

is not as pronounced as *e.g.* in the $\text{Sr}(\text{OH})\text{Cl}\cdot 4\text{H}_2\text{O}$ -type compounds (Kellersohn, Beckenkamp & Lutz, 1991) where, in addition to large differences in the hydrogen-bond lengths, the acceptor strengths of X are also very different. For a more quantitative evaluation of the situation in $\text{CoSO}_4\cdot 4\text{D}_2\text{O}$, however, further vibrational spectroscopic studies will be essential.

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Synthesis and Structure Determination of $\text{SrCa}(\text{edta})\cdot 5\text{H}_2\text{O}$

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Abstract. Tetraaqua(ethylenediaminetetraacetato)-calciumstrontium monohydrate, $[\text{SrCa}(\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8)(\text{H}_2\text{O})_4]\cdot \text{H}_2\text{O}$, $M_r = 505.9$, monoclinic, $C2/c$, $a = 19.568$ (2), $b = 11.535$ (8), $c = 16.028$ (2) Å, $\beta = 95.565$ (8)°, $V = 3600$ (3) Å³, $Z = 8$, $D_m = 1.82$ (2), $D_x = 1.86$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.7107$ Å, $\mu(\text{Mo } K\alpha) = 32.5$ cm⁻¹, $F(000) = 2064$, $T = 296$ K, $R = 0.040$ for 2918 unique observed reflections. The geometry of the compound consists of a three-dimensional

linkage of ligand-bridged metal ions and hydrogen bonds. The Ca ion is octacoordinated by four O and two N atoms of edta (ethylenediaminetetraacetic acid), one O atom of another edta molecule and one water molecule. The Sr ion displays nearly square antiprismatic coordination, being bound to three water molecules and five O atoms from different edta molecules.

Introduction. edta has long been known and studied as a calcium binding agent, not only with respect to

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practical applications but also as a classic research model for polydentate chelation (Gardiner, 1976). In recent years, X-ray structural studies of crystalline complexes of Ca²⁺ and Sr²⁺ ions with multidentate organic ligands have commonly revealed coordination numbers larger than six for both calcium and strontium (Barnett & Uchtman, 1979). The edta ligand is prototypic in the area of Ca binding. Complexes of this kind can also be used as precursors to obtain adequate superconductor oxides. Low-temperature decomposition of suitable complexes allows us to control strictly the cationic ratio in the resulting material, leading to single-phase homogeneous small sized particles.

In order to obtain precursors in the Bi–Ca–Sr–Cu–O family (Michel, Hervieu, Borel, Grandin, Deslandes, Provus & Raveau, 1987), we have prepared several complexes which can be formulated as $MM'(L).nH_2O$ [$M, M' = Ca, Cu, Pb, Sr$ and Bi ; $L = edta$ and $dtpa$ (diethylenetriaminepentaacetic acid)]. One of them, $[SrCa(edta)(H_2O)_4].H_2O$, has been obtained as colorless single crystals. Because of the wide application of such complexes, the structure reported here is deemed to be of considerable importance.

Experimental. The complex was synthesized by adding in equimolar ratio, with stirring, 1.009 g (10 mmol) CaCO₃ to 2.923 g (10 mmol) of edta solution. After a short period with stirring maintained to ensure complexation, 1.476 g (10 mmol) SrCO₃ was added. The complex was separated from solution as a colorless crystalline precipitate by slow addition of acetone.

A crystal with approximate dimensions $0.04 \times 0.03 \times 0.1$ mm was used for data collection. Preliminary oscillation and Weissenberg photographs showed a monoclinic crystal with systematic absences for the chosen cell, consistent with the space groups $C2/c$ or Cc . Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.7107$ Å). Cell dimensions obtained by least-squares refinement using 25 reflections in the range $5 \leq \theta \leq 13^\circ$. Density obtained by flotation. Intensity data for 7384 reflections (h 0:25, k 0:15, l -21:21; $2 < 2\theta < 56^\circ$) collected in ω/θ scan mode. 2918 reflections with $I > 2.5\sigma(I)$ were considered as observed and used in refinement. Two reference reflections ($\bar{2}43$ and $5\bar{1}1$) measured every 2 h exhibited no significant variation in intensity. Reflection intensities were corrected by Lorentz and polarization factors, no absorption correction was made ($\mu = 32.5$ cm⁻¹).

The Sr ion was located through Patterson methods (*SHELXS86*; Sheldrick, 1986) and was used to reveal the other atoms through *DIRDIF* (Beurkens, Bosman, Doesburg, Gould, Van der Hark, Prick, Noordik, Beurkens, Parthasanathi, Bruins &

Haltwanger, 1981). All non-H atoms were refined with anisotropic thermal parameters using full-matrix least squares on F (*SHELX76*; Sheldrick, 1976). Scattering factors for C, H, N and O as in *SHELX76*; scattering factors and anomalous-scattering factors for Sr and Ca from *International Tables for X-ray Crystallography* (1974, Vol. IV). H atoms, except those of some water molecules, which could not be found, were located in a difference map and were included in the refinement with fixed positional parameters and isotropic temperature factors. All calculations were carried out on a MicroVAX VT220 at the computer center of the Basque University. Geometric calculations with *BONDLA* (Stewart, Kruger, Ammon, Dickinson & Hall, 1972) and *PARST* (Nardelli, 1983). Weighting scheme of the form $w = 1/[\sigma^2|F_o| + p|F_o|^2]$ ($p = 0.000385$) was used and refinement of 302 parameters converged at $R = 0.040$, $wR = 0.042$. $\Delta/\sigma_{\max} < 0.01$. Maximum electron density in final difference Fourier synthesis was 1.44 e Å⁻³.

Discussion. The positional and equivalent isotropic thermal parameters are given in Table 1.* Bond distances and angles are given in Table 2. The structure of $[SrCa(edta)(H_2O)_4].H_2O$ consists of an intricate network of ligand-bridged coordinated metal ions and hydrogen bonds, such that no discrete molecules exit. A *SCHAKAL88* (Keller, 1988) drawing of the molecule illustrates the octacoordination around the two metal ions (Fig. 1).

The coordination polyhedron of the Sr ion is very close to a square antiprism. The sites occupied by the atoms O(18)ⁱ, O(14)ⁱⁱⁱ, O(17)ⁱ and OW(4) [(i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (iii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$] are in the same plane with deviations of ± 0.03 Å. The other plane is defined by the atoms O(18), OW(2), OW(3) and O(5)ⁱⁱ [(ii) $\frac{1}{2} + x, \frac{1}{2} - y, z - \frac{1}{2}$] [the maximum and minimum distances from the mean plane are 0.316 (4) Å for O(5)ⁱⁱ and -0.342 (4) Å for OW(2)]. The dihedral angle between the least-squares planes is 3.5 (1)°. The average Sr—O bond distance is 2.6 (1) Å.

The Ca ion is bound to two N and four O atoms from the edta. Two additional sites are filled by OW(1) from the water molecule and a symmetry-related edta O atom O(3)^{iv} [(iv) $-x, y, \frac{1}{2} - z$]. The coordination polyhedron, in accord with previous structures (Muetterties & Guggenberger, 1974), is intermediate between a C_{2v} geometry and a square antiprism. The deviations are probably due to the

* Lists of structure factors, anisotropic thermal parameters, torsion angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54701 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates ($\times 10^4$, Sr and Ca $\times 10^5$) and equivalent isotropic temperature factors (\AA^2) for non-H atoms with e.s.d.'s in parentheses

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	$B_{\text{eq}}(\text{\AA}^2)$
Sr	35931 (3)	30146 (5)	1312 (3)	1.71 (2)
Ca	9634 (5)	21590 (8)	25173 (6)	1.54 (4)
N(1)	1191 (2)	3731 (4)	3667 (3)	1.58 (18)
C(1)	1937 (3)	3983 (5)	3812 (4)	2.05 (24)
C(2)	2382 (3)	2939 (5)	3814 (3)	2.01 (22)
N(2)	2247 (2)	2214 (3)	3047 (2)	1.34 (16)
O(3)	52 (2)	2409 (3)	3415 (2)	1.79 (15)
C(4)	196 (3)	2709 (4)	4171 (3)	1.58 (21)
O(5)	-178 (2)	2549 (4)	4746 (2)	2.22 (16)
C(6)	886 (3)	3295 (5)	4402 (3)	1.84 (22)
C(7)	883 (3)	4785 (5)	3371 (3)	2.13 (24)
C(8)	946 (3)	5047 (5)	2456 (3)	1.78 (22)
O(9)	1067 (2)	4201 (3)	2005 (2)	2.18 (17)
O(10)	890 (2)	6083 (3)	2234 (2)	2.45 (18)
C(11)	2429 (3)	1006 (5)	3253 (4)	2.05 (23)
C(12)	1914 (3)	479 (5)	3796 (3)	1.78 (22)
O(13)	1321 (2)	898 (3)	3738 (2)	2.26 (17)
O(14)	2108 (2)	-362 (3)	4255 (2)	2.27 (17)
C(15)	2614 (3)	2610 (5)	2345 (3)	1.71 (21)
C(16)	2312 (3)	2102 (4)	1517 (3)	1.53 (19)
O(17)	1703 (2)	1777 (3)	1458 (2)	2.01 (16)
O(18)	2674 (2)	2077 (3)	921 (2)	2.09 (16)
OW(1)	720 (4)	86 (5)	2164 (4)	6.05 (33)
OW(2)	3505 (2)	937 (4)	-415 (2)	2.11 (17)
OW(3)	4258 (2)	2900 (4)	1617 (3)	2.91 (19)
OW(4)	4262 (2)	4914 (4)	-9 (3)	3.96 (24)
OW(5)	4371 (2)	2924 (4)	3775 (3)	3.25 (20)

perturbations produced by the metal—O bonds and hydrogen bonds. The average Ca—O bond is 2.44 (6) \AA , while for Ca—N the average is 2.58 (1) \AA . These values are similar to those found in another Ca(edta) complex (Barnett & Uchtman, 1979).

When the hexadentate chelation of edta is fully utilized, as it is in this structure, its geometry can be described by the conformation of five-membered chelated rings (Porai-Koshits, Pozhidaev & Polynova, 1974). These have been classified by Weakliem & Hoard (1959) into three types *E*, *G* and *R*. The four glycinate rings are fused either axially, R_1 [Ca—N(1)—C(7)—C(8)—O(9)—Ca] and R_2 [Ca—N(2)—C(11)—C(12)—O(13)—Ca] or equatorially, G_1 [Ca—N(1)—C(6)—C(4)—O(3)—Ca] and G_2 [Ca—N(2)—C(15)—C(16)—O(17)—Ca] to the central ethylenediamine ring, *E* [Ca—N(1)—C(1)—C(2)—N(2)—Ca]. The edta conformation is *E*, *G*/*R*, while the methylene groups of the *E* and *G* rings in the N(CH₂)₃ cluster lie on the same side of the N—M—M' plane and the methylene groups of the *R* rings on another plane. The interatomic distances and angles (Table 2) are, in general, in good agreement with those found in other edta complexes (Passer, White & Cheng, 1977; Barnett & Uchtman, 1979).

The edta ligand is bound to other symmetry-related metal ions by five O atoms: O(3), O(5), O(14), O(17), O(18), so that the Ca and Sr cations, along with the waters of hydration, serve to bridge

Table 2. Bond distances (\AA) and angles ($^\circ$) with e.s.d.'s in parentheses

Coordination sphere for Ca and Sr atoms				
O(18)—Sr	2.539 (4)	N(1)—Ca	2.593 (5)	
OW(2)—Sr	2.552 (4)	N(2)—Ca	2.573 (4)	
OW(3)—Sr	2.604 (4)	O(3)—Ca	2.415 (4)	
OW(4)—Sr	2.573 (5)	O(9)—Ca	2.509 (4)	
O(17)—Sr	2.568 (3)	O(13)—Ca	2.484 (3)	
O(18)—Sr	2.862 (4)	O(17)—Ca	2.376 (4)	
O(5) ^{iv} —Sr	2.622 (4)	OW(1)—Ca	2.493 (6)	
O(14) ⁱⁱⁱ —Sr	2.573 (4)	O(3) ^v —Ca	2.385 (4)	
edta molecule				
C(1)—C(2)	1.486 (8)	O(14)—C(12)	1.254 (6)	
C(1)—N(1)	1.484 (7)	O(5)—C(4)	1.245 (7)	
C(11)—N(2)	1.468 (7)	O(3)—C(4)	1.265 (6)	
C(6)—N(1)	1.461 (7)	O(13)—C(12)	1.252 (7)	
C(7)—N(1)	1.418 (7)	O(17)—C(16)	1.244 (7)	
N(2)—C(2)	1.489 (6)	O(18)—C(16)	1.244 (7)	
C(15)—N(2)	1.465 (6)			
Carboxylate groups				
	R_1	R_2	G_1	G_2
ϕ_1	117.0 (5)	117.7 (5)	117.1 (4)	118.2 (5)
ϕ_2	116.2 (5)	117.6 (5)	117.6 (5)	118.6 (5)
r_1	1.249 (7)	1.252 (7)	1.245 (7)	1.244 (7)
r_2	1.251 (6)	1.254 (6)	1.265 (6)	1.244 (7)

R_1 [Ca—N(1)—C(7)—C(8)—O(9)—Ca]; R_2 [Ca—N(2)—C(11)—C(12)—O(13)—Ca]; G_1 [Ca—N(1)—C(6)—C(4)—O(3)—Ca]; G_2 [Ca—N(2)—C(15)—C(16)—O(17)—Ca]; $\phi = \text{C—C—O}^\circ$; $r = \text{C—O } \text{\AA}$.

Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, z - \frac{1}{2}$; (iii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iv) $-x, y, \frac{1}{2} - z$; (v) $\frac{1}{2} - x, y, \frac{1}{2} - z$.

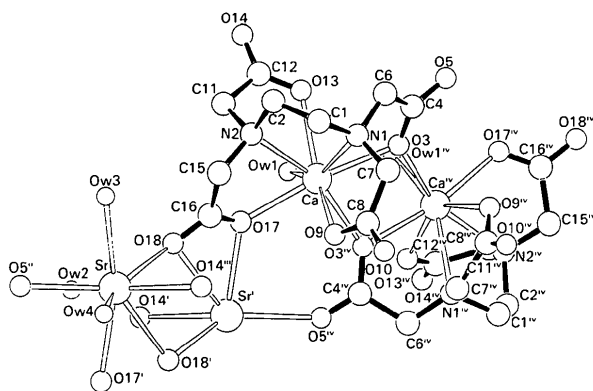


Fig. 1. A SCHAKAL (Keller, 1988) view of the molecule with octacoordination around the two metal ions.

[Ca(edta)]²⁻ complexes together. Three different links have been found for some O atoms: O(3), O(17), O(18). The atoms O(3), Ca, Ca^{iv}, O(3)^{iv}, C(4) [(iv) $-x, y, \frac{1}{2} - z$] form an approximately planar plane [the maximum distance from the mean plane is 0.412 (3) \AA]. In the planes formed by O(18)—C(16)—Srⁱ—Sr and O(17)—C(16)—Srⁱ—Ca [(i) $\frac{1}{2} -$

Table 3. Bond lengths (Å) and bond angles (°) for hydrogen bonds with *e.s.d.*'s in parentheses

OW—HW...O	OW—		OW...O	OW—
	HW	HW...O		
OW(5)—HW(5A)...O(5)	1.05 (5)	1.86 (5)	2.772 (6)	143 (4)
OW(2) ^y —HW(2B) ^y ...O(9)	1.04 (5)	1.81 (4)	2.763 (5)	149 (5)
OW(4) ^y —HW(4B) ^y ...O(13)	1.04 (5)	1.70 (6)	2.682 (6)	154 (4)

$x, \frac{1}{2} - y, -z$] the greatest deviations are for C(16) -0.236 (5) Å and O(17) -0.256 (3) Å.

It is noteworthy that the carboxylate groups are symmetric, with the angles $\varphi_1 = \varphi_2$ ($\varphi = \text{C—C—O}$) and the distance $r_1 = r_2$ ($r = \text{C—O}$ Å) (Table 2). The average C—C—O angle is 117.5 (7)°, while the average C—O bond distance is 1.250 (7) Å. The configurations of the carboxylate groups have not been greatly influenced by the perturbations produced by the different M—O bonds. Following the standard notation described by Porai-Koshits (1980) for the bridging carboxylates, four different structural functions have been distinguished. The classification for the different carboxylates is: 1-*a* for C(8), *s*-3-*sa* for C(4), *a*-2-*s* C(12), and for the last one C(16) *a*-4₃-*s*.

Some water molecules are involved in hydrogen bonds with the O atoms from carboxylate groups, providing intermolecular links. The water molecule not involved in a metal bond is linked to one O atom from a carboxylate group, O(5)...OW(5) 2.772 (6) Å (Table 3). None of the O atoms with three links form hydrogen bonds.

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Dicarbonyl(η^5 -cyclopentadienyl)(triphenylphosphite)[(triphenylphosphonio)methanide]-molybdenum *p*-Toluenesulfonate

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Abstract. [Mo(C₅H₅)(C₁₉H₁₇P)(C₁₈H₁₅O₃P)(CO)₂]-[C₇H₇O₃S]·2.6H₂O, $M_r = 1018.89$, triclinic, $P\bar{1}$, $a = 14.370$ (3), $b = 14.990$ (3), $c = 13.324$ (3) Å, $\alpha = 110.30$ (2), $\beta = 94.91$ (2), $\gamma = 110.38$ (2)°, $V = 2453.1$ Å³, $Z = 2$, $D_x = 1.39$ g cm⁻³, $\lambda(\text{Mo } K\alpha) =$

0.7093 Å, graphite monochromator, $\mu = 4.2$ cm⁻¹, $F(000) = 1062$, $T = 296$ K, $R = 0.028$, $wR = 0.032$ for 7770 observed reflections with $I > 3\sigma(I)$. The coordination environment about the Mo atom consists of a cyclopentadienyl ring, two carbonyls, a triphenylphosphite and a C-bound methylene (a triphenylphosphine unit is bound to the methylene C

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