

The Structure of Indium Tungstate $\text{In}_6\text{WO}_{12}$: Its Relation with the Fluorite Structure

BY D. MICHEL AND A. KAHN

Laboratoire de Chimie Appliquée de l'Etat Solide, LA 302, CECM, 15 rue Georges Urbain, 94400 Vitry, France

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Abstract

The crystal structure of $\text{In}_6\text{WO}_{12}$ was determined from three-dimensional X-ray diffraction data. The crystal symmetry is rhombohedral, space group $R\bar{3}$ (Y_6UO_{12} type), with lattice constants $a_R = 6.2277$ (9) Å, $\alpha = 99.01$ (1)° [hexagonal axes: $a_H = 9.472$ (2), $c_H = 8.939$ (2) Å, $c_H/a_H = 0.9438$ (2)], $Z = 1$, $d_m = 7.5$ (3), $d_x = 7.64$ Mg m⁻³. The structure was refined by least-squares methods to a final R value of 0.032 for 484 independent reflections. This structure is a fluorite superstructure in which O vacancies are paired around the W atoms. By relaxation around vacancies, atoms are shifted from ideal fluorite positions by 0.56 and 0.31 Å for the two kinds of O atoms O(1) and O(2) and by 0.26 Å for In atoms. W atoms are strongly bonded by six O(1) atoms [W–O(1) = 1.93 Å], forming octahedral $\text{WO}(1)_6$ groups isolated at corners of the cell (shortest distances between them are 6.23 and 8.09 Å). The other atoms in the cell [six O(2) and six In] build a set of $\text{In}_4\text{O}(2)$ tetrahedra sharing corners as in the fluorite or in the bixbyite structure. These tetrahedra are quite similar to those forming the bixbyite structure of In_2O_3 (mean value for In–O = 2.16 Å).

Many ternary oxides $(M, M')_7\text{O}_{12}$ are isostructural with the compound Y_6UO_{12} which possesses a rhombohedral structure, space group $R\bar{3}$ (No. 148), $Z = 1$ (Bartram, 1966).

The phases reported with this structure have different formulae depending on the nature of the elements involved in these compounds:

– $M_6M'\text{O}_{12}$ with $M'^{\text{VI}} = \text{Mo, W, Te, U}$ and $M^{\text{III}} = \text{Sc, Y, In, Ln}$ (lanthanide) (Aitken, Bartram & Juenke, 1964; Borchardt, 1963; Bartram, 1966; Blasse, 1969; McCarthy, Fischer, Johnson & Gooden, 1972; Trunov & Kovba, 1967).

– $M_{5.5}M'_{1.5}\text{O}_{12}$ with $M'^{\text{V}} = \text{Nb, Sb, Ta}$ and $M^{\text{III}} = \text{Sc}$ (Michel, Kahn & Perez y Jorba, 1976; Rossell, 1976; Varfolomeev, Spiridonov & Sotnikova, 1975).

– $M_4M'_2\text{O}_{12}$ with $M'^{\text{IV}} = \text{Zr, Hf, Ce, Pr, Tb, Cm}$ and $M^{\text{III}} = \text{Sc, Y, Ln, Cm}$ (Ferguson, Guth & Eyring, 1954; Bevan, 1955; Bevan & Kordis, 1964; Baenziger, Eick, Schuldt & Eyring, 1961; Thornber, Bevan &

Graham, 1968; Lefevre, 1963; Collongues, Queyroux, Perez y Jorba & Gilles, 1965; Thornber & Bevan, 1970; Thornber, Bevan & Summerville, 1970; Rossell, 1976; Scott, 1977; Ray & Stubican, 1977).

– $M_2M'_5\text{O}_{12}$ with $M'^{\text{IV}} = \text{Zr, Hf}$ and $M = \text{Mg}$ (Delamarre, 1972).

The Y_6UO_{12} type is related to the fluorite structure and may be described as a superstructure obtained for the O-deficient $\text{MO}_{1.714}$ composition by ordering O vacancies on $\frac{1}{4}$ of the anionic fluorite positions. The location of the vacancies along a $\langle 111 \rangle$ direction leads to a rhombohedral structure derived from that of fluorite by a slight lattice distortion and by atomic shifts from ideal fluorite sites.

Atomic positions have been determined for several $M_7\text{O}_{12}$ compounds by X-ray (Michel *et al.*, 1976; Rossell, 1976; Thornber *et al.*, 1968; Thornber & Bevan, 1970; Beaury, Faucher & Caro, 1978) or neutron (Ray & Cox, 1975; Von Dreele, Eyring, Bowman & Yarnell, 1975; Ray, Stubican & Cox, 1980) powder diffraction and only for a few cases with single crystals (Bartram, 1966; Ray & Cox, 1975).

This paper reports the determination of the rhombohedral structure of $\text{In}_6\text{WO}_{12}$ which belongs to the group considered (Trunov & Kovba, 1967), based on single-crystal data. The main structural features will be discussed with reference to the parent fluorite structure (lattice distortion, relaxation around vacancies, coordination polyhedra) and compared with other fluorite-related structures.

Experimental

Preparation of crystals

High-purity (Johnson Matthey Specpure) powders of WO_3 and In_2O_3 were mixed at the composition $3\text{In}_2\text{O}_3\text{--WO}_3$ and heated in sealed platinum tubes (volume 3 cm³). Different heat treatments were tried with best results in crystal growth for one day at 1823 K and slow cooling to room temperature (5 K h⁻¹). Crystals of the $\text{In}_6\text{WO}_{12}$ phase were obtained, with sizes ranging from 50 to 500 μm. They are transparent with well defined planar faces.

Structure determination

The powder diagram of $\text{In}_6\text{WO}_{12}$ was indexed with the rhombohedral cell: $a_R = 6.2277(9) \text{ \AA}$, $\alpha = 99.01(1)^\circ$, $U = 231.5 \text{ \AA}^3$. Pycnometric measurements gave a density $d_m \approx 7.5 \pm 0.3 \text{ Mg m}^{-3}$, in agreement with $Z = 1$ (theoretical density $d_x = 7.64 \text{ Mg m}^{-3}$).

De Jong and precession patterns confirmed that the structure belongs to group $R3$ or $R\bar{3}$ (no conditions on hkl reflections). The crystal morphology is consistent with $\bar{3}$ symmetry. The natural faces correspond to the three forms $\{100\}$, $\{11\bar{1}\}$ and $\{1\bar{1}0\}$ which delimit crystals of isometric shape. The crystal on which intensities were measured had the $[110]$ direct row parallel to the ψ axis. It was taken as spherical to a good approximation (sphere radius $R = 0.0075 \text{ cm}$).

Intensities were collected for 484 independent reflections using a Nonius CAD-3 diffractometer (Mo $K\alpha$ radiation selected by a graphite monochromator) ranging from Bragg angles 0 to 35° . Absorption corrections were made for a sphere with $\mu R \approx 2$ [$\mu(\text{Mo } K\alpha) = 277 \text{ cm}^{-1}$].

The structure refinement was undertaken with coordinates of the atoms in Wyckoff positions $6(f)$ (three adjustable parameters): six In and two sets of O(1) and O(2). The W atom is on the special position $1(a)$ at the origin of the cell. Isotropic Debye-Waller factors were assigned to all atoms. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (Cromer & Waber, 1974). Fluorite positions were introduced as initial coordinates and a few refinement steps with the program of Busing, Martin & Levy (1963) (*SAPHIR-ORFLS*) led readily to an agreement factor $R = 0.08$. Anisotropic temperature factors were then introduced and refined.

Table 1. Atomic coordinates and anisotropic thermal parameters ($\times 10^4 \text{ \AA}^2$) (expressed in terms of mean-square amplitudes of vibration)

Figures in parentheses are estimated standard deviations obtained from the least-squares analysis. Fluorite coordinates are in square brackets.

	W 1(a)	In 6(f)	O(1) 6(f)	O(2) 6(f)
x	0 [0]	0.1397 (1) [0.1429]	-0.0426 (15) [-0.1071]	0.4057 (12) [0.3929]
y	0 [0]	0.3214 (1) [0.2857]	0.0974 (13) [0.0357]	0.5838 (12) [0.5357]
z	0 [0]	0.6044 (1) [0.5714]	0.2969 (12) [0.3214]	0.8219 (12) [0.8214]
U_{11}	34 (2)	43 (3)	129 (28)	79 (25)
U_{22}	34 (2)	71 (3)	104 (27)	44 (23)
U_{33}	34 (2)	56 (3)	15 (20)	34 (22)
U_{12}	8 (2)	24 (2)	7 (15)	9 (10)
U_{13}	8 (2)	8 (2)	7 (15)	9 (10)
U_{23}	8 (2)	2 (2)	7 (15)	4 (5)

A final R value = 0.032 was obtained for the set of parameters listed in Table 1.*

Results and discussion*Comparison with the fluorite structure*

The cationic sublattice defined by W and In positions is almost face-centered cubic and, as in the fluorite structure, anions occupy tetrahedral interstices. But, according to the composition $M_7\text{O}_{12}$, two tetrahedral anionic sites per unit cell are vacant. The rhombohedral symmetry arises from the clustering of the O vacancies V_O along one of the fluorite ternary axes in Wyckoff position $2(b) \pm xxx$ ($x \approx 0.25$).

Such a distribution for vacancies corresponds to the dispersion of point defects on a cubic lattice ensuring maximal distances between them at the given composition (here one vacancy for seven sites) (Parks & Barker, 1977).

This arrangement determines two different cationic positions in the rhombohedral space group: the $1(a)$ position surrounded by six O atoms and two vacancies; and $6(f)$ position surrounded by seven O atoms and one vacancy. In $\text{In}_6\text{WO}_{12}$ the W atom occupies the sixfold-coordinated site $1(a)$. O-equivalent positions in fluorite are split into three different tetrahedral sites: $2(b)$ vacant sites defined by one W and three In atoms; $6(f)$ occupied by O(1) atoms linked to one W and three In atoms; and $6(f)$ occupied by O(2) atoms linked to four In atoms.

(a) *Lattice distortion.* The actual unit cell of $\text{In}_6\text{WO}_{12}$ will be compared to an ideal rhombohedral supercell built on three $[1, -\frac{1}{2}, \frac{1}{2}]$ fluorite vectors. The reference fluorite structure has a parameter $a_F = (4U/7)^{1/3}$ giving the same volume for the actual and ideal cell [for $\text{In}_6\text{WO}_{12}$, $a_F = 5.095(1) \text{ \AA}$]. Therefore, lattice constants for the undistorted supercell would be: $a_{R(\text{ideal})} = a_F\sqrt{6}/2$, $\alpha_{\text{ideal}} = 99.59^\circ$ ($\cos \alpha = -\frac{1}{2}$).

In fact, the actual unit cells of $M_7\text{O}_{12}$ compounds are obtained from the ideal cell by elongation along the threefold axis. This deformation results from the location of additional positive charges (with regards to the structure of MO_2 fluorites) along the ternary axis and of negative formal charges around this axis. Thus, in $\text{In}_6\text{WO}_{12}$, W atoms and vacancies take the place of tetravalent and O atoms on the threefold axis. Around this axis In atoms are present instead of tetravalent M atoms.

The lattice deformation varies with the different $M_7\text{O}_{12}$ phases without exceeding 1° for $\alpha_{\text{ideal}} - \alpha_{\text{actual}}$

* Lists of observed and calculated structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36653 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

(Michel *et al.*, 1976). The deviation from ideal values of a (or c_H/a_H) may be measured by the value ε defined by:

$$a_{H(\text{actual})} = (1 - \varepsilon) a_{H(\text{ideal})}$$

$$c_{H(\text{actual})} = (1 + 2\varepsilon) c_{H(\text{ideal})};$$

for $\text{In}_6\text{WO}_{12}$

$$\varepsilon = 6.4 \times 10^{-3}.$$

The rhombohedral unit-cell vectors for $M_7\text{O}_{12}$ compounds correspond to the three $[1, -\frac{1}{2}(1 - 3\varepsilon), \frac{1}{2}(1 + \varepsilon)]\hat{C}$ fluorite vectors.

(b) *Atomic displacements from ideal fluorite positions.* These relations allow a calculation of the atomic positions in $\text{In}_6\text{WO}_{12}$ with reference to the fluorite structure. Results are listed in Table 2 with the amplitudes and directions of atomic shifts from ideal positions.

Fig. 1 represents the $\text{In}_6\text{WO}_{12}$ asymmetric unit contained in the rhombohedral cell. The reference to the fluorite structure is given by the two cubes (edge length $a_F/2$) centered on the anionic vacancies and sharing one corner. Arrows indicate the atomic shifts from ideal positions.

Table 2. *Coordinates of $\text{In}_6\text{WO}_{12}$ atoms referred to a cubic unit cell ($a_F = 5.095 \text{ \AA}$)*

The origin is at 1(b) of $R\bar{3}$ at the center of the $\text{In}_6\text{WO}_{12}$ group represented in Fig. 1. In parentheses are indicated the ideal fluorite positions.

	x	y	z	Atomic shift	Approximate direction of displacement
W $\pm xxx$	0.5064 (0.5)	0.5064 (0.5)	0.5064 (0.5)	0.06 \AA	$[111]_f, [111]_R$
6 In $\pm xyz \hat{C}$	0.5014 (0.5)	-0.0506 (0)	-0.0107 (0)	0.26	$[0\bar{5}i]_f, [0i\bar{i}]_R$
6 O(1) $\pm xyz \hat{C}$	0.6454 (0.75)	0.2388 (0.25)	0.2792 (0.25)	0.56	$[9i3]_f, [553]_R$
6 O(2) $\pm xyz \hat{C}$	0.2101 (0.25)	-0.2919 (-0.25)	-0.2336 (-0.25)	0.31	$[155\bar{2}]_f, [130]_R$

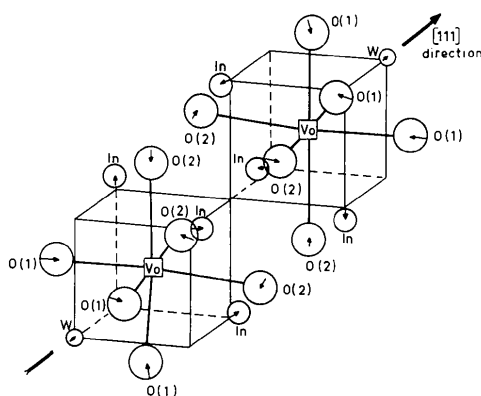


Fig. 1. The $\text{In}_6\text{WO}_{12}$ asymmetric unit with reference to the corresponding fluorite.

Table 3. *Shifts (\AA) from fluorite ideal positions for atoms neighbouring O vacancies in different fluorite-related phases*

Compounds	References	Atomic shifts for O atoms		Atomic shifts for cations	
$M_2M'_2O_7$ [pyrochlore type, $Fd\bar{3}m$ ($Z = 8$)]					
		48(f)		16(d)	
$\text{La}_2\text{Zr}_2\text{O}_7$	(a)	0.50		} No shift	
$\text{Nd}_2\text{Zr}_2\text{O}_7$	(a)	0.44			
$\text{Sm}_2\text{Zr}_2\text{O}_7$	(a)	0.40			
$\text{Gd}_2\text{Ti}_2\text{O}_7$	(b)	0.54			
$\text{Y}_2\text{Ti}_2\text{O}_7$	(b)	0.47			
$M_6M'O_{12}$ [Y_6UO_{12} type, $R\bar{3}$ ($Z = 1$)]					
		O(1) 6(f)	O(2) 6(f)	1(a)	6(f)
$\text{In}_6\text{WO}_{12}$	(c)	0.56	0.31	0.06	0.26
Y_6WO_{12}	(d)	0.43	0.39	0.10	0.29
$\text{Sc}_{3.5}\text{Nb}_{1.5}\text{O}_{12}$	(e)	0.47	0.27	0.04	0.33
Ce_7O_{12}	(f)	0.33	0.24	0.02	0.20
Pr_7O_{12}	(g)	0.33	0.24	0.03	0.21
$\text{Sc}_4\text{Zr}_3\text{O}_{12}$	(h)	0.37	0.31	0.01	0.22
$\text{Y}_4\text{Zr}_3\text{O}_{12}$	(i)	0.33	0.33	0.03	0.24
M_2O_3 [bixbyite type, $Ia\bar{3}$ ($Z = 16$)]					
		48(e)		8(b)	24(d)
Sc_2O_3	(j)	0.33		} No shift	
In_2O_3	(k)	0.35			
Y_2O_3	(l)	0.34			
Yb_2O_3	(m)	0.32			
Er_2O_3	(m)	0.32			

References: (a) Michel, Perez y Jorba & Collongues (1974). (b) Calage & Pannetier (1977). (c) This work. (d) Beaury *et al.* (1978). (e) Michel *et al.* (1976). (f) Ray & Cox (1975). (g) Von Dreele *et al.* (1975). (h) Thornber *et al.* (1968). (i) Ray *et al.* (1980). (j) Geller, Romo & Remeika (1967). (k) Marezio (1966). (l) O'Connor & Valentine (1969). (m) Moon, Koehler, Child & Raubheimer (1968).

O atoms are displaced towards vacancies; $\text{O}(1)-V_O$ and $\text{O}(2)-V_O$ distances are respectively 2.02 and 2.35 \AA , instead of 2.55 \AA for O—O distances in the corresponding fluorite. In contrast, cations are repelled from an anionic vacancy with metal—metal distances of 3.84 and 3.87 \AA for the tetrahedron around a vacancy instead of 3.60 \AA in the corresponding fluorite.

Like the Y_6UO_{12} type, other structures can be derived from that of CaF_2 by removing anions and slightly rearranging the atoms. Thus, the pyrochlore-type ($M_2M'_2O_7$) and bixbyite ($C\text{-Ln}_2\text{O}_3$) structures can be described as fluorite structures with ordered anionic vacant sites ($\frac{1}{8}$ O sites for pyrochlore, $\frac{1}{4}$ for $C\text{-Ln}_2\text{O}_3$).

The static displacements from ideal fluorite positions for different (MM') O_{2-x} compounds with fluorite-related structures are given in Table 3.

Cations are shifted by about 0.2–0.35 \AA , except for cations with two adjacent opposite vacancies which stay on fluorite positions [16(d) for pyrochlore, 8(b) for $C\text{-Ln}_2\text{O}_3$] or within 0.1 \AA [position 1(a) in $M_7\text{O}_{12}$].

Significant shifts from ideal positions are found for O atoms. There are many indications that relaxation with

comparable magnitude ($\approx 0.2\text{--}0.5 \text{ \AA}$) occurs around vacancies in disordered fluorite-like MO_{2-x} phases such as stabilized zirconias or intermediate oxides of lanthanides with variable valence: Ce, Pr, Tb. Mean displacements of O atoms from fluorite positions, ranging from 0.2 to 0.4 Å , were evaluated from neutron studies on stabilized zirconia phases (M,Zr) O_{2-x} ($M = \text{Ca}, \text{Y}, \text{Yb}$) (Carter & Roth, 1968; Steele & Fender, 1974; Faber, Mueller & Cooper, 1978).

Structural features of $\text{In}_6\text{WO}_{12}$

The coordination polyhedra for W and In atoms are given in Fig. 2 and other interatomic distances are reported in Table 4. As the $\text{In}_6\text{WO}_{12}$ structure presents common features with that of In_2O_3 (bixbyite type), distances determined on In_2O_3 by Marezio (1966) are given for comparison in the same table. Thus, the environments of the O(2) atom in $\text{In}_6\text{WO}_{12}$ and of the

O atom in In_2O_3 are nearly identical with mean distances $\text{In-O} \approx 2.16\text{--}2.18 \text{ \AA}$ and $\text{In-In} 3.50\text{--}3.51 \text{ \AA}$. In the same way, around an O vacancy, In-In distances are equal to 3.84 Å in both In_2O_3 and $\text{In}_6\text{WO}_{12}$.

The specific character of the $\text{In}_6\text{WO}_{12}$ structure lies in the presence of isolated WO_6 octahedral units. These groups are formed by the shortest bonds in the structure, $\text{W-O}(1) = 1.93 \text{ \AA}$. This length corresponds to a high bond strength ($s = 0.90$ according to the relations given by Zachariasen, 1978), compared to $s = 0.5$ for the $M\text{--O}$ bond in an MO_2 fluorite or an M_2O_3 bixbyite structure.

The $\text{WO}(1)_6$ octahedra are only slightly distorted with regard to the regular $m3m$ symmetry in $\bar{3}$ ($\text{O-W-O} = 93.2^\circ$). Each $\text{WO}(1)_6$ group is surrounded by In and O(2) atoms. The shortest distances separating two octahedral groups are 6.23 Å along $\langle 001 \rangle$ and 8.09 Å along $\langle 011 \rangle$.

The morphology of $\text{In}_6\text{WO}_{12}$ crystals may be interpreted from these structural data in terms of a 'periodic bond chain' (p.b.c.) analysis (Hartman & Perdok, 1955; Hartman, 1973).

P.b.c.'s were searched in directions along which the strongest bonds $\text{W-O}(1)$ are connected by short In-O bonds. Two p.b.c. directions were found, $\langle 001 \rangle$ and $\langle 011 \rangle$. Along $\langle 001 \rangle$ directions, two $\text{W-O}(1)_6$ groups are connected through In atoms by $\text{In-O}(1)$ bonds (2.21 and 2.28 Å). Along $\langle 011 \rangle$ directions, the octahedral groups are connected through In and O(2) atoms by $\text{In-O}(1)$ (2.21 Å) and $\text{In-O}(2)$ (2.07 and 2.11 Å) bonds. P.b.c. vectors $\langle 001 \rangle$ and $\langle 011 \rangle$ generate three forms of F faces which correspond to the natural faces $\{100\}$ $\{01\bar{1}\}$ $\{11\bar{1}\}$ defining the habit of the prepared $\text{In}_6\text{WO}_{12}$ crystals.

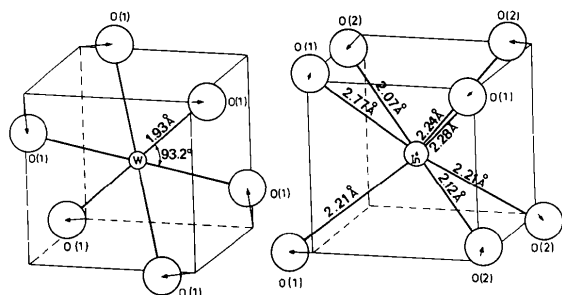


Fig. 2. The environment of the cations in $\text{In}_6\text{WO}_{12}$. Arrows show the atomic shifts from the ideal cubic coordination.

Table 4. Selected interatomic distances (Å) around O atoms and O vacancies in $\text{In}_6\text{WO}_{12}$ and In_2O_3

Estimated deviations for $\text{In}_6\text{WO}_{12}$ are lower than 0.005 Å for metal-metal distances, 0.01 Å for metal-O distances and 0.02 Å for O-O distances. The position of the O vacancy V_o is assumed to be $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ in the corresponding fluorite.

$\text{In}_6\text{WO}_{12}$			In_2O_3 (Marezio, 1966)			Corresponding MO_2 fluorite structure	
O(1)	O(2)	V_o	O	V_o	$\text{In}_6\text{WO}_{12}$ ($a_F = 5.095 \text{ \AA}$)	In_2O_3 ($a_F = 5.059 \text{ \AA}$)	
O(1)-W 1.93	O(2)-In 2.07	V_o -W 2.26	O-In(2) 2.13	V_o -In(1) 2.19	O-M 2.21 $\times 4$	O-M 2.19 $\times 4$	
O(1)-In 2.21	O(2)-In 2.12	V_o -In 2.40 $\times 3$	O-In(1) 2.16	V_o -In(2) 2.40 $\times 3$			
O(1)-In 2.28	O(2)-In 2.21		O-In(2) 2.19				
O(1)-In 2.77	O(2)-In 2.24		O-In(2) 2.25				
In-In 3.443	In-In 3.328		In(1)-In(2) 3.35		M-M 3.603 $\times 6$	M-M 3.577 $\times 6$	
W-In 3.536	In-In 3.410	In-In 3.842 $\times 3$	In(1)-In(2) 3.35	In(1)-In(2) 3.83 $\times 3$			
W-In 3.536	In-In 3.410	W-In 3.873 $\times 3$	In(2)-In(2) 3.36	In(2)-In(2) 3.84 $\times 3$			
In-In 3.552	In-In 3.443		In(2)-In(2) 3.36				
W-In 3.873	In-In 3.552		In(1)-In(2) 3.82				
In-In 4.028	In-In 3.842		In(2)-In(2) 3.84				
O(1)-O(1) 2.65 $\times 2$	O(2)-O(2) 2.71 $\times 2$		O-O 2.84 $\times 2$		O-O 2.55 $\times 6$	O-O 2.53 $\times 6$	
O(1)-O(2) 2.74	O(2)-O(1) 2.74	V_o -O(1) 2.02 $\times 3$	O-O 2.84 $\times 2$	V_o -O 2.22 $\times 3$			
O(1)-O(1) 2.80 $\times 2$	O(2)-O(2) 2.77	V_o -O(2) 2.35 $\times 3$	O-O 2.91	V_o -O 2.40 $\times 3$			
O(1)-O(2) 2.90	O(2)-O(1) 2.90						
O(1)-O(1) 2.98							

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The Structure of Diammonium Tin(II) Diphosphite, $(\text{NH}_4)_2\text{Sn}(\text{HPO}_3)_2$

BY TOSHIO YAMAGUCHI AND OLIVER LINDQVIST

*Department of Inorganic Chemistry, Chalmers University of Technology and the University of Göteborg,
S-412 96 Göteborg, Sweden*

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Abstract

$(\text{NH}_4)_2\text{Sn}(\text{HPO}_3)_2$ is triclinic, space group $P\bar{1}$ with $a = 4.799$ (1), $b = 10.060$ (6), $c = 10.338$ (6) Å, $\alpha = 107.07$ (4), $\beta = 82.18$ (4), $\gamma = 90.32$ (4)°, $V = 472.4$ (4) Å³ and $Z = 2$. The block-diagonal least-squares method gave a final $R = 0.046$ for 2364 unique

diffractometer reflections. There are three short Sn—O bonds at distances 2.111 (5), 2.115 (5) and 2.161 (6) Å, one intermediate bond at 2.696 (6) Å and one much longer interaction at 3.258 (6) Å. The phosphite ion has an approximately trigonal symmetry with P—O distances of 1.506 (5), 1.523 (5) and 1.531 (6) Å.