

utor to the sign of the CEC is C(1), which lies in the lower, right, front, negative octant. This, and the negative CEC which would be observed (*cf.*, Fig. 1) for (-)-(II) in aqueous acid is consistent with octant behavior. This is the first of the protonated amines in this series to exhibit octant behavior. However, aspects of this crystal structure suggest that the observed conformation may not be indicative of the conformation of the molecule in aqueous solution.

Ring stacking not observed in other analogs in this series, and electrostatic repulsion between O(1)T and O appear to impose a -1.1° O-C(9)-C(3)-C(2) torsion angle. Since these conformational restrictions observed in the solid state will not be characteristic of the salt in aqueous solution, the -20° rotamer is a rational choice which may be stabilized by shortening of the O...H(N) 2.4 Å distance to afford a hydrogen bond. On this basis, the observed negative CEC for (-)-(II) in aqueous acid is consistent with antiocant behavior and this conclusion is consistent with previous studies. Since two reasonable explanations provide opposite answers to the o.r.d. behavior, interest in crystal structures of other protonated analogs of (II) continues.

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The Crystal Structure of *cis*-Catena- μ -sulphato-aquotris(imidazole)cadmium(II)

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The structure of $\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)\text{SO}_4 \cdot \text{H}_2\text{O}$ has been determined from diffractometer data and refined by full-matrix least-squares calculations to a final R of 0.069 for 1856 independent reflexions. The crystals are monoclinic, space group $P2_1/n$, with $a = 11.85(1)$, $b = 9.00(1)$, $c = 14.32(1)$ Å, $\beta = 95.5(2)^\circ$, $Z = 4$. Cd exhibits distorted octahedral coordination, being bonded to three imidazole N atoms, a water molecule and two O atoms from bridging sulphates. The latter groups link the coordination polyhedra in infinite chains with Cd-O 2.32(1) and 2.37(1) Å. The mean Cd-N is 2.26(1) and the water Cd-O 2.43(1) Å. All H atoms were located in difference maps; intra- and inter-chain hydrogen bonding (O-H...O and N-H...O) is present.

Introduction

As part of a programme investigating metal ion-imidazole interaction by potentiometric and X-ray methods, we have synthesized crystals with the composition $\text{Cd}(\text{imidazole})_3\text{SO}_4 \cdot \text{H}_2\text{O}$. In view of the presence of imidazole in biological systems (*e.g.* the histidyl residue in proteins), it is of interest to establish metal-binding sites in the ligand.

The importance of Cd as a pollutant has been pointed out (Shaikh & Lucis, 1971). The metal probably functions by interactions with proteins in biological systems.

The stoichiometry of the complex suggests a four-coordinate species. However, the various possible binding modes of the sulphato group could lead to several structures and the X-ray analysis was undertaken in order to determine the Cd coordination.

Experimental

The complex was obtained by mixing 1 *M* aqueous solutions of CdSO₄ and imidazole in the molar ratio 1:2 and adjusting the pH to 7.5 with 6 *M* H₂SO₄. After 24 h colourless single crystals were isolated; micro-analysis indicated the composition Cd(C₃H₄N₂)₃SO₄·H₂O. Preliminary X-ray data were obtained by oscillation and Weissenberg methods with Ni-filtered Cu *K*α radiation; the systematic absences *h*0*l*, *h*+*l*=2*n*+1 and 0*k*0, *k*=2*n*+1 indicated the space group *P*2₁/*n*.

A roughly spherical crystal of average radius 0.25 mm was selected for intensity measurements. With graphite-monochromated Mo *K*α radiation (λ=0.7107 Å), the lattice constants were obtained from a least-squares analysis of the settings of 25 reflexions measured on a Philips PW 1100 four-circle diffractometer.

The crystal data are listed in Table 1. The density was determined by flotation in a mixture of bromobenzene and methyl iodide.

Table 1. *Crystal data*

C ₉ H ₁₄ CdN ₆ O ₅ S	<i>M</i> =430.4
Space group <i>P</i> 2 ₁ / <i>n</i> (monoclinic, 2nd setting)	
<i>a</i> = 11.85 (1) Å	<i>D_m</i> = 1.90 g cm ⁻³
<i>b</i> = 9.00 (1)	<i>D_c</i> = 1.88 for <i>Z</i> =4
<i>c</i> = 14.32 (1)	μ(Mo <i>K</i> α) = 16.1 cm ⁻¹
β = 95.5 (2)°	<i>F</i> (000) = 856
<i>V</i> = 1520.4 Å ³	

Table 2. *Fractional atomic coordinates and thermal parameters and their e.s.d.'s*

(a) Heavy atoms

Coordinates are × 10⁴, thermal parameters are of form

$$T = \exp [-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*) \times 10^3].$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cd	5768 (1)	3420 (1)	7273 (1)	9 (0)	5 (1)	12 (1)	-1 (0)	3 (0)	0 (0)
S	7468 (2)	935 (3)	8936 (2)	10 (1)	3 (1)	9 (2)	3 (1)	0 (1)	2 (1)
O(1)	6943 (8)	2232 (10)	8431 (6)	28 (5)	13 (5)	27 (5)	8 (4)	-11 (4)	8 (4)
O(2)	7698 (7)	-259 (10)	8273 (6)	21 (5)	17 (5)	26 (5)	2 (4)	4 (4)	-14 (4)
O(3)	6689 (8)	372 (10)	9591 (6)	31 (5)	24 (5)	18 (5)	-4 (4)	19 (4)	4 (4)
O(4)	8552 (7)	1380 (9)	9460 (6)	22 (5)	8 (5)	26 (5)	0 (4)	-9 (4)	-1 (4)
O(16)	4581 (8)	4831 (10)	6110 (6)	23 (5)	18 (5)	18 (5)	5 (4)	3 (4)	2 (4)
N(1)	5502 (9)	5390 (11)	8200 (7)	20 (6)	9 (6)	15 (6)	-7 (5)	5 (5)	0 (5)
C(2)	6101 (12)	6665 (18)	8270 (11)	18 (8)	31 (10)	36 (9)	-4 (7)	-1 (7)	-2 (8)
N(3)	5674 (9)	7605 (13)	8860 (8)	26 (7)	12 (6)	31 (7)	-3 (6)	7 (6)	-16 (6)
C(4)	4723 (13)	6940 (17)	9225 (11)	40 (10)	24 (9)	35 (9)	6 (8)	9 (8)	-13 (8)
C(5)	4675 (11)	5548 (17)	8818 (10)	13 (7)	30 (9)	26 (8)	-2 (7)	-4 (6)	-5 (7)
N(6)	4217 (10)	2197 (14)	7716 (8)	30 (7)	26 (7)	25 (7)	-13 (6)	-2 (6)	9 (6)
C(7)	4213 (13)	1416 (17)	8504 (11)	33 (9)	25 (9)	28 (9)	-12 (7)	-2 (7)	0 (7)
N(8)	3146 (10)	985 (14)	8637 (8)	22 (7)	34 (8)	15 (6)	-17 (6)	4 (5)	9 (6)
C(9)	2421 (14)	1545 (21)	7927 (13)	28 (9)	51 (12)	57 (12)	-19 (9)	10 (9)	14 (10)
C(10)	3092 (12)	2295 (19)	7357 (10)	17 (8)	45 (11)	31 (9)	-5 (7)	-6 (7)	16 (8)
N(11)	6086 (10)	1753 (12)	6151 (8)	29 (7)	8 (6)	22 (7)	-1 (5)	6 (5)	0 (5)
C(12)	6386 (13)	1971 (16)	5261 (10)	32 (9)	16 (8)	25 (9)	2 (7)	6 (7)	4 (7)
C(13)	6575 (14)	626 (17)	4836 (11)	44 (10)	23 (9)	26 (9)	7 (8)	5 (7)	-7 (8)
N(14)	6383 (10)	-428 (13)	5516 (10)	32 (8)	10 (7)	50 (9)	4 (6)	0 (7)	-5 (7)
C(15)	6108 (13)	270 (15)	6282 (10)	41 (9)	11 (8)	21 (8)	-4 (7)	5 (7)	0 (7)

In the 2θ range from 6 to 44°, 2010 reflexions were recorded by the ω-2θ scan technique (scan width 1.2°θ, scan speed 0.04°θ s⁻¹). Of these, 189 reflexions including systematic absences had *I*_{rel} < 1.65σ(*I*_{rel}) but some of the 'less thans' were allowed to contribute in the refinement. For the θ-range covered and for μ*R* = 0.40, *A** varied from 1.80 to 1.79 (*International Tables for X-ray Crystallography*, 1968). Absorption corrections were therefore considered negligible.

Solution and refinement of the structure

The position of the Cd atom was deduced from a Patterson map (X-RAY System, 1972). All the non-hydrogen atoms were revealed in an electron density map phased on Cd. Initially all the atoms of each imidazole ring (except that coordinated to Cd) were assigned C scattering factors. The structure was then refined by least-squares methods. Correct assignment of the second N atom was based on peak heights in a subsequent electron-density map from which the third and fourth imidazole ring atoms had been omitted. After three cycles of refinement with isotropic temperature factors, *R* was 0.127. Five cycles with anisotropic temperature factors reduced *R* to 0.083. Nine reflexions were omitted at this stage because of severe primary extinction effects. All H atoms were located in a difference map. They were then positioned at 1.08 Å from their parent atoms and given the same temperature factors as the latter. With unit weight applied to each reflexion the final *R* based on 1856 reflexions was 0.069, 'less thans' being allowed to contribute if they calcu-

Table 2 (*cont.*)(b) Fractional atomic coordinates ($\times 10^3$) for the H atoms (calculated)

	<i>x</i>	<i>y</i>	<i>z</i>
H(2)	683	689	790
H(3)	600	870	903
H(4)	417	741	970
H(5)	408	469	896
H(7)	496	116	897
H(8)	291	31	921
H(9)	151	142	783
H(10)	279	288	672
H(12)	646	305	494
H(13)	682	44	414
H(14)	645	-162	543
H(15)	593	-28	692
H(161)	512	552	592
H(162)	421	445	561

lated greater than the observed.* $\sum(|F_o| - |F_c|)^2$ was minimized and in the last cycle the average Δ/σ ratio was 0.014. A final difference map showed no prominent peaks. Scattering factors for the non-hydrogen atoms were those of Cromer & Mann (1968), and for H, those of Stewart, Davidson & Simpson (1965). Anomalous dispersion corrections (Mo $K\alpha$) were applied to the Cd and S curves (*International Tables for X-ray Crystallography*, 1968). The final positional and thermal parameters are listed in Table 2.

Description of the structure and discussion

In the asymmetric unit, the Cd atom is bonded to three N atoms from three imidazole rings, a hydrate O and the O atom of a sulphate ion. The distorted octahedron is completed by an O atom of a screw-axis related sulphate group (Fig. 1). Bond lengths and angles are listed in Tables 3 and 4 respectively. The Cd-N lengths [mean 2.26 (1) Å] are in agreement with the analogous distance [2.248 (3) Å] in catena- μ -dichloro-bisimidazolecadmium(II) (Flook, Freeman, Huq & Rosalky, 1973). The coordination polyhedra are linked by

Table 3. Bond lengths and their *e.s.d.*'s (Å)

Cd—N(1)	2.25 (1)	N(3)—C(4)	1.42 (2)
Cd—N(6)	2.28 (1)	C(4)—C(5)	1.38 (2)
Cd—N(11)	2.26 (1)	C(5)—N(1)	1.39 (2)
Cd—O(1)	2.32 (1)	N(6)—C(7)	1.33 (2)
Cd—O(2 ¹)	2.37 (1)	C(7)—N(8)	1.35 (2)
Cd—O(16)	2.43 (1)	N(8)—C(9)	1.36 (2)
S—O(1)	1.48 (1)	C(9)—C(10)	1.37 (2)
S—O(2)	1.48 (1)	C(10)—N(6)	1.39 (2)
S—O(3)	1.47 (1)	N(11)—C(12)	1.37 (2)
S—O(4)	1.48 (1)	C(12)—C(13)	1.38 (2)
N(1)—C(2)	1.35 (2)	C(13)—N(14)	1.39 (2)
C(2)—N(3)	1.33 (2)	N(14)—C(15)	1.33 (2)
		C(15)—N(11)	1.35 (2)

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31140 (20 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

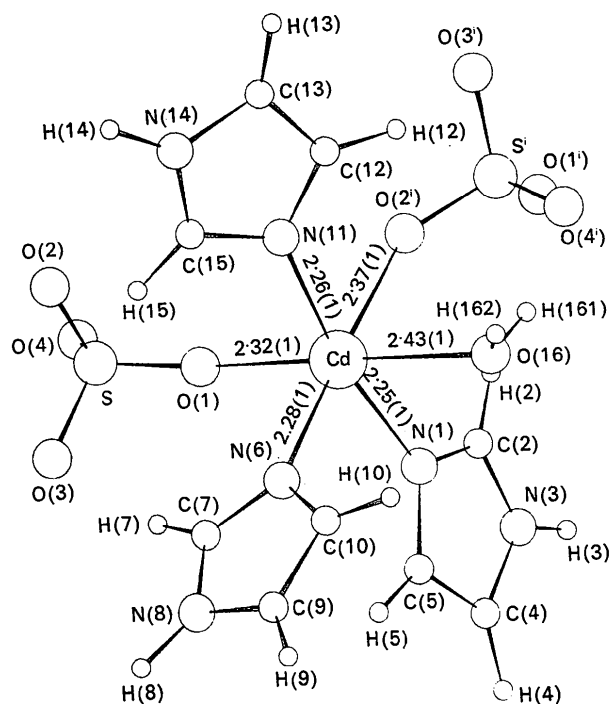
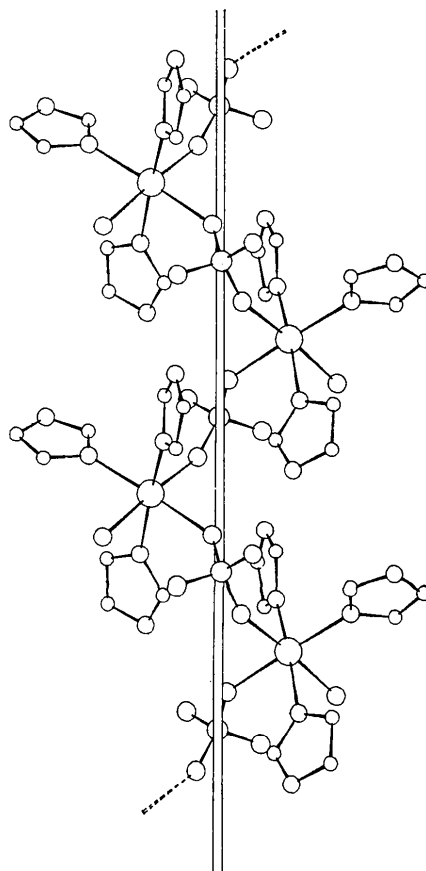


Fig. 1. Coordination about Cd.

Fig. 2. Polymer chain arranged in a helix about the 2_1 axis.

sulphato bridges with Cd—O(1) 2.32 (1) and Cd—O(2¹) 2.37 (1) Å. In monothioureacadmium sulphate dihydrate (Cavalca, Domiano, Fava Gasparri & Boldrini,

1967) the Cd coordination polyhedra are linked by an S atom of a thiourea molecule and two O atoms of each sulphate group, with Cd—O 2.27 (2) and 2.29 (2) Å.

Table 4. Bond angles and their e.s.d.'s (°)

O(1)—Cd—O(16)	175.9 (2)	S ¹ —O(2 ¹)—Cd	140.6 (5)
O(1)—Cd—O(2 ¹)	92.3 (3)	O(1)—S—O(2)	110.8 (5)
O(1)—Cd—N(1)	92.8 (2)	O(1)—S—O(3)	108.9 (5)
O(1)—Cd—N(6)	91.4 (2)	O(1)—S—O(4)	109.8 (5)
O(1)—Cd—N(11)	94.2 (2)	O(2)—S—O(3)	109.0 (5)
O(16)—Cd—N(1)	83.59 (7)	O(2)—S—O(4)	108.5 (5)
O(16)—Cd—N(6)	90.77 (6)	O(3)—S—O(4)	109.7 (5)
O(16)—Cd—N(11)	89.12 (7)	C(2)—N(1)—C(5)	105 (1)
O(16)—Cd—O(2 ¹)	85.6 (2)	N(1)—C(2)—N(3)	110 (1)
N(1)—Cd—N(6)	93.11 (6)	C(2)—N(3)—C(4)	109 (1)
N(1)—Cd—N(11)	169.82 (4)	N(3)—C(4)—C(5)	103 (1)
N(1)—Cd—O(2 ¹)	87.4 (2)	N(1)—C(5)—C(4)	111 (1)
N(6)—Cd—N(11)	94.09 (6)	C(7)—N(6)—C(10)	105 (1)
N(6)—Cd—O(2 ¹)	176.3 (2)	N(6)—C(7)—N(8)	110 (1)
N(11)—Cd—O(2 ¹)	85.0 (2)	C(7)—N(8)—C(9)	109 (1)
C(2)—N(1)—Cd	127.70 (5)	N(8)—C(9)—C(10)	105 (1)
C(5)—N(1)—Cd	126.98 (3)	N(6)—C(10)—C(9)	110 (1)
C(7)—N(6)—Cd	123.92 (3)	C(12)—N(11)—C(15)	106 (1)
C(10)—N(6)—Cd	129.62 (5)	N(11)—C(12)—C(13)	111 (1)
C(12)—N(11)—Cd	130.05 (5)	C(12)—C(13)—N(14)	104 (1)
C(15)—N(11)—Cd	124.22 (5)	C(13)—N(14)—C(15)	109 (1)
S—O(1)—Cd	155.3 (5)	N(11)—C(15)—N(14)	111 (1)

Table 5. Least-squares planes

The equations of the planes are expressed in orthogonalized space as $PI + QJ + RK = S$.

Plane I: Imidazole ring I

Equation $0.54009I - 0.37590J + 0.75299K = 9.91275$

Atoms defining plane	N(1)	C(2)	N(3)	C(4)	C(5)	Cd	N(11)
Atoms not included in plane							
Distance from plane (Å)	-0.016	0.007	0.005	-0.015	0.019	-0.106	-0.460

Plane II: Imidazole ring II

Equation $-0.15988I + 0.8365J + 0.52413K = 6.79625$

Atoms defining plane	N(6)	C(7)	N(8)	C(9)	C(10)	Cd	O(2 ¹)
Atoms not included in plane							
Distance from plane (Å)	-0.008	0.011	-0.009	0.004	0.002	0.278	0.563

Plane III: Imidazole ring III

Equation $0.93538I + 0.04591J + 0.35066K = 9.11554$

Atoms defining plane	N(11)	C(12)	C(13)	N(14)	C(15)	Cd	N(1)
Atoms not included in plane							
Distance from plane (Å)	-0.006	0.004	-0.001	-0.003	0.006	0.127	0.259

Plane IV: Coordination plane I

Equation $-0.19420I + 0.72648J + 0.65918K = 7.9640$

Atoms defining plane	O(1)	N(6)	O(16)	O(2 ¹)	Cd	N(11)	N(1)
Atoms not included in plane							
Distance from plane (Å)	0.043	-0.043	0.043	-0.043	-0.029	-2.275	2.216

Plane V: Coordination plane II

Equation $0.82748I + 0.49044J - 0.27341K = 3.60346$

Atoms defining plane	O(1)	N(1)	O(16)	N(11)	Cd	N(6)	O(2 ¹)
Atoms not included in plane							
Distance from plane (Å)	-0.047	0.050	-0.050	0.047	-0.093	-2.377	2.265

Plane VI: Coordination plane III

Equation $0.54132I - 0.46453J + 0.70084K = 8.89568$

Atoms defining plane	N(1)	O(2 ¹)	N(6)	N(11)	Cd	O(16)	O(1)
Atoms not included in plane							
Distance from plane (Å)	-0.032	0.034	0.031	-0.032	0.104	-2.323	2.426

Intersection angles

Planes I and II	89.65°	Planes IV and V	89.12°
Planes I and III	41.24	Planes IV and VI	88.89
Planes II and III	85.83	Planes V and VI	88.83

For the hydrate O atoms, Cd–O distances of 2.31 (1) and 2.27 (2) Å were reported, compared with Cd–O(16), 2.43 (1) Å, observed in the present study. Bond lengths and angles in the sulphate group are normal. There are two polymer chains in the cell, one of which is illustrated in Fig. 2. Each chain is arranged in a helix about the 2_1 axis.

Distortion of the octahedron is evident from the angles about Cd (Table 4), and from inspection of least-squares planes (Table 5) through the three sets of four ideally coplanar donor atoms. Each set of donors is fairly planar and the Cd atom lies close to one plane [O(1), N(6), O(16), O(2ⁱ)] but deviates by about 0.1 Å from each of the other two. Similarly, each imidazole ring is planar, but the Cd atom deviates from these planes by up to 0.28 Å. As observed in catena- μ -dichlorobisimidazolecadmium(II) (Flook *et al.*, 1973), there is a significant difference in the C–N lengths (for the coordinated N atoms) in all three imidazole rings. This effect is most pronounced in the second ring, in which N(6)–C(10) is 1.39 (2) Å and N(6)–C(7) 1.33 (2) Å, reflecting a greater degree of π bonding between the latter pair of atoms. The angles Cd–O–S of 140.6 (5) and 155.3 (5)° are somewhat larger than analogous angles (131.7 and 137.5°) observed in monothiourea-cadmium sulphate dihydrate (Cavalca *et al.*, 1967) but this is expected since the Cd atoms in the latter are bridged by both sulphato and thiourea groups.

Table 6. Bond lengths (Å) and angles (°) and their *e.s.d.*'s involved in hydrogen bonding

N(3)—O(3 ⁱⁱ)	2.92 (1)	N(3)—H(3)—O(3 ⁱⁱ)	166.6 (3)
N(8)—O(3 ⁱⁱⁱ)	2.81 (1)	N(8)—H(8)—O(3 ⁱⁱⁱ)	146.3 (3)
O(16)—O(4 ^{iv})	2.78 (1)	O(16)—H(162)—O(4 ^{iv})	174.1 (3)
O(16)—O(4 ⁱ)	2.80 (1)	O(16)—H(161)—O(4 ⁱ)	162.8 (3)
N(14)—O(4 ^v)	2.87 (1)	N(14)—H(14)—O(4 ^v)	167.9 (3)

Symmetry operators

(i)	$1\frac{1}{2}-x$	$\frac{1}{2}+y$	$1\frac{1}{2}-z$
(ii)	x	$y+1$	z
(iii)	$1-x$	$-y$	$2-z$
(iv)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	$z-\frac{1}{2}$
(v)	$1\frac{1}{2}-x$	$y-\frac{1}{2}$	$1\frac{1}{2}-z$

All data pertaining to hydrogen bonding are listed in Table 6. For hydrogen bonding we adopt the criterion $d(\text{H}-\text{B}) < W_{\text{H}} + W_{\text{B}} - 0.2$ Å, where W_{H} and W_{B} are the van der Waals radii for H and the acceptor B respectively (Hamilton, 1968). Within a polymer chain, there are three hydrogen bonds emanating from each asymmetric unit, between N(3) and O(3ⁱⁱ), O(16) and O(4ⁱ) and N(14) and O(4^v). Two hydrogen bonds linking the polymer chains are found between N(8) and O(3ⁱⁱⁱ) and O(16) and O(4^{iv}).

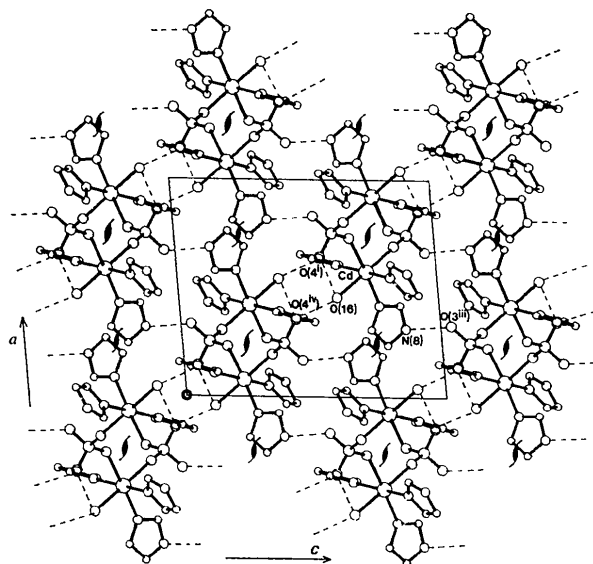


Fig. 3. [010] projection with hydrogen bonds shown as broken lines.

Fig. 3 shows the [010] projection of the structure and illustrates the polymer chains viewed down the 2_1 axes. Some of the hydrogen bonds are shown as broken lines.

All calculations were performed on a Univac 1106 computer system at the Computer Centre of the University of Cape Town.

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