Wolf, 1968) and (ii) that the angle O(2)—S—O(3) of 115·1 (3)° is smaller than the corresponding angle in sulfonic acid esters [120·0 (1)°, Wieczorek *et al.*, 1975; 119·2 (5)°, Williams *et al.*, 1979] but larger than in ionic sulfonates [112·2 (8)°, Couldwell, Prout, Robey, Taylor & Rossotti, 1978].

H of the isethionate hydroxy group, which is clearly represented by ν(OH) at 3380 cm^{-1} in the IR spectrum (same position as in sodium isethionate), was not localized. A short intermolecular O(4)···O(2)(x, $\frac{1}{2}$$-y$, $\frac{1}{2}$$+z$) distance of 2·760 (6) Å could be correlated with a hydrogen bridge between these atoms. The existence of a hydrogen bridge is also indicated by the position and broadness of ν(OH).

A linear Sb—O—Sb bridge between pentacoordinated Sb atoms was also found in μ-oxo-bis(*tert*-butylperoxotriphenylantimony) (Starikova *et al.*, 1978) and in μ-oxo-bis[tris(*p*-chlorophenyl)(1,1,1-trifluoro-2,4-pentanedionato-*O,O'*)antimony(V)]–chloroform (1/2), in which Sb, however, is hexacoordinated (Ebina, Ouchi, Yoshino, Sato & Saito, 1978). The Sb—μ-O bond lengths in these compounds are comparable [this work: 1·936 (1) Å; (Ph₃SbOO-*tert*-C₄H₉)₂O: 1·974 (2) Å; [(*p*-ClC₆H₄)₃SbCF₃C(O)CH(CO)CH₃]₂ 0·2CHCl₃: 1·943 Å, σ < 0·0004 Å].

The interesting question of whether a bent or a linear Sb—O—Sb bridge should be expected in a certain distiboxane still cannot be answered. Deviations of the Sb—O—Sb angle in distiboxanes from the tetrahedral angle have been correlated with intramolecular repulsions between the two halves of the specific molecules (Ferguson & Ridley, 1973). For linear bridges interaction of the electron pairs of O with empty d orbitals of Sb was discussed (Starikova *et al.*, 1978; see also March & Ferguson, 1975). This interpretation would be consistent with the observation of rather short Sb—μ-O bonds in the compounds with linear Sb—O—Sb bridges.

References

COULDWELL, C., PROUT, K., ROBEY, D., TAYLOR, R. & ROSSOTTI, F. J. C. (1978). *Acta Cryst.* B34, 1491–1499.
CROMER, D. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Table 2.3.1. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Table 2.2.B. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
EBINA, F., OUCHI, A., YOSHINO, Y., SATO, S. & SAITO, Y. (1978). *Acta Cryst.* B34, 2134–2138.
ENRAF-NONIUS (1978). *Structure Determination Package.* Enraf-Nonius, Delft.
FERGUSON, G. & RIDLEY, D. R. (1973). *Acta Cryst.* B29, 2221–2226.
JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.
MARCH, F. C. & FERGUSON, G. (1975). *J. Chem. Soc. Dalton Trans.* pp. 1291–1294.
SHEN, K., MCEWEN, W. E., LA PLACA, S. J., HAMILTON, W. C. & WOLF, A. P. (1968). *J. Am. Chem. Soc.* 90, 1718–1723.
STARIKOVA, Z. A., SHCHEGOLEVA, T. M., TRUNOV, V. K. & POKROVSKAYA, J. E. (1978). *Sov.-Phys. Crystallogr.* 23, 547–549.
WAAL, B. W. VAN DE (1976). *POP1*. Plot of packing program. Twente Univ. of Technology, The Netherlands.
WIECZOREK, M. W., BOKII, N. G. & STRUCHKOV, YU. T. (1975). *Acta Cryst.* B31, 2603–2606.
WILLIAMS, R. L., ANDO, D. J., BLOOR, D. & HURSTHOUSE, M. B. (1979). *Acta Cryst.* B35, 2072–2074.

Structure of Acetato(acetylacetonato)diaquacalcium, [Ca(CH₃COO)(C₅H₇O₂)(H₂O)₂]

BY J. J. SAHBARI AND M. M. OLMSTEAD*

Department of Chemistry, University of California, Davis, CA 95616, USA

Abstract. $M_r = 234\cdot27$, $P\bar{1}$, $a = 6\cdot524$ (1), $b = 6\cdot851$ (1), $c = 12\cdot504$ (1) Å, $\alpha = 87\cdot70$ (1), $\beta = 81\cdot42$ (1), $\gamma = 71\cdot21$ (1)°, $Z = 2$, $V = 523\cdot2$ (1) Å³, $D_m(298\text{ K}) = 1\cdot48$ g cm^{-3}, $D_x(140\text{ K}) = 1\cdot49$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 5\cdot74$ cm^{-1}, $T = 140$ K, $F(000) = 208$, 1953 unique observed reflections, $R = 0\cdot031$. A distorted dodecahedral arrangement of eight O atoms surrounds each Ca²⁺ ion. The ligation (average Ca—O distances in parentheses) consists of one chelating acetylacetonate (2·390 Å), two waters (2·498 Å), two monodentate acetates (2·349 Å) and one bidentate acetate (2·563 Å) which provides a cross-link to a centrosymmetrically related chain.

Introduction. The crystal structure determination of the title compound was undertaken to check the stoichiometry of the crystals, which were known to contain acetylacetonate yet differ from the previously determined structure of [Ca(acetylacetonate)₂(H₂O)₂].H₂O (Sahbari & Olmstead, 1983). The phosphorescence and

---

* Author to whom correspondence should be addressed.

triplet-state optically detected magnetic resonance (ODMR) spectra of these crystals and those of other Group II acetylacetonate complexes have been reported elsewhere (Sahbari, Bomben & Tinti, 1983).

Experimental. Colorless needles obtained by slow crystallization from an aqueous solution containing ammonium acetylacetonate and excess calcium acetate; density measured by flotation in C_6H_5Cl/CCl_4; crystal $0.10 \times 0.15 \times 0.37$ mm; Syntex $P2_1$ diffractometer, modified LT-1 low-temperature apparatus, $T = 140$ K, Mo $K\alpha$ radiation, graphite monochromator; cell dimensions from a least-squares fit of 10 reflections with $14° < 2\theta < 21°$, space group $P\bar{1}$ based on no conditions; no absorption correction (range of absorption correction factors $1.06-1.09$); data collected to $2\theta_{max} = 55°$ with h,k,l ranges 0 to 8, -8 to 8, -16 to 16, respectively; ω scans, $1°$ range, $8°$ min^{-1} speed, $1°$ offset for background; two check reflections monitored every 100 reflections displayed $<1\%$ fluctuation; 2396 unique data, 1953 observed $[I > 2.5\sigma(I)]$ used in the solution and refinement (based on F); structure solved by Patterson and Fourier methods; blocked-cascade least-squares refinement using anisotropic thermal parameters for all non-hydrogen atoms, H atoms included in the refinement, 183 parameters; $R = 0.031$, $R_w = 0.032$, $w = 1/[\sigma^2(F_o) + 0.00024F_o^2]$, $S = 1.166$, $(\Delta/\sigma)_{max} = 0.197$ for z of H(3), $(\Delta/\sigma)_{ave} = 0.018$, max. and min. $\Delta\rho$ excursions 0.23 and -0.16 e Å^{-3}, respectively; atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); computer programs from the *SHELXTL* (version 4) package (Sheldrick, 1981).

Discussion. Atom coordinates are provided in Table 1.* The results show a double-chain structure, as depicted in Fig. 1. The chains are centrosymmetrically related to each other and are propagated in the **b** direction. The Ca···Ca^{iii} distance, for example, is equal to the b axis for the crystal. Within a single chain the Ca atoms are bridged by the two O atoms of an acetate ion. Each of these O atoms $|$O(3) and O(4)$|$ uses its other set of O lone pairs to cross-link, in a bidentate fashion, to a Ca of the other chain. Thus, a single acetate actually supplies four O coordination sites per Ca, rather than the two that might be expected from the chemical formula. Four other O atoms surround each Ca: two from two water molecules and two from a bidentate acetylacetonate. These eight O atoms are shown in their arrangement around Ca in Fig. 2. Bond distances and angles are collected in Table 2.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39879 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Fig. 1 also indicates the network of H bonds that contributes to the stability of the crystal. Within a single chain a water H atom H bonds to an acetylacetonate O $|$H on O(6) to O(2)$|$. A cross-linking H bond exists between water molecules $|$H on O(5) to O(6^i)$|$. Two other H bonds link the double chain to adjacent double chains. One of these is a H on O(5) to O(1^{vi}) and the other is an H on O(6) to O(5^v). In this fashion all of the water H atoms and uncoordinated O lone pairs are involved in H bonding. Bond distances and angles for these interactions are given in Table 2.

Table 1. *Atom coordinates* $(\times 10^4, for$ H $\times 10^3)$ *and isotropic thermal parameters* $(\times 10^3, for$ H $\times 10^2)$

For non-H atoms U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

|	x	y	z	U_{eq} or U (Å^2)
Ca	569 (1)	2249 (1)	777 (1)	10 (1)
O(1)	3400 (2)	800 (2)	1862 (1)	15 (1)
O(2)	−1103 (2)	2854 (2)	2623 (1)	16 (1)
O(3)	620 (2)	5618 (2)	917 (1)	15 (1)
O(4)	220 (2)	−1081 (2)	968 (1)	15 (1)
O(5)	4032 (2)	2218 (2)	−372 (1)	15 (1)
O(6)	−3537 (2)	3578 (2)	1040 (1)	17 (1)
C(1)	5685 (4)	−543 (4)	3203 (2)	21 (1)
C(2)	3495 (3)	694 (3)	2876 (2)	15 (1)
C(3)	1762 (3)	1582 (3)	3687 (2)	17 (1)
C(4)	−431 (3)	2602 (3)	3526 (2)	16 (1)
C(5)	−2106 (4)	3439 (4)	4507 (2)	27 (1)
C(6)	709 (3)	7157 (3)	1398 (2)	11 (1)
C(7)	1427 (4)	6876 (3)	2499 (2)	18 (1)
H(1A)	597 (4)	−191 (4)	302 (2)	4 (1)
H(1B)	681 (5)	−1 (4)	285 (2)	4 (1)
H(1C)	572 (5)	−56 (4)	399 (2)	5 (1)
H(3)	204 (4)	143 (4)	443 (2)	3 (1)
H(5A)	−356 (5)	346 (5)	439 (3)	8 (1)
H(5B)	−224 (6)	484 (5)	460 (5)	8 (1)
H(5C)	−182 (6)	274 (5)	511 (3)	8 (1)
H(7A)	296 (5)	650 (5)	239 (2)	5 (1)
H(7B)	87 (4)	806 (4)	289 (2)	4 (1)
H(7C)	95 (5)	584 (5)	288 (2)	6 (1)
H(O5A)	387 (4)	344 (2)	−67 (2)	4 (1)
H(O5B)	471 (4)	129 (3)	−89 (1)	3 (1)
H(O6A)	−371 (5)	329 (4)	174 (1)	4 (1)
H(O6B)	−433 (5)	297 (5)	73 (2)	7 (1)
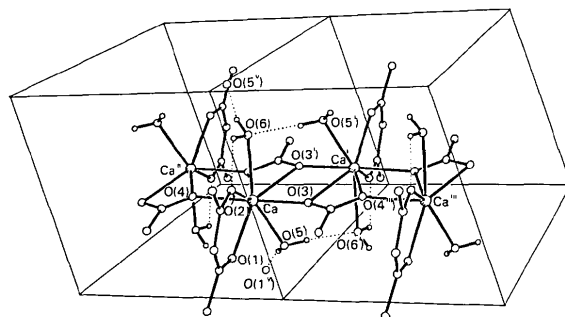
Fig. 1. The contents of two unit cells upon translation along **b**. Hydrogen bonding is indicated by dotted lines. See Table 2 for symmetry code.

Table 2. *Bond lengths* (Å) *and angles* (°) *and hydrogen-bonding dimensions*

Ca—O(3)	2·387 (1)	Ca—O(2)	2·392 (1)
Ca—O(3)	2·332 (2)	Ca—O(4)	2·365 (2)
Ca—O(5)	2·484 (1)	Ca—O(6)	2·511 (1)
Ca—O(3ⁱ)	2·595 (1)	Ca—O(4ⁱⁱ)	2·531 (2)
O(1)—C(2)	1·276 (2)	O(2)—C(4)	1·258 (3)
O(3)—C(6)	1·256 (3)	O(4)—C(6ⁱᵛ)	1·264 (2)
C(1)—C(2)	1·514 (3)	C(2)—C(3)	1·394 (3)
C(3)—C(4)	1·416 (3)	C(4)—C(5)	1·510 (3)
C(6)—C(7)	1·505 (3)		

O(1)—Ca—O(2)	73·2 (1)	O(1)—Ca—O(3)	94·7 (1)
O(2)—Ca—O(3)	82·6 (1)	O(1)—Ca—O(4)	82·2 (1)
O(2)—Ca—O(4)	87·0 (1)	O(3)—Ca—O(4)	169·6 (1)
O(1)—Ca—O(5)	74·1 (1)	O(2)—Ca—O(5)	139·1 (1)
O(3)—Ca—O(5)	76·3 (1)	O(4)—Ca—O(5)	112·1 (1)
O(1)—Ca—O(6)	137·5 (1)	O(2)—Ca—O(6)	65·4 (1)
O(3)—Ca—O(6)	89·4 (1)	O(4)—Ca—O(6)	86·3 (1)
O(5)—Ca—O(6)	147·0 (1)	O(1)—Ca—O(3ⁱ)	147·4 (1)
O(2)—Ca—O(3ⁱ)	128·6 (1)	O(3)—Ca—O(3ⁱ)	68·7 (1)
O(4)—Ca—O(3ⁱ)	118·7 (1)	O(5)—Ca—O(3ⁱ)	74·7 (1)
O(6)—Ca—O(3ⁱ)	72·4 (1)	O(1)—Ca—O(4ⁱⁱ)	132·6 (1)
O(2)—Ca—O(4ⁱⁱ)	138·4 (1)	O(3)—Ca—O(4ⁱⁱ)	119·1 (1)
O(4)—Ca—O(4ⁱⁱ)	69·4 (1)	O(5)—Ca—O(4ⁱⁱ)	82·4 (1)
O(6)—Ca—O(4ⁱⁱ)	78·9 (1)	O(3)—Ca—O(4ⁱⁱ)	50·7 (1)
Ca—O(1)—C(2)	134·9 (1)	Ca—O(2)—C(4)	135·5 (1)
Ca—O(3)—C(6)	155·4 (1)	Ca—O(3)—Caⁱ	111·3 (1)
C(6)—O(3)—Caⁱ	92·8 (1)	Ca—O(4)—Caⁱⁱ	110·6 (1)
Ca—O(4)—C(6ⁱᵛ)	150·3 (1)	Caⁱⁱ—O(4)—C(6ⁱᵛ)	95·6 (1)
O(1)—C(2)—C(1)	116·0 (2)	O(1)—C(2)—C(3)	125·5 (2)
C(1)—C(2)—C(3)	118·4 (2)	C(2)—C(3)—C(4)	125·4 (2)
O(2)—C(4)—C(3)	124·9 (2)	O(2)—C(4)—C(5)	117·0 (2)
C(3)—C(4)—C(5)	118·1 (2)	O(3)—C(6)—C(7)	119·0 (2)
O(3)—C(6)—O(4ⁱⁱⁱ)	121·0 (2)	C(7)—C(6)—O(4ⁱⁱⁱ)	120·1 (2)

Hydrogen bonding

O(6)···O(5ⁱ)	2·896 (2)	O(6)···H(O5Aⁱ)—O(5ⁱ)	168 (1)
O(6)···H(O5Aⁱ)	2·02 (2)	O(2)···H(O6A)—O(6)	119 (1)
O(2)···O(6)	2·652 (2)	O(1ᵛⁱ)···H(O5B)—O(5)	169 (1)
O(2)···H(O6A)	2·10 (2)	O(5ᵛ)···H(O6B)—O(6)	161 (1)
O(1ᵛⁱ)···O(5)	2·775 (2)		
O(1ᵛⁱ)···H(O5B)	1·90 (2)		
O(5ᵛ)···O(6)	2·903 (2)		
O(5ᵛ)···H(O6B)	2·04 (2)		

Symmetry code: (i) $-x$, $1 - y$, $-z$; (ii) $-x$, $-y$, $-z$; (iii) x, $1 + y$, z; (iv) x, $-1 + y$, z; (v) $-1 + x$, y, z; (vi) $1 - x$, $-y$, $-z$.
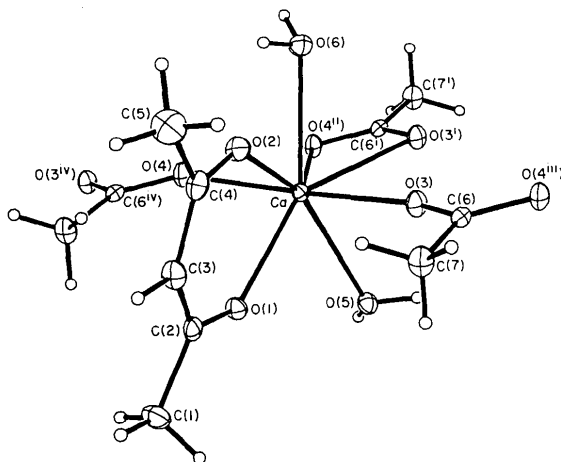

Fig. 2. A view of the stereochemistry around Ca, showing anisotropic thermal ellipsoids at the 50% level and the atom-numbering scheme. H atoms have been given an arbitrary size. See Table 2 for symmetry code.

The stereochemistry of eight coordination is an irregular dodecahedron of O atoms around a central Ca. It is useful to visualize the dodecahedron as two interpenetrating trapezoids (Kepert, 1978). This is portrayed in Fig. 3(a) and 3(b). One of the trapezoids (Fig. 3a) is described by O(3), O(4), O(3ⁱ) and O(4ⁱⁱ). The sum of the squared deviations of these atoms from the least-squares plane is 0·053 Å². The Ca is 0·128 Å out of this plane. The other trapezoid (Fig. 3b), involving O(1), O(2), O(5), O(6), is less planar, with a sum of squared deviations equal to 0·246 Å². The Ca is 0·252 Å out of this plane. The normals to the two least-squares planes make an angle of 93·8 (2)° with respect to each other. Even though vastly different chelating ligands are present, and the Ca—O bonds vary from 2·332 to 2·595 Å, the dodecahedral stereochemistry is unmistakable. No doubt a contribution to this symmetry is the *trans* arrangement of the two chelating groups, which span the '*A*' sets of positions. Acetylacetonate, with its large bite angle of 73·2° and six-membered ring, is represented in the figure by O(1) and O(2). Acetate, in its chelating form, is represented by O(4ⁱⁱ) and O(3ⁱ); here, there is only a four-membered ring and the bite angle is reduced to 50·7°. Even by computing the normalized bite angle (Kepert, 1978) $|b = O···O/(Ca—O)|$, which takes into account the longer Ca—O bond to acetate, the very different nature of acetate and acetylacetonate as chelating ligands is pointed out. The values obtained for b of 1·19 for acetylacetonate and 0·86 for acetate put them at opposite ends of the normal range for b.

A comparison of the eight-coordinate Ca complex reported here with the six-coordinate complex $|Ca(acetylacetonate)_2(H_2O)_2|$ nicely illustrates the bond lengthening that is expected to occur with higher coordination number. The average Ca—O distance is lengthened by *ca* 3% (0·06 Å) for the chelating acetylacetonate and *ca* 6% (0·14 Å) for the aqua ligand.
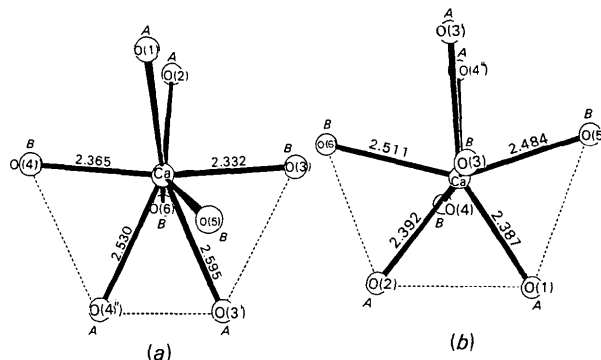

Fig. 3. Perpendicular views of the trapezoidal arrangement of four O atoms around Ca: O(1) and O(2) are from chelating acetylacetonate, O(3) and O(4) are from monodentate acetate, O(5) and O(6) are from water, O(4ⁱⁱ) and O(3ⁱ) are from chelating (cross-chain) acetate. (Distances in Å.)

References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

KEPERT, D. L. (1978). Progress in Inorganic Chemistry, edited by S. J. LIPPARD, pp. 179–249. New York: Interscience.

SAHBARI, J. J., BOMBEN, K. D. & TINTI, D. S. (1983). J. Am. Chem. Soc. 105, 5577–5583.

SAHBARI, J. J. & OLMSTEAD, M. M. (1983). Acta Cryst. C39, 208–211.

SHELDRICK, G. M. (1981). SHELXTL. An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data. Univ. of Göttingen. (Obtained from Nicolet Instruments, Madison, WI.)

Structure of Di-μ-(+)-tartrato-bis[aquazinc(II)] Trihydrate, [Zn₂(C₄H₄O₆)₂(H₂O)₂].3H₂O and Anomalous Scattering by Zinc

BY LIESELOTTE K. TEMPLETON, DAVID H. TEMPLETON, DECHUN ZHANG* AND ALLAN ZALKIN

Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720, USA

Abstract. $M_r = 517 \cdot 0$, orthorhombic, $P2_12_12_1$, $a = 11 \cdot 256$ (3), $b = 18 \cdot 021$ (7), $c = 7 \cdot 960$ (3) Å, $V = 1615$ Å^3, $Z = 4$, $D_x = 2 \cdot 126$ (2) g cm^{-3}, Mo $K\alpha$, $\lambda(\alpha_1) = 0 \cdot 70930$ Å, $\mu = 31 \cdot 3$ cm^{-1}, $F(000) = 1048$, $T = 296$ K, $R = 0 \cdot 047$ for 3728 reflections. The structure consists of cyclic double chelates which are linked by additional strong coordination of each Zn to a carboxyl O atom of an adjacent group and further by hydrogen bonds. Ave. Zn—O distances are $2 \cdot 040$ (14) (carboxyl), $2 \cdot 158$ (24) (hydroxyl), and $2 \cdot 059$ (4) Å (water). A determination of the anomalous scattering term f'' for Zn and Mo $K\alpha$ radiation gives $1 \cdot 47$ (3) e/atom.

Introduction. In search of crystals for study of anomalous X-ray scattering with synchrotron radiation (e.g. Templeton, Templeton, Phizackerley & Hodgson, 1982) we prepared crystals of this Zn salt and determined its structure. Its properties of composition, symmetry, chemical stability, and crystalline quality are suitable for this purpose, and it has been used to measure the X-ray scattering by the Zn^{2+} ion at wavelengths near its K absorption edge (Templeton & Templeton, 1984). Here we report the crystal structure parameters which we needed for analysis of the K-edge experiments, and also a determination of f'' of Zn for Mo $K\alpha$ radiation.

Experimental. Crystals of the title compound were grown by diffusion-controlled precipitation from silica gel using the technique described by Hopwood & Nicol (1972). Crystal $0 \cdot 09 \times 0 \cdot 20 \times 0 \cdot 33$ mm with 15 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 23 reflections, $20° < 2\theta < 32°$; analytical absorption correction, range $1 \cdot 26$ to $1 \cdot 41$; max. $(\sin\theta)/\lambda = 0 \cdot 651$ Å^{-1}, h 0 to 14, k 0 to 23, $l -10$ to 10; three standard reflections, $\sigma = 1 \cdot 6$, $1 \cdot 3$, $1 \cdot 4\%$, no correction for decay; 4093 data, 3730 unique (including 546, $I < \sigma$), 2 low-angle reflections deleted because of poor agreement, $R_{int} = 0 \cdot 017$; structure solved by MULTAN78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and Fourier methods, 14 H atoms located in ΔF maps; refinement on F, 301 parameters including f'' for Zn, H atoms with isotropic thermal parameters, anisotropic thermal parameters for other atoms, all O—H bond distances restrained to $0 \cdot 90$ (5) Å, water H—H to $1 \cdot 50$ (10) Å; $R = 0 \cdot 047$ for 3728 reflections (0·029 for 3182 for which $I > \sigma$), $wR = 0 \cdot 030$, $S = 0 \cdot 94$; $w = [\sigma(F)]^{-2}$, derived from $\sigma^2(F^2) = \{[\sigma(F^2),$ counting statistics only] $+ (0 \cdot 03 F^2)^2\}$; max. $\Delta/\sigma = 0 \cdot 16$; max. empirical isotropic correction for extinction 7% of F; max. and min. of ΔF synthesis $0 \cdot 6$ and $-0 \cdot 9$ e Å^{-3}; atomic f for Zn^{2+}, O$^{1/2-}$ (carboxyl, interpolated), neutral O and C, and spherical bonded H from International Tables for X-ray Crystallography (1974); local unpublished programs and ORTEP (Johnson, 1965).

Discussion. Atomic parameters are listed in Table 1.† The basic structural unit of this salt is a cyclic double chelate, Fig. 1. Similar groups occur in various tartrate

---

† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39878 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

---

* On leave from Chemistry Division, East-China Engineering Institute, Nanjing, Jiangsu, People's Republic of China.