Le site prismatique de la file unique n'est que partiellement occupé, ce qui se traduit par un allongement des distances interatomiques moyennes Sn(3)—S: 3,11 Å au lieu de Sn(1)—S: 3,04 Å et Sn(2)—S: 3,03 Å. Les deux atomes Sn(1) et Sn(2) sont par contre très semblables, leurs sites prismatiques mettent en commun trois atomes de soufre, deux sur une arête du prisme et le troisième dans le plan équatorial.

La structure du composé $In_4Sn_5S_{26}$ se révèle identique à celle du composé $Pb_3In_{6,67}S_{13}$ (soit $In_{13,33}Pb_6S_{26}$) décrite par Ginderow (1978): les positions atomiques sont sensiblement identiques et l'unique différence porte sur les taux d'occupation de deux des sites atomiques. On observe en effet, pour deux sites correspondants, Sn(3) et Pb(1) d'une part, In(6) et site I d'autre part, les taux d'occupation suivants:

$In_{14}Sn_5S_{26}$	$In_{13,33}Pb_6S_{26}$ (Ginderow, 1978)
Sn(3): $\frac{1}{2}$ Sn + $\frac{1}{2}$ □	Pb(1): $\frac{2}{3}$ Pb + $\frac{1}{3}$ □
In(6): In pur	Site I: $\frac{2}{3}$ In + $\frac{1}{3}$ Pb.

Ainsi s'expliquent les différences de composition, bien que les structures soient isotypes. Il apparaît donc que ces structures sont dominées par la stabilité de l'édifice formé par les octaèdres d'indium, dans les interstices prismatiques desquels les atomes d'étain ou de plomb viennent s'insérer. Les occupations différentes de ces sites sont difficilement explicables, et demandent pour être interprétées une étude plus approfondie de ce type structural et des types semblables où interviennent des réseaux complexes formées par les octaèdres (InS_6).

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Structure of Silver Telluryl Nitrate, $AgTeO_2NO_3$

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Abstract. $M_r = 329{\cdot}5$, orthorhombic, $Pbcn$, $a = 5{\cdot}667$ (2), $b = 14{\cdot}202$ (8), $c = 5{\cdot}232$ (2) Å, $V = 421{\cdot}1$ (3) Å^3, $Z = 4$, $D_x = 5{\cdot}19$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 114{\cdot}2$ cm^{-1}, $F(000) = 584$, $T = 290$ K, final $R = 0{\cdot}034$ for 480 independent reflexions. The structure contains infinite TeO_2 chains, parallel to the c axis, connected by Ag^+ ions forming $AgTeO_2^+$ sheets. Successive sheets are separated by layers containing discrete NO_3^- ions.

Introduction. The increased metallic character of tellurium compared with sulfur and selenium is reflected by its ability to form tetravalent cationic species in aqueous solution. Thus TeO_2 dissolves in concentrated nitric acid to form a Te^{IV} solution from which the compound $Te_2O_4HNO_3$ may be precipitated.

As part of our work on the aqueous chemistry of Te^{IV}, we discovered a related compound of composition $AgTeO_2NO_3$ which forms when Ag_2Te is treated with concentrated HNO_3(aq.).

Experimental. $AgTeO_2NO_3$ was synthesized in the following way: 0·376 g Ag_2Te was dissolved in 12 ml boiling 65% HNO_3(aq.) The colourless solution was slowly cooled to room temperature, precipitating colourless needle-shaped crystals. The crystal mass was then washed with a small amount of cold concentrated HNO_3(aq.). The compound is stable in dry air at room temperature. Ag and Te were analysed by atomic absorption spectroscopy confirming the stoichiometry of the compound. An IR study, using the KBr disc method, showed absorptions typical of the nitrate ion.

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Crystal 0·06 × 0·06 × 0·12 mm used for data collection on a Syntex $P2_1$ diffractometer. Cell dimensions determined from setting angles of 15 reflexions, $5 \leq 2\theta \leq 22°$. Intensities measured out to $2\theta = 65°$ using graphite-monochromatized Mo $K\alpha$ radiation and ω–2θ scan mode. 786 independent reflexions with *hkl* range 0→12, 0→24, 0→12, of which 480 had $I \geq 3\sigma(I)$. Two test reflexions, 202, 131, were remeasured every 20 reflexions, revealing negligible crystal decay. Corrections made for Lorentz–polarization and absorption effects (*LEOMA*; Andersen, 1985; *DIFABS*; Walker & Stuart, 1983); min., max. transmission factor 0·630, 0·806. Profile analysis according to Lehmann & Larsen (1974).

Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å^2); *e.s.d.'s are given in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Ag	0	1143 (1)	2500	2·24 (2)
Te	5000	615 (1)	7500	1·49 (1)
O(1)	7019 (9)	223 (3)	627 (9)	1·97 (8)
O(2)	1329 (11)	7168 (3)	1004 (12)	2·88 (13)
O(3)	0	8488 (5)	2500	2·98 (20)
N	0	7594 (6)	2500	1·75 (14)

Table 2. *Interatomic distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

For reference, the Te—O coordination of α-TeO_2 (Lindqvist, 1968) is given.

	$AgTeO_2NO_3$	α-TeO_2
Te—O($1^{i,iv}$)	2·072 (5)	2·082 (2)
Te—O($1^{ii,iii}$)	1·920 (5)	1·903 (2)
Te—O($2^{v,vi}$)	2·965 (5)	
Te—O(3)	3·106 (3)	
Te—Te	3·146 (2)	
Ag—O($1^{i,iv}$)	2·349 (5)	
Ag—O($2^{ii,iii}$)	3·111 (5)	
Ag—O($2^{v,vi}$)	2·658 (6)	
Ag—O($3^{ii,iii}$)	2·668 (2)	
N—O(2)	1·243 (7)	
N—O(3)	1·270 (11)	
O(1^{i})—O(1^{ii})	2·463 (7)	
O(1)—Te—O(1^{ii})	76·1 (2)	84·6 (11)
O(1^{iii})—Te—O(1^{iv})	76·1 (2)	84·6 (11)
O(1)—Te—O(1^{iii})	84·7 (2)	88·1 (5)
O(1^{ii})—Te—O(1^{iv})	84·7 (2)	88·1 (5)
O(1)—Te—O(1^{iv})	148·8 (2)	168·5 (13)
O(1^{iii})—Te—O(1^{ii})	103·4 (2)	102·0 (13)
O(1)—Ag—O(1^{iv})	112·5 (2)	
O(2)—N—O(2^{iv})	121·8 (8)	
O(2)—N—O(3)	119·1 (4)	

Symmetry code: (i) x, y, z; (ii) $-x, -y, -z$; (iii) $x, -y, z+\tfrac{1}{2}$; (iv) $-x, y, -z+\tfrac{1}{2}$; (v) $-x\ \tfrac{1}{2}, y+\tfrac{1}{2}, z$; (vi) $x+\tfrac{1}{2}, y+\tfrac{1}{2}, -z+\tfrac{1}{2}$.

The Ag- and Te-atom positions were determined from a Patterson map; all other atoms were located by subsequent difference syntheses. Full-matrix least-squares refinement (*SHELX*76; Sheldrick, 1976) minimizing $\sum w(|F_o| - |F_c|)^2$. 41 parameters refined: scale factor, positions and anisotropic temperature factors, isotropic extinction value [$g = 1·7\ (3) \times 10^{-7}$]. $R = 0·034$, $wR = 0·039$, $w = 1/[\sigma^2(F_o) + 0·0009F_o^2]$. $(\Delta/\sigma)_{max} = 0·005$, max. and min. heights in final ΔF map = 0·75 and −0·62 e Å^{-3} respectively. Scattering factors from *International Tables for X-ray Crystallography* (1974), drawings by *ORTEP* (Johnson, 1965).

Discussion. The final positional parameters and equivalent isotropic temperature factors are given in Table 1.* Important interatomic distances and angles, calculated by the program *PARST*83 (Nardelli, 1983) are listed in Table 2. Fig. 1 is an *ORTEP* stereoscopic drawing of the contents of the unit cell.

The Te coordination in $AgTeO_2NO_3$ is typical of four-valent Te—O compounds featuring a distorted trigonal bipyramidal configuration around Te with one of the equatorial positions left unoccupied (*cf.* Table 2). The next-nearest Te contacts are with nitrate O atoms at 2·965 (5) Å, clearly outside the coordination sphere.

Angles and distances within the TeO_4 unit are similar to those found for example for α-TeO_2 (Lindqvist, 1968), *cf.* Table 2. In the title compound, the TeO_4 units connect by sharing edges, thus forming TeO_2 chains parallel to **c** (*cf.* Fig. 2). In α-TeO_2, a three-dimensional

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44543 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

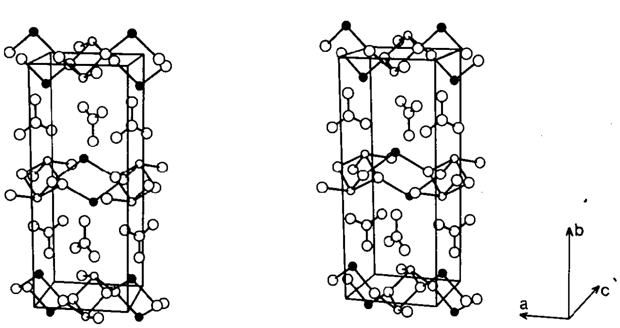

Fig. 1. A stereoscopic view of the unit cell.

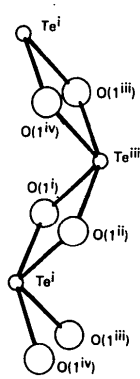

Fig. 2. Fragment of the structure, showing a TeO_2 chain.

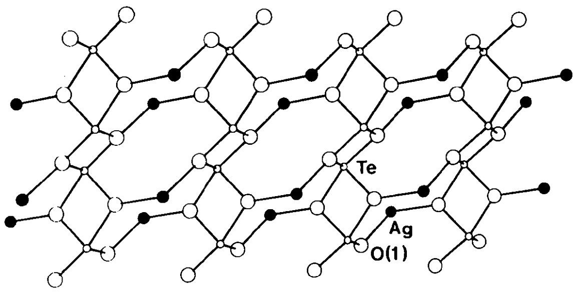

Fig. 3. The infinite cationic sheet of composition $AgTeO_2^+$.

network is formed because of the sharing of corners between the TeO_4 polyhedra, while in $Te_2O_4HNO_3$ (Anderson, 1980) the alternate sharing of edges and corners leads to the formation of Te—O sheets.

Ag forms two short bonds [2·349 (5) Å] to O atoms belonging to adjacent TeO_2 chains. In this way, the TeO_2 chains are linked to form positively charged sheets of composition $AgTeO_2^+$ parallel to *ac* (Fig. 3). The Ag coordination polyhedron is completed by four long contacts with nitrate O atoms [2·658 (6) and 2·668 (2) Å]. The nitrate ions are situated between the $AgTeO_2^+$ sheets. The nitrate ion deviates only slightly from ideal D_{3h} symmetry and distances are similar to those found for example for $NaNO_3$ [1·257 (1) Å; Paul & Pryor, 1972]. The title compound thus contains positively charged layers separated by layers of discrete nitrate ions balancing the charge. Structures containing positively charged two-dimensional networks are rare in inorganic chemistry, the only other example known to us being the related $Te_2O_4HNO_3$ (Anderson, 1980), where the positively charged network has the composition $Te_2O_4H^+$. As with the title compound, layers containing discrete nitrate ions separate the positively charged sheets.

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Structure de la Tétra(*p*-*n*-octylphényl)-5,10,15,20 Porphine de Zinc(II)

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Abstract. $C_{76}H_{92}N_4Zn$, $M_r = 1126·97$, triclinic, $P\bar{1}$, $a = 10·397$ (2), $b = 13·236$ (4), $c = 25·149$ (5) Å, $\alpha = 97·76$ (1), $\beta = 105·96$ (1), $\gamma = 84·84$ (1)°, $V = 3292$ (3) Å^3, $Z = 2$, $D_x = 1·14$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0·797$ mm^{-1}, $F(000) = 1212$. Final $R = 0·099$ for 4041 observed reflexions. The porphine skeleton is non-planar. The Zn atom is only 0·15 Å out of the plane of the core. Mean Zn···N distance is 2·024 (9) Å. The pertinent feature of the structure is the presence of four long aliphatic chains attached to the phenyl rings and lying approximately in the mean plane of the core. They adopt a centrosymmetric disposition, two of them being fully extended while the others are bent. The porphyrin nuclei are stacked in piles of dimers between which the chains are densely packed in parallel rows.

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