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CRYSTAL STRUCTURE OF A MIXED LIGAND TRINUCLEAR COMPLEX OF CADMIUM(II)

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Single crystals of a complex made from cadmium(II) acetate and the Schiff base of salicylaldehyde and 1,3-diaminopropane, and recrystallized from pyridine, was synthesized and its structure determined by single-crystal X-ray diffraction methods. It crystallizes in the monoclinic system, space group $P2_1/n$ with $a = 15.959(4)$, $b = 26.222(3)$, $c = 25.907(6)$ Å, $\beta = 101.60(2)^\circ$, $V = 10620(7)$ Å³, $M = 1652.80$, $Z = 4$, $D_c = 1.034$ g cm⁻³, $\mu = 6.34$ cm⁻¹, and $F(000) = 3360$. Refinement gave $R = 0.078$, $R_w = 0.077$ for 4990 observed reflection with $I \geq 3\sigma(I)$. Each Cd(II) atom is coordinated by two nitrogen atoms from two pyridine molecules, two oxygen atoms and one nitrogen atom from one Schiff base and one nitrogen atom from another Schiff base to form a distorted octahedron.

Keywords: Cadmium(II); crystal structure; Schiff base

INTRODUCTION

The synthesis and complexation of macrocyclic Schiff base compounds with cadmium(II) has attracted considerable attention in recent years.^{1–5} Cadmium(II) ions, being poisonous for humans and animals,⁶ can lead to diseases such as pneumonia, pulmonary edema and pulmonary emphysema.⁷ Furthermore, it can also lead to cancer, deformity, and mutation. Cd-MT (MT: metal sulfur protein) is the form of cadmium in the human body.⁸

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So far, the structure and function of Cd-MT has not been fully elucidated. Thus it has been seen as being important to study Schiff base compounds with cadmium(II) as models of Cd-MT. On the basis of previous work,⁹⁻¹⁵ we have synthesized a novel compound reported below, and determined its crystal structure.

EXPERIMENTAL

Apparatus and Measurements

Elemental analyses were carried out with a Perkin-Elmer 240C elemental analyzer and the Cd²⁺ content was determined by EDTA titration.

Preparation of Cd₂(L)(CH₃COO)₂

Some 1.05 cm³ of salicylaldehyde was dissolved in 20 cm³ of 99.5% ethanol, and then 0.42 cm³ of 1,3-diaminopropane was added. The mixture was stirred and heated on a waterbath at 50–60°C for about 1.5 h. The solution turned yellow. An aqueous solution (10 cm³) of Cd(Ac)₂·3H₂O (1.42 g), was then added with constant stirring at 60–70°C during about 4 h. A yellow precipitate of Cd₂(L)(CH₃COO)₂ was filtered off and washed with water and

TABLE I Crystal data for the compound

Empirical formula	C ₈₁ H ₇₈ Cd ₃ N ₁₂ O ₆
Space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
<i>M</i>	1652.80
<i>a</i> , Å	15.959(4)
<i>b</i> , Å	26.222(3)
<i>c</i> , Å	25.907(6)
β , deg	101.60(2)
<i>V</i> , Å ³	10620(7)
<i>Z</i>	4
<i>h</i> , <i>k</i> , <i>l</i> range collected	−15 ≤ <i>h</i> ≤ 15, 0 ≤ <i>k</i> ≤ 25, 0 ≤ <i>l</i> ≤ 24
<i>F</i> (000)	3360
μ , cm ^{−1}	6.34
No. of data measd.	10157
No. of unique data	8406 (<i>R</i> _{int} = 3.1%)
No. of obsd. data [<i>I</i> ≥ 3.0σ(<i>I</i>)]	4990
<i>R</i> , <i>R</i> _w	0.078, 0.077
Good of fit	5.70
Maximum Δ/σ	0.16
Max/min transm. factors	1.035/0.834
ρ_{calcd} , g cm ^{−3}	1.034

$$R = \frac{\sum |F_o|^2 - |F_c|^2}{\sum |F_o|^2}; R_w = \frac{\sum (|F_o|^2 - |F_c|^2)\omega^{1/2}}{\sum |F_o|^2\omega^{1/2}} \text{ and } \omega = 1.$$

TABLE II Fractional coordinates and equivalent isotropic thermal parameters for the non-hydrogen atoms

Atom	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B_{eq}</i> , Å ²	Atom	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B_{eq}</i> , Å ²
Cd(1)	0.741175(6)	0.17831(4)	0.13313(4)	4.12(2)	C(38)	0.5982(9)	0.1328(5)	0.1903(5)	4.1(3)
Cd(2)	0.29217(6)	0.17341(4)	0.19075(4)	4.26(2)	C(39)	0.5188(9)	0.1636(5)	0.1624(7)	4.6(3)
Cd(3)	0.50566(7)	0.42602(2)	0.16100(4)	4.35(2)	C(40)	0.4444(9)	0.1290(6)	0.1377(7)	4.5(4)
O(2)	0.5274(7)	0.4318(5)	0.0801(4)	6.5(3)	C(22)	0.4452(9)	0.3614(6)	0.0338(5)	4.7(3)
O(3)	0.8114(6)	0.2360(4)	0.1899(4)	5.1(2)	C(23)	0.432(1)	0.3307(7)	-0.0120(6)	5.8(4)
O(1)	0.3689(7)	0.1221(4)	0.2505(5)	6.0(3)	C(41)	0.3458(9)	0.1761(7)	0.0755(5)	5.2(3)
O(4)	0.2204(6)	0.2276(4)	0.1314(4)	4.8(2)	C(42)	0.2785(9)	0.2102(6)	0.0544(5)	4.4(3)
O(5)	0.4778(6)	0.4179(4)	0.2397(4)	4.9(2)	C(24)	0.472(2)	0.3367(7)	-0.0508(7)	6.8(5)
O(6)	0.6650(6)	0.1229(4)	0.0776(4)	4.9(2)	C(25)	0.539(1)	0.3748(8)	-0.0456(7)	6.8(5)
N(1)	0.3720(7)	0.2329(4)	0.2441(4)	3.8(2)	C(43)	0.269(1)	0.2180(7)	0.0002(7)	5.9(4)
N(2)	0.4051(7)	0.3675(5)	0.1190(5)	4.7(3)	C(26)	0.554(1)	0.4059(8)	-0.0026(7)	6.4(4)
N(3)	0.6702(8)	0.1661(5)	0.2003(5)	4.9(3)	C(27)	0.512(1)	0.4004(6)	0.0395(6)	5.1(3)
N(4)	0.3661(8)	0.1609(4)	0.1250(5)	4.6(3)	C(44)	0.213(1)	0.255(1)	-0.0254(7)	7.7(5)
N(11)	0.8303(8)	0.1073(5)	0.1669(5)	5.4(3)*	C(31)	0.7601(9)	0.2172(6)	0.2695(6)	4.6(3)
N(12)	0.8452(8)	0.1897(5)	0.0819(5)	4.9(2)*	C(32)	0.775(1)	0.2276(8)	0.3242(7)	6.0(4)
N(13)	0.1835(8)	0.1881(5)	0.2405(5)	5.2(3)*	C(45)	0.163(1)	0.2833(7)	0.0008(6)	6.3(4)
N(14)	0.207(1)	0.1000(7)	0.1583(6)	6.9(3)*	C(46)	0.168(1)	0.2743(7)	0.0526(7)	5.8(4)
N(15)	0.3877(8)	0.4872(5)	0.1493(5)	5.6(3)*	C(33)	0.830(1)	0.2614(8)	0.3495(8)	6.9(4)
N(16)	0.6050(8)	0.4940(5)	0.1730(5)	4.8(2)*	C(34)	0.878(1)	0.2889(7)	0.3203(7)	6.3(4)
C(11)	0.4686(8)	0.1777(7)	0.3040(5)	4.7(3)	C(47)	0.2233(9)	0.2357(6)	0.0824(6)	4.8(3)
C(12)	0.5426(9)	0.1806(9)	0.3441(6)	6.2(4)	C(81)	0.196(1)	0.1676(8)	0.2900(8)	7.3(4)*
C(13)	0.584(1)	0.1382(9)	0.3688(7)	7.0(5)	C(82)	0.130(2)	0.171(1)	0.319(1)	10.0(7)*
C(14)	0.555(1)	0.0923(9)	0.3494(8)	8.4(5)	C(83)	0.057(2)	0.197(1)	0.299(1)	9.3(6)*
C(15)	0.481(1)	0.0858(8)	0.3111(7)	7.2(4)	C(84)	0.047(2)	0.218(1)	0.250(1)	8.9(6)*
C(16)	0.4361(9)	0.1290(6)	0.2866(6)	4.9(3)	C(85)	0.113(1)	0.2132(7)	0.2228(7)	5.9(3)*
C(17)	0.4352(9)	0.2265(6)	0.2835(5)	4.4(3)	C(86)	0.136(2)	0.109(1)	0.126(1)	9.5(6)*
C(18)	0.353(1)	0.2869(6)	0.2294(6)	5.2(3)	C(87)	0.078(2)	0.064(2)	0.107(2)	12.7(9)*
C(19)	0.396(1)	0.3010(6)	0.1836(7)	5.2(3)	C(88)	0.110(2)	0.019(1)	0.122(1)	10.6(7)*
C(35)	0.870(1)	0.2811(6)	0.2675(7)	5.6(4)	C(36)	0.8132(9)	0.2440(6)	0.2398(6)	4.3(3)
C(37)	0.6903(8)	0.1832(6)	0.2484(7)	5.2(3)	C(51)	0.585(1)	0.3625(6)	0.2876(6)	4.9(3)
C(52)	0.616(1)	0.3374(7)	0.3334(8)	7.2(5)	C(53)	0.574(2)	0.3401(9)	0.3755(7)	8.2(5)
C(54)	0.502(1)	0.368(1)	0.3713(8)	8.2(5)	C(55)	0.469(1)	0.3929(7)	0.3258(6)	5.9(4)
C(56)	0.5086(9)	0.3923(5)	0.2829(5)	4.2(3)	C(57)	0.6335(9)	0.3546(6)	0.2466(6)	4.9(3)
C(58)	0.6694(9)	0.3540(6)	0.1646(6)	5.3(3)	C(59)	0.635(1)	0.3041(7)	0.1371(7)	5.5(4)
C(60)	0.678(1)	0.2896(7)	0.0916(6)	5.5(4)	C(61)	0.5968(8)	0.2259(7)	0.0369(5)	4.6(3)
C(62)	0.5661(9)	0.1772(6)	0.0176(6)	4.8(3)*	C(63)	0.497(1)	0.1767(7)	-0.0232(6)	5.5(3)*
C(64)	0.454(1)	0.1339(8)	-0.0454(8)	7.0(4)*	C(65)	0.484(1)	0.0876(9)	-0.0250(9)	7.8(5)*
C(66)	0.556(1)	0.0859(6)	0.0168(6)	5.0(3)*	C(67)	0.598(1)	0.1281(6)	0.0395(6)	4.9(3)*
C(80)	0.837(2)	0.168(1)	0.037(1)	9.1(6)*	C(71)	0.894(1)	0.1126(7)	0.2077(7)	6.3(4)*
C(72)	0.954(1)	0.0763(8)	0.2266(8)	7.0(4)*	C(73)	0.945(1)	0.0307(9)	0.2008(9)	7.8(5)*
C(74)	0.880(2)	0.020(1)	0.161(1)	8.5(5)*	C(75)	0.823(1)	0.0621(8)	0.1442(8)	6.9(4)*
C(76)	0.918(1)	0.213(1)	0.097(1)	8.4(5)*	C(77)	0.982(2)	0.217(1)	0.070(1)	9.6(6)*
C(78)	0.975(2)	0.194(1)	0.023(1)	10.1(7)*	C(79)	0.902(3)	0.171(2)	0.001(2)	15(1)
C(91)	0.355(1)	0.5042(8)	0.1014(8)	6.5(4)*	C(92)	0.284(1)	0.5377(9)	0.0908(9)	7.7(5)
C(93)	0.242(1)	0.5476(9)	0.1316(9)	8.0(5)*	C(94)	0.275(1)	0.5287(9)	0.1816(9)	7.6(5)*
C(95)	0.350(1)	0.4991(8)	0.1895(8)	6.5(4)*	C(96)	0.676(1)	0.4925(8)	0.2096(8)	6.7(4)*
C(97)	0.740(2)	0.531(1)	0.218(1)	9.0(6)*	C(98)	0.728(1)	0.5698(9)	0.1864(9)	7.7(4)*
C(99)	0.653(2)	0.575(1)	0.148(1)	8.9(5)*	C(100)	0.593(1)	0.5354(8)	0.1442(8)	6.7(4)*
C(20)	0.3512(9)	0.3470(6)	0.1540(7)	5.1(3)	C(89)	0.181(2)	0.009(1)	0.154(1)	11.4(9)
C(21)	0.3978(9)	0.3500(5)	0.0719(6)	4.5(3)	C(90)	0.235(1)	0.0545(9)	0.1709(9)	7.7(5)*

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as $B_{eq} = (4/3) \times [a^2 \times \beta(1,1) + b^2 \times \beta(2,2) + c^2 \times \beta(3,3) + ab(\cos \gamma) \times \beta(1,2) + ac(\cos \beta) \times \beta(1,3) + bc(\cos \alpha) \times \beta(2,3)]$.

99.5% ethanol (yield 51.3%). Anal. Calculated for $\text{Cd}_2\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}_6$ (%): C, 40.38; H, 3.52; N, 4.49; Cd, 31.54. Found: C, 39.88; H, 3.49; N, 4.48; Cd, 32.05. The *bis*(pyridine) adduct, the subject of the single-crystal X-ray analysis, was obtained by dissolving the above compound in pyridine at 80°C to give a saturated solution. The resulting solution was evaporated at room temperature in air to give light-yellow, transparent, single crystals suitable for X-ray analysis.

Crystal Structure Determination

Intensity data for a single crystal of $\text{C}_81\text{H}_{78}\text{N}_{12}\text{O}_6\text{Cd}_3$ having dimensions $0.3 \times 0.25 \times 0.3$ mm, were measured at 299 K on an Enraf-Nonius CAD4 diffractometer fitted with graphite-monochromatized $\text{MoK}\alpha$ radiation,

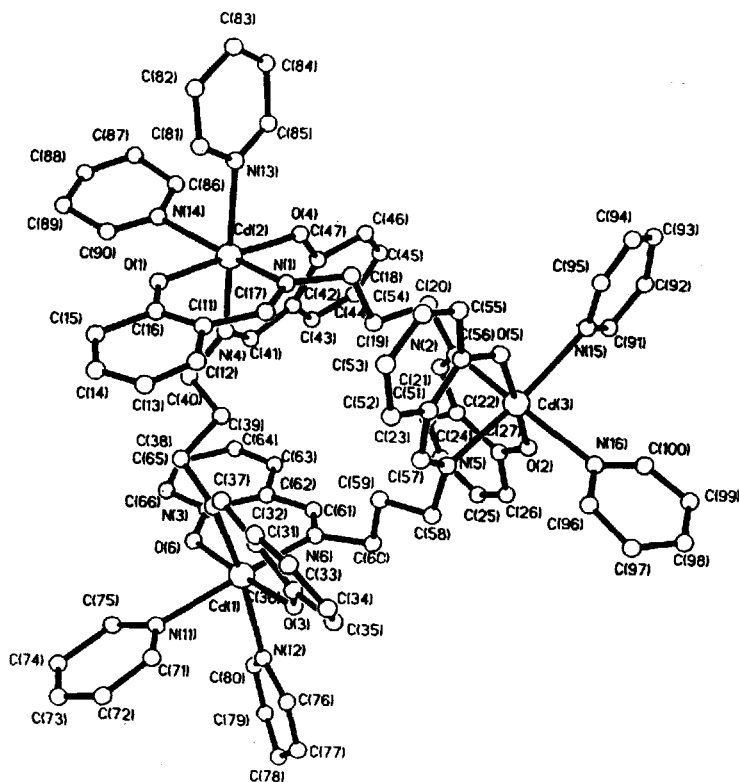


FIGURE 1 Molecular structure and crystallographic numbering scheme for the single crystal.

$\lambda = 0.71073 \text{ \AA}$; a total of 8456 independent reflexions were measured in the range $2.0^\circ \leq \theta \leq 20.0^\circ$ by the ω - 2θ scan technique. No significant decomposition of the crystal occurred during data collections, and absorption corrected data¹⁶ which satisfied the $I \geq 3.0\sigma(I)$ criterion were used in the subsequent analysis. Crystal data are summarized in Table I.

The structure was solved by direct methods using MULTAN82. All of non-hydrogen atoms were refined by full-matrix least-squares methods. At convergence $R = 0.078$ and $R_w = 0.077$; final refinement details are collected in Table I. Scattering factors for all atoms were those in the crystallographic programs.¹⁷⁻²⁰ Final fractional atomic coordinates are listed in Table II; the atom numbering scheme is shown in Figure 1, which was drawn with ORTEP.²¹

TABLE III Selected bondlengths (Å) and angles (°) for the complex

Cd(2)-N(13)	2.391(6)	Cd(2)-N(14)	2.410(8)	O(1)-C(16)	1.286(9)	O(4)-C(47)	1.298(9)
N(1)-C(17)	1.294(9)	N(1)-C(18)	1.490(1)	C(11)-C(12)	1.410(2)	C(11)-C(16)	1.420(1)
Cd(1)-N(6)	2.316(6)	Cd(1)-N(11)	2.394(6)	Cd(1)-N(12)	2.336(6)	Cd(3)-O(2)	2.198(5)
Cd(3)-O(5)	2.184(5)	Cd(3)-N(2)	2.327(6)	Cd(3)-N(5)	2.353(7)	Cd(3)-N(15)	2.445(6)
Cd(3)-N(16)	2.365(6)	O(2)-C(27)	1.318(9)	O(3)-C(36)	1.305(9)	O(5)-C(56)	1.313(9)
O(6)-C(67)	1.309(8)	N(2)-C(20)	1.47(1)	N(2)-C(21)	1.286(9)	N(3)-C(37)	1.30(1)
N(3)-C(38)	1.425(9)	N(4)-C(40)	1.486(9)	N(4)-C(41)	1.318(9)	N(5)-C(57)	1.260(9)
N(5)-C(58)	1.430(9)	N(6)-C(60)	1.48(2)	N(6)-C(61)	1.304(9)	C(21)-C(22)	1.39(2)
N(13)-C(85)	1.310(1)	Cd(2)-O(1)	2.223(5)	Cd(2)-O(4)	2.233(5)	Cd(2)-N(1)	2.294(5)
Cd(2)-N(4)	2.283(7)	Cd(1)-O(3)	2.243(5)	Cd(1)-O(6)	2.231(4)	Cd(1)-N(3)	2.288(6)
O(1)-Cd(2)-N(13)	94.6(3)	O(1)-Cd(2)-N(14)	87.2(2)	O(4)-Cd(2)-N(1)	97.3(2)		
O(4)-Cd(2)-N(4)	81.3(2)	O(4)-Cd(2)-N(14)	95.4(2)	O(4)-Cd(2)-N(13)	86.6(2)		
N(1)-Cd(2)-N(4)	103.9(2)	N(1)-Cd(2)-N(13)	86.6(2)	N(1)-Cd(2)-N(14)	163.8(2)		
N(4)-Cd(2)-N(13)	164.8(2)	N(4)-Cd(2)-N(14)	87.9(2)	N(13)-Cd(2)-N(14)	84.1(2)		
Cd(2)-O(1)-C(16)	133.0(5)	Cd(2)-O(4)-C(47)	131.5(4)	O(1)-C(16)-C(11)	123.9(6)		
Cd(2)-N(13)-C(81)	117.5(5)	Cd(2)-N(13)-C(85)	124.0(5)	C(81)-N(13)-C(85)	118.6(7)		
O(3)-Cd(1)-O(6)	176.6(2)	O(3)-Cd(1)-N(3)	81.5(2)	Cd(1)-N(1)-C(17)	129.5(5)		
Cd(2)-N(1)-C(18)	115.8(4)	O(3)-Cd(1)-N(6)	96.9(2)	O(3)-Cd(1)-N(11)	96.1(2)		
O(3)-Cd(1)-N(12)	88.4(2)	O(6)-Cd(1)-N(3)	96.2(2)	O(6)-Cd(1)-N(6)	81.2(2)		
O(6)-Cd(1)-N(11)	86.3(2)	O(6)-Cd(1)-N(12)	94.4(2)	N(3)-Cd(1)-N(6)	104.3(3)		
N(3)-Cd(1)-N(11)	87.8(2)	N(3)-Cd(1)-N(12)	165.5(2)	N(6)-Cd(1)-N(11)	163.4(2)		
N(6)-Cd(1)-N(12)	87.3(2)	N(11)-Cd(1)-N(12)	82.9(2)	O(2)-Cd(3)-O(5)	176.9(2)		
O(2)-Cd(3)-N(2)	80.0(3)	O(2)-Cd(3)-N(5)	101.6(2)	O(2)-Cd(3)-N(15)	95.8(2)		
O(2)-Cd(3)-N(16)	81.0(2)	O(5)-Cd(3)-N(2)	97.0(3)	O(5)-Cd(3)-N(5)	79.4(2)		
O(5)-Cd(3)-N(15)	83.3(2)	O(5)-Cd(3)-N(16)	102.1(2)	N(2)-Cd(3)-N(5)	100.1(2)		
N(2)-Cd(3)-N(15)	86.2(2)	N(2)-Cd(3)-N(16)	160.1(2)	N(5)-Cd(3)-N(15)	162.2(2)		
N(5)-Cd(3)-N(16)	89.3(2)	N(15)-Cd(3)-N(16)	90.0(3)	Cd(3)-O(2)-C(27)	132.7(4)		
Cd(1)-O(3)-C(36)	131.9(4)	Cd(3)-O(5)-C(56)	137.3(4)	Cd(1)-O(6)-C(67)	132.7(4)		
Cd(1)-N(11)-C(71)	121.0(5)	Cd(1)-N(11)-C(75)	122.8(5)	Cd(2)-N(14)-C(86)	115.6(7)		
Cd(2)-N(14)-C(90)	120.6(6)	C(91)-N(15)-C(95)	120.2(7)	Cd(3)-N(16)-C(100)	122.2(5)		
Cd(3)-N(15)-C(95)	120.6(5)	Cd(3)-N(16)-C(96)	121.6(5)	O(1)-Cd(2)-O(4)	177.0(1)		
O(1)-Cd(2)-N(4)	97.9(3)	O(1)-Cd(2)-N(1)	80.0(2)				

Numbers in parentheses are estimated standard deviations.

RESULTS AND DISCUSSION

Crystal Structure of the Complex

Selected bond distances and angles are listed in Table III and molecular packing in the unit cell is shown in Figure 2. The complex possesses a complicated trinuclear cadmium structure. Distances between the three Cd(II) atoms are almost equal ($d_{12}=7.616 \text{ \AA}$, $d_{23}=7.558 \text{ \AA}$, $d_{31}=7.617 \text{ \AA}$). Each Cd(II) atom is in the same coordination environment comprising two nitrogen atoms from two pyridine molecules, two oxygen atoms and one nitrogen atom from one Schiff base ligand, and one nitrogen atom from another Schiff base ligand. These form a distorted octahedron, in which the two nitrogen atoms from each Schiff base are coordinated to two cadmium atoms. The whole structure is connected by three Schiff base ligands to form a macrocyclic structure. In a complex,⁹ each cadmium atom is coordinated to two nitrogen atoms from two pyridine molecules, two oxygen atoms and

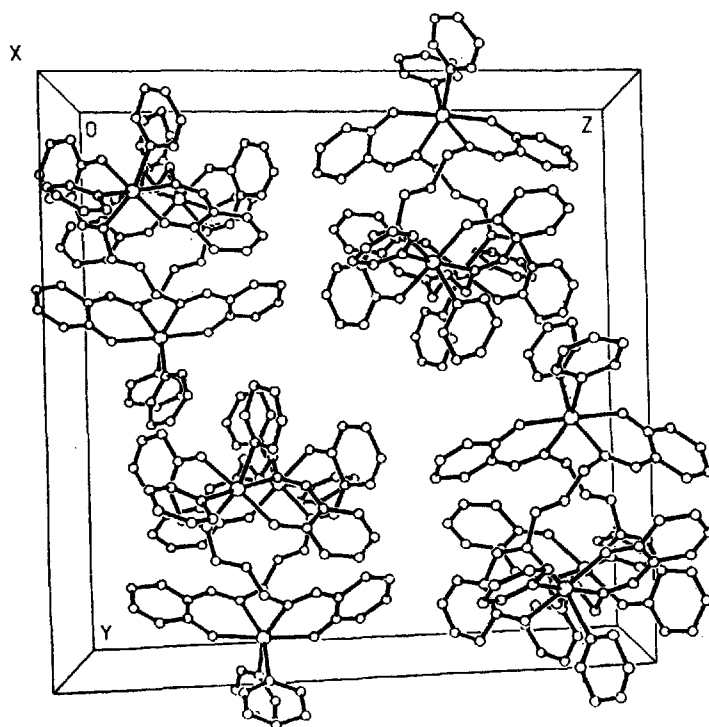


FIGURE 2 Figure of the crystal unit cell.

one nitrogen atom from one Schiff base and one oxygen atom from another Schiff base; each Cd(II) ion is connected by a μ_3 -O bridge. The large trinuclear structure is determined by the stereo-chemical demands of the whole molecule. The Schiff base has enough flexibility to coordinate the central ions such that the Cd(II) geometry is only slightly distorted from ideal octahedral values.

Though pyridine can coordinate strongly, its bonds are weaker than those of the Schiff base, as shown in their bond lengths. Appropriate lengths are 2.393 Å for Cd(II)-N pyridine and 2.286 Å for Cd-N Schiff base. This conclusion is also suggested by the thermal properties of the complex. The complex has a lower density than might be expected, and this may be traced to two factors. First, the whole molecule forms a macrocyclic structure, which has a large free space inside it (4–5 Å). Secondly, each Cd(II) atom has bulky ligands surrounding it and adjacent molecules cannot approach very closely.

Supplementary Data

Full lists of anisotropic thermal parameters, bond lengths and angles and observed and calculated structure factors are available from the authors upon request.

References

- [1] G.A. Kordosky, S.M. Olafson, R.G. Lewis, V.L. Deffner and J.E. House, *Sep. Sci. Technol.*, **22**, 215 (1987).
- [2] R. Sreenivasulu, V.S. Raghavendra Rao and K. Hussain Reddy, *J. Indian Inst. Sci.*, **65**, 127 (1984).
- [3] M.L. Duran, A. Rodriguez, J. Romero and A. Sousa, *Synth. React. Inorg. Met.-Org. Chem.*, **17**, 681 (1987).
- [4] A. Rodriguez, M.L. Duran, J. Romero and A. Sousa, *An. Quim., Ser. B*, **84**, 198 (1988).
- [5] S.K. Agarwal, Rajesh Kumar and Ramesh Chandra, *Orient. J. Chem.*, **5**, 192 (1989).
- [6] Kui Wang, "Bioinorganic Chemistry," in Chinese (Qinghua University Press, Beijing, 1988), p. 217.
- [7] Liang N. Ji, Ting H. Mo and Associates, "Bioinorganic Chemistry Introduction," in Chinese (Zhongshan University Press, Guangzhou, 1992).
- [8] M.J. Stillman, Wu H. Cai and A.J. Zelazowski, *J. Biol. Chem.*, **262**, 4538 (1987).
- [9] D.X. Liu, X.G. Cui, S.X. Hao and F.L. Li, *Chemical J. of Chin. Univ.*, **12**, 165 (1991).
- [10] S.L. Li, D.X. Liu, S.Q. Zhang, H. Wang and Z.H. Yang, *Thermochimica Acta*, **275**, 215 (1996).
- [11] S.L. Li, D.X. Liu, J.H. Zhou, F.Q. Meng and Z.H. Yang, *Acta Chimica Sinica*, **53**, 343 (1995).
- [12] S.L. Li, H. Wang, D.X. Liu, X.G. Cui and X.Y. Li, *Acta Chimica Sinica*, **53**, 455 (1995).
- [13] S.L. Li, D.X. Liu, J.H. Zhou, S.Q. Zhang, L. Liu and Z.H. Yang, *Chemical Res. in Chin. Univ.*, **12**, 194 (1996).
- [14] D.X. Liu, Y.J. Kang, S.L. Li and L. Liu, *Acta Chimica Sinica*, **54**, 1114 (1996).
- [15] Y.J. Kang, D.X. Liu, S.L. Li, Z.H. Li and L. Liu, *Acta Chimica Sinica*, **54**, 893 (1996).

- [16] N. Walker and D. Stuart, *Acta Crystallogr.*, **A39**, 158 (1983).
- [17] J.D. Schagen, L. Straver, F. van Meurs and G. Williams, "CAD4: Program for Data Collection and Cell Refinement," (Enraf-Nonius Delft, P.O. Box 483, 2600 AL Delft, The Netherlands).
- [18] B.A. Frenz and Associates, "SDP-PLUS: Program for Solution and Refinement" (College Station, Texas 77840 and Enraf-Nonius, Delft, The Netherlands).
- [19] G.M. Sheldrick, "SHELXS-86: Program for solution and refinement," *Acta Crystallogr.*, **A46**, 467 (1990).
- [20] G.M. Sheldrick, "SHELXL-93: Program for the Refinement of Crystal Structures," (Institute fuer Anorg. Chemie, Univ. of Gottingen, Tammannstrasse 4, D-37077, Gottingen, Germany).
- [21] Carroll K. Johnson, "ORTEP A Fortran Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations," (Oak Ridge National Laboratory ORNL-5138, third Revision March, 1976).