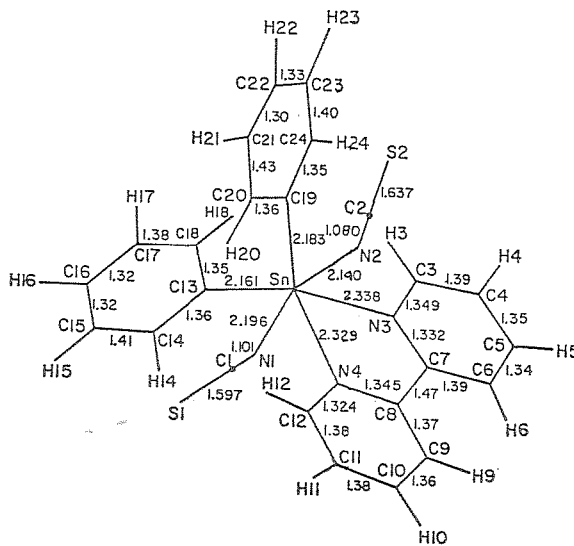
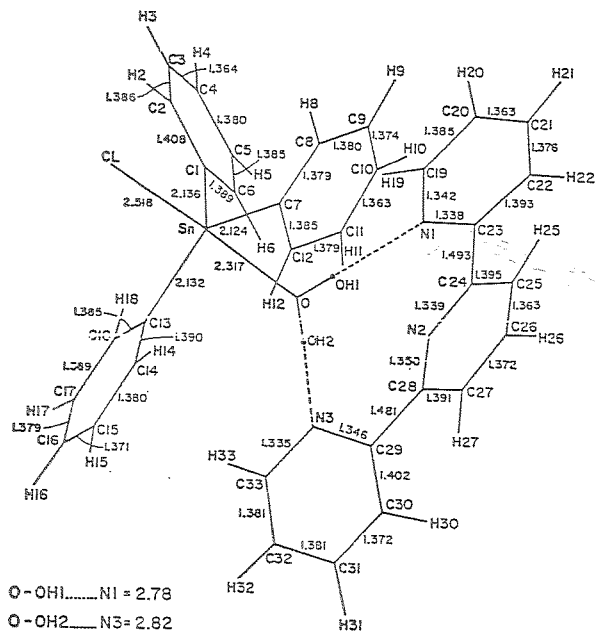


by hydrogen bonds between the N atoms of its two outer rings and the water molecule oxygen.



09.3-16 THE CRYSTAL STRUCTURE OF 2,2'-BIPYRIDYL DIPHENYL DIISOTHIOCYANATO TIN (IV). By L. Prasad, E.J. Gabe and Y. Le Page, Chemistry Division, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada and F.E. Smith, Chemistry Department, Kenyatta University College, P.O. Box 43844, Nairobi, Kenya.

White crystals of $C_{24}H_{20}N_4S_2Sn$ were obtained by adding 2,2'-bipyridyl to an ethanolic solution of diphenyl tin diisothiocyanate. The crystals are monoclinic, space group $P2_1/n$ $a = 10.722(3)$, $b = 15.752(4)$, $c = 14.131(2)$ Å $\beta = 92.32^\circ(2)$, $Z = 4$, $D_{calc} = 1.52$ Mg.m $^{-3}$. Intensities were measured with a four-circle Picker diffractometer using graphite monochromatised $MoK\alpha$ radiation. The Sn atom was found in an E-map based on phases derived by MULTAN (Germain, Main & Woolfson, Acta Cryst. (1971) A27, 368) and all the other non hydrogen atoms were located in a heavy atom phased Fourier map. The structure was refined by block diagonal least squares and the final R_F and R_{F_w} are .043 and .036 respectively.

The coordination around Sn is a distorted octahedron, similar to the structure of (2,2'-bipyridyl)-dichloro-diphenyl tin (Harrison, King & Richards, J. Chem. Soc. (1974), Dalton Transactions, 1723). The Sn atom is coordinated to the two N atoms of the bipyridyl group, the two phenyl groups and to the N atoms of the two (NCS) groups. The two phenyl groups are in the *cis* configuration. The structure confirms the earlier result obtained from dipole moment and Mössbauer data (Smith, Grant and Gray, J. Inorg. Nucl. Chem. (1979) 41, 629).

09.3-17 PRIMARY AND SECONDARY BONDING IN PHENYL TELLURIUM (IV) COMPOUNDS. By N.W. Alcock and W.D. Harrison, Department of Chemistry and Molecular Sciences, University of Warwick, Coventry, CV4 7AL, U.K.

The crystal structures of biphenyl and monophenyl nitrates and chlorides of Te(IV) have been determined. Under the preparation conditions used, both nitrates are formed as basic species. Unit cell and bond length data are as follows.

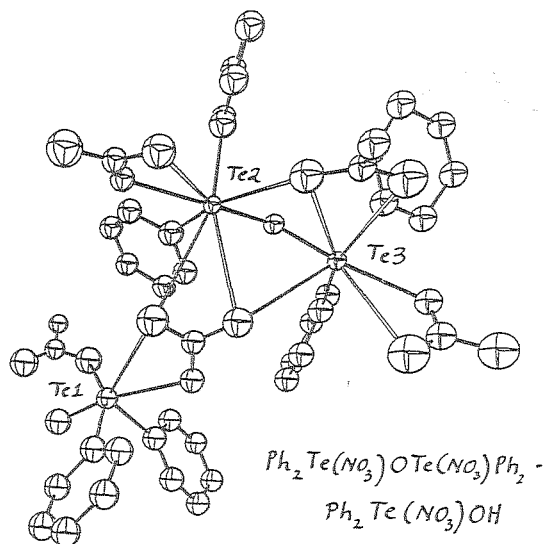
	Space Gp	Z	$a/\text{Å}$
1 $[\text{Ph}_2\text{Te}(\text{NO}_3)]_2 \cdot \text{O} \cdot \text{Ph}_2\text{Te}(\text{NO}_3)(\text{OH})$	$P\bar{1}$	2	11.839(3)
2 $[\text{PhTeO}(\text{NO}_3)]_n$	$P\bar{1}$	4	11.555(5)
3 $[\text{PhTeCl}_3]_n$	$P\bar{1}$	4	7.468(1)
4 $\text{Ph}_2\text{TeCl}_2^n$ (at 173K)	Pbca	8	7.644(2)

	$b/\text{Å}$	$c/\text{Å}$	$\alpha/^\circ$	$\beta/^\circ$	$\gamma/^\circ$
1	11.220(1)	14.793(2)	90.85(2)	100.98(2)	99.28(2)
2	5.350(2)	14.987(3)	94.89(3)	110.68(3)	106.07(3)
3	8.610(1)	13.987(2)	98.89(1)	92.10(1)	90.81(1)
4	18.160(3)	18.014(3)	90.00	90.00	90.00

R	Te-C (mean)	Te-X bridge (mean)	Te-X terminal (mean)	Te---O Te---Cl
1	2.3	2.112(6)	0: 1.978(4) OH: 1.957(5) NO $_3$: 2.479(4)	0: 317
2	4.2	2.12	0: 1.95	NO $_3$: 2.52
3	1.8	2.122(4)	Cl: 2.755(1)	Cl: 3.94
4	3.6	2.106(7)	-	Cl: 2.505(2) Cl: 3.68

Compounds (2) and (3) exist as linear polymers, involving respectively Te-O-Te and Te-Cl-Te bridges. Compounds (1) and (4) exist as molecular units in the crystal. The primary geometries about Te are trigonal bipyramidal with one vacant position for (1), (2) and (4), with the phenyl groups equatorial. Compound (3)

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\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 $3.1-3.35\text{\AA}$ 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. $\text{Th}(\text{C}_{12}\text{H}_{13})_3\text{Cl}$

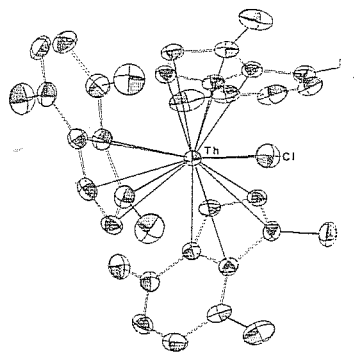
crystallizes in space group $P2_1/c$ with cell

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

$c = 18.913(2)\text{\AA}$, $\beta = 100.96(1)^\circ$ 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 α 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 $2.665(1)\text{\AA}$, and to the carbon atoms of each five-membered ring of the three indenyl moieties, with Th-C distances ranging from $2.720(5)\text{\AA}$ to $2.976(5)\text{\AA}$. 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 Vaciago, 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, $P2_1/a$, $a = 11.981(1)$, $b = 5.871(2)$, $c = 12.878(1)\text{\AA}$, $\beta = 113.62(1)^\circ$, $V = 829.9\text{\AA}^3$, $D_x = 1.434\text{ g cm}^{-3}$, $M_z = 179.24$) and $\text{LiS}_2\text{CN}(\text{CH}_2)_4 \cdot 4\text{H}_2\text{O}$ (Monoclinic, $P2_1/n$, $Z = 4$, $a = 10.279(1)$, $b = 9.989(3)$, $c = 11.291(1)\text{\AA}$, $\beta = 93.03(1)^\circ$, $V = 1157.8\text{\AA}^3$, $D_x = 1.292$, D_m (floatation) = 1.304 g cm^{-3} , $M_z = 225.25$) 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.