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Potassium Salt of a Synthetic Carboxylic Ionophore

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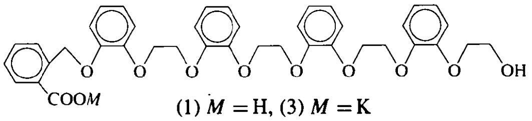
Abstract

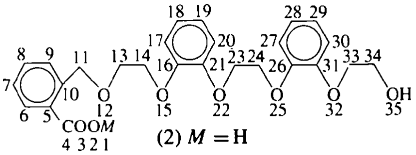
The potassium salt of an ω-hydroxycarboxylic acid with five ethereal O atoms, dipotassium bis(2-{[2-(2-{2-[2-(2-hydroxyethoxy)phenoxy]ethoxy}phenoxy)ethoxy]-methyl}benzoate) tetrahydrate, $2K^+.2C_{26}H_{27}O_8^-.4H_2O$, forms a dimeric structure with twofold symmetry, containing two polyether chains and water molecules. The water molecule lying on the twofold axis forms a bridge between the two polyether complexes by coordination to two K^+ ions. The distance between the K^+ ions is 4.231 (3) Å. Each polyether chain wraps around one cation, taking an 'S'-like conformation. The K^+ ion is ninefold coordinated by six ethereal O atoms, including one from another ether chain of the dimer, one hydroxyl group and two water molecules, one of which lies on the twofold axis. O atoms of carboxylato groups do not participate in coordination.

Comment

Naturally occurring carboxylic ionophores such as nigericin, which contain a terminal carboxylic group and one or two hydroxyl groups at the other end, connected with tetrahydrofuran and tetrahydropyran rings, mediate active ion transport across biological and artificial membranes (Pressman, 1976). To understand the complexation properties of ion carriers and how these acyclic compounds utilize conformation for optimum complexation with a guest cation, the crystal structures of various complexes have been determined using X-rays (Duesler & Paul, 1983, and references therein). We have synthesized a series of ω-hydroxycarboxylic acids as model compounds for the natural ionophores to investigate the relationship between the primary molecular structures and transport properties (Kuboniwa *et al.*, 1985; Kuboniwa, Yamaguchi, Nakahama, Hirao & Yamazaki, 1982; Yamaguchi *et al.*, 1988, 1989; Yamazaki, Hirao & Nakahama, 1979; Yamazaki, Nakahama, Hirao & Negi, 1978). Among the compounds, (1) and (2), which have eight and five ethereal O atoms, respectively, show relatively high K^+-ion selectivity. The longer ionophore, (1), exhibits higher transport ability and selectivity than the shorter one, and the crystal structure of the potassium salt of (1), (3), has been reported previously (Kuboniwa, Yamaguchi, Nakahama, Hori & Ohashi, 1988; Kasuga, Nakahama, Yamaguchi, Ohashi & Hori, 1991). The backbone of (3) forms a pseudocyclic ring by head-to-tail hydrogen bonding between the terminal carboxylato and hydroxyl groups and wraps around the cation like the seam of a tennis ball to give a complex with a lipophilic exterior. Although several crystallographic studies on similar synthetic polyethers have been reported (Chacko & Saenger, 1981; Hughes & Wingfield, 1978; Hughes, Mortimer, Parsons, Truter & Wingfield, 1977; Saenger & Reddy, 1979; Saenger & Brand, 1979; Weber & Saenger, 1979*a*,*b*, 1980; Weber, Saenger, Vögtle & Sieger, 1979), little is known about the complexation properties compared with those of the cyclic compounds (Truter, 1973).

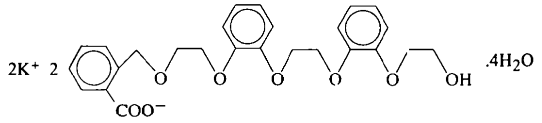


(1) *M* = H, (3) *M* = K



(2) *M* = H

This paper reports the structure of the potassium salt of the acyclic ionophore (2), dipotassium bis(2-{[2-(2-{2-[2-(2-hydroxyethoxy)phenoxy]ethoxy}phenoxy)-ethoxy]methyl}benzoate) tetrahydrate, (4).



(4)

The crystal structure of (4) is shown in Fig. 1. The coordination complex contains two polyethers and two types of water molecule, O36 and O37. The water molecule lying on the twofold axis, O37, is coordinated to two K$^+$ ions, bridging two polyether complexes to form a dimer. A solvent water molecule, O38, lies on the other twofold axis (O37 and O38 have partial occupancies, see Table 1). Both O atoms of the carboxylato group, O2 and O3, participate in intermolecular hydrogen bonding. One of the O atoms, O2, makes head-to-tail intermolecular hydrogen bonds with the hydroxyl group of the other dimer molecules, O35, and connects molecules along a screw axis. The other O atom of the carboxylato group, O3, forms hydrogen bonds with two water molecules, O36 and O38. These hydrogen bonds connect the dimeric molecules to give a network through the crystal. The structure of the polyether with K$^+$ ions is shown in Fig. 2.

The polyether chains have no head-to-tail intramolecular hydrogen bond as observed in (3). However, one K$^+$ ion is wrapped in an 'S'-like conformation, making the carboxylato groups face towards the outside of the molecule. The water molecule, O37, located on the twofold symmetry axis, links the two polyether complexes through coordination with two cations to give the dimer. Of several bis[(8-quinolyloxy)ethoxyethyl] ethers with alkali metal salts, dinuclear complexes of potassium isothiocyanate with an acyclic polyether having two 2-nitrophenoxy groups at both terminal positions form a similar 'S'-like conformation with twofold symmetry. The distance between the two K$^+$ ions of (4) is 4.231 (3) Å, which is shorter than that of the potassium complex of the oligoether with two carboxyl groups (4.74 Å) (Hughes, Mortimer, Parsons, Truter & Wingfield, 1977). The K—O37—K angle is 95.1 (7) or 96.9 (4)°. In linear and cyclic ether complexes, torsion angles around the C—O bond are usually *trans* and ethylene glycol C—C torsion angles are *gauche*. In general, this rule also holds for the present complex. Only two torsion angles, C20—C21—O22—C23 and C21—O22—C23—C24, are *gauche* [−77.4 (6) and −77.3 (6)°, respectively]. Sequential *gauche* conformers around the C—O bond make a kink in the backbone. This enables O atoms in the backbone to coordinate with the cation spherically. This is also observed in the structure of (3).

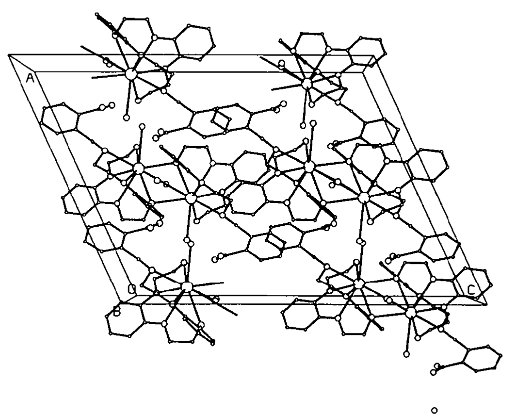


Fig. 1. The crystal structure of (4) viewed along the *b* axis.

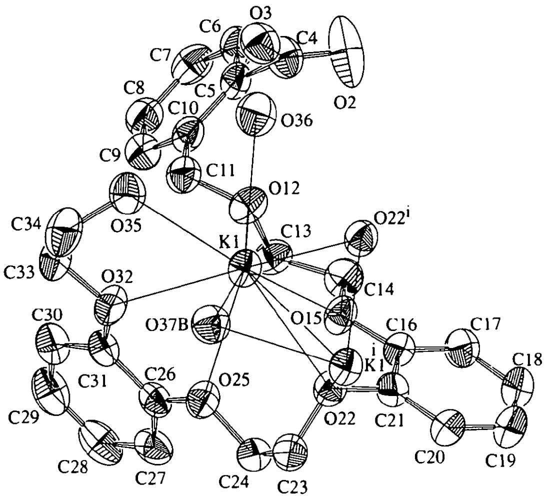


Fig. 2. *ORTEP*II drawing (Johnson, 1976) of the polyether with K$^+$ ions with 50% probability displacement ellipsoids. O37*A* is omitted because it lies close to O37*B*. O38*A* and O38*B* are not shown because they exist between the salt molecules.

The K—O distances indicate that each cation is ninefold coordinated with six ethereal O atoms, including one, O22^i [symmetry code: (i) $-x, y, \frac{3}{2} - z$], from the other polyether chain in the dimer, two water molecules and a terminal hydroxy group, O35. Atom O35 has the shortest K—O distance. The four O atoms O22, O25, O32 and O35 are coplanar within experimental error. The K$^+$ ion is located 0.79 Å above this plane. The salt of the longer polyether, (3), displays tenfold coordination without any coordination of water molecules. The complex of the diol described above (Hughes & Wingfield, 1978) also shows tenfold coordination. Interestingly, both O atoms in the carboxylato group of (4) do not coordinate to the K$^+$ ion but participate in intermolecular hydrogen bonding. Although a carboxylato group that is not coordinated to a metal ion is also seen in the structures of the sodium salts of 5-bromolasalocid, which is a natural ionophore with a short backbone (Schmidt, Wang & Paul, 1974; Chiang & Paul, 1977), most of the carboxylato groups in the related structures coordinate to the cation.

In conclusion, the overall structure of (4) is different from that of the 1:1 potassium salt of the ω-hydroxycarboxylic acid with eight ethereal O atoms, (3). In (4), hydrophilic carboxylato groups face towards the outside of the dimer and the water molecules located around the salt make the hydrophobicity much less than that of (3). Although one polyether chain of (4) coordinates with one K^+ cation, the coordination of water molecules would be essential when (2) transports a cation through hydrophobic membranes. On the other hand, the longer ionophore, (1), can effectively carry the cation through the membrane since one acid molecule can wrap the cation with a more hydrophobic exterior without coordination of water molecules. This may be a reason why (1) has higher ion-transport ability than (2).

Experimental

Crystal data

$2K^+.2C_{26}H_{27}O_8^-.4H_2O$
$M_r = 1085.25$
Monoclinic
$C2/c$
$a = 17.729\ (11)$ Å
$b = 13.521\ (13)$ Å
$c = 23.842\ (6)$ Å
$\beta = 114.64\ (2)°$
$V = 5194\ (4)$ Å^3
$Z = 4$
$D_x = 1.411$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 30.08$–$38.04°$
$\mu = 2.275$ mm^{-1}
$T = 296.0$ K
Plate
0.40 × 0.40 × 0.20 mm
Colourless

Data collection

AFC-5*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan
$T_{min} = 0.62$, $T_{max} = 1.00$
4513 measured reflections
4354 independent reflections
2446 observed reflections [$I > 3\sigma(I)$]

$R_{int} = 0.045$
$\theta_{max} = 62.6°$
$h = 0 \rightarrow 20$
$k = 0 \rightarrow 16$
$l = -27 \rightarrow 27$
3 standard reflections monitored every 150 reflections
intensity decay: 0.7%

Refinement

Refinement on F
$R = 0.051$
$wR = 0.065$
$S = 1.703$
2446 reflections
409 parameters
All H-atom parameters refined
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{max} = 0.4870$

$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: Zachariasen (1967) type 2 Gaussian isotropic
Extinction coefficient: 6.19244
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters* (Å^2)

U_{iso} for O37 and O38; $U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ for others.

	x	y	z	U_{eq}/U_{iso}
K1	0.06407 (7)	0.20095 (9)	0.69241 (5)	0.0482 (3)
O2	0.3102 (4)	−0.0852 (3)	0.6767 (2)	0.103 (2)
O3	0.3281 (2)	0.0735 (3)	0.7017 (2)	0.061 (1)
C4	0.3092 (4)	0.0044 (5)	0.6641 (3)	0.058 (2)
C5	0.2868 (3)	0.0287 (4)	0.5967 (3)	0.045 (2)
C6	0.3277 (4)	−0.0210 (4)	0.5666 (3)	0.055 (2)
C7	0.3114 (4)	0.0008 (5)	0.5061 (3)	0.062 (2)
C8	0.2540 (4)	0.0729 (5)	0.4748 (3)	0.058 (2)
C9	0.2125 (4)	0.1213 (5)	0.5041 (3)	0.053 (2)
C10	0.2283 (3)	0.1008 (4)	0.5654 (3)	0.045 (2)
C11	0.1807 (3)	0.1566 (4)	0.5949 (3)	0.052 (2)
O12	0.1382 (2)	0.0941 (3)	0.6211 (2)	0.050 (1)
C13	0.0755 (4)	0.0357 (5)	0.5760 (3)	0.051 (2)
C14	0.0439 (4)	−0.0365 (5)	0.6082 (3)	0.056 (2)
O15	−0.0002 (2)	0.0163 (3)	0.6377 (2)	0.052 (1)
C16	−0.0471 (3)	−0.0386 (4)	0.6595 (3)	0.046 (2)
C17	−0.0515 (4)	−0.1407 (5)	0.6588 (3)	0.062 (2)
C18	−0.1037 (5)	−0.1877 (5)	0.6809 (4)	0.077 (2)
C19	−0.1490 (4)	−0.1341 (5)	0.7044 (3)	0.073 (2)
C20	−0.1443 (4)	−0.0321 (5)	0.7059 (3)	0.058 (2)
C21	−0.0941 (3)	0.0151 (4)	0.6832 (3)	0.046 (2)
O22	−0.0871 (2)	0.1179 (3)	0.6865 (2)	0.048 (1)
C23	−0.1578 (4)	0.1681 (5)	0.6400 (3)	0.057 (2)
C24	−0.1564 (4)	0.1661 (5)	0.5780 (3)	0.054 (2)
O25	−0.0872 (2)	0.2245 (3)	0.5815 (2)	0.049 (1)
C26	−0.0821 (3)	0.2477 (4)	0.5275 (2)	0.044 (2)
C27	−0.1361 (4)	0.2161 (4)	0.4696 (3)	0.053 (2)
C28	−0.1258 (4)	0.2476 (5)	0.4174 (3)	0.065 (2)
C29	−0.0610 (5)	0.3081 (5)	0.4237 (3)	0.064 (2)
C30	−0.0052 (4)	0.3383 (4)	0.4820 (3)	0.055 (2)
C31	−0.0161 (3)	0.3096 (4)	0.5330 (2)	0.043 (1)
O32	0.0340 (2)	0.3356 (3)	0.5928 (2)	0.055 (1)
C33	0.0941 (4)	0.4107 (4)	0.6032 (3)	0.063 (2)
C34	0.1243 (5)	0.4473 (5)	0.6675 (3)	0.067 (2)
O35	0.1631 (2)	0.3695 (3)	0.7108 (2)	0.059 (1)
O36	0.2435 (3)	0.1728 (3)	0.7599 (2)	0.067 (1)
O37*A*†	−0.028 (1)	0.339 (2)	0.7298 (9)	0.039 (5)
O37*B*	0	0.340 (1)	3/4	0.059 (4)
O38*A*	0.502 (1)	0.066 (2)	0.7891 (9)	0.127 (6)
O38*B*	1/2	0.032 (2)	3/4	0.126 (9)

† Site occupancies: 037*A* 0.4, O37*B* 0.3, O38*A* 0.34, O38*B* 0.17.

Table 2. *Selected geometric parameters* (Å, °)

K1—O12	2.927 (4)	C10—C11	1.506 (7)
K1—O15	2.827 (4)	C11—O12	1.437 (6)
K1—O22	2.855 (4)	O12—C13	1.420 (6)
K1—O22^{i}	2.963 (4)	C13—C14	1.489 (8)
K1—O25	2.893 (4)	C14—O15	1.440 (7)
K1—O32	2.861 (4)	O15—C16	1.370 (6)
K1—O35	2.798 (4)	O22—C23	1.451 (7)
K1—O36	2.930 (5)	C23—C24	1.489 (9)
K1—O37*A*	2.85 (2)	C24—O25	1.432 (7)
K1—O37*A*^{i}	2.88 (2)	O25—C26	1.366 (6)
K1—O37*B*	2.83 (1)	C31—O32	1.375 (6)
K1···K1^{i}	4.231 (3)	O32—C33	1.416 (6)
O2—C4	1.247 (7)	C33—C34	1.483 (9)
O3—C4	1.240 (6)	C34—O35	1.432 (8)
C4—C5	1.522 (8)	O35···O36	3.015 (6)
C5—C6	1.387 (8)	O2···O35^{ii}	2.596 (6)
C5—C10	1.392 (7)	O2···O37*A*^{iii}	2.81 (2)
C6—C7	1.381 (8)	O3···O36	2.777 (6)
C7—C8	1.382 (9)	O3···O38*A*	2.91 (2)
C8—C9	1.374 (8)	O3···O38*A*^{iv}	2.94 (2)
C9—C10	1.397 (7)	O3···O38*B*	2.829 (7)
O2—C4—O3	125.9 (6)	C23—C24—O25	107.5 (5)
C4—C5—C6	118.6 (5)	C24—O25—C26	117.6 (4)
C10—C11—O12	113.9 (4)	O25—C26—C27	125.5 (5)
C11—O12—C13	112.6 (4)	C31—O32—C33	118.6 (4)
O12—C13—C14	108.6 (5)	O32—C33—C34	109.9 (5)
C13—C14—O15	108.8 (5)	C33—C34—O35	111.0 (5)

C14—O15—C16	117.1 (4)	O36—K1—O37A	122.9 (5)
O15—C16—C17	125.3 (6)	O36—K1—O37$A^{\rm i}$	102.3 (4)
C21—O22—C23	113.3 (4)	K1—O37A—K1$^{\rm i}$	95.1 (7)
O22—C23—C24	112.6 (5)	K1—O37B—K1$^{\rm i}$	96.9 (4)

Symmetry codes: (i) $-x, y, \frac{3}{2}-z$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$; (iii) $\frac{1}{2}+x, y-\frac{1}{2}, z$; (iv) $1-x, y, \frac{3}{2}-z$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *TEXSAN LS*. Software used to prepare material for publication: *TEXSAN FINISH*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AS1158). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Alkyne Coupling Induced by a Trinuclear Ruthenium Cluster: Synthesis and Structure of Di-μ-carbonyl-hexacarbonyl-μ_3-(1,2,3,4-tetraphenyl-1,3-butadiene-1,4-diyl)-triruthenium(2 *Ru*—*Ru*), [$Ru_3(CO)_8(C_4Ph_4)$]

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Abstract

The reaction of PhC$\equiv$CPh with [$Ru_3(CO)_{10}(MeCN)_2$] affords two [$Ru_3(CO)_8(C_2Ph_2)_2$] complexes, one red–violet containing only terminal carbonyl groups and the other the orange–yellow title compound, di-μ-carbonyl-1:2κ^2C;1:3κ^2C-hexacarbonyl-1κ^2C,2κ^2C,3κ^2C-μ_3-[1,2,3,4-tetraphenyl-2(η^4):3(η^4)-1,3-butadiene-1,4-diyl-1κ^2C]-triruthenium(2 *Ru*—*Ru*). The structure of the latter isomer consists of an open Ru_3 cluster [Ru—Ru 2.6696 (8) and 2.6717 (6), Ru$\cdots$Ru 3.7461 (7) Å] coordinated to the C_4Ph_4 ligand, formed by the dimerization of PhC$\equiv$CPh, and to eight CO groups, six terminal and two bridging. The central Ru atom is σ-bonded to the butadiene moiety to form an RuC_4 metallacyclopentadiene ring [Ru—C 2.219 (4) and 2.216 (4); mean C—C 1.461 Å]. Each of the other two metal atoms is η^4-bonded to the C atoms of the RuC_4 ring [mean Ru—C 2.322 Å] to form a pentagonal bipyramidal Ru_3C_4 core.

Comment

Dodecacarbonyltriruthenium has been shown to react with alkynes to give good yields of complexes containing a metallacyclopentadiene ring, RuC_4, with σ metal–carbon bonds (Sears & Stone, 1968; Cetini, Gambino, Sappa & Valle, 1969; Sappa, Manotti Lanfredi & Tiripicchio, 1980; Rosenberg *et al.*, 1981), where two or three alkynes join to form the heterocyclic five-membered ring.