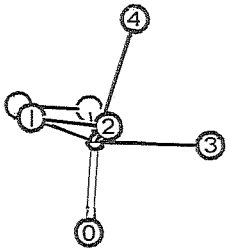
the "free" H_2O and the other the apical H_2O of the Mo moiety. A fifth oxygen of the crown is hydrogen bonded to the equatorial H_2O of the Mo moiety, which is itself also hydrogen bonded to the "free" H_2O; the sixth crown oxygen does not participate in hydrogen bonding.

Computational support from the OSU Computer Center is acknowledged.



Mo-O distances (Å) :		
=O (ap.)	(0)	1.647(5)
-O (peroxo)	(1)	1.900(4)
-O (peroxo)	(2)	1.920(3)
$-OH_2$ (eq.)	(3)	2.084(5)
$-OH_2$ (ap.)	(4)	2.325(4)
Mo to L.S. plane of equatorial O and H_2O (Å)		0.359

09.4–27 CRYSTAL STRUCTURE OF A BASIC THORIUM DICHLOROACETATE $[Th_6(O_2CCHCl_2)_{12}(OH)_{12}(OH_2)_2]$, A NOVEL OLIGOMERIC STRUCTURE. By E.Towns and A.J. Smith, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, England.

While studying carboxylate compounds of thorium, we obtained crystals of the title compound by reacting thorium hydroxide with excess dichloroacetic acid and recrystallising the product from ethanol. *Crystal data* Monoclinic $P2_1/n$, a = 15.087(9)Å, b = 15.111(11), c = 16.084(5) Å, β = 99.73(4)°, V = 3614 Å^3, Z = 4, μ = 158.6 cm^{-1} D_m = 2.85, D_x = 2.90 g cm^{-3}; 1950 unique data with $2\theta < 50°$ and $I > 3\sigma(I)$ collected on Syntex R3 diffractometer and corrected for crystal decay and X-ray absorption. The structure was solved by Patterson and difference Fourier methods and refined to a current R of 0.061. H atoms have not been detected and so OH and H_2O are distinguished only on chemical grounds.

The complex forms discrete molecules (Fig.3). The thorium atoms are at the vertices of a nearly regular octahedron, with an oxygen (presumed to be OH) above the centre of each face. These thorium and oxygen atoms together mark the 14 vertices of a rhombic dodecahedron (Fig.1). Each edge of the octahedron is spanned by a dichloroacetate group (Fig.5). The relationship of these bridges is more clearly seen in Fig.2 (carbon and chlorine omitted). Each of the remaining 6 oxygens (4OH & $2H_2O$) is attached to one of the octahedron vertices. The 6 thorium atoms with all their attached oxygens are shown in Fig.4. Each thorium atom is coordinated to 9 oxygens at the vertices of a monocapped square antiprism (1.4/4) having $\theta_1 = 64.9°$ and $\theta_2 = 127.5°$.

We thank the SERC and the Chemistry Division of AERE Harwell for a CASE Studentship awarded to one of us (ET).

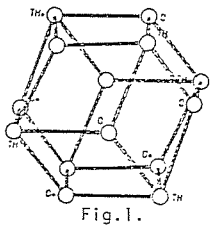


Fig.1.

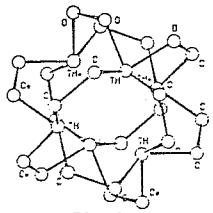


Fig.2.

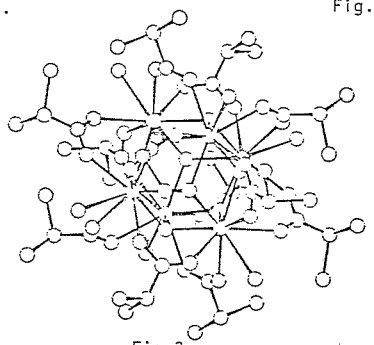


Fig.3.

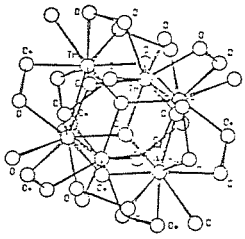


Fig.4.

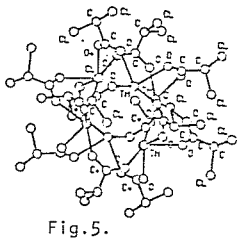


Fig.5.