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Synthesis and Structure of Thorium Chloride–1,4,7,10,13-Pentaoxacyclopentadecane–Water–Methanol–Acetonitrile (1/1/2/2/1), [ThCl₄(OHMe)₂(OH₂)₂].15-Crown-5.CH₃CN*

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Abstract. Diaquatetrachlorobis(methanol)thorium(IV)–15-crown-5–acetonitrile, [ThCl₄(CH₃O)₂(OH₂)₂].C₁₀H₂₀O₅.C₂H₃N, *M_r* = 735.3, monoclinic, *P*2₁/*n*, *a* = 8.686 (1), *b* = 18.620 (2), *c* = 16.043 (3) Å, β = 99.56 (1)°, *V* = 2558 Å³, *Z* = 4, *D_x* = 1.91 g cm⁻³, λ(Mo Kα) = 0.71073 Å, μ = 59.9 cm⁻¹, *F*(000) = 1424, *T* = 123 K, *R* = 0.045 for 3387 independent observed [*F_o* ≥ 5σ(*F_o*)] reflections. The Th^{IV} ion is eight-coordinate with approximate dodecahedral geometry. The four Cl atoms occupy *A* sites [Th–Cl average = 2.710 (7) Å] with the remaining *B* sites occupied by two water molecules [Th–O average = 2.527 (4) Å] and two methanol groups [Th–O average = 2.562 (3) Å]. The water and methanol groups are hydrogen-bonded to symmetry-related crown-ether molecules forming polymeric chains. One O atom of the crown molecule accepts two hydrogen bonds which has an interesting effect on this molecule's conformation. The acetonitrile molecule has close contacts suggesting hydrogen bonds with two of the Cl atoms from different asymmetric units, thus bridging the polymeric chains.

Introduction. In our investigation into *f*-element/crown-ether complexation we have tried to find clues to the effects of such variables as metal-ion size, crown-

ether-cavity size, crown-ether conformation, anion, solvent, conditions of reaction, and method of crystallization on the actual complexation of the crown ether directly to the metal ion. Since a study of various metal-ion sizes in the actinide series is difficult for us to accomplish limited to thorium and uranium, we have concentrated on investigations of changing the anion and solvent for these metals. Although examples of crown ethers coordinated directly to uranium have been reported (see, for example, de Villardi, Charpin, Costes, Folcher, Plurien, Rigny & de Rango, 1978; Navaza, Villain & Charpin, 1984; Dejean, Charpin, Folcher, Rigny, Navaza & Tsoucaris, 1987), we have only managed to crystallize second-sphere hydrogen-bonded complexes such as [Th(NO₃)₄(OH₂)₃].18-crown-6 (Rogers, Kurihara & Benning, 1987*a*), [ThCl₄(OH₂)₃(OH₂)].18-crown-6.H₂O (Rogers, Kurihara & Benning, 1988), [UO₂(OH₂)₅](ClO₄)₂.2(18-crown-6).H₂O.CH₃CN, and [UO₂(OH₂)₃](ClO₄)₂.3(15-crown-5).CH₃CN (Rogers, Kurihara & Benning, 1987*b*). The isolation and structural characterization of the title complex gives us this opportunity to compare the effects of methanol *versus* ethanol in the primary coordination sphere of similar complexes – [ThCl₄(OHMe)₂(OH₂)₂].15-crown-5.CH₃CN and [ThCl₄(OH₂)₃(OH₂)].18-crown-6.H₂O.

Experimental. Under Ar, 10 mmol of 15-crown-5 in 25 mL of a 3:1 mixture of acetonitrile:methanol was added to a stirring solution of 10 mmol of ThCl₄.*n*H₂O

* *f*-Element/Crown Ether Complexes. 19. Part 18: Rogers (1988).

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in 25 mL of the same solvent. The reaction mixture was heated to 333 K for 24 h, cooled to 295 K, and concentrated to 25 mL. Contents were transferred to a capped flask and stored at 278 K. A greyish crust formed at the bottom of the flask after 10 days and transparent single crystals of the title complex were found embedded in this crust. Crystals of the title complex decompose slowly over a period of 24 h.

Crystal 0.15 × 0.20 × 0.20 mm. D_m not measured. Enraf-Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$. Cell constants from setting angles of 25 reflections ($\theta > 20^\circ$). Corrections for Lorentz-polarization effects and for absorption (empirical), range of relative transmission factors 82.3/100%. $\theta_{\max} = 25^\circ$; h 0–10, k 0–22, l –19–19. Three standard reflections, no intensity variation. 4923 reflections measured, 3387 independent observed reflections [$F_o \geq 5\sigma(F_o)$]. Structure solved *via* Patterson function and subsequent difference Fourier techniques. Crown-ether H atoms placed 0.95 Å from the bonded C atom with a fixed isotropic thermal parameter $B = 5.5 \text{ \AA}^2$ and allowed to ride with the C–H distance fixed. The remaining H atoms were not located. Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); structure refined with *SHELX76* (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ was minimized, weights = $[\sigma(F_o)]^{-1}$, 257 parameters varied. $R = 0.045$, $wR = 0.050$, $S = 1.6$. Δ/σ in final least-squares refinement cycle < 0.01 , $\Delta\rho < 1.2 \text{ e \AA}^{-3}$ (near Th) in final difference map.

Discussion. The final atomic coordinates are given in Table 1,* the interatomic distances and angles in Table 2. The thorium coordination environment and hydrogen-bonding contacts are depicted in the *ORTEP* (Johnson, 1976) illustration, Fig. 1, with the overall polymeric nature of the complex revealed in the cell packing diagram Fig. 2.

The Th atom is eight-coordinate with approximate dodecahedral geometry, the Cl atoms in *A* sites, the O atoms in *B* sites. The two trapezoids are planar to within 0.096 [Cl(2), Cl(3), O(2), O(4)] and 0.012 Å [Cl(1), Cl(4), O(1), O(3)] with a dihedral angle between the two of 89.8°. Cl(1) and Cl(4) have close contacts with C(14) indicative of interaction with the CH₃CN molecule [Cl...C(14) = 3.26 (3) Å average]; however, the Th–Cl distances seem to be paired irrespective of this with average distances of 2.716 (1) [Cl(1), Cl(2)] and 2.702 (2) Å [Cl(3), Cl(4)]. In [ThCl₄(OH₂)₃-

Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters for [ThCl₄(OHMe)₂(OH₂)₂].15-crown-5.CH₃CN*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}^*(\text{\AA}^2)$
Th	0.24017 (5)	0.32043 (2)	0.13721 (2)	0.012
Cl(1)	0.1364 (3)	0.3887 (2)	0.2669 (2)	0.019
Cl(2)	0.0736 (4)	0.1992 (2)	0.1535 (2)	0.023
Cl(3)	0.2939 (4)	0.4332 (2)	0.0398 (2)	0.028
Cl(4)	0.4729 (3)	0.2412 (2)	0.0914 (2)	0.021
O(1)	–0.0387 (9)	0.3623 (4)	0.0820 (5)	0.021
O(2)	0.4759 (9)	0.3903 (4)	0.2146 (5)	0.020
O(3)	0.1347 (9)	0.2829 (4)	–0.0125 (4)	0.016
O(4)	0.3809 (9)	0.2602 (4)	0.2697 (5)	†
O(5)	0.3906 (9)	0.3087 (4)	0.4354 (5)	0.019
O(6)	0.301 (1)	0.1721 (4)	0.4266 (5)	0.024
O(7)	0.4955 (9)	0.1221 (4)	0.3130 (5)	0.020
O(8)	0.7526 (9)	0.2134 (4)	0.3379 (4)	0.016
O(9)	0.6364 (9)	0.3524 (4)	0.3686 (5)	0.018
C(1)	0.247 (1)	0.2915 (7)	0.4688 (7)	0.023
C(2)	0.178 (1)	0.2235 (6)	0.4219 (7)	0.018
C(3)	0.259 (1)	0.1119 (6)	0.3727 (7)	0.021
C(4)	0.408 (1)	0.0748 (7)	0.3614 (7)	0.026
C(5)	0.648 (1)	0.0974 (7)	0.3139 (7)	0.022
C(6)	0.741 (2)	0.1559 (7)	0.2782 (8)	0.032
C(7)	0.801 (2)	0.2779 (7)	0.3015 (8)	0.029
C(8)	0.795 (1)	0.3376 (7)	0.3656 (8)	0.030
C(9)	0.608 (1)	0.3875 (7)	0.4472 (7)	0.022
C(10)	0.440 (1)	0.3827 (6)	0.4492 (8)	0.022
C(11)	–0.174 (1)	0.3933 (7)	0.1109 (7)	0.024
C(12)	0.514 (2)	0.4663 (7)	0.2209 (8)	0.033
N	–0.176 (2)	0.5408 (7)	0.4143 (8)	0.051
C(13)	–0.053 (2)	0.5465 (7)	0.4006 (9)	0.035
C(14)	0.107 (2)	0.5503 (8)	0.3849 (9)	0.038

* $U_{eq} = (U_{11} + U_{22} + U_{33})/3$.

† Refined isotropically.

(OH₂).18-crown-6.H₂O (Rogers *et al.*, 1988), two of the three ethanol moieties form bifurcated inter- and intramolecular hydrogen bonds with only two of the four unique Cl atoms resulting in a square antiprismatic geometry and inequivalence in the average Th–Cl separations [2.790 (4) Å for the hydrogen-bonded Cl atoms and 2.694 (3) Å for the remaining two]. The third ethanol group and the coordinated water molecule are hydrogen-bonded to the non-coordinated water molecule and to the 18-crown-6 molecule, as are all of the hydrogen-bond donors in the coordination sphere of the title complex. The average of all four Th–Cl distances in the title complex [2.710 (7) Å] is shorter than observed in [ThCl₄(OH₂)₃(OH₂).18-crown-6.H₂O [2.74 (5) Å] and the Th–O separations are correspondingly longer: Th–OHMe = 2.562 (3), Th–OH₂ = 2.527 (4) Å in the title complex *versus* Th–OH₂ = 2.52 (2), Th–OH₂ = 2.453 (7) Å in the above-mentioned 18-crown-6 complex.

One of the more interesting aspects of the title complex involves the crown-ether conformation. There are three hydrogen bonds (from one water molecule and one methanol group) on each side of the crown molecule. O(5) accepts two hydrogen bonds (one on each side) from the water molecules. When 15-crown-5 accepts hydrogen bonds on each side it can adopt a near D_{3d} conformation as usually observed for 18-

* Lists of structure factors, anisotropic thermal parameters, calculated H-atom coordinates, least-squares-planes results, torsion angles and hydrogen-bonding-contact geometries have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44639 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Bond distances (Å) and angles (°) for $[\text{ThCl}_4(\text{OHMe})_2(\text{OH}_2)_2] \cdot 15\text{-crown-5} \cdot \text{CH}_3\text{CN}$

Th-Cl(1)	2.716 (3)	Th-Cl(2)	2.717 (3)
Th-Cl(3)	2.704 (3)	Th-Cl(4)	2.701 (3)
Th-O(1)	2.559 (8)	Th-O(2)	2.565 (8)
Th-O(3)	2.523 (7)	Th-O(4)	2.531 (7)
O(1)-C(11)	1.46 (1)	O(2)-C(12)	1.45 (1)
O(5)-C(1)	1.47 (1)	O(5)-C(10)	1.45 (1)
O(6)-C(2)	1.43 (1)	O(6)-C(3)	1.43 (1)
O(7)-C(4)	1.47 (1)	O(7)-C(5)	1.40 (1)
O(8)-C(6)	1.43 (1)	O(8)-C(7)	1.43 (1)
O(9)-C(8)	1.41 (1)	O(9)-C(9)	1.48 (1)
C(1)-C(2)	1.54 (2)	C(3)-C(4)	1.50 (2)
C(5)-C(6)	1.52 (2)	C(7)-C(8)	1.52 (2)
C(9)-C(10)	1.47 (2)	N-C(13)	1.12 (2)
C(13)-C(14)	1.46 (2)		
Cl(1)-Th-Cl(2)	93.74 (9)	Cl(1)-Th-Cl(3)	101.0 (1)
Cl(2)-Th-Cl(3)	147.84 (9)	Cl(1)-Th-Cl(4)	145.34 (8)
Cl(2)-Th-Cl(4)	90.4 (1)	Cl(3)-Th-Cl(4)	93.3 (1)
Cl(1)-Th-O(1)	72.9 (2)	Cl(2)-Th-O(1)	78.4 (2)
Cl(3)-Th-O(1)	78.9 (2)	Cl(4)-Th-O(1)	141.3 (2)
Cl(1)-Th-O(2)	74.4 (2)	Cl(2)-Th-O(2)	140.3 (2)
Cl(3)-Th-O(2)	71.7 (2)	Cl(4)-Th-O(2)	80.5 (2)
O(1)-Th-O(2)	130.3 (3)	Cl(1)-Th-O(3)	138.1 (2)
Cl(2)-Th-O(3)	75.3 (2)	Cl(3)-Th-O(3)	74.6 (2)
Cl(4)-Th-O(3)	76.1 (2)	O(1)-Th-O(3)	65.3 (2)
O(2)-Th-O(3)	137.3 (2)	Cl(1)-Th-O(4)	74.9 (2)
Cl(2)-Th-O(4)	75.0 (2)	Cl(3)-Th-O(4)	136.4 (2)
Cl(4)-Th-O(4)	73.0 (2)	O(1)-Th-O(4)	136.3 (2)
O(2)-Th-O(4)	65.4 (2)	O(3)-Th-O(4)	136.5 (2)
Th-O(1)-C(11)	141.3 (6)	Th-O(2)-C(12)	133.0 (7)
C(1)-O(5)-C(10)	113.4 (9)	C(2)-O(6)-C(3)	112.1 (9)
C(4)-O(7)-C(5)	111.8 (9)	C(6)-O(8)-C(7)	110.4 (9)
C(8)-O(9)-C(9)	114.6 (9)	O(5)-C(1)-C(2)	106.8 (9)
O(6)-C(2)-C(1)	107.1 (9)	O(6)-C(3)-C(4)	107 (1)
O(7)-C(4)-C(3)	109 (1)	O(7)-C(5)-C(6)	109 (1)
O(8)-C(6)-C(5)	106 (1)	O(8)-C(7)-C(8)	107 (1)
O(9)-C(8)-C(7)	108 (1)	O(9)-C(9)-C(10)	107.4 (9)
O(5)-C(10)-C(9)	109 (1)	N-C(13)-C(14)	177 (2)

crown-6 [where all O-C-C-O torsion angles alternate $\pm g$ ($\pm 60^\circ$) and all C-O-C-C angles are *anti* (180°)]. The lower symmetry of 15-crown-5 requires two consecutive O-C-C-O angles to be of the same sign and this occurs for O(5)-C(1)-C(2)-O(6) (49.6°) and O(9)-C(9)-C(10)-O(5) (51.5°). Typically one of the two C-O-C-C angles between two such C-C angles of like sign deviates toward a *gauche* conformation. See, for example, $[\text{Y}(\text{OH}_2)_8]\text{Cl}_3 \cdot 15\text{-crown-5}$ (Rogers & Kurihara, 1987), $[\text{Y}(\text{NO}_3)_3(\text{OH}_2)_3] \cdot 1.5\text{-}(15\text{-crown-5}) \cdot \text{Me}_2\text{CO}$ (Rogers, Royal & Bolton, 1987), and $[\text{CuBr}_2(\text{OH}_2)_2] \cdot 15\text{-crown-5}$ (Arte, Feneau-Dupont, Declercq, Germain & Van Meerssche, 1979). In the title complex, both angles around O(5) are much closer to an *anti* conformation and both are distorted by approximately the same amount [C(9)-C(10)-O(5)-C(1) = 156.8° , C(10)-O(5)-C(1)-C(2) = 159.2°]. A greater distortion of crown conformation in $[\text{Dy}(\text{OH}_2)_8]\text{Cl}_3 \cdot 18\text{-crown-6} \cdot 4\text{H}_2\text{O}$ (Rogers, 1987b) allows one O atom to accept two hydrogen bonds on the same side of the ether ring. The conformational changes in the 15-crown-5 molecule in the title complex have little effect on overall bonding parameters: C-O = 1.44 (3), C-C = 1.51 (2) Å average, C-O-C = 112 (1), and O-C-C = 108 (1)° average.

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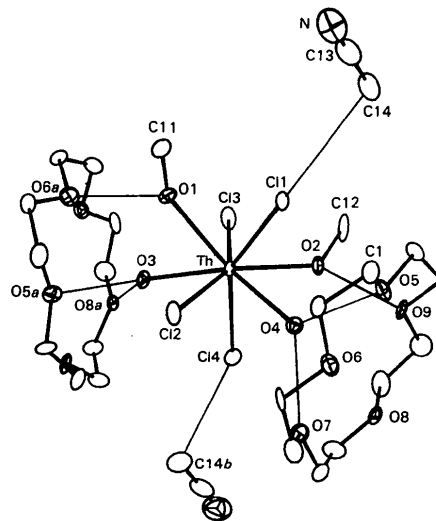
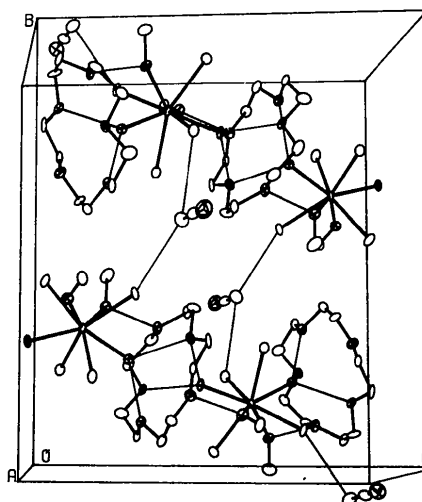
Fig. 1. $[\text{ThCl}_4(\text{OHMe})_2(\text{OH}_2)_2] \cdot 15\text{-crown-5} \cdot \text{CH}_3\text{CN}$. 50% probability ellipsoids for thermal motion. H atoms omitted.

Fig. 2. Cell packing diagram.

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Structure of Diaqua[1,6-bis(4-imidazolyl)-2,5-dithiahexane]nickel(II) Dinitrate

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Abstract. [Ni(C₁₀H₁₄N₄S₂)(H₂O)₂](NO₃)₂, $M_r = 473.12$, triclinic, $P\bar{1}$, $a = 10.306$ (2), $b = 10.483$ (2), $c = 10.791$ (2) Å, $\alpha = 62.46$ (1), $\beta = 64.66$ (1), $\gamma = 65.22$ (1)°, $V = 897.9$ (3) Å³, $Z = 2$, $D_x = 1.750$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 13.6$ cm⁻¹, $F(000) = 448$, $T = 293$ K, final $R = 0.036$ for 2666 observed reflections. The Ni^{II} ion is octahedrally coordinated by two imidazole N atoms and two thioether S atoms of the ligand 1,6-bis(4-imidazolyl)-2,5-dithiahexane, and two O atoms of coordinating water molecules. The Ni–N distances are 2.027 (3) and 2.050 (3) Å, the Ni–S distances 2.448 (1) and 2.453 (1) Å, and the Ni–O(aqua) distances 2.077 (2) and 2.084 (3) Å. The non-coordinating nitrate ions are hydrogen-bonded to the nitrogen H atoms of the imidazole groups of the ligand and to the water molecules, forming chains of cations in the structure.

Introduction. Coordination compounds with imidazole- and thioether-containing ligands are important as model systems for type I copper proteins. Recently a new method of synthesizing this kind of ligand has been developed (Bouwman & Driessen, 1988). One of the first ligands of this new series used in the preparation of coordination compounds is 1,6-bis(4-imidazolyl)-2,5-dithiahexane (bhdhx). The synthesis and characterization of several transition-metal compounds of bhdhx have been described recently (Bouwman, ten Hove, Driessen & Reedijk, 1988). The complexes with copper and nickel nitrates appeared to be X-ray isomorphous and the crystal structure of the copper compound [Cu(bhdhx)(NO₃)₂] has been determined (Bouwman, ten Hove, Driessen & Reedijk, 1988). A second modification of the nickel nitrate compound has been crystallized, and shows Weissenberg photographs different from those of the copper nitrate compound. The crystal structure of this compound, with stoichiom-

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