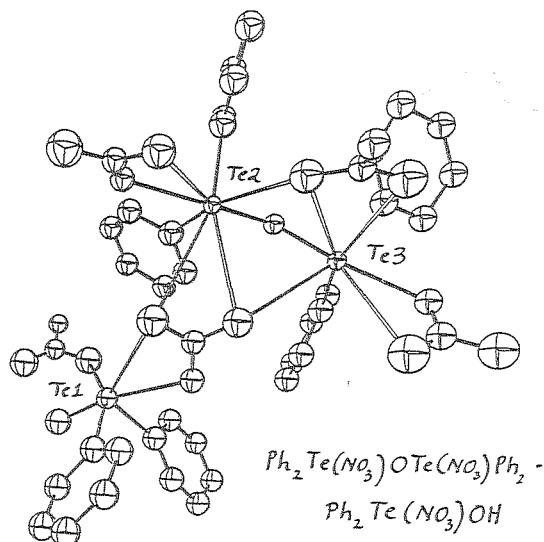


has square pyramidal coordination about Te (apical phenyl, 4 basal chlorines). This shows only long intermolecular non-directed Te-Cl contacts. In (4) a secondary Te---Cl bond occurs ( $3.68\text{\AA}$ ), *trans* to a phenyl group. Both (1) and (2) have complex arrangements of Te---O interactions around the vacant position of the trigonal bipyramid (Te---O  $3.1\text{--}3.35\text{\AA}$  in (1)). These are illustrated in the diagram showing the molecular structure of (1).



**09.3-18** THE CRYSTAL STRUCTURE OF TRIS-(4,7,9-TRIMETHYLINDENYL)THORIUM CHLORIDE. By M.R. Spirlet, Laboratoire de Physique Expérimentale, Université de Liège au Sart Tilman, B.4000, Liège, Belgium, J. Rebizant, Commission of the European Communities, Joint Research Centre, Karlsruhe Establishment, European Institute for Transuranium Elements, Postfach 2266, D-7500, Karlsruhe, F.R.G. and J. Goffart, Institut de Radiochimie, Université de Liège au Sart Tilman, B.4000, Liège, Belgium.

Within the field of coordination chemistry of the actinide elements, the X-ray crystal structure analysis of the title compound was undertaken to clarify the role of the thorium atom in an environment of five- and six-membered conjugated ring systems.  $\text{Th}(\text{C}_{12}\text{H}_{13})_3\text{Cl}$

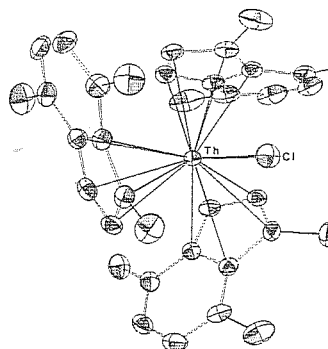
crystallizes in space group  $P2_1/c$  with cell

dimensions  $a = 9.781(2)$ ,  $b = 16.565(2)$ ,

$c = 18.913(2)$  Å,  $\beta = 100.96(1)^\circ$  and

$\rho_{\text{calc}} = 1.632\text{ g cm}^{-3}$  for  $Z = 4$ . Intensities of 5451 independent reflections were measured with an ENRAF-NONIUS CAD4 diffractometer using MoK $\alpha$  radiation. The structure was solved by direct method. Full-matrix least-squares refinement, on 3792 reflections for which  $I \geq 3\sigma(I)$ , with all atoms treated anisotropically, except H atoms gave a conventional R factor of 0.03. Coordination about the thorium atom is a slightly distorted tetrahedron: The tho-

rium atom is bonded to the chlorine atom, with a Th-Cl bond length of  $2.665(1)$  Å, and to the carbon atoms of each five-membered ring of the three indenyl moieties, with Th-C distances ranging from  $2.720(5)$  Å to  $2.976(5)$  Å. The character of the metal-ligand bonding will be discussed and compared with that found in similar organoactinides and-lanthanides compounds.



**09.4-01** A STRUCTURAL COMPARISON BETWEEN FOUR ALKALI-METAL DITHIOCARBAMATE HYDRATES. By I. Ymén. *Inorganic Chemistry, Chemical Center, University of Lund, P.O.B. 740, S-220 07 Lund, Sweden.*

The crystal structures of metal-dithiocarbamate complexes have been extensively studied during the past 10-20 years. So far, however, only two alkali-metal dithiocarbamate structures have been published;  $\text{NaS}_2\text{CN}(\text{C}_2\text{H}_5)_2 \cdot 3\text{H}_2\text{O}$  (Colapietro, Domenicano and Vaciano, *Chem. Comm.* (1968) 572-573) and  $\text{NaS}_2\text{CN}(\text{CH}_2)_4 \cdot 2\text{H}_2\text{O}$  (Albertsson, Oskarsson, Ståhl, Svensson and Ymén, *Acta Cryst.* (1980) B36, 3072-3078). These compounds provide information on the geometry of the dithiocarbamate ligand in structures with small metal-ligand interactions.  $\text{NaS}_2\text{CN}(\text{CH}_2)_4 \cdot 2\text{H}_2\text{O}$  has also been refined using neutron data collected at 295 K to an R-value of 0.069. The heavy atom structure is almost identical to the X-ray structure.

The crystal structures of  $\text{NaS}_2\text{CN}(\text{CH}_3)_2 \cdot 2\text{H}_2\text{O}$  (Monoclinic,  $P2_1/a$ ,  $a = 11.981(1)$ ,  $b = 5.871(2)$ ,  $c = 12.878(1)$  Å,  $\beta = 113.62(1)^\circ$ ,  $V = 829.9$  Å<sup>3</sup>,  $D_x = 1.434$  g·cm<sup>-3</sup>,  $M_r = 179.24$ ) and  $\text{LiS}_2\text{CN}(\text{CH}_2)_4 \cdot 4\text{H}_2\text{O}$  (Monoclinic,  $P2_1/n$ ,  $Z = 4$ ,  $a = 10.279(1)$ ,  $b = 9.989(3)$ ,  $c = 11.291(1)$  Å,  $\beta = 93.03(1)^\circ$ ,  $V = 1157.8$  Å<sup>3</sup>,  $D_x = 1.292$ ,  $D_m$  (flotation) =  $1.304$  g·cm<sup>-3</sup>,  $M_r = 225.25$ ) have now been determined from X-ray intensities and refined to  $R = 0.034$  and  $0.032$  respectively. The first compound is very similar to  $\text{NaS}_2\text{CN}(\text{CH}_2)_4 \cdot 2\text{H}_2\text{O}$  while the other consists of  $\text{Li}(\text{H}_2\text{O})_4^+$  tetrahedra and  $\text{S}_2\text{CN}(\text{CH}_2)_4^-$  units kept together by O-H...S hydrogen bonds. The four alkali-metal dithiocarbamate hydrates so far investigated will be compared. The discussion will include geometric features, thermal motion and O-H...S hydrogen bonds.