

I (2.70 Å), indicative of some ionic bond character. While the Te(1)—C bond lengths are comparable with those for the other Te atoms, the bond angle C(1)—Te(1)—C(11) is significantly greater than the other corresponding values. This difference can be a result of the different bond modes, namely *sp*<sup>3</sup>*d* hybridization for Te(1) and nearly pure *p* orbitals adopted for the other Te atoms. Moreover, Te—C bond lengths involving central carbons are slightly longer than those involving side ones, which can be ascribed to the steric repulsion between the Te atoms around the linkage of two central C atoms. In the charge-transfer salts of HMTTeF the C=C bond lengths were found to be increased on oxidation (Kikuchi *et al.*, 1985). A comparison of C=C bond lengths between this compound and the neutral HMTTeF molecule (Carroll, Lakshminantham, Cava, Wudl, Aharon-Shalom & Cox, 1982) shows little difference and suggests that oxidation is not occurring at the C=C bonds.

The molecules of (HMTTeF)<sub>2</sub> are partly stacked in the **b** direction, which is different from the complete stacking in (HMTTeF)<sub>4</sub>(PF<sub>6</sub>)<sub>2</sub> where three HMTTeF molecules with partially oxidized C=C bonds are stacked in a column with particular benefit for  $\pi$ -electron transfer. As seen in Fig. 2, a layer arrangement is formed in the direction perpendicular to the molecular planes. The Te(2) atom is in contact with C(21) and C(22) [3.86 (1) and 3.84 (1) Å] of the upper molecule ( $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ) and with C(12) [3.89 (1) Å] of the lower molecule ( $2 - x, -y, 1 - z$ ). The shortest intermolecular Te—I contact is 3.717 (1) Å.

In summary, the oxidation takes place mainly on the Te(1) atom in the title compound resulting in no  $\pi$ -electron transfer from the C=C bonds. This is why the compound does not exhibit the expected conductivity. Despite all this, the compound provides an interesting example of the iodides of HMTTeF and further supports the proposal that the oxidation of HMTTeF may originate from the tellurium lone pairs (Wudl & Aharon-Shalom, 1982). For the plate-like crystal of the other I salt (Matsuzaki, Li & Sano, 1986), however, it may be that oxidation results from  $\pi$ -electron transfer on the basis of its Raman spectrum and metallic conduction. Because of different crystallization conditions for the two compounds, it is clear that the oxidation of HMTTeF is related to the solvents and electrolytes used in electrocrystallization.

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## Structure of the Cryptate (2.1.1) Dihydrochloride Dihydrate at 120 K

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**Abstract.** 4,7,13,18-Tetraoxa-1,10-diazabicyclo[8.5.5]-icosane dihydrochloride dihydrate, C<sub>14</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub><sup>2+</sup>·2Cl<sup>-</sup>·2H<sub>2</sub>O, *M<sub>r</sub>* = 397.34, monoclinic, *P*2<sub>1</sub>/*n*, *a* = 18.956 (11), *b* = 12.939 (8), *c* = 8.338 (5) Å,  $\beta$  = 102.62 (5)°, *V* = 1995.7 Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* =

1.322 Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 0.36$  mm<sup>-1</sup>, *F*(000) = 856, *T* = 120 K, final *R*(*F*) = 0.063 for 2632 independent observed reflections. In the crystal the cryptate dication has the *endo-endo* conformation with the protons on both N atoms

pointing inwards to make three close contacts each with the cryptand O atoms.

**Introduction.** This work is part of a program to study the kinetic and thermodynamic data of configuration equilibria of different protonated aminopolyethers (APE). In this paper we present the structure of the cryptate (2.1.1).2HCl.2H<sub>2</sub>O. So far only one X-ray structural investigation of a diprotonated (2.1.1) cryptate has been made by Cox, Murray-Rust, Murray-Rust, van Truong & Schneider (1982) with a perchlorate anion. In solution an effect of the anion on the configuration equilibria of diprotonated APE was observed by high-resolution NMR studies. It was thus of special interest to know whether an effect of the anion on the solid-state conformation of the cryptate could be observed.

**Experimental.** Single crystals of the title compound were grown from methanol/water. X-ray experiments were made at a temperature of 120 K on a Siemens four-circle diffractometer which was equipped with an N<sub>2</sub> gas stream cooling device built according to the design of Dietrich & Dierks (1970). Inspection of several reflection profiles indicated only moderate crystal quality. However, since only few single crystals were available this crystal quality had to be accepted. Crystal dimensions 0.4 × 0.4 × 0.4 mm. Lattice parameters from least-squares refinement of 24 reflections with 20 < 2θ < 27°. 3911 reflections of a quadrant measured in ω-2θ scan mode up to (sin θ/λ)<sub>max</sub> = 0.615 Å<sup>-1</sup> with Zr-filtered Mo Kα radiation, reduced to 3589 independent reflections (R<sub>int</sub> = 7.2%), 957 unobserved reflections with I < 2σ(I), h, k, l 0 to 22, 0 to 15, -9 to 10. Three standard reflections, measured every 40 min, showed insignificant statistical intensity variation. Reflection intensities corrected by Lorentz and polarization factors, no absorption or extinction corrections. Structure solution easily obtained with SHELXS86 (Sheldrick, 1986). Two water molecules identified, so that the complex is present as a dihydrate. Isotropic, later anisotropic atomic parameters submitted to full-matrix least-squares refinement with the XTAL system (Hall & Stewart, 1987). Quantity minimized  $\sum w(|F_o| - |F_c|)^2$ . Unobserved reflections included if |F<sub>c</sub>| > |F<sub>o</sub>|. All H atoms from difference synthesis refined isotropically. Final R = 0.063 and wR = 0.037, based on 2632 reflections and 353 variables, w = 1/σ<sup>2</sup>(F<sub>o</sub>), σ<sup>2</sup>(F<sub>o</sub>) values from counting statistics, S = 1.90 (3). Average (Δ/σ) = 0.07, maximum (Δ/σ) = 0.39, largest peak in final difference map = 0.67 e Å<sup>-3</sup>, largest hole = 0.44 e Å<sup>-3</sup>. Atomic scattering factors for Cl<sup>-</sup>, C, O and N atoms from Cromer & Mann (1968), H-atom scattering factors from Stewart, Davidson & Simpson (1965) and dis-

Table 1. Atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup> × 10<sup>2</sup>)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U <sub>eq</sub>
N(1)	0.0376 (2)	0.2177 (3)	-0.1690 (4)	1.9 (1)
C(2)	-0.0391 (3)	0.2324 (4)	-0.2663 (6)	2.9 (2)
C(3)	-0.0634 (3)	0.3395 (4)	-0.2407 (6)	3.2 (2)
O(4)	-0.0093 (2)	0.4057 (2)	-0.2782 (4)	2.7 (1)
C(5)	-0.0219 (3)	0.5140 (4)	-0.2588 (7)	3.0 (2)
C(6)	0.0458 (3)	0.5716 (4)	-0.2595 (6)	3.0 (2)
O(7)	0.0989 (2)	0.5443 (2)	-0.1185 (3)	2.33 (9)
C(8)	0.1669 (3)	0.5938 (4)	-0.1073 (6)	2.8 (2)
C(9)	0.2215 (3)	0.5338 (3)	0.0142 (6)	2.7 (2)
N(10)	0.2172 (2)	0.4209 (3)	-0.0298 (4)	1.7 (1)
C(11)	0.2539 (3)	0.3979 (3)	-0.1697 (6)	2.3 (2)
C(12)	0.2214 (2)	0.3018 (4)	-0.2602 (6)	2.2 (1)
O(13)	0.1452 (1)	0.3179 (2)	-0.3081 (3)	2.13 (9)
C(14)	0.1065 (3)	0.2304 (4)	-0.3887 (6)	2.6 (2)
C(15)	0.0851 (3)	0.1594 (3)	-0.2614 (5)	2.3 (1)
C(16)	0.0401 (3)	0.1747 (4)	-0.0025 (6)	2.8 (2)
C(17)	0.1105 (3)	0.1980 (4)	0.1155 (6)	2.5 (2)
O(18)	0.1194 (1)	0.3079 (2)	0.1171 (3)	2.1 (1)
C(19)	0.1872 (2)	0.3403 (4)	0.2162 (6)	2.4 (2)
C(20)	0.2437 (2)	0.3513 (4)	0.1146 (5)	2.3 (1)
O(1W)	0.1579 (2)	-0.1233 (4)	0.0271 (5)	5.1 (2)
O(2W)	0.4022 (2)	0.5032 (3)	0.0903 (5)	3.4 (1)
Cl(1)	0.26437 (6)	0.06873 (8)	0.0165 (1)	2.50 (3)
Cl(2)	0.54848 (6)	0.63251 (8)	0.1837 (1)	2.63 (4)

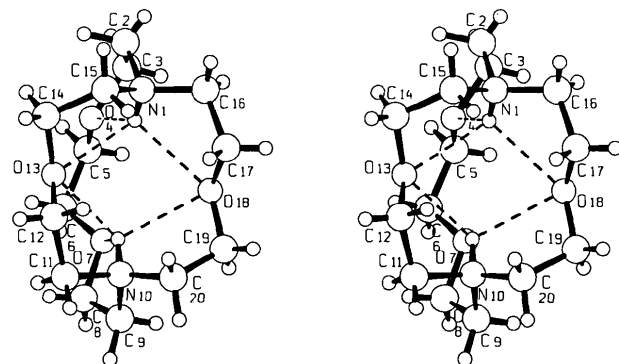


Fig. 1. Structure and atomic notation of the (2.1.1) cryptate dihydrate in the crystal. Intramolecular N—H...O contacts are represented by dashed lines (SCHAKAL drawing, Keller, 1980).

persion corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV).

**Discussion.** Final atomic coordinates and equivalent isotropic displacement factors (Hamilton, 1959) are given in Table 1.\* A stereo representation by SCHAKAL (Keller, 1980) of the cryptate molecular structure in the crystal is shown in Fig. 1, giving the atomic-numbering scheme. Table 2 lists bond lengths, bond angles and the ring torsion angles.

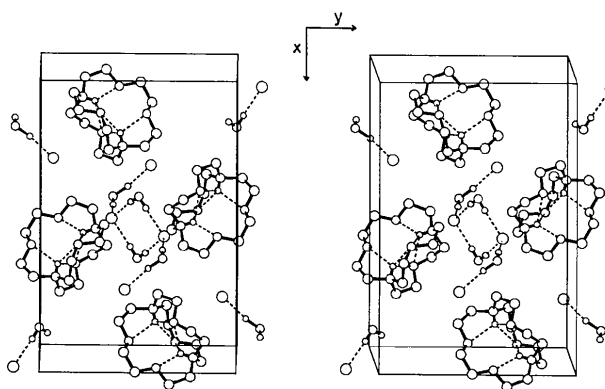
\* Lists of structure factors, anisotropic displacement parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53872 (39 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Bond lengths, bond angles and torsion angles (Å, °) with *e.s.d.*'s in parentheses

N(1)—C(2)	1.514 (6)	N(1)—C(15)	1.509 (6)
N(1)—C(16)	1.487 (6)	C(2)—C(3)	1.491 (7)
C(3)—O(4)	1.422 (6)	O(4)—C(5)	1.437 (5)
C(5)—C(6)	1.485 (7)	C(6)—O(7)	1.415 (5)
O(7)—C(8)	1.425 (6)	C(8)—C(9)	1.497 (6)
C(9)—N(10)	1.504 (6)	N(10)—C(11)	1.512 (6)
N(10)—C(20)	1.500 (5)	C(11)—C(12)	1.514 (6)
C(12)—O(13)	1.427 (5)	O(13)—C(14)	1.435 (5)
C(14)—C(15)	1.524 (7)	C(16)—C(17)	1.505 (6)
C(17)—O(18)	1.432 (5)	O(18)—C(19)	1.431 (5)
C(19)—C(20)	1.510 (7)		
C(2)—N(1)—C(15)	113.5 (3)	C(9)—N(10)—C(20)	113.4 (3)
C(2)—N(1)—C(16)	112.2 (4)	C(11)—N(10)—C(20)	111.8 (3)
C(15)—N(1)—C(16)	112.9 (3)	N(10)—C(11)—C(12)	109.9 (4)
N(1)—C(2)—C(3)	109.3 (4)	C(11)—C(12)—O(13)	107.2 (4)
C(2)—C(3)—O(4)	105.5 (4)	C(12)—O(13)—C(14)	113.5 (3)
C(3)—O(4)—C(5)	114.7 (4)	O(13)—C(14)—C(15)	109.7 (4)
O(4)—C(5)—C(6)	108.9 (4)	N(1)—C(15)—C(14)	109.5 (4)
C(5)—C(6)—O(7)	109.3 (4)	N(1)—C(16)—C(17)	112.2 (4)
C(6)—O(7)—C(8)	114.3 (4)	C(16)—C(17)—O(18)	106.9 (4)
O(7)—C(8)—C(9)	107.0 (4)	C(17)—O(18)—C(19)	112.7 (3)
C(8)—C(9)—N(10)	110.3 (3)	O(18)—C(19)—C(20)	111.2 (4)
C(9)—N(10)—C(11)	111.7 (3)	N(10)—C(20)—C(19)	110.7 (4)
C(15)—N(1)—C(2)—C(3)	-138.1 (4)	N(10)—C(11)—C(12)—O(13)	54.6 (4)
C(16)—N(1)—C(2)—C(3)	92.4 (5)	C(11)—C(12)—O(13)—C(14)	-177.0 (4)
N(1)—C(2)—C(3)—O(4)	52.9 (5)	C(12)—O(13)—C(14)—C(15)	89.3 (4)
C(2)—C(3)—O(4)—C(5)	-179.1 (4)	O(13)—C(14)—C(15)—N(1)	59.9 (4)
C(3)—O(4)—C(5)—C(6)	165.7 (4)	C(14)—C(15)—N(1)—C(16)	-155.0 (3)
O(4)—C(5)—C(6)—O(7)	-66.1 (5)	C(14)—C(15)—N(1)—C(2)	75.8 (4)
C(5)—C(6)—O(7)—C(8)	179.0 (4)	C(15)—N(1)—C(16)—C(17)	72.5 (5)
C(6)—O(7)—C(8)—C(9)	-162.7 (4)	N(1)—C(16)—C(17)—O(18)	56.1 (5)
O(7)—C(8)—C(9)—N(10)	51.9 (5)	C(16)—C(17)—O(18)—C(19)	-175.8 (4)
C(8)—C(9)—N(10)—C(11)	77.9 (5)	C(17)—O(18)—C(19)—C(20)	93.0 (4)
C(8)—C(9)—N(10)—C(20)	-154.6 (4)	O(18)—C(19)—C(20)—N(10)	53.8 (5)
C(9)—N(10)—C(11)—C(12)	-154.4 (3)	C(19)—C(20)—N(10)—C(11)	-154.6 (4)
C(20)—N(10)—C(11)—C(12)	77.3 (4)	C(19)—C(20)—N(10)—C(9)	78.0 (4)

Table 3. Close contacts involving H atoms (Å) with *e.s.d.*'s in parentheses

X—H...Y	X...Y	Y—H	H...Y	Symmetry operator for Y
<b>(a) Intramolecular</b>				
N(1)—H(1)...O(4)	2.680 (5)	0.86 (3)	2.11 (3)	$x, y, z$
N(1)—H(1)...O(13)	2.868 (5)	0.86 (3)	2.43 (4)	$x, y, z$
N(1)—H(1)...O(18)	2.800 (4)	0.86 (3)	2.39 (3)	$x, y, z$
N(10)—H(10)...O(7)	2.721 (4)	0.91 (3)	2.18 (3)	$x, y, z$
N(10)—H(10)...O(13)	2.764 (4)	0.91 (3)	2.24 (3)	$x, y, z$
N(10)—H(10)...O(18)	2.841 (5)	0.91 (3)	2.41 (4)	$x, y, z$
<b>(b) Intermolecular</b>				
O(1W)—H(11W)...Cl(2)	3.150 (4)	1.04 (5)	2.11 (5)	$-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$
O(1W)—H(12W)...Cl(1)	3.214 (5)	1.26 (8)	2.12 (6)	$x, y, z$
O(2W)—H(21W)...Cl(2)	3.179 (4)	0.81 (6)	2.38 (6)	$1 - x, 1 - y, -z$
O(2W)—H(22W)...Cl(2)	3.186 (4)	0.92 (5)	2.27 (5)	$x, y, z$

Fig. 2. Unit cell of the cryptate (2.1.1).2HCl.2H<sub>2</sub>O projected onto the *xy* plane (SCHAKAL stereo representation).

The average lengths of the C—C, C—O and C—N bonds are 1.504 (11), 1.427 (8) and 1.504 (10) Å, respectively. In a previously determined (2.1.1) cryptate diperchlorate (Cox *et al.*, 1982), these quantities were very similar for C—O and C—N [1.419 (11) and 1.501 (4) Å], but significantly smaller for C—C [1.486 (11) Å]. In a LiI (2.1.1) complex with non-protonated N atoms (Moras & Weiss, 1973) C—N was smaller [1.474 (17) Å] as expected, whereas C—C and C—O had averages of 1.505 (3) and 1.420 (4) Å.

The cryptate cation has the *endo-endo* conformation with the N—H bonds pointing inwards. This clearly most stable conformation has already been found for both (2.1.1) cryptates mentioned above. The conformation around all C—C bonds in the cryptate is *gauche* so as to avoid steric hindrance between the methylene H atoms. There are pure *trans* arrangements along C(3)—O(4) and O(7)—C(8) of the eight-membered chain C(2)...C(9) and a total of four *trans* arrangements in the twelve-membered ring containing N(1), O(13), N(10) and O(18), being located at N(1)—C(15), O(13)—C(12), N(10)—C(20) and O(18)—C(17). So the twelve-membered ring has the same conformation as free cyclododecane, as was previously mentioned by Cox

*et al.* (1982). A comparison of the present cryptate spatial structure with its diperchlorate salt shows almost no difference. This also holds for the non-protonated LiI complex (Moras & Weiss, 1973). This complex has crystallographic C<sub>2</sub> symmetry, which is also present in the two protonated complexes to a good approximation but is not crystallographically active.

The two protons on N(1) (Fig. 1) and N(10) have three close contacts to the four oxygen atoms inside the cryptate, so that O(13) and O(18) are engaged in two N—H...O contacts. As shown in Table 3, the N(1)—H(1)...O(4) and N(10)—H(10)...O(7) contacts are the stronger ones with smaller H...O and N...O distances. With respect to these contacts the O atoms in the cryptate play a different role, so that O(13) and O(18) in the twelve-membered ring are distinguishable from O(4) and O(7) in the eight-membered chain. In this connection it may be noticed that the bond angles at O(13) and O(18) are 1.5° smaller than those at O(4) and O(7), which is just at the significance limit.

The two Cl<sup>-</sup> anions and the two water molecules are related by a total of four hydrogen bonds (see Table 3) with all water H atoms acting as donors, with Cl(2) being the acceptor in three cases but Cl(1) only once (see Fig. 2). The differences of the anion-cation interactions in the chloride and perchlorate complex are obviously too small to cause a difference in the conformation of the macrocation. This result corresponds to the experiments of high-resolution NMR investigations in solution (to be published). In contrast, the NMR spectra of the diprotonated (2.2.2.) cryptate show a significant anion effect. Unfortunately no single crystals of these complexes suitable for X-ray structure analysis have been obtained up to now.

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## Structure of Hexamethylhexahydropyrropetrocarpan

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**Abstract.** 1,2,7a,10,11,14a-Hexahydro-3,3,7,7,9,9-hexamethyl-3*H*,7*H*,9*H*-[1]benzopyrano[8',7':4,5]furo[3,2-*c*]pyrano[3,2-*g*][1]benzopyran, C<sub>27</sub>H<sub>32</sub>O<sub>4</sub>, m.p. 422–423 K, *M<sub>r</sub>* = 420.55, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 9.984 (2), *b* = 17.632 (1), *c* = 13.223 (1) Å, β = 100.57 (1)°, *V* = 2288.25 (4) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.220, *D<sub>m</sub>* = 1.235 Mg m<sup>-3</sup> (by flotation in CCl<sub>4</sub>/C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>), λ(Cu Kα) = 1.5418 Å, μ = 0.56 mm<sup>-1</sup>, *F*(000) = 904, *T* = 296 K, final *R*, *wR* 0.0401, 0.0506, respectively, for 2665 observed reflections. The benzofuro-benzopyran (*C/D*) ring junction is *cis* and the conformation is staggered looking from C(7) to C(7*a*). Three atoms in ring *F* occupy two positions each with s.o.f.'s 0.7 and 0.3. The dihedral angle between the aromatic rings [37.3 (2)°] is close to that reported for analogous antifungal-active natural products.

**Introduction.** Heterocyclic compounds with the basic benzofuro-benzopyran structure have two asymmetric centers [C(7*a*), C(14*a*)]. At the junction the

conformation can be *H,H-cis* or *-trans*. From <sup>1</sup>H NMR, the coupling constant between two protons (7.3 Hz) characterizes the *H,H-cis* conformation. A *cis*-fused benzofuro-benzopyran (*C/D*) ring junction can have two possible conformations, corresponding to the relative orientations of the methyl group attached to C(7) and the H atom attached to C(7*a*); the most stable is the staggered one (Pachler & Underwood, 1967). A number of structurally related oxygen heterocyclic compounds have been reported to be biologically active, exhibiting antifungal and antitumor activity (Vanetten, 1976; Kojima, Fukushima, Ueno & Saiki, 1970). This activity may depend on the molecular geometry (Perrin & Cruickshank, 1969).

The basic interest in analysing the detailed crystal structure of the title compound by X-ray diffraction methods was to confirm the geometry of the benzofuro-benzopyran system when affected by two pyran rings attached to their sides (Fig. 1). The structure is compared with analogous reported structures.

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