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Dibromodiphenylstannane: isolated centrosymmetric dimers as a new structure motif for the intermolecular association of diorganotin(IV) dihalides

Fei Ye and Hans Reuter*

Institut für Chemie, Anorganische Chemie II, Universität Osnabrück, Barbarastrasse 7, 49069, Osnabrück, Germany Correspondence e-mail: hreuter@uni-osnabrueck.de

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In the crystalline state, the low-melting title compound [common name: diphenyltin(IV) dibromide], $[SnBr_2(C_6H_5)_2]$, consists of distorted tetrahedral molecules with compressed halide and enlarged carbon opening angles of 102.741 (9) and 123.53 (8)°, respectively, and Sn-C and Sn-Br bond lengths of 2.109 (2)/2.113 (2) and 2.4710 (3)/2.4947 (3) Å, respectively. Intermolecular Sn...Br interactions, typical for diorganotin(IV) dihalides, R_2 SnHal₂ (with Hal = Cl, Br, I), and sterically less demanding organic groups lead to the formation of a hitherto unknown association pattern consisting of centrosymmetric dimers with an antiparallel orientation of the dipole moments and two weak intermolecular Sn...Br distances of 3.8482 (3) Å between one of the two Br atoms and its neighbouring Sn atom, and vice versa. The second Br atom is not involved in intermolecular interactions and lies somewhat outside the association plane that, therefore, is not coplanar [interplanar angle = $1.750 (2)^{\circ}$] with the tin-halide plane. The new structure motif of intermolecular tin-halide interaction can be classified as $2a_i$, which indicates the number of molecules (i.e. '2') composing the oligomer, the antiparallel orientation (i.e. 'a') of their dipole moments and the centre of symmetry (i.e. 'i') giving rise to the association pattern.

Comment

Diorganotin(IV) dihalides, denoted R_2 SnHal₂ (Hal = Cl, Br, I; R = nonfunctionalized organic groups), are easy to prepare and versatile starting materials for the preparation of many other diorganotin derivatives, such as alkoxides (Bradley *et al.*, 1978), hydrides (Ingham *et al.*, 1960), tetraorganodistannoxanes (Jurkschat, 2008), carboxylates (Mehrotra & Bohra, 1980) or different coordination monomers and polymers, that are not only important in basic research for the formation of, for example, supramolecular assemblies (Dakternieks & Duthie, 2003; Haiduc, 2007) or metal-organic frameworks (MOFs) (Shankar *et al.*, 2011), but are also used in industry as PVC stabilizers (Arkis, 2008) or catalysts (Evans & Karpel, 1985).



In the gas phase, diorganotin(IV) dihalides consist of monomeric molecules of point-group symmetry $C_{2\nu}$ with a considerable dipole moment (Lorberth & Nöth, 1965) in the direction of the twofold axis of symmetry. For dimethyltin(IV) dichloride, Me₂SnCl₂ (Fujii & Kimura, 1971), and di-*tert*-butyltin(IV) dichloride, ¹Bu₂SnCl₂ (Belyakov *et al.*, 1988), the four main structural parameters (Sn-Hal, Sn-C, Hal-Sn-Hal and C-Sn-C) were determined by electron diffraction experiments. Deviations from a tetrahedral bond arrangement at the Sn atom mainly result from bond-angle distortions, which are small in the case of Me₂SnCl₂ (Cl-Sn-Cl = 107.5±3.9°) but considerable for ¹Bu₂SnCl₂ (C-Sn-C = 118.6±4.2° and Cl-Sn-Cl = 103.1±4.5°).

In different noncoordinating organic solvents, such as toluene or chloroform, they also represent monomeric molecules, whereas coordination compounds are formed in the case of solvent molecules with donor atoms such as N [*e.g.* N,N-dimethylformamide (DMF) or dimethyl sulfoxide (DMSO)] as a result of Lewis base–Lewis acid adduct formation between the solvent molecule and the diorgano-tin(IV) dihalide unit.

In the solid state, diorganotin(IV) dichlorides, dibromides and diiodides with large organic residuals like *tert*-butyl ('Bu₂SnCl₂; Dakternieks *et al.*, 1994), 2-methyl-2-phenylpropyl [(MePhPr)PhSnBr₂; Bomfim *et al.*, 2003] or mesityl (Mes₂-SnBr₂; Chandrasekhar & Thirumoorthi, 2010) are monomeric also, with large respective carbon and small halide opening angles, *viz.* 133.1 (2) and 101.86 (5)° in 'Bu₂SnCl₂, 127.0 (1) and 102.18 (1)° in (MePhPr)PhSnBr₂, and 118.7 (2) and 100.51 (2)° in Mes₂SnBr₂.

The corresponding diorganotin(IV) dihalides with organic ligands having small steric requirements, however, show a strong tendency for intermolecular association as a result of intermolecular tin (Lewis acid)-halide (Lewis base) interactions for which such terms as 'secondary bonding' (Alcock & Sawyer, 1977), 'supramolecular architecture' (Buntine *et al.*, 2003) or 'soft-soft interactions' (Haiduc, 2007) have been used. Usually, these additional (sec) bonds are considerably longer than normal (cov) ones, but shorter than van der Waals (vdW) contacts: $d(Sn-Hal)_{cov} < d(Sn\cdots Hal)_{sec} < d(Sn\cdots Hal)_{vdW}$. Furthermore, they are accompanied by an increase in the coordination number at tin from four to five or six, resulting in a distorted trigonal bipyramid or a distorted octahedron as the coordination polyhedron.

In the case of small organic ligands, predominantly infinite polymeric chains are formed which we propose to term einersingle chains following the terminology of silicates (Liebau, 1985) in order to delimit these structures from others. There are two main structure-type families in this area: one with an antiparallel (A) or nearly antiparallel ordering of the dipole moments of neighbouring molecules and the other where they are parallel (P) or nearly parallel to each other. The aristotypes of these structure-type families (Fig. 1) are represented by dimethyltin(IV) dichloride (Me₂SnCl₂; Reuter & Pawlak, 2001a) as type A and diethyltin(IV) diiodide (Et₂SnI₂; Alcock & Sawyer, 1977) as type P. The less symmetrical members of both structure-type families can be further classified according to the symmetry elements responsible for the chain propagation. Other structure types based on an infinite polymeric association pattern can be classified as einer-double chains or bands (β -Cy₂SnCl₂; Ganis *et al.*, 1986), zweier-single chains (Ph₂SnCl₂; Greene & Bryan, 1971) or sheets (EtPhSnCl₂; Casas et al., 2003).

On the other hand, finite oligomeric association patterns are rare. Applying the bond criteria defined above, there is only one example of a noncentrosymmetric dimer, *viz. trans*-Myr₂SnCl₂ (Myr = myrtanyl; Beckmann *et al.*, 2008), with an antiparallel orientation of the dipole moments, and one example of a centrosymmetric tetramer (MePhSnCl₂; Amini *et al.*, 1987), also with an antiparallel orientation of the dipole moments.

With the crystal structure of dibromodiphenylstannane, Ph_2SnBr_2 , (I), we present the first example of a diorganotin(IV) dihalide exhibiting a centrosymmetric dimeric association pattern in the solid state.

Me₂SnCl₂



Figure 1

Schematic representation of the tin-halide interactions (broken bonds) and the orientation of the dipole moments (red arrows of arbitrary units) in the crystal structures Me_2SnCl_2 and Et_2SnI_2 . In both cases, the halide atoms of one molecule are individually labelled although they are symmetry related in the real structures. Organic groups have been omitted for clarity.

(I) is a colourless low-melting solid (m.p. 309-311 K) that can easily be prepared (Chambers & Scherer, 1926) from commercially available tetraphenylstannane and bromine using carbon tetrachloride as solvent. Yields are usually moderate ($\simeq 35\%$) because of the formation of the side products bromotriphenylstannane and bromobenzene.

The asymmetric unit of (I) (Fig. 2) consists of one molecule of local point-group symmetry C_1 . Both phenyl groups are almost planar [maximum deviation from the least-squares plane = ± 0.002 (2) Å for the C11–C16 ring and ± 0.003 (2) Å for the C21-C26 ring] and bond lengths within the phenyl groups, covering the range 1.375 (4)-1.395 (3) Å, with a mean value of 1.385 (7) Å, are as expected (Allen et al., 1987). Distortions of the bond angles within the organic groups are small and in the range 119.1 (2)-120.9 (2)°; an ipso effect (Domenicano et al., 1983) is not recognizable, but the Sn atom lies significantly outside [0.038 (3) and -0.044 (3) Å] the leastsquares planes through both phenyl groups. Both Sn-C bonds (Table 1) are very similar [mean value = 2.111 (3) Å] and comparable with other tin-phenyl bond lengths with tin in a predominantly tetrahedral environment, such as in triphenyltin(IV) bromide (Ph₃SnBr; Preut & Huber, 1979), where a mean value of 2.114 (8) Å (T = 293 K) was found.

Both Sn-Br bond lengths are also very similar [Δ = 0.0237 Å and mean value = 2.483 (17) Å] but considerably shorter ($\simeq 0.1$ Å) than the sum (2.59 Å) of the covalent radii (Cordero et al., 2008) of tin (1.39 Å) and bromine (1.20 Å). They fit very well into the range (2.44–2.54 Å) of Sn–Br bond lengths found in other diorganotin(IV) dibromides with nonfunctionalized hydrocarbon groups [ten compounds with 14 individual values; Cambridge Structural Database (Allen, 2002)], even if the literature data cover all kinds of intermolecular association patterns and are derived from X-ray diffraction measurements at different temperatures. They are, however, longer than the corresponding bond lengths [mean value = 2.423 (4) Å, T = 249 K] in tin(IV) bromide (Reuter & Pawlak, 2001b). Because of the low symmetry of the molecule, the tin-halide plane is not exactly perpendicular to the tincarbon plane, but the deviation of $0.14 (4)^{\circ}$ is negligible.

The bromine and carbon opening angles (Table 1) of (I) are compressed and significantly enlarged, respectively. A detailed comparison with the corresponding values of other



Figure 2

A view of the molecule of (I) in parallel projection, showing the atomlabelling scheme. Displacement ellipsoids are drawn at the 50% probability level.



Figure 3

(a) Capped sticks model of the centrosymmetric dimers resulting from intermolecular Sn...Br interactions [3.8482 (3) Å, broken sticks] in the crystal structure of (I). (b) A detailed view of the centrosymmetric dimers projected (above) on the association plane $[Sn1-Br2-Sn1^i-Br2^i, grey; i = centre of inversion]$ and a view (below) showing the antiparallel orientation of the dipole moments (arrows of arbitrary units) and the out-of-plane positions of the exocyclic Br1 and Br1ⁱ atoms. The positions of the phenyl groups are indicated by shortened sticks. Ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) -x + 1, -y, -z.]

diorganotin(IV) dibromides, however, is difficult because other association patterns will give clearly different values. In addition, monomeric diorganotin(IV) dibromides show a similar broad spectrum of carbon and bromine opening angles, as can be seen from the examples Mes₂SnBr₂ and (MePhPr)-PhSnBr₂ above.

In looking for intermolecular $Sn \cdots Br$ interactions, we have taken into account all intermolecular $Sn \cdots Br$ distances shorter than the sum (4.00 Å) of the van der Waals radii (Mantina *et al.*, 2009) of tin (2.17 Å) and bromine (1.83 Å). Indeed, there are only two intermolecular $Sn \cdots Br$ contacts of 3.8482 (3) Å fulfilling this criterion. These contacts exist between the Sn and Br atoms (Br2) of two molecules related to each other by a crystallographic ($\frac{1}{2}$,0,0; Wyckoff letter *b*) centre of symmetry (Fig. 3). The intermolecular bond angles within the four-membered centrosymmetric tin-bromine ring are $Sn-Br \cdots Sn = 101.92$ (1)° and $Br-Sn \cdots Br = 78.08$ (1)°.

For further discussion of the association pattern of oligomeric diorganotin(IV) dihalides, it seems helpful to treat the four-membered tin-halide ring as an aggregation plane. Because of the centre of symmetry, this reference plane is





The crystal packing of (I), viewed down the *b* axis, showing the isolated centrosymmetric dimers formed by intermolecular $Sn \cdots Br$ interactions. H atoms have been omitted for clarity.

almost planar in the present case, in contrast to the nonplanar aggregation plane in trans-Myr₂SnCl₂. In relation to the aggregation plane, atom Br1 is 0.0742 (3) Å below it. As a consequence, the tin-halide plane is not coplanar with the reference plane, resulting in an interplanar angle of $1.750 (2)^{\circ}$. Furthermore, the dipole moments of both molecules, which are exactly antiparallel to each other (inversion centre), will be situated somewhat outside the association plane. Taking the weak intermolecular interactions into account, the Sn atoms adopt a fivefold trigonal-bipyramidal coordination with the organic groups in equatorial and atoms Br1 and Br2ⁱ in axial positions [symmetry code: (i) -x + 1, -y, -z]. This may be the reason why the Sn-Br distance to Br1 is somewhat longer than to Br2, although this atom interacts with the neighbouring Sn atom. The crystal packing (Fig. 4) reveals that the phenyl groups completing the dimers inhibit further intermolecular Sn...Br interactions.

In order to classify the association pattern of diorganotin(IV) dihalides more rationally, we propose to denote the new association pattern as $2a_i$, where '2' indicates the number of molecules comprising the oligomer, 'a' represents the antiparallel orientation of the dipole moments of both molecules and the subscript 'i' represents the symmetry element leading to the association pattern. In doing this, the noncentrosymmetric dimers of *trans*-Myr₂SnCl₂ (see above) can be classified as $2a_1$.

In addition, the new structure motif for the intermolecular $Sn \cdots Br$ interaction in Ph_2SnBr_2 shows some important relationships to other structure types in the field of diorganotin(IV) dihalides: for one thing, dimers with an antiparallel orientation of dipole moments are the shortest possible oligomeric sections within the structure family of Me_2SnCl_2 , and for another thing, the structure type of Ph_2SnCl_2 , which is characterized as a zweier-single chain, is built up of two different centrosymmetric dimers of type $2a_i$ with each Sn atom undergoing an additional interaction to the exocyclic Cl atom of a neighbouring dimer, and *vice versa*. Applying our

classification scheme, this structure type can be expressed by the term $C2(2a_i)$, with the letter C being an abbreviation for the chain structure motif and $2(2a_i)$ denoting the repeat unit.

Experimental

A solution of tetraphenyltin (21.36 g, 50 mmol, Janssen Chimica) and bromine (15.98 g, 100 mmol, Fluka) in carbon tetrachloride (150 ml, Fluka) was heated for 3 h under reflux. After filtration, the solvent was removed under reduced pressure. The residue was purified by fractional distillation of PhBr (300 K, 37 kbar; 1 bar = 100 kPa), PhSnBr₃ (358-361 K, 17 kbar) and Ph₂SnBr₂ (396-402 K, 16 kbar). After cooling, colourless crystals of the title compound were obtained in a vield of 33.09%. Elemental data (Elementar vario MICRO Cube, calculated/found, %): C 33.31/32.91, H 2.33/2.26.

ATR-FT-IR (Bruker VERTEX 70, cm⁻¹): 3068.0 [w, ν (CH)], 1576.2 [w, v(CC)], 1479.0 [w, v(CC)], 1430.6 [s, v(CC)], 1331.8 [m, $\nu(CC)$ and $\delta(CH)_{ip}$], 1301.5 [w, $\delta(CH)_{ip}$], 1189.3 [w, $\delta(CH)_{ip}$], 1159.8 $\delta(\text{ring})$], 913.2 [*m*, $\delta(\text{CH})_{\text{oop}}$], 724.5 [*s s*, $\delta(\text{CH})_{\text{oop}}$], 688.0 [*s s*, $\delta(CH)_{oop}$]; assignments according to Poller (1962).

¹H NMR (Bruker AVANCE DPX, 250 MHz, CDCl₃): δ 7.34–7.51 (m, 3H, meta, para), 7.55-7.62 (m, 2H, ortho).

 1 H 13 C NMR (Bruker AVANCE DPX, 250 MHz, CDCl₃): δ [ⁿJ (Hz) 128.1 [C_{meta} , ${}^{3}J({}^{13}C-{}^{119}Sn/{}^{117}Sn) = 84.2/80.6$], 130.2 [C_{para} , ${}^{4}J({}^{13}C-{}^{119/117}Sn) = 17.3$], 133.4 [C_{ortho} , ${}^{2}J({}^{13}C-{}^{119}Sn/{}^{117}Sn) = 63.9/$ 61.5], 135.8 [C_{ipso} , ${}^{1}J({}^{13}C-{}^{119}Sn/{}^{117}Sn) = 728.8/696.5$]; for literature data, see Holeček et al. (1990).

A suitable single crystal was selected under a polarization microsope and mounted on a 50 µm MicroMesh MiTeGen Micromount using Fromblin Y perfluoropolyether (LVAC 16/6, Aldrich).

Crystal data

$[SnBr_2(C_6H_5)_2]$	$V = 1317.71 (12) \text{ Å}^3$
$M_r = 432.71$	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 8.9553 (5) Å	$\mu = 7.97 \text{ mm}^{-1}$
b = 8.7468 (5) Å	$T = 100 { m K}$
c = 17.0671 (8) Å	$0.23 \times 0.17 \times 0.13 \text{ mm}$
$\beta = 99.713 \ (2)^{\circ}$	

46736 measured reflections

 $R_{\rm int} = 0.031$

3182 independent reflections

2856 reflections with $I > 2\sigma(I)$

Data collection

Bruker APEXII CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2009) $T_{\min} = 0.262, T_{\max} = 0.419$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$	138 parameters	
$wR(F^2) = 0.039$	H-atom parameters constrained	
S = 1.05	$\Delta \rho_{\rm max} = 0.43 \ {\rm e} \ {\rm \AA}^{-3}$	
3182 reflections	$\Delta \rho_{\rm min} = -0.48 \text{ e } \text{\AA}^{-3}$	

All H atoms were found in a difference Fourier synthesis, but were placed in geometrically idealized positions, with C-H = 0.95 Å, and constrained to ride on their parent atoms, with one common isotropic displacement parameter for each of the two phenyl groups.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics:

Table 1

Selected geometric parameters (Å, °).

Sn1-C21	2.109 (2)	Sn1-Br2	2.4710 (3)
Sn1-C11	2.113 (2)	Sn1-Br1	2.4947 (3)
C21-Sn1-C11	123.53 (8)	C21-Sn1-Br1	105.46 (5)
C21-Sn1-Br2	107.70 (5)	C11-Sn1-Br1	106.33 (5)
C11-Sn1-Br2	109.12 (6)	Br2-Sn1-Br1	102.741 (9)

DIAMOND (Brandenburg, 2006) and Mercury (Macrae et al., 2008); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG3245). Services for accessing these data are described at the back of the journal.

References

- Alcock, N. W. & Sawyer, J. F. (1977). J. Chem. Soc. Dalton Trans. pp. 1090-1095
- Allen, F. H. (2002). Acta Cryst. B58, 380-388.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). J. Chem. Soc. Perkin Trans. 2, pp. S1-19.
- Amini, M. M., Holt, E. M. & Zuckerman, J. J. (1987). J. Organomet. Chem. 327, 147-155.
- Arkis, E. (2008). Organotin Compounds as PVC Stabilizers, in Tin Chemistry -Fundamentals, Frontiers and Applications, edited by A. G. Davies, M. Gielen, K. H. Pannell & E. R. T. Tiekink, pp. 312-322. Chichester: Wiley.
- Beckmann, J., Duthie, A., Grassmann, M. & Semisch, A. (2008). Organometallics, 27, 1495-1500.
- Belyakov, A. V., Litvinov, O. A., Bogoradovskii, E. T., Girbasova, N. V. & Zavgorodnii, V. S. (1988). J. Struct. Chem. 29, 36-42.
- Bomfim, J. A. S., Filgueiras, C. A. L., Howie, R. A., Skakle, J. M. S. & Wardell, J. L. (2003). Acta Cryst. C59, m526-m529.
- Bradley, D. C., Mehrotra, R. C. & Gaur, D. P. (1978). In Metal Alkoxides. London, New York, San Francisco: Academic Press
- Brandenburg, K. (2006). DIAMOND. Crystal Impact GbR, Bonn, Germany.
- Bruker (2009). APEX2, including SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Buntine, M. A., Kosovel, F. J. & Tiekink, E. R. T. (2003). CrystEngComm, 5, 331-336.
- Casas, J. S., Castellano, E. E., Ellena, J., Garcia-Tasende, M. S., Sanchez, A., Sordo, J., Toboada, C. & Vidarte, M. J. (2003). Appl. Organomet. Chem. 17, 940-944.
- Chambers, R. F. & Scherer, P. C. (1926). J. Am. Chem. Soc. 48, 1054-1062.
- Chandrasekhar, V. & Thirumoorthi, R. (2010). J. Chem. Sci. 122, 687-695.
- Cordero, B., Gomez, V., Platero-Plats, A. E., Reves, M., Echeverria, J., Cremades, E., Barragan, F. & Alvarez, S. (2008). Dalton Trans. pp. 2832-2838
- Dakternieks, D. & Duthie, A. (2003). Organometallics, 22, 4599-4603.
- Dakternieks, D., Jurkschat, K. & Tiekink, E. R. T. (1994). Main Group Met. Chem. 17, 471-480.
- Domenicano, A., Murray-Rust, P. & Vaciago, A. (1983). Acta Cryst. B39, 457-468
- Evans, C. J. & Karpel, S. (1985). In Organotin Compounds in Modern Technology. Amsterdam, New York: Elsevier Science.
- Fujii, H. & Kimura, M. (1971). Bull. Chem. Soc. Jpn, 44, 2643-2647.
- Ganis, P., Valle, G., Furlani, D. & Tagliavini, G. (1986). J. Organomet. Chem. 302, 165-170.
- Greene, P. T. & Bryan, R. F. (1971). J. Chem. Soc. A, pp. 2549-2554.
- Haiduc, I. (2007). Appl. Organomet. Chem. 21, 476-482.
- Holeček, J., Lyčka, A., Handlíř, K. & Nádvorník, M. (1990). Collect. Czech. Chem. Commun. 55, 1193-1207.

Ingham, R. K., Rosenberg, S. D. & Gilman, H. (1960). Chem. Rev. 60, 459-539.

Jurkschat, K. (2008). Tetraorganodistannoxanes: Simple Chemistry From a Personal Perspective, in Tin Chemistry - Fundamentals, Frontiers and Applications, edited by A. G. Davies, M. Gielen, K. H. Pannell & E. R. T. Tiekink, pp. 201-230. Chichester: Wiley.

Liebau, F. (1985). In Structural Chemistry of Silicates – Structure, Bonding and Classifications. Berlin, Heidelberg, New York, Tokyo: Springer.

Lorberth, J. & Nöth, H. (1965). Chem. Ber. 98, 969–976.

- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). J. Appl. Cryst. 41, 466–470.
- Mantina, M., Chamberlin, A. C., Valero, R., Cramer, C. J. & Truhlar, D. G. (2009). J. Phys. Chem. A, 113, 5806–5812.
- Mehrotra, R. C. & Bohra, R. (1980). In *Metal Carboxylates*. London, New York, San Francisco: Academic Press.
- Poller, R. C. (1962). J. Inorg. Nucl. Chem. 24, 593-600.
- Preut, H. & Huber, F. (1979). Acta Cryst. B35, 744-746.
- Reuter, H. & Pawlak, R. (2001a). Z. Kristallogr. 216, 56-59.
- Reuter, H. & Pawlak, R. (2001b). Z. Kristallogr. 216, 34-38.
- Shankar, R., Jain, A., Singh, A. P. & Molloy, K. (2011). Phosphorus Sulfur Silicon Relat. Elem. 186, 1375–1378.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.