O6	0.2303 (2)	0.0372 (3)	0.3254 (2)	0.033 (1)
N1	0.0948 (2)	0.0722 (4)	−0.0335 (2)	0.026 (1)
N2	0.1681 (2)	0.2022 (3)	0.1120 (2)	0.028 (1)
N3	0.4008 (2)	−0.0918 (4)	0.1716 (2)	0.029 (1)
N4	0.3215 (2)	0.0001 (4)	0.2551 (2)	0.024 (1)
C1	0.0938 (2)	0.1910 (4)	0.0304 (3)	0.025 (1)
C2	0.0228 (2)	0.2818 (4)	0.0032 (3)	0.034 (1)
C3	−0.0466 (2)	0.2474 (5)	−0.0839 (3)	0.041 (1)
C4	−0.0432 (2)	0.1208 (4)	−0.1432 (3)	0.034 (1)
C5	0.0273 (3)	0.0368 (4)	−0.1200 (3)	0.032 (2)
C6	0.0372 (2)	−0.0969 (5)	−0.1810 (3)	0.039 (2)
C7	0.1766 (2)	0.3176 (4)	0.1823 (3)	0.034 (1)
C8	0.2762 (3)	0.4457 (5)	0.3242 (4)	0.042 (2)
C9	0.2868 (4)	0.6069 (6)	0.2880 (5)	0.085 (3)
C10	0.4008 (2)	−0.0555 (4)	0.2646 (3)	0.026 (1)
C11	0.4735 (3)	−0.0823 (5)	0.3480 (3)	0.039 (2)
C12	0.5412 (3)	−0.1408 (5)	0.3354 (4)	0.046 (2)
C13	0.5395 (3)	−0.1774 (5)	0.2401 (3)	0.039 (2)
C14	0.4687 (2)	−0.1513 (5)	0.1581 (3)	0.035 (2)
C15	0.4585 (3)	−0.1852 (6)	0.0526 (3)	0.049 (2)
C16	0.3112 (3)	0.0369 (4)	0.3430 (4)	0.032 (2)
C17	0.2073 (3)	0.0793 (6)	0.4080 (4)	0.041 (2)
C18	0.2118 (5)	−0.0554 (9)	0.4762 (5)	0.081 (3)

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

Cu—O1	1.899 (3)	N3—C10	1.375 (5)
Cu—O4	1.912 (3)	N3—C14	1.365 (5)
Cu—N2	1.941 (3)	N4—C10	1.411 (5)
Cu—N4	1.916 (3)	N4—C16	1.380 (6)
O1—N1	1.330 (4)	C1—C2	1.381 (5)
O2—C7	1.189 (5)	C2—C3	1.394 (6)
O3—C7	1.345 (5)	C3—C4	1.395 (6)
O3—C8	1.459 (5)	C4—C5	1.346 (6)
O4—N3	1.357 (4)	C5—C6	1.493 (6)
O5—C16	1.231 (6)	C8—C9	1.512 (7)
O6—C16	1.327 (5)	C10—C11	1.384 (5)
O6—C17	1.438 (5)	C11—C12	1.353 (6)
N1—C1	1.376 (5)	C12—C13	1.396 (7)
N1—C5	1.374 (5)	C13—C14	1.354 (6)
N2—C1	1.372 (5)	C14—C15	1.486 (6)
N2—C7	1.380 (5)	C17—C18	1.496 (8)
O1—Cu—O4	91.6 (1)	C1—N2—C7	118.4 (3)
O1—Cu—N2	82.2 (1)	O4—N3—C10	119.7 (3)
O4—Cu—N2	154.9 (1)	O4—N3—C14	117.1 (3)
O1—Cu—N4	157.9 (2)	C10—N3—C14	123.2 (3)
O4—Cu—N4	83.3 (1)	Cu—N4—C10	114.2 (3)
N2—Cu—N4	110.9 (1)	Cu—N4—C16	128.4 (3)
Cu—O1—N1	113.0 (2)	C10—N4—C16	117.0 (3)
Cu—O4—N3	111.7 (2)	N1—C1—N2	111.9 (3)
O1—N1—C1	118.5 (3)	N1—C1—C2	117.9 (3)
O1—N1—C5	118.7 (3)	N2—C1—C2	130.2 (3)
C1—N1—C5	122.8 (3)	N3—C10—N4	110.4 (3)
Cu—N2—C1	113.5 (2)	N3—C10—C11	117.6 (3)
Cu—N2—C7	127.8 (3)	N4—C10—C11	131.9 (4)

Cell-constant data were collected by + and -2θ scans and parameters were determined from least-squares calculations that accounted for $K(\alpha_1-\alpha_2)$ splitting. All H atoms were found in subsequent difference Fourier maps. During refinement the H atoms were fixed in positions of idealized geometry with C—H = 0.95 Å and U(H) = 0.04, 0.05 and 0.06 Å^2 for the aromatic, methylene and methyl H atoms, respectively. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71602 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1043]

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Polyol Metal Complexes. V.† Structure of (2,2′-Bipyridyl-$\kappa^2 N,N'$)[*meso*-oxolane-3,4-diolato(2−)-$\kappa^2 O,O'$]palladium(II) 6.5-Hydrate

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Abstract

In the title compound, $[Pd(C_4H_6O_3)(C_{10}H_8N_2)].6.5H_2O$, an oxolanediolato ligand forms a chelate complex with palladium(II). The dianion is formed by double deprotonation of anhydroerythritol in alkaline aqueous solution. The square-planar $[(2,2'\text{-bipyridyl})Pd(C_4H_6O_4)]$ complex acts as a multiple acceptor in a hydrogen-bond system *via* its alkoxide and ether O atoms. A special feature of the hydrogen-bond system is a homodromic helix, formed by four of the 6.5 water molecules of the asymmetric unit.

Comment

Multiply charged polyolato ligands derived from simple polyalcohols or carbohydrates are formed in alkaline aqueous solution by deprotonation in the presence of copper(II) ions (Habermann, Klaassen & Klüfers, 1993; Habermann, Jung, Klaassen & Klüfers, 1992; Klaassen & Klüfers, 1993; Fuchs, Habermann & Klüfers, 1993). Diols are deprotonated twice in such solutions to form

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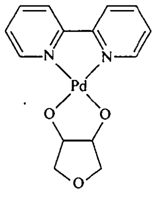
† Part IV: Fuchs, Habermann & Klüfers (1993).

either amine diolato(2−) copper complexes (in the presence of amine) or bis-diolato(2−) cuprates.

We now report the structure of (2,2′-bipyridyl-κ^2N,N')-[*meso*-oxolane-3,4-diolato(2−)-κ^2O,O']palladium(II) 6.5-hydrate (1). To our knowledge, the title compound is the first structurally characterized polyolato complex of palladium. The *meso*-oxolane-3,4-diolato(2−) ligand is derived from anhydroerythritol (*meso*-oxolane-3,4-diol) by double deprotonation in aqueous solution. Compound (1) was prepared by the reaction of 0.333 g (1 mmol) of (2,2′-bipyridyl)palladium(II) hydroxide dihydrate and 0.105 g of anhydroerythritol in 5 ml of water and crystallized by saturation with diethyl ether. Yellow crystals were obtained after several days at 278 K.



(1)

In the crystals, disc-shaped molecules of the coordination compound are stacked along the crystallographic *c* axis. A perspective view of the square-planar complex is shown in Fig. 1. The $[Pd(C_4H_6O_3)]$ moiety is characterized by the distances and angles given in Table 2 and by the puckering parameters (Cremer & Pople, 1975) of the chelate and the oxolane five-membered rings: Q = 0.346 (3) and 0.382 (3) Å and φ = 264.9 (3) and 262.6 (5)° for the rings Pd—O2—C2—C3—O3 and O1—C1—C2—C3—C4, respectively. The values indicate a normal puckering amplitude. The conformations of both rings are approximately $^4T_3$, indicating twist conformations with the twist axes of the individual rings running through Pd and O1, respectively. The ideal φ value for this conformation is 270°. The observed phase angles indicate a distortion towards an envelope conformation, E_3, indicating that the C2 atoms of the rings deviate the most from the respective best-fit planes.

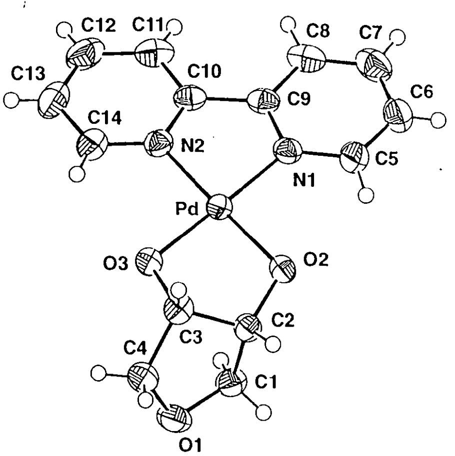


Fig. 1. Structure of (2,2′-bipyridyl-κ^2N,N')[*meso*-oxolane-3,4-diolato(2−)-κ^2O,O']palladium(II) (50% probability displacement ellipsoids).

The alkoxide O atoms are each acceptors of two hydrogen bonds, as also found in related copper compounds. The hydrogen-bond system is depicted in Fig. 2. Four of the 6.5 water molecules constitute a homodromic helix along the 2_1 axis parallel to [001], to which the other water molecules are attached [for the definition of the term 'homodromic', see Jeffrey & Saenger (1991)]. The ether O atom (O1) also acts as an acceptor in the system.

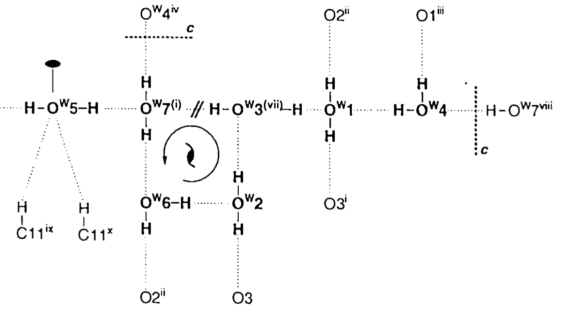


Fig. 2. The hydrogen-bond structure in (1). Water molecules in the asymmetric unit are indicated in bold with all nearest neighbours. Symmetry indicators are given in Table 3; further codes: (vi) $-x, y, \frac{3}{2} - z$; (vii) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z$; (viii) $x, 1 - y, -\frac{1}{2} + z$; (ix) $-\frac{1}{2} + x, -\frac{1}{2} + y, \frac{3}{2} + z$; (x) $\frac{1}{2} - x, -\frac{1}{2} + y, z$. The four water molecules around the 2_1 axis are part of a homodromic helix; at O*W*3 and O*W*7 the symmetry indicator of the respective neighbour in the helix is given in parentheses. The twofold axis at O*W*5 and *c*-glide planes between O*W*4 and O*W*7 are also indicated.

Experimental

Crystal data

$[Pd(C_4H_6O_3)(C_{10}H_8N_2)]$.-
$6.5H_2O$
M_r = 481.78
Orthorhombic
Pbcn
a = 17.723 (3) Å
b = 15.126 (3) Å
c = 14.796 (3) Å
V = 3966.5 (13) Å^3
Z = 8
D_x = 1.6136 (5) Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 132 reflections
θ = 10–26°
μ = 0.985 mm^{-1}
T = 221 (3) K
Prism
0.50 × 0.28 × 0.20 mm
Yellow

Data collection

Stoe Stadi-4 diffractometer
ω/θ scans
Absorption correction: empirical
T_{min} = 0.70, T_{max} = 0.78
3898 measured reflections
3898 independent reflections
2793 observed reflections [$I > 2\sigma(I)$]

θ_{max} = 26.06°
$h = 0 \rightarrow 21$
$k = 0 \rightarrow 18$
$l = -18 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0266$
$wR(F^2) = 0.0704$
$S = 1.046$
3898 reflections
349 parameters
All H-atom parameters refined
Calculated weights $w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 3.0616P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.407$ e Å^{-3}
$\Delta\rho_{\min} = -0.326$ e Å^{-3}
Extinction correction: $F_c^* = kF_c\{1 + 0.001F_c^2\lambda^3 \times [\sin(2\theta)]^{-1}\}^{-1/4}$
Extinction coefficient: 0.00011 (5)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

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

$$U_{\text{eq}} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Pd	0.486481 (12)	0.305683 (14)	0.609808 (15)	0.02894 (8)
O1	0.39435 (13)	0.0750 (2)	0.4830 (2)	0.0460 (6)
O2	0.54980 (11)	0.20750 (13)	0.56459 (15)	0.0345 (5)
O3	0.40966 (11)	0.21263 (13)	0.63431 (14)	0.0318 (5)
N1	0.56230 (14)	0.4012 (2)	0.5874 (2)	0.0338 (6)
N2	0.42577 (14)	0.4104 (2)	0.6505 (2)	0.0337 (6)
C1	0.4577 (2)	0.1315 (2)	0.4656 (2)	0.0397 (8)
C2	0.5037 (2)	0.1318 (2)	0.5523 (2)	0.0329 (7)
C3	0.4417 (2)	0.1260 (2)	0.6226 (2)	0.0335 (7)
C4	0.3862 (2)	0.0638 (2)	0.5795 (2)	0.0405 (8)
C5	0.6335 (2)	0.3877 (3)	0.5577 (2)	0.0416 (8)
C6	0.6824 (2)	0.4572 (3)	0.5453 (3)	0.0502 (10)
C7	0.6587 (2)	0.5418 (3)	0.5625 (3)	0.0518 (10)
C8	0.5863 (2)	0.5559 (2)	0.5925 (2)	0.0458 (9)
C9	0.5386 (2)	0.4848 (2)	0.6056 (2)	0.0347 (7)
C10	0.4600 (2)	0.4897 (2)	0.6401 (2)	0.0350 (7)
C11	0.4235 (2)	0.5664 (3)	0.6611 (3)	0.0497 (10)
C12	0.3505 (2)	0.5631 (3)	0.6936 (3)	0.0546 (11)
C13	0.3158 (2)	0.4837 (3)	0.7039 (3)	0.0513 (10)
C14	0.3553 (2)	0.4073 (3)	0.6819 (2)	0.0424 (8)
H11	0.4455 (22)	0.611 (2)	0.655 (3)	0.049 (12)
O*W*1	0.1527 (2)	0.3115 (2)	0.2991 (2)	0.0431 (6)
O*W*2	0.2818 (2)	0.2405 (3)	0.5300 (3)	0.0681 (10)
O*W*3	0.2984 (2)	0.2621 (3)	0.3473 (3)	0.0708 (10)
O*W*4	0.1527 (2)	0.4956 (2)	0.3206 (2)	0.0679 (9)
O*W*5	0	0.2393 (3)	3/4	0.084 (2)
O*W*6	0.1645 (2)	0.3465 (2)	0.5537 (2)	0.0847 (11)
O*W*7	0.1268 (2)	0.3498 (2)	0.7320 (3)	0.0720 (10)
H*W*11	0.135 (2)	0.296 (2)	0.245 (3)	0.060 (13)
H*W*12	0.125 (2)	0.305 (3)	0.330 (3)	0.033 (12)
H*W*21	0.316 (2)	0.235 (3)	0.561 (3)	0.051 (13)
H*W*22	0.289 (4)	0.246 (5)	0.481 (5)	0.17 (4)
H*W*31	0.287 (2)	0.216 (3)	0.349 (3)	0.037 (13)
H*W*32	0.255 (4)	0.273 (4)	0.332 (4)	0.11 (2)
H*W*41	0.151 (2)	0.445 (3)	0.315 (3)	0.062 (15)
H*W*42	0.148 (3)	0.509 (3)	0.369 (3)	0.083 (19)
H*W*5	0.047 (3)	0.274 (3)	0.746 (3)	0.092 (16)
H*W*61	0.1345 (14)	0.2823 (17)	0.5844 (17)	0.010 (6)
H*W*62	0.209 (5)	0.284 (6)	0.553 (6)	0.23 (4)
H*W*71	0.128 (3)	0.395 (4)	0.752 (4)	0.11 (2)
H*W*72	0.143 (3)	0.349 (3)	0.671 (3)	0.077 (16)

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

Pd—O2	1.978 (2)	O2—C2	1.419 (4)
Pd—O3	1.992 (2)	O3—C3	1.439 (4)
Pd—N1	2.000 (3)	C1—C2	1.520 (5)
Pd—N2	2.007 (3)	C2—C3	1.514 (4)
O1—C1	1.435 (4)	C3—C4	1.503 (5)
O1—C4	1.446 (4)		
O2—Pd—O3	85.34 (9)	O2—C2—C1	114.8 (3)
N1—Pd—N2	80.80 (10)	C3—C2—C1	101.0 (3)
C1—O1—C4	109.0 (2)	O3—C3—C4	111.2 (3)
C2—O2—Pd	108.8 (2)	O3—C3—C2	108.5 (2)
C3—O3—Pd	110.6 (2)	C4—C3—C2	102.7 (3)
O1—C1—C2	105.7 (3)	O1—C4—C3	106.3 (3)
O2—C2—C3	112.1 (2)		
O2—C2—C3—O3	43.0 (3)	N1—C9—C10—N2	2.0 (4)
C1—C2—C3—C4	38.2 (3)		

Table 3. *Hydrogen-bonding geometry* (Å, °)

D	H	*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*1	H*W*11	O3$^{\text{i}}$	0.90 (4)	1.81 (4)	2.702 (4)	168 (3)
O*W*1	H*W*12	O2$^{\text{ii}}$	0.68 (4)	2.06 (4)	2.733 (3)	173 (4)
O*W*2	H*W*21	O3	0.77 (4)	2.01 (4)	2.775 (4)	175 (4)
O*W*2	H*W*22	O*W*3	0.74 (7)	2.00 (7)	2.737 (6)	175 (8)
O*W*3	H*W*31	O*W*7$^{\text{i}}$	0.73 (5)	2.51 (4)	2.745 (6)	101 (3)
O*W*3	H*W*32	O*W*1	0.82 (7)	1.97 (7)	2.782 (5)	174 (6)
O*W*4	H*W*41	O*W*1	0.77 (5)	2.03 (5)	2.804 (4)	177 (4)
O*W*4	H*W*42	O1$^{\text{iii}}$	0.75 (4)	2.10 (5)	2.812 (5)	159 (5)
O*W*5	H*W*5	O*W*7	0.99 (5)	1.83 (5)	2.815 (4)	173 (4)
O*W*6		O2$^{\text{ii}}$			2.804 (4)	
O*W*6	H*W*62	O*W*2	1.23 (9)	1.49 (9)	2.648 (5)	154 (7)
O*W*7	H*W*71	O*W*4$^{\text{iv}}$	0.75 (6)	1.99 (6)	2.718 (5)	166 (6)
O*W*7	H*W*72	O*W*6	0.95 (4)	1.78 (4)	2.721 (5)	175 (5)
C11	H11	O*W*5$^{\text{v}}$	0.79 (3)	2.58 (3)	3.226 (5)	140 (4)

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

All e.s.d.'s (except the e.s.d. in the dihedral angle between two LS planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving LS planes.

The localization of the H atoms at O*W*6, which has the largest value of a main axis component of the vibrational tensor of all atoms, was not successful. Only H*W*62 refines near the expected position, as derived from the O···O distances. The H atom in the hydrogen bond to O2 can be detected in the difference map, but least-squares refinement shifts it to the reported coordinates, which cannot be regarded as an H-atom position. For this reason, the O*W*6···O2$^{\text{ii}}$ hydrogen bond is given without an H atom in Table 3.

Data collection: *DIF*4 (Stoe & Cie, 1988*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1988*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*92 (Sheldrick, 1992). Molecular graphics: *ORTEP*II (Johnson, 1976) and *PLATON* (Spek, 1982).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71493 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1065]

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Disodium Bis(*o*-chloranilato)uranyl(VI) Hexahydrate

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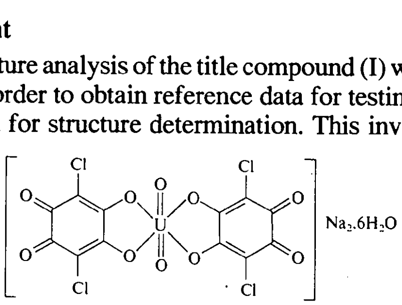
Abstract

In the title compound, disodium bis[3,6-dichloro-4,5-dihydroxy-3,5-cyclohexadiene-1,2-dionato(2−)]dioxouranium hexahydrate, Na$_2$[UO$_2$(C$_6$Cl$_2$O$_4$)$_2$].6H$_2$O, the coordination polyhedra for both uranium and sodium are pentagonal bipyramids. The uranyl anilate groups are organized in planes parallel to $(\bar{3}01)$ and are connected by Na ions which also lie in these planes. The arrangement produces channels in the [010] and [001] directions which are filled with water molecules at the intersection points. A pseudo orthorhombic F cell can be found by the transformation $a' = a - c$, $b' = b$, $c' = a + 3c$. In this cell, the anilate planes are parallel to (100). The three water molecules, O(21), O(25) and its symmetrically equivalent O(25)′, form an H$_2$O cluster connected by hydrogen bonding.

Comment

The structure analysis of the title compound (I) was undertaken in order to obtain reference data for testing powder data used for structure determination. This investigation is the first of a series studying the behaviour of different metals in anilate compounds. All angles and distances are in good agreement with values found in the literature (Krough Andersen, 1967; Krough Andersen & Krough Andersen, 1975).



(I)

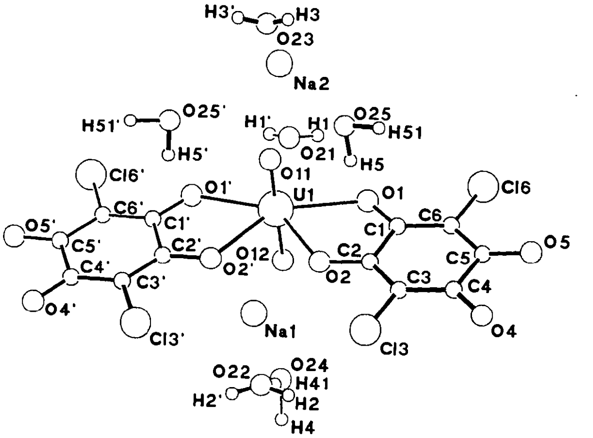
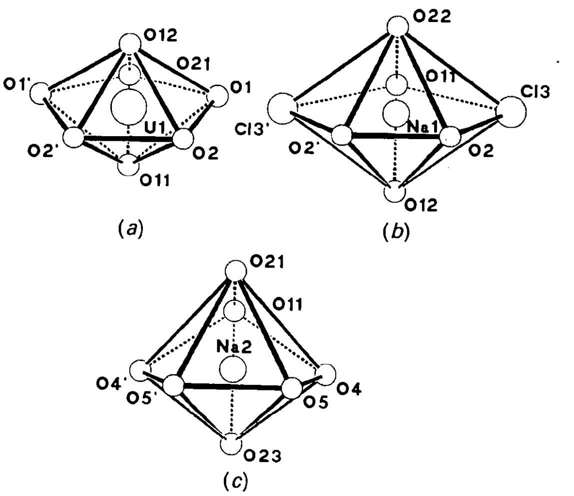


Fig. 1. View of the title compound showing the atomic numbering system; only one of the two formula units in the cell is plotted.



(*a*) (*b*)

(*c*)

Fig. 2. Coordination polyhedra of (*a*) U(1), (*b*) Na(1) and (*c*) Na(2).

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