(1)	6.0(6)
CN(8)	0.318(1)	0.021(1)	0.475(2)	6.4(7)
N	0.169(1)	0.068(1)	0.358(1)	5.9(6)
C	0.112(1)	0.054(1)	0.319(1)	5.1(7)
O(1)	0.030(2)	0.208(2)	0.209(2)	8(1)*
O(2)	0.072(1)	0.080(1)	0.095(2)	3.8(7)*
O(3)	0.065(2)	-0.072(2)	0.158(2)	7.3(9)*
O(4)	-0.071(2)	0.168(2)	0.344(2)	8(1)*
O(5)	-0.080(2)	0.010(2)	0.408(2)	8(1)*
O(6)	-0.029(2)	-0.102(2)	0.300(2)	7(1)*
C(1)	-0.017(4)	0.261(3)	0.216(4)	10(2)*
C(2)	0.043(3)	0.221(3)	0.141(3)	19(2)*
C(3)	0.090(3)	0.163(2)	0.081(3)	4(1)*
C(4)	0.125(3)	0.138(3)	0.084(3)	7(1)*
C(5)	0.134(2)	0.053(2)	0.076(2)	14(1)*
C(6)	0.117(3)	-0.046(3)	0.085(3)	7(1)*
C(7)	0.074(3)	-0.063(2)	0.069(3)	5(1)*
C(8)	0.045(3)	-0.109(4)	0.126(4)	9(2)*
C(9)	0.020(5)	-0.148(5)	0.167(5)	17(3)*
C(10)	-0.025(3)	-0.163(3)	0.241(5)	8(2)*
O(7)	0.491(8)	0.001(5)	0.271(6)	29(3)*
C(11)	0.004(6)	0.452(5)	0.323(5)	22(3)*
C(12)	0.037(5)	0.493(7)	0.163(6)	15(4)*
O(8)	0.214(3)	0.363(3)	0.200(3)	39(3)*
C(13)	0.192(5)	0.431(4)	0.270(5)	34(4)*
C(14)	0.247(4)	0.351(3)	0.292(3)	24(2)*

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\mathbf{a}_j$
Starred atoms were refined isotropically.

the 3-fold axis passing through the N-C-Cd-C-N bonds and with the Cd atom sitting on the inversion center. The crystallographic asymmetric unit includes an N-C-Cd unit and a -CH_2CH_2O- unit of the crown ether. The cadmium ion in **1** has a hexagonal bipyramidal geometry containing six equatorial oxygen atoms from the crown ether and two axial CN ligands. The symmetry requires that the N-C-Cd-C-N 'rod' is perfectly linear with an end-to-end distance of 6.509 (12) Å. The Cd ion sits at the center of the hexagon defined by six oxygen atoms and the N-C-Cd-C-N 'rod' is normal to the plane defined by six oxygen atoms. The Cd-O distance 2.749 (3) Å is the same as that in $CdCl_2\cdot$(18-crown-6), 2.752 (1) Å within experimental error.

As mentioned earlier, 4,4'-bipyridine can serve as a 'coordinating template' to generate a new 3-D $[Cd(CN)_2]_n$ framework: the $[Cd(CN)_2]_n$ framework in $Cd(CN)_2\cdot 1/2$(4,4'-bipy) is composed of fused-adamantane-like cavities each of which includes a bipyridine molecule forming a bridge between two cadmium centers across the cavity.[7] Although the NC-Cd-CN rod of **1** (6.51 Å) is somewhat

Table 4 Selected bond distances (Å) and angles (°) for **1**

	Bond Distances		
Cd-O	2.749(3)	N-C	1.131(12)
Cd-C	2.123(8)	Cd----C(1)	3.568(5)
O-(1)	1.409(8)	Cd----C(2)	3.626(4)
O-C(2)	1.428(8)	Cd----N	3.255(9)
C(1)-C(2)	1.482(10)		
	Bond Angles		
O-Cd-O′	60.37(13)	C(1)--O--C(2)	112.4(4)
O-Cd-C	86.52(8)	Cd-C-N	180.00
O-Cd-C′	93.48(8)	C-Cd-C′	180.00
Cd-O-C(1)	114.3(3)	O-C(1)-C(2)	108.3(5)
Cd-O-C(2)	116.9(3)		

shorter than the N···N distance of 4,4'-bipyridine (7.00 Å), the macrocylic ligand coordinated to the metal center makes the molecular volume of **1** much larger than that of bipyridine. Therefore, we decided to study what type of $[Cd(CN)_2]_n$ framework could be created with the coordination compound $Cd(CN)_2 \cdot$(18-crown-6) as 'coordinating template'.

Structure of $[Cd(CN)_2] \cdot 1/2[(Cd(CN)_2 \cdot (18\text{-crown-}6)] \cdot 3/2EtOH$ *(2)*

The infinite coordination compound **2** was formed when **1** was allowed to diffuse into a cadmium cyanide aqueous solution. The asymmetric unit of the crystal structure of **2** is shown in Fig. 2. Selected bond distances and angles are given in Table 5. There are three unique cadmium ions in **2**: Cd(1) is for the metal center of $Cd(CN)_2 \cdot$(18-crown-6) and Cd(2) and Cd(3) are for those in the $[Cd(CN)_2]_n$ framework. The Cd(1) center is linked to two Cd(3) atoms *via* the axial cyanide

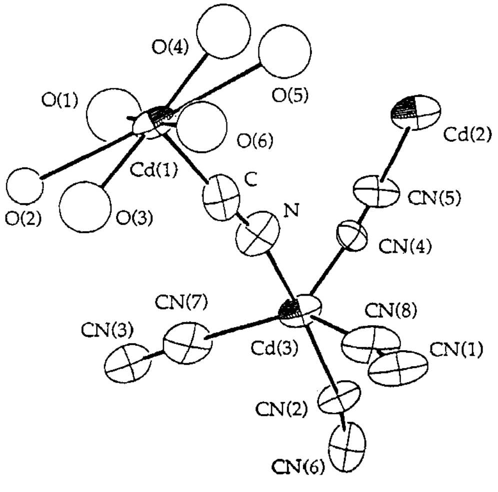

Figure 2 Asymmetric unit of **2** with atomic labels. Only oxygen atoms of 18-crown-6 are shown. The included ethanol molecules are also omitted.

Table 5 Selected bond distances (Å) and angles (°) for **2**

Bond Distances			
Cd(1)–O(1)	2.90(3)	Cd(3)–N	2.35(2)
Cd(1)–O(2)	2.77(3)	Cd(3)–CN(2)	2.37(2)
Cd(1)–O(3)	2.75(3)	Cd(3)–CN(4)	2.22(2)
Cd(1)–O(4)	2.82(4)	Cd(3)–CN(7)	2.17(2)
Cd(1)–O(5)	2.88(4)	Cd(3)–CN(8)	2.18(2)
Cd(1)–O(6)	2.76(3)	N–C	1.15(3)
Cd(1)–C	2.16(2)	CN(1)–CN(8)	1.11(3)
Cd(2)–CN(1)	2.26(2)	CN(2)–CN(6)	1.08(3)
Cd(2)–CN(3)	2.21(2)	CN(3)–CN(7)	1.16(3)
Cd(2)–CN(5)	2.20(2)	CN(4)–CN(5)	1.16(3)
Cd(2)–CN(6)	2.23(2)		
Bond Angles			
O(1)–Cd(1)–O(2)	62.4(8)	O(1)–Cd(1)–O(4)	58.2(10)
O(2)–Cd(1)–O(3)	61.4(9)	O(3)–Cd(1)–O(6)	60.4(10)
O(4)–Cd(1)–O(5)	61.8(10)	O(5)–Cd(1)–O(6)	57.5(10)
O(1)–Cd(1)–C	84.8(9)	O(1)–Cd(1)–C′	89.0(9)
O(2)–Cd(1)–C	93.4(8)	O(2)–Cd(1)–C′	85.3(8)
O(3)–Cd(1)–C	88.2(9)	O(3)–Cd(1)–C′	96.7(9)
O(4)–Cd(1)–C	93.2(10)	O(4)–Cd(1)–C′	82.0(9)
O(5)–Cd(1)–C	88.7(9)	O(5)–Cd(1)–C′	92.7(9)
O(6)–Cd(1)–C	93.3(9)	O(6)–Cd(1)–C′	92.7(9)
C–Cd(1)–C′	173.6(8)	CN(1)–Cd(2)–CN(3)	108.8(8)
CN(1)–Cd(2)–CN(5)	108.4(8)	CN(1)–Cd(2)–CN(6)	115.5(7)
CN(3)–Cd(2)–CN(5)	101.3(8)	CN(3)–Cd(2)–CN(6)	108.9(7)
CN(5)–Cd(2)–CN(6)	113.0(7)	N–Cd(3)–CN(2)	174.1(7)
N–Cd(3)–CN(4)	91.7(7)	N–Cd(3)–CN(7)	88.1(7)
N–Cd(3)–CN(8)	89.5(7)	CN(2)–Cd(3)–CN(4)	94.1(7)
CN(2)–Cd(3)–CN(7)	90.0(7)	CN(2)–Cd(3)–CN(9)	87.2(7)
CN(4)–Cd(3)–CN(7)	118.3(8)	CN(4)–Cd(3)–CN(8)	114.8(8)
CN(7)–Cd(3)–CN(8)	127.0(8)	Cd(2)–CN(1)–CN(8)	178(2)
Cd(3)–CN(8)–CN(1)	169(2)	Cd(2)–CN(6)–CN(2)	172(2)
Cd(3)–CN(2)–CN(6)	156(2)	Cd(2)–CN(3)–CN(7)	170(2)
Cd(3)–CN(7)–CN(3)	176(2)	Cd(2)–CN(5)–CN(4)	171(2)
Cd(3)–CN(4)–CN(5)	171(2)	Cd(1)–C–N	171(2)
Cd(3)–N–C	162(2)		

Primed atoms were generated by a symmetry code, (–*x*, *y*, 0.5–*z*).

ligands. The tetrahedral Cd(2) is linked to four Cd(3) metal centers whereas the trigonal bipyramidal Cd(3) is connected to four Cd(2) metal centers and a Cd(1) center all *via* cyanide bridges. The discrimination of C and N of the cyanides between Cd(2) and Cd(3) was not possible on the basis of the present X-ray data.

The macrocycle of the $Cd(CN)_2$·(18-crown-6) unit in **2** takes two different orientations. One orientation is rotated around the NC-Cd-CN rod by ~30° with respect to the other. The structure of the $Cd(CN)_2$·(18-crown-6) unit in 2 is somewhat distorted compared with that in **1**. The NC-Cd(1)-CN unit is no longer linear; the angles C-Cd(1)-C and N-C-Cd(1) are 173.6 (8) and 171.1 (19), respectively. The Cd(1)-O distances are in the range 2.76–2.90 Å and the average value (2.81 Å) is somewhat longer than that in **1** (2.749 Å).

The $Cd(CN)_2$·(18-crown-6) unit is trapped in a 10-faced-cage formed in the $[Cd(CN)_2]_n$ framework as shown in Fig. 3. The $Cd(CN)_2$·(18-crown-6) unit is

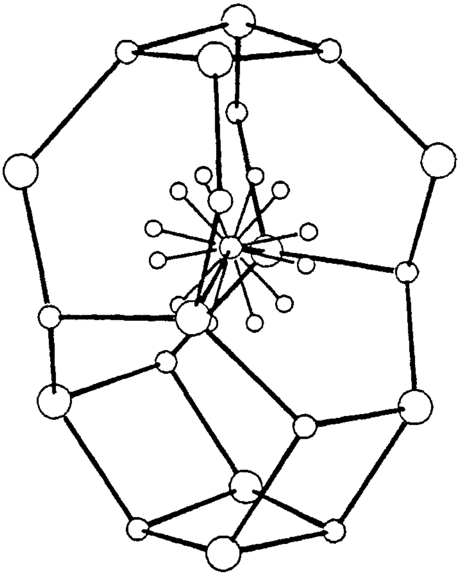

Figure 3 A 10-faced-cage built of ten tetrahedral Cd ions (smaller circles), ten trigonal bipyramidal Cd ions (larger circles) and bridging cyanide ligands (bold sticks). Only cadmium and oxygen atoms of the disordered $Cd(CN)_2$(18-crown-6) molecules trapped inside the cage are shown.

coordinated to two Cd(3) centers across the cage through the axial cyanide groups. The cage with dimensions of ~11.2 × 17.4 × 7.8 Å has 4 rectangular, 4 hexagonal and two octagonal faces. The size of the cage is the largest among all the known $[Cd(CN)_2]_n$ frameworks. A two-fold axis passes through the centers of the top and bottom rectangular faces and the Cd center of $Cd(CN)_2$·(18-crown-6) which is trapped in the cage. The space at the bottom of the cage is filled with ethanol molecules. The cages are fused together in an anti-parallel fashion through the octagonal window stacked along the *c* axis direction (Fig. 4). The $[Cd(CN)_2]_n$ framework viewed down the *c* axis shows two types of channels, one octagonal and

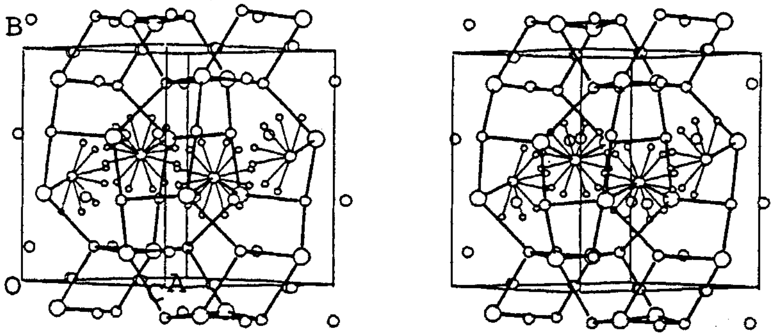

Figure 4 A stereoview for the two cages fused in an antiparallel fashion. The circles not connected to other ones represent the oxygen atoms of ethanol molecules.

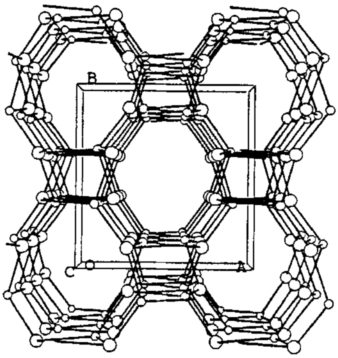

Figure 5 Perspective view of $[Cd(CN)_2]_n$ frameworks in **2** down the *c*-axis. Only Cd centres are shown.

one tetragonal (Fig. 5) whose dimensions are ~11.2 × 12.6 and 5.6 × 4.8 Å, respectively. These channels are filled with $Cd(CN)_2 \cdot$(18-crown-6) and ethanol molecules, respectively.

In summary, we have determined the crystal structure of the infinite coordination compound **2** formed when the coordination compound **1** was allowed to diffuse into the cadmium cyanide solution. The cadmium macrocycle is trapped in a cage formed by the $[Cd(CN)_2]_n$ framework of **2**. The cage is the largest among those in the known $[Cd(CN)_2]_n$ frameworks. This work demonstrated that coordination compounds may serve as 'templates' to generate new $[Cd(CN)_2]_n$ frameworks in the same manner that simple organic guest molecules do in the cadmium cyanide inclusion compounds.

Acknowledgements

This research was kindly supported by the Basic Science Research Institute Program, Ministry of Education (BSRI-94-3436), and Korea Science and Engineering Foundation (KOSEF). We also thank Pohang University of Science and Technology (POSTECH) for partial support of the X-ray analysis.

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