distance of 3·40 Å. This close contact may be attributed to a dipole interaction between O(2) and C on the ligand which has acquired a positive charge due to electron withdrawal from the ligand by Al. The effect of this dipolar interaction is to bring the layers of 'free' dioxane closer to the halogens. Cl(1) and Cl(3) which point towards layers of dioxane molecules are affected more than Cl(2), resulting in a large angle.

References

ATWOOD, J. L. & STUCKY, G. D. (1967). J. Am. Chem. Soc. 89, 5362–5366.

BEAMISH, J. C., SMALL, R. W. H. & WORRALL, I. J. (1979). Inorg. Chem. 18, 220–223.

BREWER, F. M., CHADWICK, J. R. & GARTON, G. (1961). J. Inorg. Nucl. Chem. pp. 45–52.

COWLEY, A. H., CUSHNER, M. C., DAVIS, R. E. & RILEY, P. E. (1981). Inorg. Chem. 20, 1179–1181.

CROMER, D. T. & LIBERMAN, D. (1970). J. Chem. Phys. 53, 1891–1898.

CROMER, D. T. & MANN, J. B. (1968). Acta Cryst. A24, 321–324.

GREENE, P. T., RUSS, B. J. & WOOD, J. S. (1971). J. Chem. Soc. A, pp. 3636–3639.

KULISHOV, V. I., BOKII, N. G., STRUCHKOV, Y. T. NEFEDOV, O. M., KOLESNIKOV, S. P. & PERL'MUTTER, B. L. (1970). J. Struct. Chem. (USSR), 11, 61–64.

LOBKOVSKII, E. B., KOROBOV, I. I. & SEMENKO, K. N. (1978). J. Struct. Chem. (USSR), 19, 908–914.

MAIN, P., LESSINGER, L., WOOLFSON, M. M., GERMAIN, G. & DECLERCQ, J. P. (1977). MULTAN. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. Univs. of York, England, and Louvain, Belgium.

SHELDRICK, G. M. (1976). SHELX 76. Program for crystal structure determination. Univ. of Cambridge, England.

SMALL, R. W. H. & WORRALL, I. J. (1982). Acta Cryst. B38, 250–251.

Crystal Structures of Ethylenediaminetetraacetato Metal Complexes. I. A Comparison of Crystal Structures Containing Hexacoordinated Metal Ions, $[(H_2O)_4X(C_{10}H_{12}N_2O_8)Y]_n.2nH_2O$

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Abstract. (1) $X = Mn$, $Y = Cu$, $n = 1$, $M_r = 514·8$, orthorhombic, space group $Pn2_1a$, $a = 14·626$ (3), $b = 13·068$ (4), $c = 9·969$ (3) Å, $V = 1905$ (2) Å³, $Z = 4$, $D_x = 1·79$ Mg m⁻³, $F(000) = 1056$, final $R = 0·044$ for 1658 observed reflections; (2) $X = Mn$, $Y = Co$, $n = 1$, $M_r = 510·3$, orthorhombic, space group $Pn2_1a$, $a = 14·584$ (3), $b = 13·366$ (4), $c = 9·799$ (3) Å, $V = 1910$ (2) Å³, $Z = 4$, $D_x = 1·77$ Mg m⁻³, $F(000) = 1048$, final $R = 0·059$ for 1633 observed reflections; (3) $X = Mg$, $Y = Zn$, $n = 1$, $M_r = 486·1$, orthorhombic, space group $Pn2_1a$, $a = 14·476$ (4), $b = 13·237$ (4), $c = 9·746$ (3) Å, $V = 1886$ (2) Å³, $Z = 4$, $D_x = 1·71$ Mg m⁻³, $F(000) = 1008$, final $R = 0·049$ for 1617 observed reflections. A half-normal-probability-plot comparison of these structures and others from the literature show that the main differences are essentially due to the different ionic radii of X and Y. [For the isostructural Mn–Zn and Mn–Ni compounds the following cell parameters were determined by automatic diffractometer: $a = 14·594$ (4), $b = 13·294$ (4), $c = 9·841$ (3) Å and $a = 14·499$ (4), $b = 13·250$ (4), $c = 9·768$ (3) Å respectively.]

Introduction. A systematic structural study of metal coordination compounds with the ethylenediaminetetraacetato (EDTA) ligand is being carried out by the Departments of Crystallography and Mineralogy (Faculty of Geology) and Inorganic Chemistry (Faculty of Pharmacy) of the University of Barcelona, in order to determine the influence of the different metals on coordination of EDTA. Thereby the crystal structures of the isostructural compounds $[(H_2O)_4Mn(EDTA)Co]_n.2nH_2O$ (Mn–Cu), $[(H_2O)_4Mn(EDTA)Co]_n.2nH_2O$ (Mn–Co) and $[(H_2O)_4Mg(EDTA)Zn]_n.2nH_2O$ (Mg–Zn) were determined.

Experimental. A small crystal of each compound was selected; Philips PW1100 four-circle diffractometer; unit cells determined by centring 25 independent reflections and refining orientation matrix and unit-cell parameters by least squares; intensities collected with Mo $K\alpha$ radiation $(\lambda = 0.71069$ Å), monochromatized by reflection from a graphite crystal; no absorption correction; $\theta_{max} = 25°$; number of reflections measured for Mn–Cu, Mn–Co and Mg–Zn 1678, 1677 and 1637 respectively, 1658, 1633 and 1617 considered observed with $I \geq 2.5\sigma(I)$; structure of Mn–Cu compound solved with *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), remaining structures solved by isomorphous replacement from the atomic coordinates of the Mn–Cu structure; each structure refined isotropically and anisotropically by full-matrix least squares using *SHELX* 76 (Sheldrick, 1976); $R = 0.044, R_w = 0.047$ for Mn–Cu, $R = 0.059$, $R_w = 0.061$ for Mn–Co, $R = 0.049$, $R_w = 0.052$ for Mg–Zn; function minimized was $w||F_o| - |F_c||^2$, where $w = [\sigma^2(F_o) + k|F_o|^2]^{-1}$, k being equal to 0.0067, 0.0162 and 0.0070 for Mn–Cu, Mn–Co and Mg–Zn, respectively; a difference synthesis for the first compound revealed the position of 21 H atoms, which were refined isotropically and the remaining atoms anisotropically; 22 H atoms located in Mg–Zn structure, which was refined using the same method; scattering factors taken from *International Tables for X-ray Crystallography* (1974).

Half-normal-probability-plot comparison

In order to compare the influence of the different metals on the structures, the half-normal-probability plot (Abrahams & Keve, 1971) was used. Two different analyses were carried out, including interatomic distances less than 4 Å. In the first analysis the Mn–Cu, Mn–Co, Mg–Zn, Co–Co (Candlish, Michael, Neal, Lingafelter & Rose, 1978) and K–Mn [K(EDTA)Mn.2H₂O; Lis, 1978] crystal structures were compared, considering only the Y–O and O–O distances. The results of the first plots are shown in Table 1,* where the number of the included distances, the maximum δp value, the slope and intercept obtained by least squares, the agreement factor R between related distances and the factor which indicates the linearity of the plot are indicated. Several trial plots were made with successive exclusion of the distances with largest δp, which were considered responsible for the distortions in the previous plot. Plots were terminated to best value of γ^2_{min}, where $\gamma^2_{min} = (\langle y^2 \rangle - \langle y \rangle^2)(1 - p^2)$. The final calculated plots are given in the same table. The same method was used in the second analysis, where the remaining distances less than 4 Å were compared in the Mn–Cu, Mn–Co, Mg–Zn, and Co–Co crystal structures. Results are given in the same table.

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* See deposition footnote.

Discussion. Final atomic parameters are listed in Table 2.* Fig. 1 shows views of the X and Y coordination and the numbering of atoms.

The study of the distances excluded from the 'best' plots (Table 3) shows that the differences among the five metal–EDTA coordination polyhedra are mainly found in the bond distances involving metal and in the $O(11) \cdots O(21)$ interatomic contacts. It shows, also, that if exception is made for the distance Co–O(41) and the angle O(11)–Co–O(21), the Co–EDTA coordination polyhedra are not significantly different indicating no particular influence of the hydrated cation on them.

Considering the averaged values of Table 4, some regular trends in bond distances involving the Y^{2+} ion are observed for the $X^{II}-Y^{II}$ series. If, following Lind, Hamor, Hamor & Hoard (1964), we indicate as O_G the oxygen-ligand atoms roughly lying in the $N(10)-Y-N(20)$ coordination plane and O_R those in an apical position with respect to this plane, the distances $Y-O_G$ and $Y-N$ increase while the $Y-O_R$ distances decrease with the increase in the ionic radius r_Y of the metal. These opposite effects tend to produce an elongation, in the axial direction of the coordination octahedron, which is maximum for Cu^{II} as indicated by the $Y-O_R/Y-O_G$ ratio whose values decrease with the increase in r_Y. Also the angle O_G-Y-O_G is affected by the metal ionic radius as it increases with the increase in r_Y. This behaviour could be related to a decrease in the ability of the EDTA ligand to completely encircle the metal ion, such that a further coordination site can
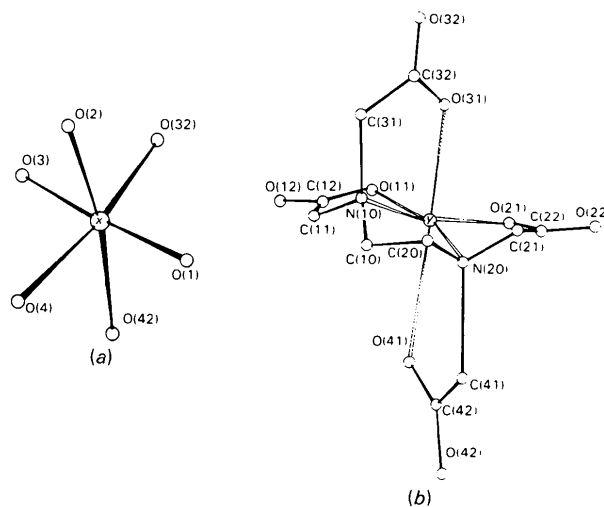

Fig. 1. View of (a) X and (b) Y coordination with numbering of the atoms.

Table 2. *Final atomic coordinates* ($\times 10^4$, $\times 10^3$ *for* H) *and equivalent isotropic temperature factors with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	$B_{eq}(\text{Å}^2)$
$|(H_2O)_4Mn(EDTA)Cu|_n \cdot 2nH_2O$				
Mn	7319(1)	−72(1)	8009(1)	2.0(1)
O(1)	6759(5)	1346(6)	8981(8)	2.7(7)
O(2)	7517(6)	673(8)	6072(8)	3.6(7)
O(3)	7945(6)	−1410(7)	7134(9)	3.4(7)
O(4)	5969(6)	−529(8)	7264(8)	3.5(7)
O(5)	4649(7)	964(13)	8653(12)	6.4(7)
O(6)	6875(6)	2461(7)	5110(8)	3.6(7)
Cu	5581(1)	97	3143(1)	1.7(1)
N(10)	4269(5)	450(6)	2616(8)	2.0(7)
C(10)	3992(8)	−440(10)	1769(10)	2.8(7)
C(20)	4330(7)	1419(9)	2404(12)	2.7(7)
N(20)	5334(6)	1374(6)	2555(7)	2.1(7)
C(11)	4363(7)	1423(9)	1877(11)	2.3(7)
O(11)	5724(5)	1592(6)	3181(7)	2.4(7)
C(12)	5169(6)	2043(8)	2432(10)	2.5(7)
O(12)	5238(5)	2951(6)	2049(9)	3.4(7)
C(21)	5710(6)	−1991(8)	3675(11)	2.2(7)
O(21)	6699(4)	−544(6)	3978(6)	2.3(7)
C(22)	6594(6)	−1492(6)	4185(9)	2.3(7)
O(22)	7139(6)	−2046(6)	4795(8)	3.5(7)
C(31)	3680(7)	564(10)	3843(9)	2.8(7)
O(31)	4943(5)	−3(8)	5153(6)	3.2(7)
C(32)	4124(6)	254(7)	5154(9)	2.1(7)
O(32)	3636(4)	281(6)	6188(6)	3.1(7)
C(41)	5833(8)	−1620(8)	1294(10)	2.8(7)
O(41)	6159(5)	155(5)	1010(7)	3.1(7)
C(42)	6317(6)	−724(7)	633(8)	2.1(7)
O(42)	6854(4)	−966(6)	−298(6)	2.7(7)
H(O1)	717(9)	200(14)	911(14)	3.6(8)
H(O1)'	673(12)	130(15)	1009(18)	
H(O2)	726(9)	124(14)	591(15)	
H(O2)'	746(9)	51(13)	524(18)	
H(O3)	780(1)	−158(12)	633(17)	
H(O4)	580(10)	−108(14)	748(14)	
H(O5)	517(9)	63(13)	835(18)	
H(O5)'	477(9)	93(13)	747(18)	
H(O6)	732(9)	293(12)	483(15)	
H(O6)'	668(9)	245(12)	422(15)	
H(C10)	355(11)	−46(13)	173(14)	
H(C20)	421(10)	−198(14)	201(14)	
H(C20)'	411(10)	−159(13)	325(15)	
H(C11)	435(8)	136(13)	101(15)	
H(C11)'	389(11)	191(14)	193(13)	
H(C21)	584(9)	−274(14)	349(15)	
H(C21)'	518(9)	−196(12)	443(15)	
H(C31)	311(9)	10(13)	369(14)	
H(C31)'	352(9)	123(13)	388(14)	
H(C41)	615(10)	−207(14)	141(15)	
H(C41)'	547(10)	−180(14)	54(15)	
$|(H_2O)_4Mn(EDTA)Co|_n \cdot 2nH_2O$				
Mn	7406(1)	−131(2)	8030(2)	1.7(1)
O(1)	6845(7)	1222(8)	9066(10)	2.5(7)
O(2)	7575(8)	626(12)	6076(11)	3.2(7)
O(3)	8036(7)	−1430(10)	7087(11)	3.3(7)
O(4)	6043(7)	−568(9)	7290(13)	3.1(7)
O(5)	4781(11)	999(19)	8552(19)	6.5(11)
O(6)	6888(10)	2336(9)	5066(13)	4.2(11)
Co	5685(1)	97	3170(2)	1.4(1)
N(10)	4307(6)	412(8)	2555(11)	1.9(7)
C(10)	4006(12)	−457(12)	1722(15)	2.3(7)
C(20)	4349(9)	−1450(11)	2396(19)	2.4(7)
N(20)	5356(11)	−1416(10)	2560(13)	1.5(11)
C(11)	4352(8)	1349(12)	1799(15)	2.1(11)
O(11)	5709(5)	1631(7)	3075(10)	2.2(7)
C(12)	5126(9)	2036(10)	2318(14)	2.0(11)
O(12)	5145(8)	2918(8)	1981(12)	3.0(7)
C(21)	5690(8)	−2023(11)	3735(16)	2.0(11)
O(21)	6750(6)	−693(7)	4095(9)	2.0(7)
C(22)	6596(8)	−1596(10)	4260(12)	2.0(7)
O(22)	7104(8)	−2196(8)	4902(11)	3.3(7)
C(31)	3718(8)	511(14)	3810(13)	2.5(7)
O(31)	5068(6)	90(9)	5087(3)	2.1(7)
C(32)	4222(8)	231(9)	5137(12)	1.8(7)
O(32)	3771(6)	210(9)	6211(9)	2.7(7)
C(41)	5847(8)	−1677(10)	1310(14)	2.3(7)
O(41)	6316(6)	64(8)	1242(8)	2.2(7)
C(42)	6416(8)	−792(9)	756(12)	1.7(7)
O(42)	6941(6)	−1014(8)	−249(9)	2.4(7)

Table 2 (*cont.*)

	x	y	z	$B_{eq}(\text{Å}^2)$
$|(H_2O)_4Mg(EDTA)Zn|_n \cdot 2nH_2O$				
Mg	7380(2)	27(5)	8058(2)	0.8(1)
O(1)	6846(4)	1346	8981(8)	2.7(7)
O(2)	7596(5)	778(8)	6224(7)	3.0(7)
O(3)	7969(4)	1233(7)	7174(7)	2.9(7)
O(4)	6080(4)	372(8)	7317(7)	2.7(7)
O(5)	4724(7)	1163(10)	8559(10)	5.3(11)
O(6)	6940(6)	2519(8)	5126(9)	4.0(9)
Zn	5678(1)	246(5)	3212(1)	1.4(1)
N(10)	4282(4)	592(7)	2574(7)	1.8(7)
C(10)	4004(6)	287(9)	1718(8)	2.4(7)
C(20)	4341(6)	−1283(10)	2342(12)	2.2(7)
N(20)	5355(6)	1268(7)	2589(7)	1.8(7)
C(11)	4356(6)	1566(10)	1842(10)	2.4(7)
O(11)	5746(5)	1817(7)	3144(7)	2.7(7)
C(12)	5164(6)	2210(8)	2396(8)	2.2(7)
O(12)	5178(5)	3129(7)	2055(8)	3.3(7)
C(21)	5678(5)	−1851(9)	3729(10)	2.2(7)
O(21)	6741(4)	−494(6)	4107(6)	1.9(7)
C(22)	6594(6)	1432(8)	4290(8)	2.0(7)
O(22)	7124(5)	−2011(7)	4896(8)	1.6(7)
C(31)	3694(6)	678(9)	3828(8)	2.1(7)
O(31)	5020(4)	211(8)	5136(5)	2.4(7)
C(32)	4171(5)	376(8)	5146(7)	1.8(7)
O(32)	3686(5)	324(8)	6198(5)	2.4(7)
C(41)	5865(6)	−1489(9)	1288(9)	2.5(7)
O(41)	6279(4)	268(7)	1219(5)	2.1(7)
C(42)	6400(5)	−603(8)	733(7)	1.8(7)
O(42)	6931(4)	−802(7)	−252(6)	2.1(7)
H(O1)	715(9)	157(13)	919(14)	3.8(7)
H(O1)'	653(8)	67(12)	924(12)	
H(O2)	738(7)	94(13)	537(13)	
H(O2)'	755(9)	122(13)	572(14)	
H(O3)	799(8)	152(12)	637(16)	
H(O4)	635(9)	−70(13)	730(17)	
H(O4)'	570(7)	23(13)	653(14)	
H(O5)	53(13)	98(17)	666(17)	
H(O6)	715(11)	273(15)	484(16)	
H(O6)'	7183(10)	274(12)	619(16)	
H(C10)	907(9)	−37(13)	420(14)	
H(C10)'	794(12)	−42(13)	344(13)	
H(C20)	893(11)	−83(16)	177(19)	
H(C20)'	883(12)	−172(13)	332(15)	
H(C11)	926(11)	218(13)	338(14)	
H(C11)'	923(10)	131(13)	412(16)	
H(C21)	496(10)	−175(11)	444(13)	
H(C21)'	552(11)	−224(14)	355(16)	
H(C31)	788(10)	37(15)	144(4)	
H(C31)'	833(10)	121(14)	138(14)	
H(C41)	541(8)	−218(12)	81(16)	
H(C41)'	658(10)	−218(12)	160(15)	

Table 3. *Bond distances* (Å) *and bond angles* (°) *showing significant differences*

$X-Y$	Mn–Cu	Mg–Zn	Mn–Co	Co–Co	K–Mn
Y–N(10)	2.043(5)	2.164(6)	2.140(6)	2.158(3)	2.176(10)
Y–N(20)	2.042(5)	2.163(8)		2.161(4)	2.220(9)
Y–O(11)	1.965(5)	2.083(8)	2.053(6)	2.039(4)	2.020(8)
Y–O(21)	2.016(4)	2.022(6)	2.086(5)	2.082(3)	2.004(8)
Y–O(31)	2.215(4)	2.103(5)	2.083(5)	2.087(3)	1.907(8)
Y–O(41)	2.289(4)	2.129(5)	2.103(5)	2.123(3)	1.909(8)
O(11)–Y–O(21)	108.6(2)	117.5(3)	120.8(2)	119.3(1)	125.0(4)
X–O(1)	2.246(8)	2.119(7)	2.229(11)	2.127(4)	
X–O(2)	2.182(9)	2.069(9)	2.180(12)	2.116(3)	
X–O(3)	2.158(9)	2.062(10)	2.171(13)	2.091(4)	
X–O(4)	2.193(4)	2.084(6)	2.195(6)	2.102(3)	
X–O(32)	2.136(6)	2.063(5)	2.173(9)	2.084(3)	
X–O(42)	2.162(7)	2.083(8)	2.167(10)	2.105(3)	

Table 4. *Averaged values for the* Y *coordination polyhedra*

Y	Cu^{II}	Zn^{II}	Co^{II}	Mn^{III}
Y–N (Å)	2.043(4)	2.157(9)	2.157(4)	2.200(22)
Y–O$_G$ (Å)	2.00(2)	2.04(3)	2.07(1)	2.012(8)
Y–O$_R$ (Å)	2.25(4)	2.12(1)	2.10(1)	1.908(6)
O$_G$–Y–O$_G$ (Å)	108.6(2)	117.5(3)	120.0(7)	125.0(4)
Y–O$_R$/Y–O$_G$	1.125(23)	1.039(16)	1.014(7)	0.948(5)
Ionic radius (Å)	0.69	0.74	0.78	0.66

become available as observed in $\{[(H_2O)_4Mn]_2[(EDTA)Cd]_2\}_n.4nH_2O$ (Solans, Font-Altaba, Oliva & Herrera, 1983) where Cd is heptacoordinated.

Comparing the distances in the coordination polyhedra of the hydrate ions it appears that the differences between related distances of different polyhedra (Table 4) are essentially related to the different ionic radii, while the differences between the X–O distances for the same metal are determined by the hydrogen bonds in which the coordinated O atoms are involved; thus, the shortest values correspond to the X–O(acetato) and X–O(aqua) distances, the latter when the water coordinating to metal is linked by weak hydrogen bonds to the uncoordinated water, while the largest values correspond to X–O(aqua) when the coordinated water molecule is linked by two strong hydrogen bonds to the acetato O atoms. From the distances excluded it can also be deduced that the different cationic radii produce variations in intrachain distances greater than 3·5 Å, but do not produce differences in interchain distances or intrachain hydrogen bonds.

References

ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A27, 157–165.
CANDLISH, E. F. K., MICHAEL, T. K., NEAL, J. A., LINGAFELTER, E. C. & ROSE, N. J. (1978). *Inorg. Chem.* 17, 1383–1394.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.
LIND, M. D., HAMOR, M. J., HAMOR, T. A. & HOARD, J. L. (1964). *Inorg. Chem.* 3, 34–43.
LIS, T. (1978). *Acta Cryst.* B34, 1342–1344.
MAIN, P., FISKE, S. L., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J. P. & WOOLFSON, M. M. (1980). *MULTAN. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.
SHELDRICK, G. M. (1976). *SHELX. A program for crystal structure determination.* Univ. of Cambridge, England.
SOLANS, X., FONT-ALTABA, M., OLIVA, J. & HERRERA, J. (1983). *Acta Cryst.* To be published.

Crystal Structures of Ethylenediaminetetraacetato Metal Complexes. III. Hexaaquamagnesium(II) Aquaethylenediaminetetraacetatocadmium(II) Trihydrate, $[(H_2O)_6Mg(C_{10}H_{12}N_2O_8)(H_2O)Cd]_n.3nH_2O$

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Abstract. $M_r = 605·1$, triclinic, $P\bar{1}$, $a = 20·594$ (4), $b = 7·755$ (2), $c = 7·619$ (2) Å, $\alpha = 102·25$ (3), $\beta = 102·01$ (3), $\gamma = 82·52$ (4)°, $V = 1158$ (2) Å³, $Z = 2$, $D_x = 1·73$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0·71069$ Å, $\mu = 1·052$ mm⁻¹, $F(000) = 620$. Final $R = 0·047$ for 4011 observed reflections. The crystal structure consists of discrete ions linked by hydrogen bonds. There are two independent sets of Mg atoms located on inversion centres separated by $\frac{1}{2}a$ and displaying a distorted octahedral coordination. The Cd atom is coordinated to a water and an ethylenediaminetetraacetato molecule, the latter ligand acting in a hexadentate fashion.

Introduction. A systematic study on crystal structures with ethylenediaminetetraacetato (EDTA) as a ligand is being carried out by the Departments of Crystallography and Mineralogy (Faculty of Geology) and Inorganic Chemistry (Faculty of Pharmacy) of the University of Barcelona (preceding papers: Solans, Font-Altaba, Oliva & Herrera, 1983a,b).

In general, as can be observed from the literature, the crystal structures of compounds with the formula $(H_2O)_nX(EDTA)(H_2O)_mY.pH_2O$ consist of infinite chains of X and Y atoms, where the EDTA ligand acts as bridge between the two metals (Candlish, Michael,