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Acta Cryst. (1992). **C48**, 1782–1785

Structure of $[Ca(triethylene\ glycol)_2]Cl_2.4H_2O$

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(*Received* 13 *November* 1991; *accepted* 20 *February* 1992)

Abstract. Bis{2,2′-[1,2-ethanediylbis(oxy)]bisethanol}calcium dichloride tetrahydrate, $[Ca(C_6H_{14}O_4)_2]Cl_2.4H_2O$, $M_r = 483.40$, triclinic, $P\bar{1}$, $a = 8.471\ (1)$, $b = 10.157\ (1)$, $c = 14.821\ (3)$ Å, $\alpha = 102.81\ (1)$, $\beta = 97.74\ (1)$, $\gamma = 103.52\ (1)°$, $V = 1185.4\ (3)$ Å^3, $Z = 2$, $D_x = 1.35$ g cm^{-3}, $\lambda(Mo\ K\alpha) = 0.71073$ Å, $\mu = 5.32$ cm^{-1}, $F(000) = 516$, $T = 293$ K, final $R = 0.048$ for 2098 observed $[F_o \geq 5\sigma(F_o)]$ reflections. The cation is 8-coordinate dodecahedral with the alcoholic O atoms in B sites [average Ca—O = 2.41 (1) Å] and the etheric O atoms in A sites [average Ca—O = 2.458 (9) Å]. The counter ions and water molecules are hydrogen bonded with the alcoholic ends of the glycol chains in a three-dimensional network.

Introduction. Lanthanide podates are reported to be less stable than the corresponding crown ether complexes owing to a size-related macrocycle effect (Bünzli & Pilloud, 1989; Barthelemy, Desreux & Massaux, 1986). Our efforts to study competitive crystallization of the hard lanthanide(III) ions between crown ethers and the related polyethylene glycols (PEG's) have always resulted in crystalline complexes of the acyclic PEG's (Rogers, Rollins, Henry, Murdoch, Etzenhouser, Huggins & Nuñez, 1991) or complexes consisting of a directly coordinated PEG and a hydrogen bonded crown ether (Rogers, Voss & Etzenhouser, 1988). There are some indications that the flexibility of the PEG and the added stability of hydrogen bonding from the terminal glycols may be responsible for the observed crystal structures.

This report continues our investigations of structural features which may lead to the preferential crystallization of PEG complexes. Competitive crystallization of $CaCl_2.2H_2O$ with 3-methylene-16-crown-5 and traces of triethylene glycol (EO3) resulted in isolation of the title complex.

Experimental. 0.1467 g of $CaCl_2.2H_2O$ was added to 5 mL of a 3:1 solution of CH_3CN:CH_3OH. To this was added 0.15 mL of a mixture of 3-methylene-16-crown-5 contaminated with triethylene glycol. The resulting solution was stirred at 333 K for 1 h followed by storage at 268 K for 20 h. Evaporation of the reaction solution initially gave a powder. Dissolution of the solid in a new aliquot of the solvent mixture followed by slow evaporation afforded diffraction-quality crystals. Analysis: calculated C 29.82, H 7.51; found for precipitate C 37.45, H 3.29; found for crystals C 31.99, H 5.29. A crystal of 0.13 × 0.13 × 0.40 mm was used for data collection on an Enraf–Nonius CAD-4 diffractometer, with graphite-monochromated Mo $K\alpha$ radiation. Cell constants were determined from setting angles of 25 reflections ($\theta > 19°$). Intensities were measured using ω–2θ scans, to $\theta_{max} = 50°$ and for h 0 to 10,

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Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters* (Å^2) *for* [Ca(EO3)$_2$]Cl$_2$.4H$_2$O

$$B_{eq} = (4/3)[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + ab(\cos\gamma)\beta_{12} + ac(\cos\beta)\beta_{13} + bc(\cos\alpha)\beta_{23}].$$

	x	*y*	*z*	B_{eq}
Ca	0.5258 (1)	0.7418 (1)	0.25412 (8)	1.96
Cl(1)	0.1155 (2)	0.7953 (2)	−0.0048 (1)	3.06
Cl(2)	0.9331 (2)	1.3668 (2)	0.3554 (1)	3.79
O(1)	0.2681 (5)	0.6684 (4)	0.1416 (3)	3.27
O(2)	0.3353 (5)	0.5208 (4)	0.2612 (3)	2.49
O(3)	0.6459 (5)	0.6155 (4)	0.3566 (3)	2.63
O(4)	0.7943 (5)	0.8753 (5)	0.3485 (3)	3.41
O(5)	0.6340 (6)	0.5952 (5)	0.1439 (3)	3.78
O(6)	0.6350 (5)	0.8548 (4)	0.1371 (3)	3.21
O(7)	0.4723 (5)	0.9698 (4)	0.2585 (3)	2.92
O(8)	0.4051 (5)	0.8255 (4)	0.3869 (3)	3.13
O(9)	0.2095 (6)	0.6487 (5)	0.4605 (3)	3.87
O(10)	0.7279 (6)	0.3694 (5)	0.1614 (3)	3.86
O(11)	1.0246 (6)	1.0799 (5)	0.3167 (4)	4.17
O(12)	1.1145 (7)	1.0799 (6)	0.1408 (4)	5.13
C(1)	0.1353 (7)	0.5637 (6)	0.1540 (4)	2.84
C(2)	0.2030 (8)	0.4536 (6)	0.1819 (4)	2.90
C(3)	0.4072 (8)	0.4238 (7)	0.2959 (5)	3.42
C(4)	0.5336 (8)	0.5065 (7)	0.3817 (5)	3.57
C(5)	0.7744 (8)	0.7023 (7)	0.4336 (5)	3.51
C(6)	0.8883 (8)	0.8015 (8)	0.3954 (5)	3.79
C(7)	0.728 (1)	0.6562 (9)	0.0852 (6)	5.27
C(8)	0.655 (1)	0.7612 (9)	0.0537 (5)	4.88
C(9)	0.5748 (8)	0.9695 (7)	0.1200 (5)	3.69
C(10)	0.5638 (9)	1.0574 (7)	0.2094 (5)	3.76
C(11)	0.447 (1)	1.0420 (7)	0.3469 (5)	4.05
C(12)	0.3371 (9)	0.9417 (7)	0.3842 (6)	3.96

Table 2. *Distances* (Å) *and angles* (°) *for the* Ca^{2+} *ion coordination sphere and the hydrogen-bonding contacts*

Ca^{2+} coordination sphere			
Ca—O(1)	2.411 (4)	Ca—O(2)	2.472 (4)
Ca—O(3)	2.458 (4)	Ca—O(4)	2.414 (4)
Ca—O(5)	2.385 (4)	Ca—O(6)	2.450 (4)
Ca—O(7)	2.450 (4)	Ca—O(8)	2.418 (4)
O(1)—Ca—O(2)	65.7 (1)	O(1)—Ca—O(3)	130.2 (1)
O(2)—Ca—O(3)	65.2 (1)	O(1)—Ca—O(4)	163.0 (1)
O(2)—Ca—O(4)	131.1 (1)	O(3)—Ca—O(4)	66.8 (1)
O(1)—Ca—O(5)	88.6 (2)	O(2)—Ca—O(5)	85.5 (1)
O(3)—Ca—O(5)	79.6 (1)	O(4)—Ca—O(5)	94.4 (2)
O(1)—Ca—O(6)	84.2 (1)	O(2)—Ca—O(6)	139.6 (2)
O(3)—Ca—O(6)	131.5 (1)	O(4)—Ca—O(6)	81.7 (2)
O(5)—Ca—O(6)	66.7 (1)	O(1)—Ca—O(7)	79.8 (1)
O(2)—Ca—O(7)	129.2 (1)	O(3)—Ca—O(7)	141.2 (1)
O(4)—Ca—O(7)	85.7 (1)	O(5)—Ca—O(7)	131.5 (1)
O(6)—Ca—O(7)	65.3 (1)	O(1)—Ca—O(8)	94.3 (2)
O(2)—Ca—O(8)	79.1 (1)	O(3)—Ca—O(8)	84.6 (1)
O(4)—Ca—O(8)	88.2 (2)	O(5)—Ca—O(8)	161.4 (1)
O(6)—Ca—O(8)	131.8 (1)	O(7)—Ca—O(8)	67.0 (1)
Hydrogen-bonding contacts			
O(1)···Cl(1)	3.051 (5)	O(4)···O(11)	2.671 (7)
O(5)···O(10)	2.649 (8)	O(8)···O(9)	2.669 (7)
O(9)···Cl(2^a)	3.164 (4)	O(9)···Cl(2^b)	3.150 (6)
O(10)···Cl(1^c)	3.176 (5)	O(10)···Cl(2^d)	3.162 (5)
O(11)···Cl(2)	3.141 (6)	O(11)···O(12)	2.814 (8)
O(12)···Cl(1^e)	3.271 (7)	O(12)···Cl(1^f)	3.203 (6)
C(1)···O(1)···Cl(1)	105.6 (3)	C(6)···O(4)···O(11)	103.7 (4)
C(7)···O(5)···O(10)	107.5 (5)	C(12)···O(8)···O(9)	108.6 (4)
Cl(2^a)···O(9)···Cl(2^b)	87.6 (1)	Cl(1^c)···O(10)···Cl(2^d)	104.7 (2)
Cl(2)···O(11)···O(12)	98.1 (2)	Cl(1^e)···O(12)···Cl(1^f)	100.5 (1)

Symmetry code: (*a*) $x-1, y-1, z$; (*b*) $1-x, 2-y, 1-z$; (*c*) $1-x, 1-y, -z$; (*d*) $x, y-1, z$; (*e*) $1-x, 2-y, -z$; (*f*) $x+1, y, z$.

k − 12 to 12, *l* − 17 to 17. Corrections were made for Lorentz–polarization effects, but not for absorption. Standard reflections observed every 3600 s of data-collection time (200, 030, 008) showed a variation of ± 2%. 4170 reflections were measured (3247 unique, $R_{int} = 0.019$), of which 2098 were independent observed reflections [$F_o \geq 5\sigma(F_o)$]. The structure was solved utilizing the *SHELXS*86 (Sheldrick, 1985) direct-methods program. The geometrically constrained H atoms were placed in calculated positions 0.95 Å from the bonded C atom and allowed to ride

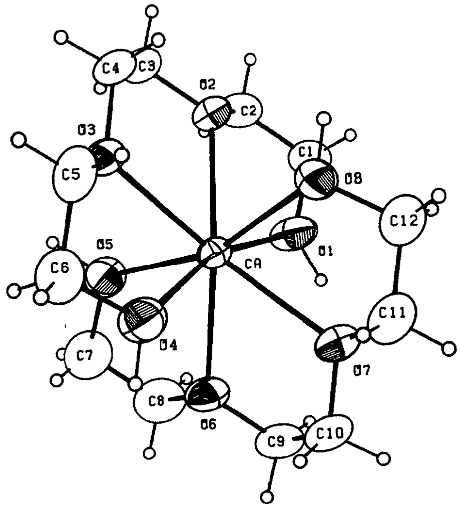

Fig. 1. Illustration of the [Ca(EO3)$_2$]$^{2+}$ cation with 50% probability thermal ellipsoids. H atoms are arbitrarily reduced.

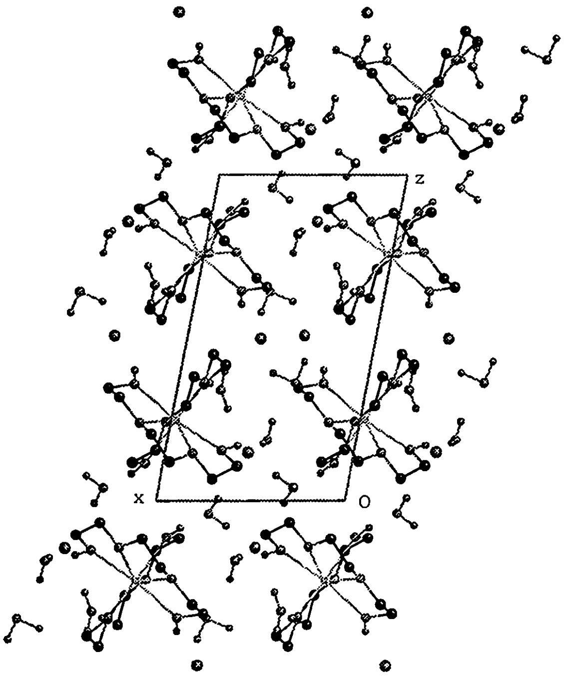

Fig. 2. *SYBYL* (Tripos Associates, 1992) illustration of the unit-cell packing (2 × 2 representation of the *xz* plane). Ethyl H atoms have been omitted. C atoms are black, alcoholic and aquo H atoms have smaller radii. Uncoordinated Cl anions appear as unconnected grey spheres.

Table 3. *Comparison of bonding parameters in* Ca^{2+} *complexes of crown ethers, glymes and glycols*

Compound	Coordination No.	No. of tight* ion pairs	Average Ca—OH(alcoholic) (Å)	Average Ca—O(etheric) (Å)	Reference
[Ca(NCS)$_2$(OH$_2$)$_2$(12-crown-4)]	8	2		2.53 (1)	Wei, Tinant, Declercq, Van Meerssche & Dale (1988*a*)
[Ca(OH$_2$)$_4$(12-crown-4)]Cl$_2$.4H$_2$O	8	0		2.52 (2)	North, Steiner, van Remoortere & Boer (1976)
[Ca(NCS)$_2$(OH$_2$)(15-crown-5)]	8	2		2.54 (3)	Wei, Tinant, Declercq, Van Meerssche & Dale (1988*b*)
[Ca(NCS)$_2$(OHMe)(benzo-15-crown-5)]	8	2		2.53 (5)	Owen (1978)
[Ca(NCS)$_2$(OH$_2$)(EG3)]	7	2		2.45 (2)	Wei, Tinant, Declercq, Van Meerssche & Dale (1987*b*)
[Ca(NCS)$_2$(OH$_2$)(EG4)]	8	2		2.49 (1)	Wei, Tinant, Declercq, Van Meerssche & Dale (1987*a*)
[Ca(NCS)$_2$(EG5)]	8	2		2.50 (3)	Wei, Tinant, Declercq, Van Meerssche & Dale (1987*c*)
[Ca(OH$_2$)$_2$(EG6)]$_2$[Ca(NCS)$_6$].H$_2$O	8	0		2.46 (5)	Wei, Tinant, Declercq, Van Meerssche & Dale (1987*d*)
[Ca(EO3)$_2$]Cl$_2$.4H$_2$O	8	0	2.41 (1)	2.458 (9)	This study
[Ca(picrate)$_2$(OH$_2$)(EO4)]	8	2	2.40 (1)	2.46 (3)	Singh, Reinhardt & Poonia (1980, 1984)

* Tight ion pairs refer to anions in the primary coordination sphere of Ca^{2+}.

on that atom with B fixed at 5.5 Å^2. The remaining H atoms were located from a difference Fourier map and included with fixed contributions ($B = 5.5$ Å^2). Scattering factors and anomalous-dispersion corrections were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 72, 99, 149). The structure was refined with *SHELX*76 (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ was minimized, with weights $= [\sigma(F_o)^2 + 0.003F_o^2]^{-1}$; 244 parameters were varied. $R = 0.048$, $wR = 0.070$, $S = 0.74$. $\Delta/\sigma <$ 0.01 in the final least-squares refinement cycle; $\Delta\rho <$ 0.3 e Å^{-3} in the final difference map.

Discussion. Fractional coordinates and B_{eq} values are given in Table 1,* bond distances and angles and contact geometries in Table 2, an *ORTEP*II (Johnson, 1976) illustration of the cation environment is in Fig. 1, and a cell-packing diagram in Fig. 2.

The Ca^{2+} ion is 8-coordinate dodecahedral, complexed by two EO3 molecules. The four alcoholic terminal ends are in B coordination sites and average 2.41 (1) Å from Ca^{2+}. All four etheric O atoms are in A sites with an average Ca—O separation of 2.458 (9) Å. The two chloride anions and four water molecules in the asymmetric unit are hydrogen bonded together and with the alcoholic EO3 ends in a three-dimensional network.

The two glycol ligands adopt a crown-ether-like conformation rather than the helical conformation often observed for glycol complexes (Rogers, Rollins, Henry, Murdoch, Etzenhouser, Huggins & Nuñez, 1991). The O—C—C—O torsion angles alternate ±*gauche* (±60°) and the C—O—C—C angles are all *anti* (180°) as found for the common D_{3d} form of 18-crown-6. Taken together, however, an overall helical wrapping of the Ca^{2+} ion is observed.

Only three 2/1 PEG/metal complexes have been crystallographically characterized: [MCl(OH$_2$)(EO3)$_2$]Cl$_2$, M = La, Ce (Rogers, Etzenhouser & Murdoch, 1992), and [Nd(EO4)$_2$]$_4$[NdCl$_6$]Cl$_9$ (Rogers, Rollins, Henry, Murdoch, Etzenhouser, Huggins & Nuñez, 1991). Several 1/1 crown ether and glyme structures and one PEG complex of Ca^{2+} have appeared in the literature (Table 3).

The one Ca^{2+}/PEG complex in the literature, [Ca(picrate)$_2$(OH$_2$)(EO4)], has bonding parameters to the PEG which are nearly identical to those in the title complex. The Ca^{2+} ion in the EO4 complex is 8-coordinate with Ca—O(alcoholic) distances which average 2.40 (1) Å [*vs* 2.41 (1) Å in the title complex] and average Ca—O(etheric) separations of 2.46 (3) Å [*vs* 2.458 (9) Å].

The Ca—O separations in the crown ether (12-crown-4, 15-crown-5 and benzo-15-crown-5) structures, all of which are 8-coordinate, are longer than the Ca—O(etheric) distances in the title complex by an average of 0.07 Å. The range in average Ca—O(crown ether) distances is only 0.02 Å despite the differences in the number of tight ion pairs (2 or 0).

The Ca—O(etheric) separations in the glyme structures bracket the 2.458 (9) Å observed in the title complex; however, all of these are shorter than the Ca—O values found for the crown ether complexes. The 7-coordinate triethylene glycol dimethyl ether (EG3) complex, [Ca(NCS)$_2$(OH$_2$)(EG3)], exhibits the smallest Ca—O average, perhaps owing to its lower coordination number. The EG6 complex, [Ca(OH$_2$)$_2$(EG6)]$_2$[Ca(NCS)$_6$].H$_2$O, is next at 2.46 (5) Å. This is essentially the same as the title

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* Lists of bond distances and angles, H-atom coordinates, thermal parameters, torsion angles, least-squares-planes results, and observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55214 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD0085]

complex, both of which do not have any tight ion pairs. The longest Ca—O distances of this type are observed for two 8-coordinate complexes [Ca(NCS)$_2$(OH$_2$)(EG4)] and [Ca(NCS)$_2$(EG5)], each of which has two tight ion pairs.

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Acta Cryst. (1992). C**48**, 1785–1788

Mixed Chelate Complexes. III.
Structures of (L-Alaninato)(aqua)(2,2′-bipyridine)copper(II) Nitrate Monohydrate and Aqua(2,2′-bipyridine)(L-tyrosinato)copper(II) Chloride Trihydrate

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(*Received* 19 *March* 1991; *accepted* 14 *April* 1992)

Abstract. (I) [Cu(C$_3$H$_6$NO$_2$)(C$_{10}$H$_8$N$_2$)(H$_2$O)]-NO$_3$.H$_2$O, $M_r = 405.9$, orthorhombic, $P2_12_12_1$, $a = 19.113\,(3)$, $b = 15.079\,(2)$, $c = 5.782\,(1)$ Å, $V = 1666.4\,(8)$ Å^3, $Z = 4$, $D_x = 1.617$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 1.409$ mm^{-1}, $F(000) = 836.0$, $T = 288$ K, $R = 0.042$ for 1595 reflections. (II) [Cu(C$_9$H$_{10}$NO$_3$)(C$_{10}$H$_8$N$_2$)(H$_2$O)]Cl.3H$_2$O, $M_r = 507.4$, hexagonal, $P6_1$, $a = 9.307\,(2)$, $c = 44.432$ Å, $V = 3333\,(3)$ Å^3, $Z = 6$, $D_x = 1.516$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 1.188$ mm^{-1}, $F(000) = 1578.0$, $T = 288$ K, $R = 0.053$ for 2048 reflections. In each complex the Cu ion displays a square pyramidal coordination with an apical water molecule. The apical Cu—OH$_2$ bond lengths are 2.230 (4) Å for (I) and 2.308 (6) Å for (II). The results obtained are compared with those for other aminoacidate copper(II) complexes.

Introduction. Compounds with general formula [Cu(N–N)(O–N)]$^+$, where (N–N) = 2,2′-bipyridine and (O–N) = alaninato or tyrosinato, have been synthesized and characterized by Ruíz-Ramírez, Martínez & Gasque (1992) who also determined their stability constants potentiometrically. The compounds are obtained from 1:1 mmol solutions of Cu$^{\rm II}$ ion and the (N–N) ligand in water, followed by the

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0108-2701/92/101785-04$06.00