Table 2. *Selected bond distances* (Å) *and angles* (°)

Numbers in parentheses are e.s.d.'s of the least significant digits.

Mo—S(1)	2·3452 (9)	Mo—N(31)	2·216 (2)
Mo—S(2)	2·3702 (9)	S(1)—C(41)	1·769 (3)
Mo—N	1·766 (2)	S(2)—C(51)	1·770 (3)
Mo—N(11)	2·244 (2)	O—N	1·193 (3)
Mo—N(21)	2·205 (2)		

S(1)—Mo—S(2)	102·92 (3)	N—Mo—N(11)	177·4 (1)
S(1)—Mo—N	94·80 (9)	N—Mo—N(21)	95·7 (1)
S(1)—Mo—N(11)	82·72 (6)	N—Mo—N(31)	94·2 (1)
S(1)—Mo—N(21)	89·23 (7)	N(11)—Mo—N(21)	83·53 (9)
S(1)—Mo—N(31)	164·75 (7)	N(11)—Mo—N(31)	88·03 (9)
S(2)—Mo—N	86·38 (8)	N(21)—Mo—N(31)	77·66 (9)
S(2)—Mo—N(11)	94·93 (6)	Mo—S(1)—C(41)	112·2 (1)
S(2)—Mo—N(21)	167·49 (7)	Mo—S(2)—C(51)	114·2 (1)
S(2)—Mo—N(31)	89·89 (7)	Mo—N—O	179·1 (2)

the complex. Whenever filled d_{xz} and d_{yz} orbitals exist, as in the $\{Mo(NO)\}^4$ complexes, the torsional angles adopt values near 0 and 180° to maximize d_{xy}–p overlap (Ashby & Enemark, 1986).

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Table 3. *Torsion angles X*—Mo—S—C (°) *in selected complexes*

			Reference
$[\{HB(Me_2pz]_3\}Mo(NO)(SC_6H_5)_2]$	−16	−168	This work
$[(\eta^5\text{-}C_5H_5)Mo(NO)(SC_6H_5)_2]$	12	−174	(1)
$[\{HB(Me_2pz)_3\}MoO(SC_6H_5)_2]$	−34	−110	(2)
$[\{HB(Me_2pz)_3\}MoO(OC_6H_5)_2]$	−49	−90	(3)

References: (1) Ashby & Enemark (1986). (2) Cleland *et al.* (1987). (3) Kipke *et al.* (1989).

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Structure of Triphenyltin(IV) 2-Aminophenyl Sulfide

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Abstract. (2-Aminobenzenethiolato-*S*)triphenyltin(IV), $[Sn(C_6H_5)_3(C_6H_6NS)]$, $M_r = 474{\cdot}17$, monoclinic, $P2_1/a$, $a = 9{\cdot}074\,(1)$, $b = 19{\cdot}062\,(1)$, $c = 13{\cdot}119\,(1)$ Å, $\beta = 106{\cdot}78\,(1)°$, $V = 2172{\cdot}5\,(4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}44$ Mg m^{-3}, $\lambda(\text{Cu } K\alpha_1) = 1{\cdot}54056$ Å, $\mu = 10{\cdot}55$ mm^{-1}, $F(000) = 952$, $R = 0{\cdot}044$, $wR = 0{\cdot}037$ for 2360 $[I_{\text{net}} > 2{\cdot}5\sigma(I_{\text{net}})]$ reflections. The geometry at the Sn atom is tetrahedral and the 2-aminobenzenethiol ligand is monodentate. The compound is an uncommon example of a molecule containing an $^-$S—CH═CH—NH$_2$ ligand grouping that is neither chelating nor bridging.

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Introduction. The sulfido linkage generally reduces the Lewis acidity of tin in triorganotin sulfides; for example, triorganotin thiocarbamates are four-coordinate molecules (Chandra, James, Magee, Patalinghug, Skelton & White, 1988; Holt, Nasser, Wilson & Zuckerman, 1985; Srivastava, Gupta, Nöth & Rattay, 1988) despite the known ability of the thiocarbamato ligand to chelate to metals. The Sn atom in triphenyltin 4-pyridyl sulfide, on the other hand, is five coordinate with a trigonal-bipyramidal geometry: the imino N atom bridges the molecules to give a *trans*-C_3SnNO chain (Bokii, Struchkov, Kravtsov & Rokhlina, 1973*b*). In contrast, in triphenyltin 8-quinolinyl sulfide, the ligand adopts a chelating bonding mode which results in a monomeric *cis*-C_3SnNS trigonal-bipyramidal configuration for the compound (Furmanova, Struchkov, Rokhlina & Kravtsov, 1980). An unusual square-pyramidal geometry has been found in tribenzyltin 2-pyridyl sulfide *N*-oxide (Ng, Chen Wei, Kumar Das & Mak, 1987) but unfortunately a diffraction study on triphenyltin 2-pyridyl sulfide *N*-oxide (Boehringer Ingelheim GmbH, 1966), for which a similar geometry is anticipated, could not be carried out as the compound was not crystalline. The present study was initiated because triphenyltin 2-pyridyl sulfide *N*-oxide and triphenyltin 2-aminophenyl sulfide (Poller & Ruddick, 1972) are isoelectronic, and therefore conceivably also isostructural.

Experimental. The title compound was prepared by a literature procedure (Poller & Ruddick, 1972). The cell dimensions were obtained from 38 reflections with 2θ in the range 100·0–120·0° on a 0·10 × 0·20 × 0·30 mm crystal. The intensity data were collected to $2\theta_{\max} = 119{\cdot}9°$ with graphite-monochromatized Cu $K\alpha_1$ radiation on a Picker diffractometer using the $\theta/2\theta$ scan technique with profile analysis (Grant & Gabe, 1978); the h, k, l ranges were -10 to 9, 0 to 21 and 0 to 14; 3236 measured reflections, 2360 with $I_{\rm net} > 2{\cdot}5\sigma(I_{\rm net})$. Absorption corrections were applied. The minimum and maximum transmission factors are 0·274251 and 0·494713, respectively. The structure was solved by direct methods and refined by full-matrix least-squares techniques using the *NRC VAX* program system (Gabe, Lee & Le Page, 1985). The H-atom positions of the phenyl groups were calculated. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). The final least-squares cycle was calculated with 46 atoms, 245 parameters; weights were based on counting statistics. The residuals are: for significant reflections, $R = 0{\cdot}044$, $wR = 0{\cdot}037$, goodness-of-fit = 2·153; for all reflections, $R = 0{\cdot}065$, $wR = 0{\cdot}038$. The maximum Δ/σ ratio was 0·051. In the last $\Delta\rho$ map, the deepest hole was $-0{\cdot}400$ e Å^{-3} and the highest peak was 0·380 e Å^{-3}. The secondary-extinction coefficient was 8·149453. The final atomic positions and equivalent isotropic temperature factors are listed in Table 1. Distances and angles for triphenyltin 2-aminophenyl sulfide are listed in Table 2. Fig. 1 is a view of the molecule.*

Table 1. *Atomic coordinates and equivalent isotropic temperature factors*

	x	y	z	$B_{\rm eq}$*(Å^2)
Sn	0·79213 (6)	0·56123 (3)	0·30763 (4)	4·34 (3)
S	0·6095 (3)	0·6226 (1)	0·1621 (2)	5·7 (1)
N	0·8111 (11)	0·7405 (4)	0·1193 (7)	10·0 (7)
C(11)	0·7704 (9)	0·4538 (4)	0·2683 (6)	4·2 (4)
C(12)	0·6283 (10)	0·4244 (5)	0·2113 (7)	5·9 (5)
C(13)	0·6168 (12)	0·3540 (5)	0·1823 (8)	7·2 (6)
C(14)	0·7442 (13)	0·3108 (5)	0·2092 (8)	7·2 (7)
C(15)	0·8828 (11)	0·3381 (5)	0·2669 (7)	6·1 (6)
C(16)	0·8948 (9)	0·4097 (5)	0·2954 (6)	4·9 (5)
C(21)	0·7304 (9)	0·5908 (4)	0·4460 (6)	4·4 (4)
C(22)	0·6896 (9)	0·5410 (4)	0·5131 (7)	4·9 (5)
C(23)	0·6519 (10)	0·5633 (6)	0·6041 (7)	6·0 (6)
C(24)	0·6527 (11)	0·6318 (6)	0·6303 (7)	6·3 (6)
C(25)	0·6927 (11)	0·6816 (5)	0·5659 (7)	6·2 (6)
C(26)	0·7317 (10)	0·6609 (4)	0·4731 (7)	5·4 (5)
C(31)	1·0177 (9)	0·5971 (4)	0·3208 (6)	4·2 (4)
C(32)	1·1041 (11)	0·6291 (5)	0·4136 (7)	5·5 (5)
C(33)	1·2490 (13)	0·6525 (5)	0·4247 (8)	6·9 (7)
C(34)	1·3130 (11)	0·6436 (5)	0·3422 (11)	7·6 (8)
C(35)	1·2305 (12)	0·6113 (5)	0·2488 (8)	6·5 (7)
C(36)	1·0830 (10)	0·5881 (4)	0·2395 (7)	5·2 (5)
C(41)	0·7199 (9)	0·6199 (5)	0·0718 (6)	4·8 (5)
C(42)	0·8086 (12)	0·6805 (7)	0·0639 (9)	7·1 (7)
C(43)	0·9009 (17)	0·6734 (8)	−0·0070 (11)	10·0 (9)
C(44)	0·8988 (17)	0·6140 (10)	−0·0638 (11)	10·7 (13)
C(45)	0·8114 (15)	0·5552 (9)	−0·0565 (9)	10·6 (10)
C(46)	0·7204 (10)	0·5580 (6)	0·0120 (7)	6·2 (5)

* $B_{\rm eq}$ is the mean of the principal axes of the thermal ellipsoid.

Discussion. The Sn atom in triphenyltin 2-aminophenyl sulfide is four coordinate, with the *ipso* C atoms of the three phenyl rings and the S atom occupying the corners of the tetrahedron around the metal. The aromatic plane of the ligand is twisted around the C_{ipso}—C_{para}—S axis so that the *ortho* substituents, the amino group and an H atom, appear to be as far as possible from the metal atom [Sn—S—C(41)—C(42) −97·7 (6), Sn—S—C(41)—C(46) 80·9 (5)°]; the Sn···N distance exceeds 4 Å. A similar ligand arrangement is found in triphenyltin 2-methylphenyl sulfide (Bokii, Struchkov, Kravtsov & Rokhlina, 1974). The Sn—S bond is similar in length to those found in other four-coordinate triphenyltin aryl sulfides (Bokii, Struchkov, Kravtsov & Rokhlina, 1973*a*, 1974; Clarke, Cradwick & Wardell, 1973), but is slightly longer than the bond in bis(triphenyltin) sulfide (D'yachenko, Zolotoi, Atovmyan,

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51868 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å) *and angles* (°)

Sn—S	2·436 (2)	Sn—C(11)	2·108 (8)
Sn—C(21)	2·124 (8)	Sn—C(31)	2.118 (8)
S—C(41)	1·760 (9)	N—C(42)	1·35 (2)
C(11)—C(12)	1·41 (1)	C(11)—C(16)	1·37 (1)
C(12)—C(13)	1·39 (1)	C(13)—C(14)	1·38 (2)
C(14)—C(15)	1·37 (1)	C(15)—C(16)	1·41 (1)
C(21)—C(22)	1·42 (1)	C(21)—C(26)	1·38 (1)
C(22)—C(23)	1·40 (1)	C(23)—C(24)	1·35 (2)
C(24)—C(25)	1·39 (2)	C(25)—C(26)	1·42 (1)
C(31)—C(32)	1·39 (1)	C(31)—C(36)	1·37 (1)
C(32)—C(33)	1·36 (2)	C(33)—C(34)	1·38 (2)
C(34)—C(35)	1·38 (2)	C(35)—C(36)	1·38 (1)
C(41)—C(42)	1·43 (2)	C(41)—C(46)	1·42 (2)
C(42)—C(43)	1·43 (2)	C(43)—C(44)	1·35 (3)
C(44)—C(45)	1·39 (3)	C(45)—C(46)	1·39 (2)

S—Sn—C(11)	106·3 (2)	S—Sn—C(21)	104·8 (2)
S—Sn—C(31)	109·4 (2)	C(11)—Sn—C(21)	116·0 (3)
C(11)—Sn—C(31)	110·7 (3)	C(21)—Sn—C(31)	109·4 (3)
Sn—S—C(41)	97·1 (3)	Sn—C(11)—C(12)	121·6 (6)
Sn—C(11)—C(16)	121·4 (6)	C(12)—C(11)—C(16)	117·0 (7)
C(11)—C(12)—C(13)	121·0 (8)	C(12)—C(13)—C(14)	121·0 (8)
C(13)—C(14)—C(15)	118·8 (9)	C(14)—C(15)—C(16)	120·2 (8)
C(11)—C(16)—C(15)	122·0 (7)	Sn—C(21)—C(22)	122·4 (6)
Sn—C(21)—C(26)	119·4 (6)	C(22)—C(21)—C(26)	118·2 (7)
C(21)—C(22)—C(23)	120·0 (8)	C(22)—C(23)—C(24)	121·7 (8)
C(23)—C(24)—C(25)	119·4 (8)	C(24)—C(25)—C(26)	120·3 (8)
C(21)—C(26)—C(25)	120·3 (8)	Sn—C(31)—C(32)	120·2 (6)
Sn—C(31)—C(36)	121·3 (6)	C(32)—C(31)—C(36)	118·5 (7)
C(31)—C(32)—C(33)	121·7 (8)	C(32)—C(33)—C(34)	119·3 (9)
C(33)—C(34)—C(35)	120·5 (9)	C(34)—C(35)—C(36)	118·9 (9)
C(31)—C(36)—C(35)	121·1 (8)	S—C(41)—C(42)	117·9 (8)
S—C(41)—C(46)	119·3 (7)	C(42)—C(41)—C(46)	122·8 (9)
N—C(42)—C(41)	125 (1)	N—C(42)—C(43)	121 (1)
C(41)—C(42)—C(43)	115 (1)	C(42)—C(43)—C(44)	121 (1)
C(43)—C(44)—C(45)	124 (1)	C(44)—C(45)—C(46)	118 (1)
C(41)—C(46)—C(45)	119 (1)		

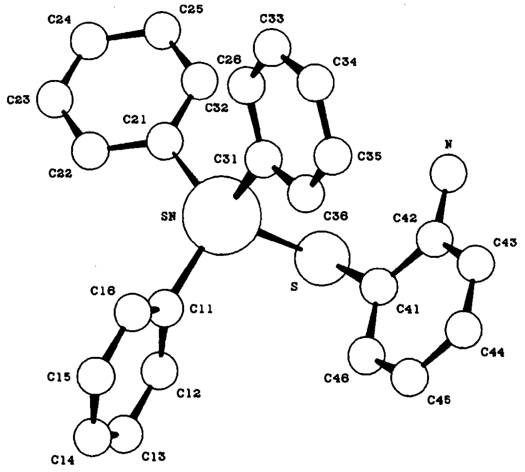

Fig. 1. Triphenyltin 2-aminophenyl sulfide, with atomic labeling.

Mirskov & Voronkov, 1977). The 97·1 (3)° Sn—S—C angle in 2-aminobenzenethiol is of a similar size compared to the angle at sulfur found in the 2-methyl (98·6°), 2,6-dibromo-4-fluoro (101·0°) (Bokii, Struchkov, Kravtsov & Rokhlina, 1974) and 2,4,6-trimethyl (100·2°) (Bokii, Struchkov, Kravtsov & Rokhlina, 1973*a*) benzenethiols, but is smaller than the angle in triphenyltin 4-*tert*-butylphenyl sulfide (105·0°) (Clarke, Cradwick & Wardell, 1973). In these structures, this Sn—S—C angle opens up in response to the steric bulk of the substituents in the ligand, and the packing of the molecules in the unit cell appears to be dictated largely by steric factors. The S atom raises the average C—Sn—C angle in the title compound from the tetrahedral 109·5 to 112·0°, in accordance with Bent's (1961) rule, which predicts that the more electronegative S atom will tend to concentrate *p* character along the Sn—S bond, thereby imparting more *s* character to the Sn—C bonds. The average C—Sn—C angle in the related four-coordinate (2-aminobenzoato)triphenyltin (Swisher, Vollano, Chandrasekhar, Day & Holmes, 1984) is also 112·0°; the amino group is hydrogen bonded to the carboxyl O atom, precluding a bridging or a chelating mode for the ligand. The N and S atoms in the title compound are presumably also hydrogen bonded.

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