Crystal and Molecular Structure of Cadmium(II) Maleate Dihydrate

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Crystals of the title compound are monoclinic, $a = 8{\cdot}729(2)$, $b = 14{\cdot}285(6)$, $c = 11{\cdot}622(4)$ Å, $\beta = 102{\cdot}66(2)°$, $Z = 8$, space group $P2_1/c$. The structure was determined from *X*-ray diffractometer data by Patterson and Fourier syntheses, and refined by full-matrix least-squares calculations to *R* 0·045 for 2401 observed reflections. The structure contains two cadmium atoms and two maleate ligands, both pairs of which are crystallographically and chemically distinct. One cadmium atom is six-co-ordinate through four water molecules and two bridging maleate oxygen atoms while the other is eight-co-ordinate, in distorted dodecahedral geometry, through four chelated carboxy-groups from the two maleate ligands. The maleate ligands link cadmium atoms into a three-dimensional polymer which is further strengthened by extensive hydrogen bonding through the water molecules. Cd–O distances are 2·199(5)—2·843(5) Å, while the bridging Cd–O bonds [2·289(4) and 2·285(4) Å] suggest relatively high interaction. The structure exhibits chelation and bridging by two separate carboxy-groups, a mode of co-ordination uncommon in carboxylates.

CADMIUM is known to form complexes with acetates and carboxy-ligands to yield both charged[1] and neutral[2,3] compounds. The possibility of forming structures with higher co-ordination numbers[2] has resulted in the observation of some of the more unusual co-ordination geometries about the metal atom, and the formation of polymeric species.[2,3] The present work studies the structural effects when the carboxy-ligand has more than one functional group, since under such conditions the formation of polymeric and, possibly, higher co-ordination number complexes should be favoured, as has been reported for some copper(II) dicarboxylates.[4,5]

EXPERIMENTAL

The title compound was prepared by the addition of an aqueous solution of maleic acid to an excess of finely divided cadmium(II) carbonate, in suspension in water, followed by heating to near boiling point. After filtration the complex precipitated on cooling. Crystals from water were transparent, approximately rectangular prisms elongated slightly along *a*, with {011} well developed. The space group and initial unit-cell parameters were determined from Weissenberg and precession photographs, accurate unit-cell parameters being obtained later by a least-squares treatment of the 2θ values of 25 general (*hkl*) reflections measured on a General Electric XRD 6 diffractometer.

Crystal Data.—$C_4H_6CdO_6$, $M = 262{\cdot}49$, Monoclinic, $a = 8{\cdot}729(2)$, $b = 14{\cdot}285(6)$, $c = 11{\cdot}622(4)$ Å, $\beta = 102{\cdot}66(2)°$, $U = 1413{\cdot}96$ Å^3, $Z = 8$, $D_c = 2{\cdot}47$, $F(000) = 960$. Mo-K_α radiation, $\lambda = 0{\cdot}71069$ Å, μ(Mo-K_α) $= 30{\cdot}6$ cm^{-1}. Space group $P2_1/c$ from absent spectra: $0k0$, k odd; $h0l$, l odd.

For cell refinement and data collection, a crystal of size *ca.* $0{\cdot}40 \times 0{\cdot}35 \times 0{\cdot}30$ mm was mounted with the a^* direction coincident with the instrument ϕ axis of a Datex-automated General Electric XRD 6 diffractometer. Reflections with 2θ(Mo-K_α) $\leqslant 55°$ were measured by use of a θ—2θ scan at 2° min^{-1} in 2θ, and of the 3059 measured, 658 were considered unobserved, having intensities $< 3\sigma(I)$ above background, [$\sigma(I)$ is defined by: $\sigma^2(I) = S + B + (0{\cdot}05S)^2$, where S = scan count and B = background], and were treated as unobserved. A check and scaling reflection was monitored every 45 reflections and its intensity had dropped by 18% by the end of data collection. Lorentz and polarisation corrections were made and relative structure factors derived. No absorption correction was applied.

Structure Solution and Refinement.—The positions of the two independent cadmium atoms were determined from a Patterson synthesis. Using these atoms and refining the scale only, a structure-factor calculation yielded *R* 0·247. A Fourier synthesis at this stage showed the positions of the remaining non-hydrogen atoms, and after two cycles of full-matrix least-squares refinement of all the atoms with isotropic thermal parameters, *R* was 0·069. Refinement was continued with anisotropic temperature factors, those for the cadmium atoms being corrected for the real and imaginary components of anomalous dispersion. Subsequent difference-Fourier syntheses indicated sites for all the hydrogen atoms, and these were included in following structure-factor calculations, although their positional and thermal (B_{iso} 6·0 Å^2) parameters were held fixed during refinement. During the final stages of refinement, a weighting scheme of the form $w = [A + B|F_o| + C|F_o|^2 + D|F_o|^3]^{-1}$ with $A = 3{\cdot}767$, $B = -0{\cdot}1018$, $C = 0{\cdot}0017$, and $D = 0{\cdot}00001$ was employed, and convergence was attained at *R* 0·045 (weighted *R'* 0·055) for 2401 observed reflections. No parameter shift was $> 0{\cdot}5\sigma$ during the final cycle. Final positional and thermal parameters are given in Tables 1 and 2. Measured and calculated structure factors are listed in Supplementary Publication No. SUP 20885 (30 pp., 1 microfiche).*

DISCUSSION

Details of the structure are shown in Figure 1 and a clearer view of the co-ordination geometry around Cd(2) in Figure 2, where atoms not bonded to Cd are omitted. Bond lengths and bond and co-ordination angles are presented in Tables 3 and 4, while distances and angles involving the water molecules are listed in Table 5.

Each of the cadmium atoms is crystallographically

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* For details see Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue.

[1] D. A. Langs and C. R. Hare, *Chem. Comm.*, 1967, 890.

[2] W. Harrison and J. Trotter, *J.C.S. Dalton*, 1972, 956.

[3] M. L. Post and J. Trotter, *J.C.S. Dalton*, 1974, 285.

[4] B. H. O'Connor and E. N. Maslen, *Acta Cryst.*, 1966, **20**, 824.

[5] O. Asai, M. Kishita, and M. Kubo, *J. Phys. Chem.*, 1959, **63**, 96.

and chemically distinct. Atom Cd(1) is six-co-ordinate through four water molecules [O(9)—(12)] and through two carboxy-oxygen atoms, O(3), and O(1), which also bridge to Cd(2). The geometry around Cd(1) is best described as distorted octahedral (Figure 1). Atom Cd(2), however, is eight-co-ordinate through four chelated carboxy-groups (Figure 2), the co-ordination geometry being a considerably distorted dodecahedron with no other recognised polyhedron [6] discernible. The

TABLE 1

Final positional parameters ($\times 10^4$), with standard deviations in parentheses

Atom	x	y	z
Cd(1)	7304·8(5)	7067·2(3)	3654·0(4)
Cd(2)	3430·9(5)	6183·4(3)	6647·3(4)
O(1)	6205(5)	6590(3)	7763(4)
O(2)	5718(5)	5517(4)	6371(5)
O(3)	7709(6)	5569(3)	4343(4)
O(4)	7916(6)	4202(3)	5210(4)
O(5)	1259(6)	7457(4)	6175(5)
O(6)	3720(5)	7699(4)	6194(5)
O(7)	2542(7)	8219(4)	3684(5)
O(8)	2946(7)	9646(3)	3122(4)
O(9)	9829(5)	6942(4)	3342(5)
O(10)	6521(5)	6489(3)	1788(4)
O(11)	4883(6)	6769(4)	3993(4)
O(12)	8300(7)	7914(4)	5250(6)
C(1)	6669(7)	6003(4)	7098(5)
C(2)	8373(7)	5881(4)	7190(6)
C(3)	8987(7)	5482(4)	6377(6)
C(4)	8108(7)	5077(4)	5244(5)
C(5)	2334(8)	7988(4)	6061(5)
C(6)	2018(10)	9014(5)	5867(6)
C(7)	2128(10)	9483(5)	4909(7)
C(8)	2587(8)	9070(4)	3857(5)
H(1)	10170	5400	6450
H(2)	9140	6100	7930
H(3)	1630	9380	6510
H(4)	1970	10220	4820
H(5)	10530	6520	3840
H(6)	10510	7340	3390
H(7)	6450	5910	1790
H(8)	6730	6470	1100
H(9)	4150	7150	3850
H(10)	4760	6260	4400
H(11)	9200	7770	5670
H(12)	7700	7970	5930

TABLE 2

Final anisotropic thermal parameters * (Å $\times 10^3$), with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	36·3(3)	32·4(3)	33·8(3)	2·1(2)	6·7(2)	3·6(2)
Cd(2)	34·3(3)	36·6(3)	37·3(3)	−1·4(2)	5·3(2)	2·2(2)
O(1)	38(2)	32(2)	43(2)	−3(2)	7(2)	−12(2)
O(2)	34(2)	57(3)	52(3)	−7(2)	5(2)	−26(2)
O(3)	48(3)	33(2)	39(2)	3(2)	9(2)	7(2)
O(4)	46(3)	29(2)	43(3)	−1(2)	−1(2)	0(2)
O(5)	42(3)	44(3)	57(3)	−5(2)	9(2)	7(2)
O(6)	35(2)	39(3)	64(3)	−1(2)	−4(2)	2(2)
O(7)	75(4)	38(3)	46(3)	−3(2)	23(3)	−8(2)
O(8)	71(3)	35(3)	41(3)	2(2)	23(2)	5(2)
O(9)	32(2)	46(3)	56(3)	2(2)	10(2)	10(2)
O(10)	42(2)	38(2)	34(2)	2(2)	7(2)	−3(2)
O(11)	51(3)	54(3)	89(3)	14(2)	37(2)	27(2)
O(12)	40(3)	65(3)	41(4)	6(3)	5(3)	−12(3)
C(1)	37(3)	29(3)	37(3)	−2(2)	7(2)	−2(2)
C(2)	32(3)	33(3)	39(3)	−8(2)	−1(2)	−11(3)
C(3)	29(3)	32(3)	41(3)	−6(2)	5(2)	−2(3)
C(4)	30(3)	32(3)	36(3)	3(2)	8(2)	2(2)
C(5)	44(3)	35(3)	27(3)	−1(3)	6(2)	−3(2)
C(6)	71(5)	33(3)	42(4)	9(3)	22(3)	−2(3)
C(7)	69(5)	33(4)	46(4)	11(3)	23(3)	5(3)
C(8)	40(3)	33(3)	31(3)	4(3)	9(2)	3(2)

* Thermal parameters are in the form: $\exp[-2\pi^2(U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{12}a^*b^*hk + 2U_{13}a^*c^*hl + 2U_{23}b^*c^*kl)]$.

TABLE 3

Bond distances (Å), with standard deviations in parentheses

Cd(1)–O(1^{III})	2·289(4)	C(1)–O(1)	1·265(8)
Cd(1)–O(3)	2·285(4)	C(1)–O(2)	1·256(8)
Cd(1)–O(9)	2·317(5)	C(1)–C(2)	1·478(9)
Cd(1)–O(10)	2·281(5)	C(2)–C(3)	1·314(9)
Cd(1)–O(11)	2·274(5)	C(4)–O(3)	1·246(7)
Cd(1)–O(12)	2·226(5)	C(4)–O(4)	1·262(8)
Cd(2)–O(1)	2·550(4)	C(4)–C(3)	1·488(8)
Cd(2)–O(2)	2·297(4)	C(5)–O(5)	1·236(8)
Cd(2)–O(3^{II})	2·843(5)	C(5)–O(6)	1·255(8)
Cd(2)–O(4^{II})	2·287(5)	C(5)–C(6)	1·490(9)
Cd(2)–O(5)	2·598(5)	C(6)–C(7)	1·321(10)
Cd(2)–O(6)	2·255(5)	C(8)–O(7)	1·231(8)
Cd(2)–O(7^{I})	2·782(5)	C(8)–O(8)	1·274(8)
Cd(2)–O(8^{I})	2·199(5)	C(8)–C(7)	1·499(9)

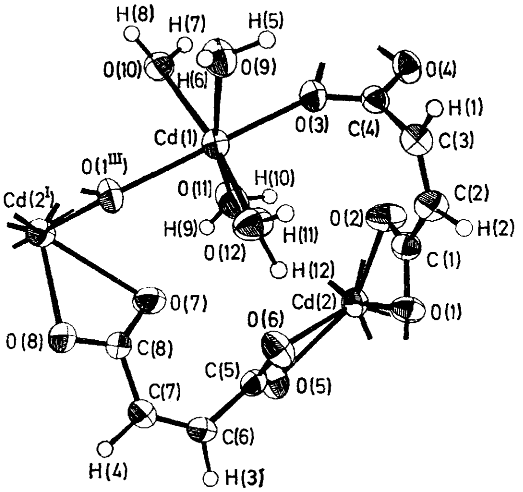

FIGURE 1 Perspective view of cadmium(II) maleate dihydrate with all non-hydrogen atoms represented by 50% probability, thermal ellipsoids

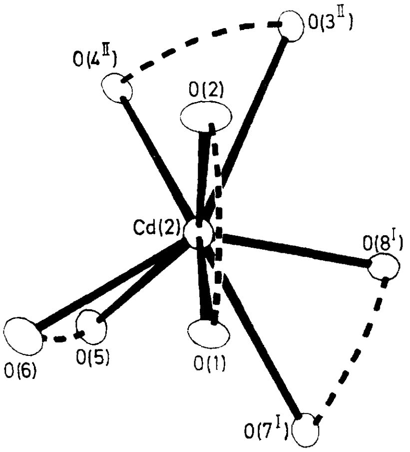

FIGURE 2 Perspective view of the co-ordination around Cd(2). Broken lines connect pairs of chelating atoms

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[6] R. B. King, *J. Amer. Chem. Soc.*, 1969, **91**, 7211.

TABLE 4

Co-ordination and bond angles with standard deviations in parentheses

O(9)–Cd(1)–O(1^{III})	108·3(2)	O(4^{II})–Cd(2)–O(8^{I})	117·3(2)
O(9)–Cd(1)–O(3)	84·5(2)	O(5)–Cd(2)–O(6)	52·6(2)
O(9)–Cd(1)–O(10)	85·4(2)	O(5)–Cd(2)–O(7^{I})	68·8(2)
O(9)–Cd(1)–O(11)	164·7(2)	O(5)–Cd(2)–O(8^{I})	106·6(2)
O(9)–Cd(1)–O(12)	87·8(2)	O(6)–Cd(2)–O(7^{I})	88·3(2)
O(10)–Cd(1)–O(1^{III})	82·2(2)	O(6)–Cd(2)–O(8^{I})	138·5(2)
O(10)–Cd(1)–O(3)	89·2(2)	O(7^{I})–Cd(2)–O(8^{I})	50·6(2)
O(10)–Cd(1)–O(11)	90·0(2)	Cd(2)–O(1)–Cd(1^{I})	132·7(3)
O(10)–Cd(1)–O(12)	166·0(2)	Cd(2)–O(1)–C(1)	86·2(4)
O(11)–Cd(1)–O(1^{III})	85·5(2)	C(1)–O(1)–Cd(1^{I})	132·3(4)
O(11)–Cd(1)–O(3)	80·9(2)	Cd(2)–O(2)–C(1)	98·3(4)
O(11)–Cd(1)–O(12)	99·5(2)	O(1)–C(1)–O(2)	121·6(6)
O(12)–Cd(1)–O(1^{III})	88·3(2)	O(1)–C(1)–C(2)	119·1(5)
O(12)–Cd(1)–O(3)	102·4(2)	O(2)–C(1)–C(2)	119·4(5)
O(1^{III})–Cd(1)–O(3)	163·9(2)	C(1)–C(2)–C(3)	124·1(5)
O(1)–Cd(2)–O(2)	53·7(1)	C(2)–C(3)–C(4)	126·3(5)
O(1)–Cd(2)–O(3^{II})	128·1(1)	O(3)–C(4)–C(3)	121·3(5)
O(1)–Cd(2)–O(4^{II})	140·3(2)	O(4)–C(4)–C(3)	116·9(5)
O(1)–Cd(2)–O(5)	121·1(2)	O(3)–C(4)–O(3)	121·5(6)
O(1)–Cd(2)–O(6)	76·0(2)	Cd(2^{II})–O(4)–C(4)	107·8(4)
O(1)–Cd(2)–O(7^{I})	84·7(2)	Cd(2^{II})–O(3)–C(4)	81·5(3)
O(1)–Cd(2)–O(8^{I})	92·8(2)	Cd(1)–O(3)–C(4)	144·7(4)
O(2)–Cd(2)–O(3^{II})	79·4(2)	Cd(1)–O(3)–Cd(2^{II})	132·0(3)
O(2)–Cd(2)–O(4^{II})	92·9(2)	Cd(2)–O(5)–C(5)	85·2(4)
O(2)–Cd(2)–O(5)	151·3(2)	Cd(2)–O(6)–C(5)	101·0(4)
O(2)–Cd(2)–O(6)	102·7(2)	O(5)–C(5)–O(6)	121·2(8)
O(2)–Cd(2)–O(7^{I})	131·2(2)	O(5)–C(5)–C(6)	119·8(6)
O(2)–Cd(2)–O(8^{I})	102·0(2)	O(6)–C(5)–C(6)	118·8(6)
O(3^{II})–Cd(2)–O(4^{II})	49·0(1)	C(5)–C(6)–C(7)	125·4(6)
O(3^{II})–Cd(2)–O(5)	110·9(2)	C(6)–C(7)–C(8)	124·9(6)
O(3^{II})–Cd(2)–O(6)	149·9(2)	O(7)–C(8)–O(8)	122·1(6)
O(3^{II})–Cd(2)–O(7^{I})	118·5(2)	O(7)–C(8)–C(7)	121·4(6)
O(3^{II})–Cd(2)–O(8^{I})	74·4(2)	O(8)–C(8)–C(7)	116·4(5)
O(4^{II})–Cd(2)–O(5)	76·6(2)	Cd(2^{III})–O(7)–C(8)	80·3(4)
O(4^{II})–Cd(2)–O(6)	94·1(2)	Cd(2^{III})–O(8)–C(8)	107·0(4)
O(4^{II})–Cd(2)–O(7^{I})	134·1(2)		

Roman numerals refer to the following equivalent positions, relative to x, y, z:

I $x, 1{\cdot}5 - y, 0{\cdot}5 + z$ II $1 - x, 1 - y, 1 - z$

midpoints between the oxygen atoms of each carboxy-chelate lie very close to the vertices of a tetrahedron, an effect which has been noted in a few other eight-co-ordinate compounds[7] where the ligand bite distances were <2·2 Å. In the present compound these distances are: O(1) · · · O(2) 2·200(6), O(3) · · · O(4) 2·188(6), O(5) · · · O(6) 2·171(7), and O(7) · · · O(8) 2·192(7) Å.

TABLE 5

Distances (Å) and angles (°) involving the water molecules

O(9)–H(5)	0·96	O(11)–H(9)	0·83
O(9)–H(6)	0·82	O(11)–H(10)	0·89
H(5)–O(9)–H(6)	92·2	H(9)–O(11)–H(10)	117·8
Cd(1)–O(9)–H(5)	117·2	Cd(1)–O(11)–H(9)	123·8
Cd(1)–O(9)–H(6)	129·7	Cd(1)–O(11)–H(10)	118·2
O(10)–H(7)	0·83	O(12)–H(11)	0·85
O(10)–H(8)	0·86	O(12)–H(12)	1·04
H(7)–O(10)–H(8)	90·1	H(11)–O(12)–H(12)	97·9
Cd(1)–O(10)–H(7)	111·4	Cd(1)–O(12)–H(11)	119·1
Cd(1)–O(10)–H(8)	144·7	Cd(1)–O(12)–H(12)	120·3

This type of behaviour has also been reported for the twelve-co-ordinate anion[8] $[Ce(NO)_3)_6]^{2-}$ where an octahedral arrangement of bisector points occurs and the ligand bites are 2·14 and 2·15 Å. In common with the present structure, the set of isomorphous formate dihydrates[9,10] of Mg^{II}, Mn^{II}, Cu^{II}, and Zn^{II} also have two metal atoms in different chemical environments, although in these cases each metal atom is six-co-ordinate.

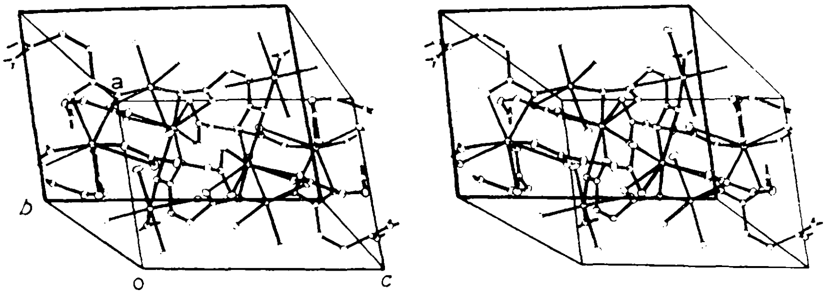

FIGURE 3 Stereoscopic view of the polymeric lattice. Slightly more than the unit cell is shown

In the compound there are also two distinct maleate ligands. One of these [O(1)—(4), C(1)—(4), *A*] chelates Cd(2) atoms related by a centre of symmetry and links them *via* the maleate carbon chain. Ligand *A* also has two trigonal oxygen atoms, O(1) and O(3), which bridge to two Cd(1) atoms which are related by the *c* glide plane. It is apparent, therefore, that Cd(1) atoms link *A* type ligands related by the *c* glide. This mode of co-ordination by *A*, with both chelation and bridging by the carboxy-groups, is the most rarely encountered with carboxylate ligands,[11] and has been reported in only a few other cases, namely $Ca[M(OAc)_4],6H_2O$ (M = Cd or Cu),[1] uranium(IV) acetate,[12] acetato(dimethyl)indium(III),[13] and cadmium diacetate dihydrate.[2] That cadmium is involved in two of these compounds is, possibly, significant with regard to its behaviour with carboxy-ligands in general. The other maleate ligand, *B*, chelates Cd(2) atoms related by the *c* glide plane and links them *via* the carbon chain in a manner similar to

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[7] J. G. Bergman, jun., and F. A. Cotton, *Inorg. Chem.*, 1966, **5**, 1208.

[8] A. Zalkin, J. D. Forrester, and D. H. Templeton, *J. Chem. Phys.*, 1963, **39**,, 2881.

[9] K. Osaki, Y. Nakai, and T. Watanabé, *J. Phys. Soc. Japan*, 1963, **18**, 919.

[10] K. Osaki, Y. Nakai, and T. Watanabé, *J. Phys. Soc. Japan*, 1964, **19**, 717.

[11] C. Oldham, *Progr. Inorg. Chem.*, 1968, **10**, 223.

[12] I. Jelenić, D. Grdenić, and A. Bezjak, *Acta Cryst.*, 1964, **17**, 758.

[13] F. W. B. Einstein, M. M. Gilbert, and D. G. Tuck, *J.C.S. Dalton*, 1973, 248.

A. Unlike *A*, however, ligand *B* does not have any trigonal bridging oxygen atoms. The crystal lattice thus formed is polymeric (Figure 3). Figure 3 also shows that the maleate ligands form sets of polymeric chains and loops which, predominantly, cross the *ab* and *ac* planes. There is extensive hydrogen bonding across the *bc* plane, and between some atoms with positions as shown in Figure 1, thus ensuring the integrity of the polymer in three dimensions. Each water molecule is involved in at least two hydrogen bonds (Table 6), with atom H(10) in such a position that it forms a slightly weaker bifurcated bond. The O · · · O and O–H · · · O distances and angles all have reasonable values. Only three maleate oxygen atoms, O(1), O(3), and O(6), are not involved in hydrogen bonding. Of these O(1) and O(3) are involved in a bridging interaction with Cd(1) leaving O(6) as the only oxygen atom which is exactly bivalent.

TABLE 6

Hydrogen-bond distances (Å) and angles (°)

Bond	O · · · O	O–H · · · O
O(9)–H(5) · · · O(4$^{\mathrm{IV}}$)	2·815	173·1
O(9)–H(6) · · · O(7$^{\mathrm{V}}$)	2·946	170·6
O(10)–H(7) · · · O(8$^{\mathrm{VI}}$)	2·672	159·9
O(10)–H(8) · · · O(12$^{\mathrm{III}}$)	2·747	137·3
O(11)–H(9) · · · O(7)	2·876	171·4
O(11)–H(10) · · · O(2)	3·238	141·5
O(11)–H(10) · · · O(4$^{\mathrm{II}}$)	3·121	121·8
O(12)–H(11) · · · O(5$^{\mathrm{V}}$)	2·653	164·4
O(12)–H(12) · · · O(10$^{\mathrm{I}}$)	2·747	156·4

Roman numeral superscripts refer to the following equivalent positions

I and II see footnote to Table 4

III $x, 1·5 - y, -0·5 + z$ V $1 + x, y, z$

IV $2 - x, 1 - y, 1 - z$ VI $1 - x, -0·5 + y, 0·5 - z$

The Cd–O distances vary from 2·199 [Cd(2$^{\mathrm{III}}$)–O(8)] to 2·843 Å [Cd(2$^{\mathrm{II}}$)–O(3)], which encompasses very nearly the whole range of those reported elsewhere (see ref. 2 and refs. therein). Although most of the variation, particularly for ligand *B*, can be better explained in terms of steric restrictions imposed by the complexity of the polymeric lattice rather than inherent chemical differences, the comparatively short and similar distances for Cd(1$^{\mathrm{I}}$)–O(1) and Cd(2)–O(2) (2·289 and 2·297 Å), and Cd(1)–O(3) and Cd(2$^{\mathrm{II}}$)–O(4) (2·285 and 2·287 Å) could be the result of electron delocalisation involving the bridged Cd atoms and the carboxy-groups of ligand *A*. Both cadmium atoms have a formal dipositive charge and it is apparent from the mode of co-ordination that Cd(2) atoms could receive excess negative charge by co-ordination with four carboxy-groups. The case would be reversed for Cd(1) atoms, however, with electron donation occurring through atoms O(1) and O(3) alone. The delocalisation process would tend to decrease the charge differential between Cd(1) and Cd(2) and to equalise the lengths of equivalent bonds in the system, as is found for the Cd–O distances involved. The C–O distances in the carboxy-groups of *A* are not identical, however, but do lie within 2σ of one another. The longer Cd(2$^{\mathrm{II}}$)–O(3) and Cd(2)–O(1) bonds (2·843 and 2·550 Å), would be expected in such a system, since O(1) and O(3) would be predominantly involved in co-ordination with Cd(1), and only weakly bonded to Cd(2).

TABLE 7

Equations of some least-squares mean planes (X, Y, Z, in Å based on orthogonal co-ordinate system a, b, c^*), and distances (Å) of some atoms from the planes in square brackets

Plane (1):
O(1), O(2), C(1), C(2)
$$0·1307X + 0·7087Y - 0·6933Z - 1·0181 = 0$$
[O(1) −0·0006, O(2) −0·0008, C(1) 0·0035, C(2) 0·0010, Cd(2) 0·1860]

Plane (2):
O(3), O(4), C(3), C(4)
$$0·9558X - 0·1476Y - 0·2542Z - 2·9406 = 0$$
[O(3) 0·0074, O(4) 0·0075, C(3) 0·0105, C(4) −0·0348, Cd(2$^{\mathrm{II}}$) −0·0476]

Plane (3):
O(5), O(6), C(5), C(6)
$$0·0376X - 0·1690Y - 0·9849Z + 8·7066 = 0$$
[O(5) −0·0069, O(6) −0·0065, C(5) 0·0280, C(6) −0·0117, Cd(2) −0·1606]

Plane (4):
O(7), O(8), C(7), C(8)
$$-0·8682X + 0·0567Y - 0·4929Z + 2·5110 = 0$$
[O(7) 0·0052, O(8) 0·0041, C(7) 0·0076, C(8) −0·0184, Cd(2$^{\mathrm{I}}$) 0·0680]

Plane (5):
C(1)—(4) $0·1343X + 0·8853Y - 0·4453Z - 4·5450 = 0$
[C(1) 0·0013, C(2) −0·0030, C(3) 0·0028, C(4) −0·0012]

Plane (6):
C(5)—(8) $-0·8937X - 0·1986Y - 0·4024Z + 5·4726 = 0$
[C(5) 0·0001, C(6) −0·0002, C(7) 0·0002, C(8) −0·0001]

The maleate ligands exhibit expected carbon–carbon bond lengths. All the acetato-groups, [O(1), O(2), C(1), C(2), *etc.*], are close to planar (Table 7), with the bridging groups exhibiting similar planar deviations to those which are non-bridging, an effect found previously[2] and further confirming the ability of carboxy-groups to take part in simultaneous chelation and bridging without any marked effect upon configuration. The carbon chains of the ligands lie very close to their respective planes (Table 7), but at an angle to the planes defined by the acetato-moieties. The crystal structure of maleic acid[14] shows the molecules to be planar, and thus the configuration of the ligands in the present structure can be described, with reference to maleic acid, by a rotation about the carbon–carbon bond of each acetato-moiety. These angles are: 17·5° O(1)–O(2)–C(1)–C(2), 83·6° O(3)–O(4)–C(3)–C(4), 66·7° O(5)–O(6)–C(5)–C(6), and 15·6° O(7)–O(8)–C(7)–C(8), the variation between values for each ligand indicating well the range of free rotation possible for a single carbon–carbon bond while the actual values are almost certainly the result of optimisation of bonding contacts and lattice packing. In

[14] M. Shahat, *Acta Cryst.*, 1952, **5**, 763.

copper(II) maleate hydrate[15] the corresponding angles are both close to 46°.

We thank Dr. F. G. Herring for suggesting the problem and the National Research Council of Canada for financial support.

[3/1599 *Received, 30th July*, 1973]

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[15] C. K. Prout, J. R. Carruthers, and F. J. C. Rossotti, *J. Chem. Soc. (A)*, 1971, 3342.