

tween the planes is 84° , while the corresponding angle is 72° in the acid and 60° in the Li compound. Table 5 lists the dihedral angles as well as the interatomic distances and angles in the oxydiacetate ion, and the deviations from planarity in the two halves are shown in Table 6.

The O—O distances in the hydrogen-bond system are given in Table 7. Two of the three independent water molecules are coordinated by Cd, while the third is situated between the layers, holding them together to form the three-dimensional structure. All water H atoms except two, marked —H— in the table, can be assigned to definite O atoms by geometrical considerations.

A comparison between the three Cd oxydiacetate structures is postponed to a later publication.

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The Structure of Cadmium Oxydiacetate–Water (2 : 7)

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The structure of $2\text{CdO}(\text{CH}_2\text{COO})_2 \cdot 7\text{H}_2\text{O}$ has been determined by Patterson and Fourier methods and refined to $R = 0.110$ for 1814 visual intensities. The space group is $P2_1/c$ with $a = 7.3215$ (11), $b = 7.3012$ (8), $c = 37.1411$ (38) Å, $\beta = 90.673$ (11)°, $Z = 4$. The crystals are built up from broad, endless chains of composition $2\text{CdO}(\text{CH}_2\text{COO})_2 \cdot 5\text{H}_2\text{O}$ parallel to **b**. The chains are linked together by an extensive hydrogen-bond system. The two independent Cd atoms coordinate seven O atoms each. The coordination polyhedra are in both cases somewhat distorted pentagonal bipyramids, which are held together two by two with one vertex shared. The coordination distances range from 2.278 (15) to 2.491 (14) Å. The shortest Cd—Cd distance is 4.738 (2) Å. The two independent oxydiacetate ions are both slightly twisted about their ether O atoms, but the non-hydrogen atoms in the oxydiacetate halves are coplanar with angles of 20° and 9° between the planes.

Introduction

Preliminary data were reported for three different phases of Cd oxydiacetate by Boman (1974). One of them, the orthorhombic trihydrate denoted CDOXY III, has been described in detail (Boman, 1977). In this paper one of the two monoclinic phases, CDOXY I, will be described.

Crystal data

Cadmium oxydiacetate–water (2 : 7) or *catena- μ -oxydiacetato-pentaaquaoxydiacetatodicadmium dihydrate*, $\text{Cd}_2\text{C}_8\text{H}_{22}\text{O}_{17}$ (CDOXY I); F.W. 615.1 g mol^{-1} ; monoclinic, space group $P2_1/c$; $a = 7.3215$ (11), $b = 7.3012$ (8), $c = 37.1411$ (38) Å, $\beta = 90.673$ (11)°; $V = 1985.3 \text{ Å}^3$; $Z = 4$; $\mu(\text{Cu K}\alpha) = 185.6 \text{ cm}^{-1}$; $D_m =$

2.02, $D_x = 2.06 \text{ g cm}^{-3}$. Numbers in parentheses are estimated standard deviations.

Experimental

The preparation of the colourless crystals, prismatic b , has been described (Boman, 1974). Elemental analyses and complexometric titration of Cd gave values in good agreement with those calculated from the formula. The density was determined from the loss of weight in carbon tetrachloride. Weissenberg photographs showed that the crystals are monoclinic; the only space group consistent with the systematic extinctions is $P2_1/c$. The preliminary unit-cell dimensions obtained from Weissenberg photographs were refined by least squares from powder data from a Guinier-Hägg camera of radius 5.00 cm (Cu $K\alpha_1$ radiation, $\lambda = 1.54051 \text{ \AA}$) with Al (cubic, $a = 4.04934 \text{ \AA}$, 22°C) as internal standard.

A single crystal, $0.20 \times 0.80 \times 0.05 \text{ mm}$, was mounted along b and non-integrated equi-inclination Weissenberg photographs were taken with Cu $K\alpha$ radiation. 1814 independent reflexions, *i.e.* 40% of those possible ($\sin \theta/\lambda \leq 0.640$; layers $h0l-h\bar{5}l$), were estimated visually by comparison with a calibrated scale. The intensities were corrected for absorption, polarization and the Lorentz effect. The transmission factors evaluated by numerical integration varied from 0.081 to 0.586.

Structure determination and refinement

The positions of the two independent Cd atoms were determined from a Patterson synthesis. The remaining

non-hydrogen atoms were located in subsequent difference syntheses. The H atoms could not be found. Full-matrix least-squares refinement minimizing $\Sigma w(|F_o| - |F_c|)^2$ was performed with $w = 1/(a + |F_o| + c|F_o|^2 + d|F_o|^3)$ according to Cruickshank. In the last cycles of refinement the constants were $a = 10.0$, $c = 0.010$ and $d = 0.00050$. The convergence was

Table 1. Atomic coordinates with standard deviations ($\times 10^4$) and isotropic temperature factors

	x	y	z	$B (\text{\AA}^2)$
Cd(1)	960 (2)	1360 (2)	1985 (1)	3.7
Cd(2)	2016 (2)	-429 (2)	779 (1)	3.8
O(1)	-961 (20)	3539 (19)	1672 (3)	4.4
O(2)	-331 (21)	3755 (28)	2359 (3)	5.4
O(3)	-2225 (16)	6027 (19)	2446 (3)	3.8
O(4)	899 (20)	1050 (26)	1339 (3)	5.3
O(5)	523 (20)	2406 (22)	813 (3)	5.0
C(1)	-1835 (34)	4899 (40)	1854 (6)	6.1 (5)
C(2)	-1489 (27)	4794 (33)	2254 (5)	4.3 (4)
C(3)	-841 (24)	3900 (29)	1303 (4)	3.6 (3)
C(4)	217 (24)	2429 (30)	1145 (4)	4.1 (3)
O(6)	3683 (21)	7395 (22)	491 (3)	4.5
O(7)	2820 (19)	7207 (26)	1163 (3)	5.3
O(8)	4099 (19)	4387 (23)	1231 (3)	5.0
O(9)	2185 (22)	10152 (26)	169 (4)	5.8
O(10)	3067 (24)	9375 (27)	-359 (3)	5.9
C(5)	4228 (24)	5699 (29)	665 (4)	3.8 (3)
C(6)	3628 (23)	5851 (30)	1046 (4)	3.5 (3)
C(7)	3876 (27)	7407 (32)	94 (5)	4.8 (4)
C(8)	3001 (30)	9104 (35)	-47 (5)	4.9 (4)
O(11)	4003 (19)	6243 (23)	2388 (4)	5.1
O(12)	2298 (32)	-1490 (30)	1875 (4)	7.8
O(13)	4695 (16)	1102 (22)	919 (3)	4.4
O(14)	3351 (20)	3322 (24)	1911 (4)	5.3
O(15)	-1807 (21)	-134 (27)	2052 (3)	5.5
O(16)	-884 (22)	-1730 (20)	708 (4)	4.4
O(17)	6891 (35)	8688 (35)	1372 (5)	8.6

Table 2. Anisotropic thermal parameters with standard deviations ($\times 10^4$ for Cd; $\times 10^3$ for O and C)

The form of the temperature factor is $\exp(-\beta_{11}h^2 - \dots - 2\beta_{12}hk - \dots)$. The r.m.s. components R_i ($\times 10^3 \text{ \AA}$) of thermal displacement along the ellipsoid axes are also listed.

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	R_1	R_2	R_3
Cd(1)	186 (3)	186 (5)	6 (1)	20 (2)	-1 (1)	-1 (1)	237	203	212
Cd(2)	221 (3)	181 (5)	6 (1)	-43 (2)	5 (1)	2 (1)	260	191	216
O(1)	30 (3)	16 (4)	1 (1)	4 (3)	1 (1)	-1 (1)	298	167	262
O(2)	26 (3)	50 (6)	1 (1)	17 (4)	-2 (1)	-1 (1)	402	177	253
O(3)	17 (2)	17 (3)	1 (1)	5 (2)	0 (1)	-1 (1)	272	175	223
O(4)	27 (3)	31 (5)	1 (1)	7 (3)	0 (1)	0 (1)	315	223	251
O(5)	32 (3)	25 (5)	1 (1)	4 (3)	0 (1)	1 (1)	304	203	254
O(6)	39 (4)	25 (5)	1 (1)	3 (3)	2 (1)	0 (1)	337	158	255
O(7)	25 (3)	36 (5)	1 (1)	3 (3)	1 (1)	0 (1)	317	212	262
O(8)	22 (3)	34 (5)	1 (1)	-4 (3)	0 (1)	2 (1)	322	199	250
O(9)	29 (4)	37 (5)	1 (1)	12 (4)	2 (1)	-1 (1)	353	198	282
O(10)	36 (4)	42 (6)	1 (1)	1 (4)	2 (1)	1 (1)	350	180	322
O(11)	22 (3)	26 (4)	1 (1)	-2 (3)	0 (1)	-1 (1)	293	234	238
O(12)	56 (7)	35 (7)	1 (1)	5 (5)	0 (1)	-1 (1)	395	259	306
O(13)	20 (3)	26 (4)	1 (1)	0 (2)	0 (1)	-1 (1)	270	204	236
O(14)	26 (3)	25 (5)	1 (1)	1 (3)	1 (1)	1 (1)	302	225	257
O(15)	26 (3)	47 (6)	1 (1)	-2 (3)	0 (1)	0 (1)	359	191	266
O(16)	34 (4)	8 (4)	1 (1)	-2 (3)	-2 (1)	0 (1)	351	149	255
O(17)	53 (7)	42 (7)	1 (1)	-10 (5)	-2 (1)	0 (1)	404	273	328

checked by $R = \Sigma |F_o| - |F_c| / \Sigma |F_o|$ and $R_w = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w|F_o|^2]^{1/2}$. Anisotropic temperature factors were used for the Cd and O but not for the C atoms. The scattering factors used for Cd were those given by Cromer & Waber (1965) and for C and O by Hanson, Herman, Lea & Skillman (1964), in all cases for the neutral atoms. The final R was 0.110 and R_w 0.129 with 204 parameters varied and with shifts less than 1% of the estimated standard deviations. A final difference map showed electron density maxima of about $3 \text{ e } \text{Å}^{-3}$ in the vicinity of the Cd positions but was otherwise featureless. No correction for extinction was made. Table 1 gives the atomic coordinates. The thermal parameters and the r.m.s. components along the principal axes of thermal displacement ellipsoids for the anisotropic atoms are listed in Table 2.*

All computations were made on the Univac 1108 in Lund, Sweden (Oskarsson, 1973).

Description of the structure

The independent unit consists of two Cd atoms, two oxydiacetate ions and seven water molecules. The structure is composed of broad, infinite zigzag chains of composition $2\text{CdO}(\text{CH}_2\text{COO})_2 \cdot 5\text{H}_2\text{O}$ parallel to (102) and running in the *b* direction. The chains are about 21 Å broad and 5 Å thick. Fig. 1, which is a projection along *b*, shows how the chains are linked together by hydrogen bonds *via* the water O(11) to O(17). The construction of the chains is shown in Fig. 2, and the coordination about the Cd atoms in Fig. 3. The two independent Cd atoms are each surrounded by seven O atoms. The polyhedra are both somewhat distorted pentagonal bipyramids. As seen from Fig. 2, the Cd(1) polyhedra are joined to zigzag chains through the carboxylate group O(2)—C(2)—O(3). Alternately to one side and the other, a Cd(2) polyhedron is linked to each Cd(1) polyhedron through an oxydiacetate ion with the formation of an oxygen bridge. The pentagonal bipyramids around Cd(1) and Cd(2) are thus connected in pairs by sharing a corner formed by the carboxylate O(4) common to the two pentagons. Distances and angles for the two coordination polyhedra are given in Table 3. The first five Cd—O distances are in both cases those to the O atoms in the pentagon. The coordination distances range between 2.280 (16) and 2.433 (18) Å for Cd(1) and between 2.278 (15) and 2.491 (14) Å for Cd(2). The distance Cd(1)—Cd(2) in a pair is 4.738 (2) Å, and the closest distance between the Cd(1) atoms in

the chain is 5.483 (2) Å. Deviations from the least-squares plane through the five equatorial O atoms are listed in Table 4 for both pentagonal bipyramids. The angle between the planes through the two pentagons in a pair is 20°.

Table 3. *Interatomic distances (Å) and angles (°) in the coordination polyhedra*

The superscripts indicate transformations applied to the coordinates given in Table 1: (i) $-x, -1 + (\frac{1}{2} + y), \frac{1}{2} - z$; (ii) $x, -1 + y, z$.

Cd(1)—O(1)	2.412 (14)	O(1)—Cd(1)—O(2)	64.7 (5)
Cd(1)—O(2)	2.433 (18)	O(2)—Cd(1)—O(3 ⁱ)	73.0 (5)
Cd(1)—O(3 ⁱ)	2.310 (12)	O(3 ⁱ)—Cd(1)—O(12)	84.3 (5)
Cd(1)—O(12)	2.338 (22)	O(12)—Cd(1)—O(4)	75.3 (6)
Cd(1)—O(4)	2.408 (13)	O(4)—Cd(1)—O(1)	65.1 (5)
Cd(1)—O(14)	2.280 (16)	O(14)—Cd(1)—O(15)	169.1 (6)
Cd(1)—O(15)	2.317 (16)		
O(1)—O(2)	2.592 (18)	O(4)—O(1)—O(2)	115.1 (7)
O(2)—O(3 ⁱ)	2.821 (22)	O(1)—O(2)—O(3 ⁱ)	108.6 (7)
O(3 ⁱ)—O(12)	3.120 (22)	O(2)—O(3 ⁱ)—O(12)	103.1 (6)
O(12)—O(4)	2.899 (25)	O(3 ⁱ)—O(12)—O(4)	99.7 (8)
O(4)—O(1)	2.594 (21)	O(12)—O(4)—O(1)	107.7 (6)
O(14)—O(1)	3.273 (21)	O(15)—O(1)	3.096 (23)
O(14)—O(2)	3.200 (21)	O(15)—O(2)	3.242 (27)
O(14)—O(3 ⁱ)	3.038 (20)	O(15)—O(3 ⁱ)	3.575 (19)
O(14)—O(12)	3.599 (28)	O(15)—O(12)	3.239 (28)
O(14)—O(4)	3.224 (21)	O(15)—O(4)	3.435 (19)
Cd(2)—O(7 ⁱⁱ)	2.310 (17)	O(7 ⁱⁱ)—Cd(2)—O(6 ⁱⁱ)	68.6 (5)
Cd(2)—O(6 ⁱⁱ)	2.278 (15)	O(6 ⁱⁱ)—Cd(2)—O(9 ⁱⁱ)	68.4 (5)
Cd(2)—O(9 ⁱⁱ)	2.310 (14)	O(9 ⁱⁱ)—Cd(2)—O(5)	85.5 (5)
Cd(2)—O(5)	2.345 (16)	O(5)—Cd(2)—O(4)	54.1 (5)
Cd(2)—O(4)	2.491 (14)	O(4)—Cd(2)—O(7 ⁱⁱ)	83.8 (5)
Cd(2)—O(13)	2.312 (13)	O(13)—Cd(2)—O(16)	171.5 (5)
Cd(2)—O(16)	2.338 (16)		
O(7 ⁱⁱ)—O(6 ⁱⁱ)	2.584 (16)	O(4)—O(7 ⁱⁱ)—O(6 ⁱⁱ)	105.3 (7)
O(6 ⁱⁱ)—O(9 ⁱⁱ)	2.580 (23)	O(7 ⁱⁱ)—O(6 ⁱⁱ)—O(9 ⁱⁱ)	112.4 (7)
O(9 ⁱⁱ)—O(5)	3.160 (21)	O(6 ⁱⁱ)—O(9 ⁱⁱ)—O(5)	102.8 (6)
O(5)—O(4)	2.203 (19)	O(9 ⁱⁱ)—O(5)—O(4)	113.1 (8)
O(4)—O(7 ⁱⁱ)	3.209 (25)	O(5)—O(4)—O(7 ⁱⁱ)	105.2 (7)
O(13)—O(7 ⁱⁱ)	3.289 (23)	O(16)—O(7 ⁱⁱ)	3.272 (21)
O(13)—O(6 ⁱⁱ)	3.221 (21)	O(16)—O(6 ⁱⁱ)	3.507 (22)
O(13)—O(9 ⁱⁱ)	3.390 (19)	O(16)—O(9 ⁱⁱ)	3.323 (22)
O(13)—O(5)	3.219 (19)	O(16)—O(5)	3.213 (22)
O(13)—O(4)	3.203 (19)	O(16)—O(4)	3.355 (22)

Table 4. *Deviations (Å) from the least-squares planes through the pentagons*

	Plane I		Plane II
O(1)	-0.104	O(7 ⁱⁱ)	0.112
O(2)	-0.101	O(6 ⁱⁱ)	-0.126
O(3 ⁱ)	0.225	O(9 ⁱⁱ)	0.073
O(12)	-0.273	O(5)	0.007
O(4)	0.252	O(4)	-0.066
Cd(1)*	-0.022	Cd(2)*	0.037
O(14)*	2.245	O(13)*	-2.269
O(15)*	-2.325	O(16)*	2.367

* Atoms not defining the plane.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32116 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

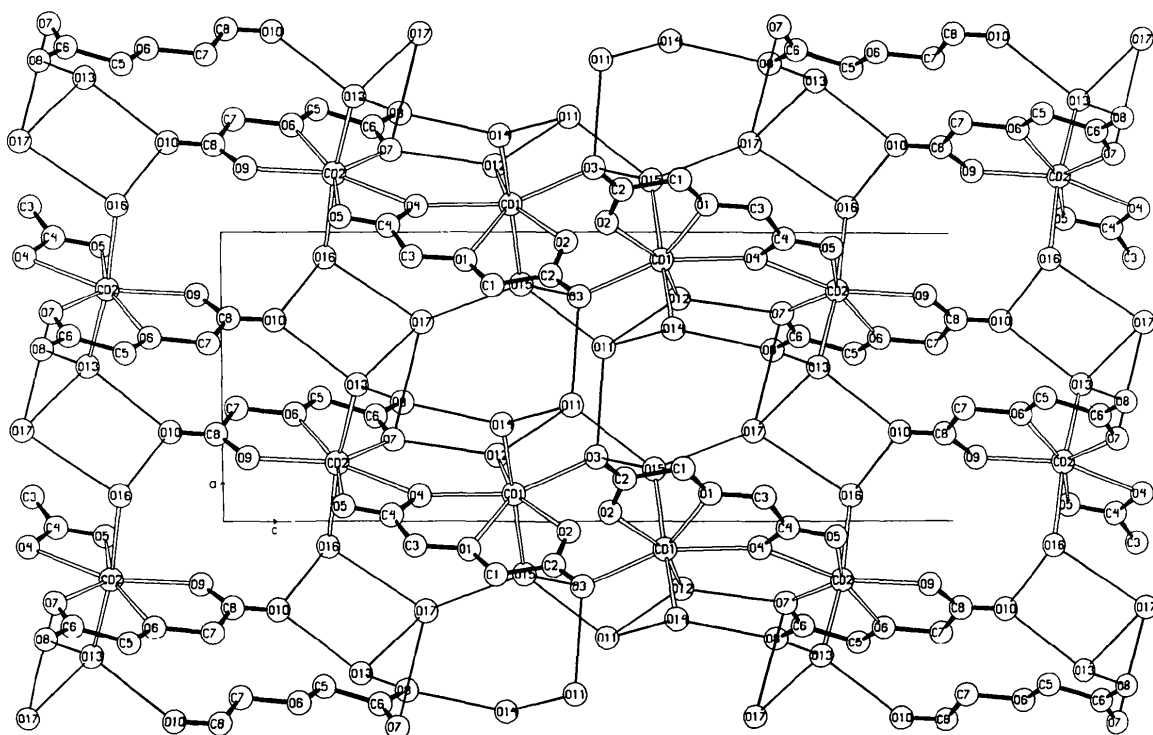


Fig. 1. Part of the structure projected along *b* with half the unit cell indicated. The hydrogen bonds are marked by thin lines. Figs. 1–5 were drawn by the program *ORTEP*.

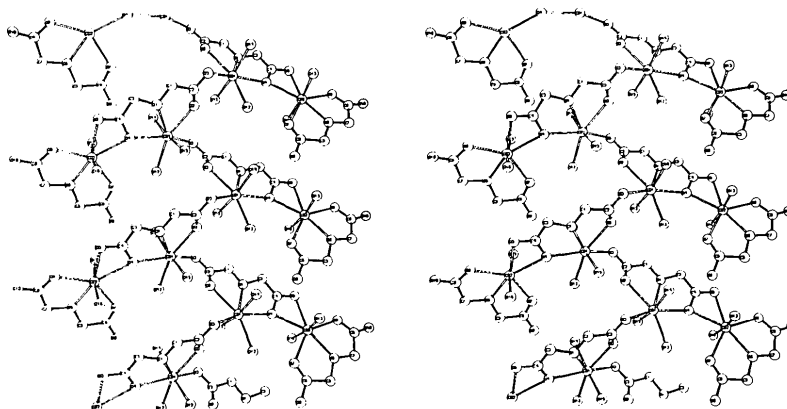


Fig. 2. A stereoscopic view showing part of a zigzag chain in detail.

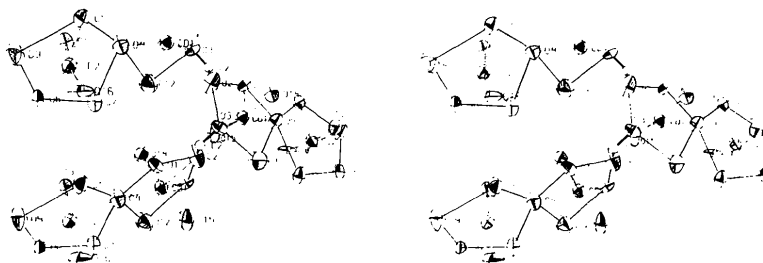


Fig. 3. Fragment of the chain showing the coordination about the two Cd atoms. In Figs. 3, 4 and 5 thermal ellipsoids were used.

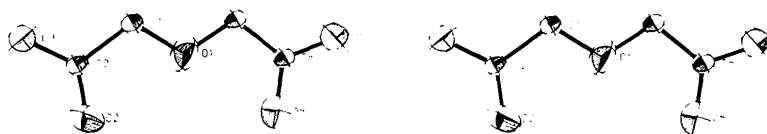


Fig. 4. A stereoscopic view of oxydiacetate ion I.

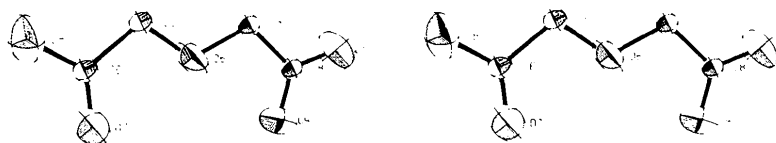


Fig. 5. A stereoscopic view of oxydiacetate ion II.

Table 5. Interatomic distances (Å) and angles (°) for the oxydiacetate ions

O(1)—C(1)	1.364 (30)	C(1)—O(1)—C(3)	112.5 (1.6)
O(1)—C(3)	1.401 (20)	O(1)—C(1)—C(2)	112.1 (2.0)
C(1)—C(2)	1.508 (30)	O(1)—C(3)—C(4)	107.2 (1.5)
C(3)—C(4)	1.452 (28)	C(1)—C(2)—O(2)	117.6 (1.9)
C(2)—O(2)	1.200 (27)	C(1)—C(2)—O(3)	116.7 (1.9)
C(2)—O(3)	1.272 (25)	O(2)—C(2)—O(3)	124.6 (1.7)
C(4)—O(4)	1.332 (26)	C(3)—C(4)—O(4)	122.6 (1.5)
C(4)—O(5)	1.254 (20)	C(3)—C(4)—O(5)	120.6 (1.8)
O(2)—O(3)	2.188 (23)	O(4)—C(4)—O(5)	116.8 (1.8)
O(4)—O(5)	2.203 (19)		
O(1)—O(2)	2.592 (18)		
O(1)—O(4)	2.594 (21)		
O(2)—O(4)	4.376 (21)		
O(6)—C(5)	1.451 (25)	C(5)—O(6)—C(7)	114.8 (1.5)
O(6)—C(7)	1.485 (21)	O(6)—C(5)—C(6)	106.1 (1.5)
C(5)—C(6)	1.491 (23)	O(6)—C(7)—C(8)	108.0 (1.6)
C(7)—C(8)	1.487 (33)	C(5)—C(6)—O(7)	122.7 (1.7)
C(6)—O(7)	1.234 (26)	C(5)—C(6)—O(8)	110.9 (1.6)
C(6)—O(8)	1.314 (25)	O(7)—C(6)—O(8)	126.4 (1.5)
C(8)—O(9)	1.264 (28)	C(7)—C(8)—O(9)	119.1 (1.8)
C(8)—O(10)	1.177 (23)	C(7)—C(8)—O(10)	117.6 (2.1)
O(7)—O(8)	2.275 (25)	O(9)—C(8)—O(10)	123.2 (2.3)
O(9)—O(10)	2.148 (20)		
O(6)—O(7)	2.584 (16)		
O(6)—O(9)	2.580 (23)		
O(7)—O(9)	4.292 (21)		

Dihedral angles

O(1)—C(1)—C(2)—O(2)	10.3	O(6)—C(5)—C(6)—O(7)	0.6
O(1)—C(1)—C(2)—O(3)	178.9	O(6)—C(5)—C(6)—O(8)	-178.5
O(1)—C(3)—C(4)—O(4)	-0.2	O(6)—C(7)—C(8)—O(9)	-4.1
O(1)—C(3)—C(4)—O(5)	179.5	O(6)—C(7)—C(8)—O(10)	177.9

The two independent oxydiacetate ions in the structure are shown in Figs. 4 and 5. Their interatomic distances and angles are normal, as can be seen in Table 5, where the dihedral angles are also given. The oxydiacetate ions are both slightly twisted, but the non-hydrogen atoms in each oxydiacetate half are coplanar. The deviations from the least-squares planes are listed in Table 6. The planes form an angle of 20° in one oxydiacetate ion and 9° in the other.

Table 6. Deviations (Å) from the least-squares planes through the independent halves in the oxydiacetate ions

Atoms defining the planes are those listed. The angle between the planes I and II is 20° and between III and IV 9°.

Plane I		Plane II	
O(1)	-0.017	O(1)	0.003
C(1)	0.037	C(3)	-0.003
C(2)	-0.056	C(4)	-0.002
O(2)	0.029	O(4)	-0.001
O(3)	0.008	O(5)	0.003
Plane III		Plane IV	
O(6)	-0.009	O(6)	-0.021
C(5)	0.010	C(7)	0.027
C(6)	0.006	C(8)	-0.006
O(7)	0.002	O(9)	0.013
O(8)	-0.009	O(10)	-0.014

Table 7. Hydrogen-bond distances (Å)

O(11)—H...O(3)	2.772 (18)
O(11)—H...O(15)	2.829 (20)
O(11)...H—O(12)	2.806 (25)
O(11)...H—O(14)	2.810 (22)
O(12)—H...O(7)	2.841 (22)
O(12)—H...O(11)	2.806 (25)
O(13)—H...O(8)	2.702 (22)
O(13)—H...O(10)	2.685 (19)
O(13)...H—O(17)	2.908 (27)
O(14)—H...O(8)	2.705 (19)
O(14)—H...O(11)	2.810 (22)
O(15)—H...O(3)	3.179 (23)
O(15)—H...O(17)	2.822 (24)
O(15)...H—O(11)	2.829 (20)
O(16)—H...O(10)	2.671 (23)
O(16)—H...O(17)	2.988 (27)
O(17)—H...O(7)	3.256 (29)
O(17)—H...O(13)	2.908 (27)
O(17)...H—O(15)	2.822 (24)
O(17)...H—O(16)	2.988 (27)

The Cd(1) atom coordinates three water molecules, O(12), O(14) and O(15), and two oxydiacetate ions, one tridentate and one monodentate; Cd(2) coordinates two water molecules, O(13) and O(16), and two oxydiacetate ions, one tridentate and one bidentate. In both the pentagonal bipyramids the apices are formed by water O atoms. The O(4) atom common to the two bipyramids in a pair is involved in a tridentate chelate with Cd(1) and in a carboxylate chelate with Cd(2), the bite O(4)–O(5) of the latter being 2.203 (19) Å.

An extensive hydrogen-bond system joins the chains to form a three-dimensional network, Fig. 1. The linking occurs *via* the two non-coordinated water molecules, O(11) and O(17), situated between the chains, but also directly between the chains through all the coordinated water molecules. Though no H atoms could be located, it was possible to assign all water H

atoms to definite O atoms from geometrical considerations. The result is shown in Table 7, which also lists the O–O distances in the hydrogen bonds.

A comparison between the three different Cd oxydiacetate structures will be given in the paper dealing with monoclinic cadmium oxydiacetate trihydrate, CDOXY II.

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The Crystal Structures of Free Radical Salts and Complexes. VIII. The Crystal Structure of and Electrical Anisotropy in [1,4-Di(*N*-quinolinium-methyl)benzene]²⁺ (7,7,8,8-Tetracyanoquinodimethane)₃⁻

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The 3:1 complex salt formed between 7,7,8,8-tetracyanoquinodimethane (TCNQ) and 1,4-di(*N*-quinolinium-methyl)benzene²⁺ is triclinic, space group *P* $\bar{1}$, with $a = 7.50$, $b = 10.07$, $c = 17.75$ Å, $\alpha = 102.79$, $\beta = 106.17$, $\gamma = 98.91^\circ$, $Z = 1$. The structure was solved by the Patterson method and refined to $R = 0.038$ for 2143 reflexions. The TCNQ moieties are stacked plane-to-plane in groups of three along **b** with almost no direct overlap between adjacent triads. The molecular geometries of the two independent TCNQ moieties indicate that the negative charge is delocalized within the triads. Anisotropic conductivities of 2×10^{-4} , 1×10^{-4} and $1 \times 10^{-6} \Omega^{-1} \text{cm}^{-1}$ at 300 K were observed along **a**, **b** and **c** respectively. The temperature dependence of conductivity along all three directions is isotropic and varies as $\exp(-E_a/kT)$ where $E_a = 0.27 \pm 0.02$ eV.

Introduction

The radical anion salts of TCNQ possess interesting electrical and magnetic properties which can be related to their crystal structures. A common feature is a characteristic parallel plane-to-plane stacking of the TCNQ molecules in columns. In a few salts, with favourable overlap and a regular short interplanar separation, metallic behaviour is observed. In the majority, however, different overlaps and intermolecular distances at different points in the stack give rise to

intermediate conductivities. In an attempt to elucidate further this relation, the crystal structure and electrical conductivity of 1,4-di(*N*-quinoliniummethyl)benzene-(TCNQ)₃ have been studied.

Experimental

Crystal data

(C₂₆H₂₂N₂)(C₁₂H₄N₄)₃, $M_r = 975.1$, triclinic, $a = 7.50$ (2), $b = 10.07$ (3), $c = 17.75$ (4) Å, $\alpha =$