Portions of the solution were placed in screw-capped vials, overlain with ethanol, closed and allowed to stand at room temperature. Small colorless prisms formed in about one week.

Diffraction data were corrected for Lorentz and polarization effects and an empirical absorption correction was applied (North, Phillips & Mathews, 1968). The positions of the K atoms were obtained using the direct methods program *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declerq & Woolfson, 1980) and a structure-factor calculation using these gave a Fourier map from which the remaining non-H atoms were located. Refinement of the structure on *F*, first with isotropic and then anisotropic thermal parameters, using a full-matrix least-squares procedure, gave parameters for the calculation of a difference Fourier map from which the locations of the H atoms were found. These H atoms were included in the final refinement cycles with isotropic thermal factors equivalent to those of the atoms to which they were bonded. All crystallographic calculations were made with in-house programs (Carrell, Shieh & Takusagawa, 1981). Thermal ellipsoid diagrams were produced with the program *SNOOPI* (Davies, 1983) and other diagrams with the program *VIEW* (Carrell, 1976).

This research was supported by grants GM-44360 and CA-06927 from the National Institutes of Health and by an appropriation from the Commonwealth of Pennsylvania.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances, bond angles and torsion angles involving H atoms, and direction cosines of non-H-atom thermal ellipsoids have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71070 (58 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1033]

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Structure of Strontium Citrate Pentahydrate

David E. Zacharias and Jenny P. Glusker

The Institute for Cancer Research, The Fox Chase Cancer Center, Philadelphia, PA 19111, USA

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Abstract

The crystal structure of tristrontium bis(2-hydroxy-1,2,3-propanetricarboxylate) pentahydrate has been determined. One Sr ion is coordinated with eight O atoms, another with nine and the third with ten at distances ranging from 2.498 (2) to 2.781 (2) Å. Two Sr ions are bound to citrate ions in a tridentate manner. Both citrate ions in the asymmetric unit are in an extended conformation. There are 11 hydrogen bonds in one asymmetric unit of the crystal structure.

Comment

The crystal structure of strontium citrate has been determined in order to establish the conformation of the citrate ion and the manner by which it is chelated by the metal ion, for comparison with data from other citrate ions (Glusker, 1980).

This crystal structure determination shows that the citrate ion is in an extended conformation. As in other citrates the plane of the central carboxyl group is almost perpendicular to the plane of the C-atom backbone [C(1) to C(5)]. The O atom of the hydroxyl group lies in the plane of the central carboxyl group [C(6), O(5), O(6) on C(3)]. Both citrate ions are chelated in a tridentate manner to an Sr cation; Sr(1) binds O(5*A*), O(7*A*) and O(4*A*) while Sr(3) binds O(5*B*), O(7*B*) and O(2*B*) (Table 2). Sr ions share both O atoms of the central carboxyl group [O(5) and O(6) bound by Sr($1^{\rm ii}$) and Sr($3^{\rm viii}$)] and the carboxyl group not involved in tridentate chelation [O(1*A*) and O(2*A*) to Sr($3^{\rm vii}$) and O(3*B*) and O(4*B*) to Sr($1^{\rm iii}$)]. This type of binding is particularly characteristic of divalent ions with metal–oxygen distances of approximately 2.6 Å (Carrell, Carrell, Erlebacher & Glusker, 1988), the range here being 2.650–2.772 Å. The hydroxyl group H atoms act as bridges between different citrate ions through hydrogen bonding (see Table 2 and Fig. 2).

The Sr—O distances vary from 2.498 (2) to 2.781 (2) Å, with average values of 2.58 Å for coordination number 8 [Sr(2)], 2.67 Å for coordination number 9 [Sr(1)], and 2.68 Å for coordination number 10 [Sr(3)]. These values are considerably longer than the seven-coordinate Ca—O distances of 2.372 to 2.490 Å found in calcium hydrogen citrate (Sheldrick, 1974).

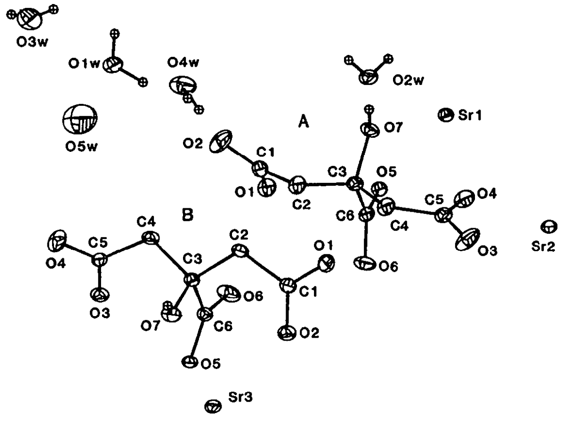

Fig. 1. Atomic numbering and representation, at 50% probability level, of the thermal ellipsoids (*ORTEP*; Johnson, 1965).

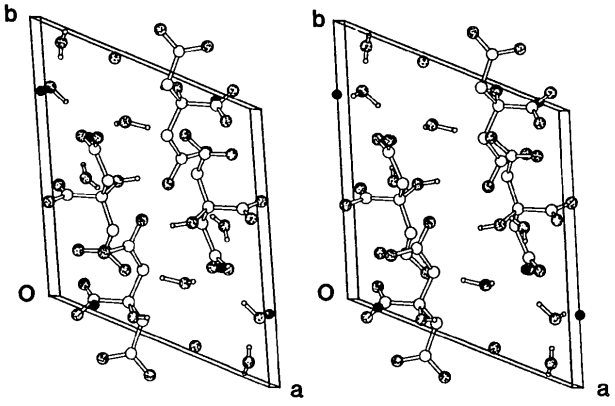

Fig. 2. Stereoview of the crystal packing projected down the *c* axis. Metal ions are black, O atoms are stippled.

Experimental

Crystal data

$3Sr^{2+}.2C_6H_5O_7^{3-}.5H_2O$
M_r = 731.14
Triclinic
$P\bar{1}$
a = 10.720 (2) Å
b = 12.467 (2) Å
c = 9.124 (2) Å
α = 104.77 (2)°
β = 100.12 (2)°
γ = 111.19 (2)°
V = 1049.4 (4) Å^3
Z = 2

D_x = 2.31 Mg m^{-3}
Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 14 reflections with
θ = 40-45°
μ = 10.842 mm^{-1}
T = 293 K
Prism
0.5 × 0.08 × 0.08 mm
Colorless

Data collection

Siemens-Nicolet *P*3*m* diffractometer
Variable θ-2θ scans of rate 2.02-58.6° min^{-1}
Absorption correction: empirical
T_{min} = 0.795, T_{max} = 1.000
4147 measured reflections
3951 independent reflections
3924 observed reflections [$I \geq 3.0\sigma(I)$]

R_{int} = 0.016
θ_{max} = 69.5°
$h = -13 \rightarrow 12$
$k = -15 \rightarrow 14$
$l = 0 \rightarrow 11$
4 standard reflections monitored every 92 reflections
intensity variation: <1%

Refinement

Refinement on F
Final R = 0.031 (R_{all} = 0.030)
wR = 0.042 (wR_{all} = 0.042)
S = 1.25
3924 reflections
379 parameters
All H-atom parameters refined
$w = [\sigma^2(F)]^{-1}$; $\sigma(F) = (F/2)[\sigma^2(I)/(I)^2 + \delta^2]^{1/2}$, δ = 0.021 (instrumental uncertainty)

$(\Delta/\sigma)_{max}$ = 0.6 for Sr,O,C;
= 0.9 for H
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic thermal parameters* (Å^2)

For non-H atoms U_{eq} = 1/3(trace of the orthogonalized U_{ij} matrix).

	x	y	z	U_{iso}/U_{eq}
Sr(1)	0.78833 (2)	0.35978 (2)	0.47373 (3)	0.0166 (1)
Sr(2)	1.01216 (2)	0.26785 (2)	0.21363 (3)	0.0161 (1)
Sr(3)	0.85298 (2)	0.98377 (2)	−0.22866 (3)	0.0186 (1)
O(1*W*)	0.0684 (3)	0.7719 (2)	0.0970 (3)	0.028 (1)
O(2*W*)	0.8027 (3)	0.5141 (2)	0.7548 (3)	0.027 (1)
O(3*W*)	0.1154 (3)	0.9473 (3)	0.4654 (4)	0.042 (1)
O(4*W*)	0.3917 (3)	0.7540 (3)	0.3904 (4)	0.035 (1)
O(5*W*)	0.3643 (4)	0.9719 (4)	0.3701 (6)	0.082 (2)
O(1*A*)	0.8705 (2)	0.7943 (2)	0.5733 (3)	0.021 (1)
O(2*A*)	0.6627 (3)	0.7963 (3)	0.5174 (3)	0.033 (1)
O(3*A*)	0.7761 (3)	0.3571 (3)	−0.0629 (3)	0.039 (1)
O(4*A*)	0.8366 (2)	0.3711 (2)	0.1893 (3)	0.026 (1)
O(5*A*)	0.9426 (2)	0.5855 (2)	0.5089 (3)	0.0171 (8)
O(6*A*)	1.0046 (2)	0.6669 (2)	0.3299 (3)	0.025 (1)
O(7*A*)	0.6755 (2)	0.4830 (2)	0.3622 (3)	0.0223 (9)
C(1*A*)	0.7498 (3)	0.7568 (3)	0.4791 (4)	0.019 (1)
C(2*A*)	0.7162 (3)	0.6721 (3)	0.3119 (4)	0.022 (1)
C(3*A*)	0.7580 (3)	0.5661 (3)	0.2944 (4)	0.018 (1)
C(4*A*)	0.7320 (3)	0.4994 (3)	0.1197 (4)	0.021 (1)
C(5*A*)	0.7854 (3)	0.4019 (3)	0.0808 (4)	0.020 (1)
C(6*A*)	0.9139 (3)	0.6111 (3)	0.3852 (4)	0.017 (1)
O(1*B*)	0.6027 (2)	0.5983 (2)	−0.2037 (4)	0.027 (1)
O(2*B*)	0.7875 (2)	0.7759 (2)	−0.1428 (3)	0.025 (1)
O(3*B*)	0.8049 (2)	1.1603 (2)	0.3043 (3)	0.021 (1)
O(4*B*)	0.5923 (2)	1.1502 (2)	0.2609 (4)	0.028 (1)
O(5*B*)	0.9220 (2)	1.0411 (2)	0.0841 (3)	0.0151 (9)
O(6*B*)	0.8723 (3)	0.9149 (2)	0.2189 (3)	0.028 (1)
O(7*B*)	0.6677 (2)	0.9667 (2)	−0.0784 (3)	0.0197 (9)
C(1*B*)	0.6699 (3)	0.7122 (3)	−0.1340 (4)	0.018 (1)
C(2*B*)	0.6042 (3)	0.7754 (3)	−0.0261 (4)	0.018 (1)
C(3*B*)	0.6797 (3)	0.9157 (3)	0.0437 (4)	0.016 (1)
C(4*B*)	0.6126 (3)	0.9608 (3)	0.1674 (4)	0.020 (1)
C(5*B*)	0.6736 (3)	1.0991 (3)	0.2463 (4)	0.017 (1)
C(6*B*)	0.8366 (3)	0.9595 (3)	0.1219 (4)	0.016 (1)
H(O7*A*)	0.584 (5)	0.443 (5)	0.309 (7)	0.07 (2)
H(O7*B*)	0.606 (4)	0.948 (4)	−0.132 (5)	0.04 (1)
H(1O1*W*)	0.136 (5)	0.741 (5)	0.086 (7)	0.07 (2)
H(2O1*W*)	0.031 (5)	0.742 (5)	0.159 (7)	0.07 (2)

H(1O2W)	0.750 (6)	0.530 (6)	0.774 (8)	0.09 (2)
H(2O2W)	0.808 (5)	0.468 (5)	0.806 (7)	0.06 (2)
H(1O3W)	0.133 (4)	0.991 (4)	0.537 (6)	0.04 (1)
H(2O3W)	0.108 (6)	0.891 (6)	0.458 (8)	0.07 (2)
H(1O4W)	0.494 (6)	0.768 (5)	0.424 (8)	0.07 (2)
H(2O4W)	0.357 (6)	0.736 (5)	0.284 (7)	0.07 (2)

Table 2. *Geometric parameters* (Å, °)

For torsion angles e.s.d.'s are 0.2°.

O(1A)—C(1A)	1.265 (3)	O(1B)—C(1B)	1.257 (3)
O(2A)—C(1A)	1.263 (2)	O(2B)—C(1B)	1.253 (2)
O(3A)—C(5A)	1.257 (4)	O(3B)—C(5B)	1.264 (2)
O(4A)—C(5A)	1.259 (3)	O(4B)—C(5B)	1.259 (2)
O(5A)—C(6A)	1.267 (4)	O(5B)—C(6B)	1.269 (2)
O(6A)—C(6A)	1.244 (3)	O(6B)—C(6B)	1.235 (3)
O(7A)—C(3A)	1.447 (3)	O(7B)—C(3B)	1.426 (3)
C(1A)—C(2A)	1.511 (5)	C(1B)—C(2B)	1.529 (3)
C(2A)—C(3A)	1.523 (3)	C(2B)—C(3B)	1.532 (3)
C(3A)—C(4A)	1.520 (5)	C(3B)—C(4B)	1.537 (4)
C(3A)—C(6A)	1.546 (3)	C(3B)—C(6B)	1.533 (3)
C(4A)—C(5A)	1.511 (3)	C(4B)—C(5B)	1.518 (3)
O(7A)—H(O7A)	0.90 (4)	O(7B)—H(O7B)	0.67 (3)
O(1W)—H(1O1W)	0.95 (2)	O(3W)—H(1O3W)	0.68 (4)
O(1W)—H(2O1W)	0.83 (4)	O(3W)—H(2O3W)	0.66 (4)
O(2W)—H(1O2W)	0.69 (3)	O(4W)—H(1O4W)	1.02 (3)
O(2W)—H(2O2W)	0.84 (4)	O(4W)—H(2O4W)	0.91 (6)
Sr(1)—O(2W)	2.726 (2)	Sr(2)—O(2$B^{\rm v}$)	2.546 (1)
Sr(1)—O(4$W^{\rm i}$)	2.652 (2)	Sr(2)—O(3$B^{\rm iii}$)	2.545 (1)
Sr(1)—O(4A)	2.762 (2)	Sr(2)—O(5$B^{\rm iii}$)	2.498 (2)
Sr(1)—O(5$A^{\rm ii}$)	2.678 (1)	Sr(3)—O(1$W^{\rm vi}$)	2.712 (2)
Sr(1)—O(5A)	2.597 (1)	Sr(3)—O(3$W^{\rm vi}$)	2.552 (3)
Sr(1)—O(6$A^{\rm ii}$)	2.772 (2)	Sr(3)—O(5$W^{\rm vi}$)	2.762 (3)
Sr(1)—O(7A)	2.563 (2)	Sr(3)—O(1$A^{\rm vii}$)	2.673 (2)
Sr(1)—O(3$B^{\rm iii}$)	2.658 (2)	Sr(3)—O(2$A^{\rm vii}$)	2.669 (3)
Sr(1)—O(4$B^{\rm iii}$)	2.650 (2)	Sr(3)—O(2B)	2.781 (2)
Sr(2)—O(1$W^{\rm iv}$)	2.672 (3)	Sr(3)—O(6$B^{\rm viii}$)	2.728 (1)
Sr(2)—O(2$W^{\rm ii}$)	2.629 (1)	Sr(3)—O(5$B^{\rm viii}$)	2.699 (1)
Sr(2)—O(1$A^{\rm ii}$)	2.564 (2)	Sr(3)—O(5B)	2.652 (2)
Sr(2)—O(4A)	2.645 (1)	Sr(3)—O(7B)	2.583 (1)
Sr(2)—O(5$A^{\rm ii}$)	2.560 (2)		
O(1A)—C(1A)—O(2A)	121.7 (3)	O(1B)—C(1B)—O(2B)	124.9 (2)
O(1A)—C(1A)—C(2A)	118.1 (1)	O(1B)—C(1B)—C(2B)	116.7 (2)
O(2A)—C(1A)—C(2A)	119.9 (2)	O(2B)—C(1B)—C(2B)	118.4 (2)
C(1A)—C(2A)—C(3A)	116.6 (2)	C(1B)—C(2B)—C(3B)	115.8 (2)
O(7A)—C(3A)—C(2A)	108.8 (2)	O(7B)—C(3B)—C(2B)	110.3 (2)
O(7A)—C(3A)—C(4A)	110.1 (2)	O(7B)—C(3B)—C(4B)	110.1 (2)
O(7A)—C(3A)—C(6A)	107.3 (2)	O(7B)—C(3B)—C(6B)	107.1 (2)
C(2A)—C(3A)—C(4A)	109.6 (2)	C(2B)—C(3B)—C(4B)	108.2 (2)
C(2A)—C(3A)—C(6A)	111.6 (2)	C(2B)—C(3B)—C(6B)	111.3 (2)
C(4A)—C(3A)—C(6A)	109.5 (2)	C(4B)—C(3B)—C(6B)	109.9 (2)
C(3A)—C(4A)—C(5A)	116.9 (2)	C(3B)—C(4B)—C(5B)	115.1 (2)
O(3A)—C(5A)—O(4A)	123.9 (2)	O(3B)—C(5B)—O(4B)	120.9 (2)
O(3A)—C(5A)—C(4A)	115.8 (2)	O(3B)—C(5B)—C(4B)	119.6 (1)
O(4A)—C(5A)—C(4A)	120.2 (3)	O(4B)—C(5B)—C(4B)	119.4 (2)
O(5A)—C(6A)—O(6A)	123.2 (2)	O(5B)—C(6B)—O(6B)	124.0 (2)
O(5A)—C(6A)—C(3A)	118.4 (2)	O(5B)—C(6B)—C(3B)	117.5 (2)
O(6A)—C(6A)—C(3A)	118.3 (2)	O(6B)—C(6B)—C(3B)	118.4 (2)
C(3A)—O(7A)—H(O7A)	114 (3)	C(3B)—O(7B)—H(O7B)	121 (3)

H(1O1W)—O(1W)—H(2O1W)	105 (3)
H(1O2W)—O(2W)—H(2O2W)	104 (5)
H(1O3W)—O(3W)—H(2O3W)	123 (6)
H(1O4W)—O(4W)—H(2O4W)	113 (4)
O(7A)—C(3A)—C(6A)—O(5A)	−9.5
O(7A)—C(3A)—C(6A)—O(6A)	168.0
C(2A)—C(3A)—C(6A)—O(5A)	109.6
C(2A)—C(3A)—C(6A)—O(6A)	−73.0
C(4A)—C(3A)—C(6A)—O(5A)	−128.9
C(4A)—C(3A)—C(6A)—O(6A)	48.6
O(7B)—C(3B)—C(6B)—O(5B)	9.5
O(7B)—C(3B)—C(6B)—O(6B)	−171.6
C(2B)—C(3B)—C(6B)—O(5B)	130.1
C(2B)—C(3B)—C(6B)—O(6B)	−50.9
C(4B)—C(3B)—C(6B)—O(5B)	−110.1
C(4B)—C(3B)—C(6B)—O(6B)	68.9

D—H···A	D—H	H···A	D···A	D—H···A
O(7A)—H···O(1$B^{\rm iv}$)	0.90 (4)	1.88 (3)	2.750 (2)	165 (3)
O(7B)—H···O(4$B^{\rm vi}$)	0.67 (3)	1.97 (3)	2.619 (3)	162 (3)
O(1W)—H1···O(3$A^{\rm iv}$)	0.95 (2)	1.79 (3)	2.706 (2)	163 (3)
O(1W)—H2···O(6$A^{\rm ix}$)	0.83 (4)	2.03 (5)	2.825 (3)	160 (3)
O(2W)—H1···O(1$B^{\rm x}$)	0.69 (3)	2.07 (3)	2.748 (2)	167 (6)
O(2W)—H2···O(3$A^{\rm x}$)	0.84 (4)	2.02 (4)	2.846 (3)	165 (2)
O(3W)—H1···O(6$B^{\rm xi}$)	0.68 (4)	2.26 (4)	2.905 (4)	159 (3)
O(3W)—H2···O(6$A^{\rm ix}$)	0.66 (4)	2.46 (5)	3.072 (3)	155 (6)
O(3W)—H2···O(3$B^{\rm xi}$)	0.66 (4)	2.53 (6)	2.929 (3)	121 (7)
O(4W)—H1···O(2A)	1.02 (3)	1.72 (4)	2.730 (2)	169 (5)
O(4W)—H2···O(3$A^{\rm iv}$)	0.91 (6)	2.01 (6)	2.878 (4)	158 (3)

Symmetry code: (i) $1-x, 1-y, 1-z$; (ii) $2-x, 1-y, 1-z$; (iii) $x, y-1, z$; (iv) $1-x, 1-y, -z$; (v) $2-x, 1-y, -z$; (vi) $1-x, 2-y, -z$; (vii) $x, y, z-1$; (viii) $2-x, 2-y, -z$; (ix) $x-1, y, z$; (x) $x, y, 1+z$; (xi) $1-x, 2-y, 1-z$.

An aqueous solution of strontium chloride and trisodium citrate in the approximate molar ratio of 3:2 was warmed with stirring, and then slowly reduced in volume by warming without stirring. Clear colorless prismatic crystals of strontium citrate pentahydrate formed over 15 d.

Diffraction data were corrected for Lorentz and polarization effects and an empirical absorption correction was applied (North, Phillips & Mathews, 1968). The positions of the Sr atoms were deduced from the highest peaks in a Patterson map; a structure-factor calculation using these and the ensuing Fourier map revealed the positions of all non-H atoms. Refinement of the structure on F, first with isotropic and then anisotropic thermal parameters, using a full-matrix least-squares procedure, followed by calculation of a difference Fourier map, led to the location of most of the H atoms. These were included in the final refinement cycles with isotropic thermal parameters equivalent to those of the atoms to which they were bonded. The H atoms of one water molecule, O(5W), were not located. All crystallographic calculations were made with in-house programs (Carrell, Shieh & Takusagawa, 1981). Thermal ellipsoid diagrams were produced with the program *SNOOPI* (Davies, 1983) and other diagrams with the program *VIEW* (Carrell, 1976).

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances, bond angles and torsion angles involving H atoms, and direction cosines of non-H-atom thermal ellipsoids have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71072 (41 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1034]

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Diphenylbis(2-pyridinethiolato)tin(IV)

RALF SCHMIEDGEN, FRIEDO HUBER* AND HANS PREUT

Lehrstuhl für Anorganische Chemie II,
Universität Dortmund, Otto-Hahn-Strasse 6,
D-4600 Dortmund 50, Germany

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Abstract

The polyhedron around tin in the title compound is a distorted trapezoidal bipyramid with the two C(phenyl) atoms in axial positions. The trapezoidal plane is formed by the two 2-pyridinethiolato residues which act as bidentate ligands with *cis* Sn—S and *cis* Sn—N bonds. Sn—N coordination is indicated by short intramolecular Sn—N distances [Sn—N(1) = 2.636 (4), Sn—N(2) = 2.698 (4) Å]. The axial C atoms are shifted towards the half-sphere occupied by two N atoms resulting in a C—Sn—C angle of 125.5 (1)°. No short intermolecular interactions are observed.

Comment

Predictions of the coordination number of tin in diorganotin complexes with S,N chelate ligands from ^{119}Sn NMR shift data are, in contrast to other types of organotin compounds, still unreliable since knowledge of the structure of such compounds is insufficient. To improve this situation we started to study the structures of various types of diorganotin compounds with S,N ligands, for instance, diorganobis(2-pyridinethiolato)tin(IV) compounds, both in solution and in the solid state. From IR and Mössbauer spectra, a distorted octahedral coordination polyhedron could be inferred, but a decision as to whether the chelate ligands are arranged *cis* or *trans* was only possible by single-crystal structure determination. We report here the structure of the title compound which was first prepared by Mullins (1979).

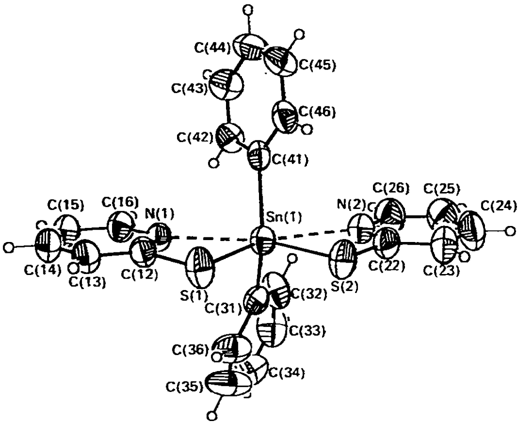

Fig. 1. The title molecule and numbering scheme.

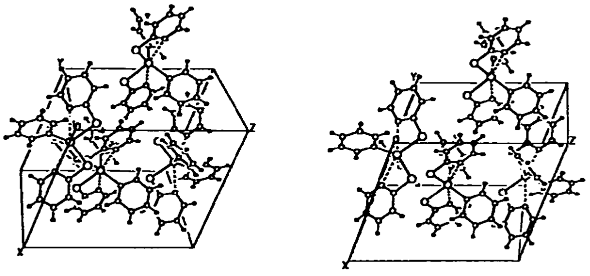

Fig. 2. Stereoscopic view of the unit cell.

The polyhedron around Sn in $Ph_2Sn(2\text{-}SPy)_2$ (2-SPy = 2-pyridinethiolate) corresponds to that found in ^{n}$Bu_2Sn(2\text{-}SPy\text{-}5\text{-}NO_2)_2$ (Domazetis, James, Mackay & Magee, 1979). It is a distorted trapezoidal bipyramid with S(1), S(2), N(1) and N(2) in the trapezoidal plane, and the two C(phenyl) atoms in apical positions. The trapezoidal plane containing the two 2-SPy ligands and tin is nearly planar. The bond distances Sn—N(1) and Sn—N(2) [mean 2.667 (4) Å] are appreciably shorter than the sum of the appropriate van der Waals radii of 3.75 Å (Bondi, 1964) and indicate the bidentate chelating nature of the 2-SPy ligands. Similar distances exist in ^{n}$Bu_2Sn(2\text{-}SPy\text{-}5\text{-}NO_2)_2$ [Sn—N = 2.77 (1) Å; Domazetis, James, Mackay & Magee, 1979] and shorter values are found in $Cl_2Sn(2\text{-}SPy)_2$ [Sn—N = 2.271 (9) and 2.256 (9) Å; Masaki, Matsunami & Ueda, 1978]. The Sn—S bond distances [Sn—S = 2.485 (1) and 2.476 (2) Å] are essentially the same as in ^{n}$Bu_2Sn(2\text{-}SPy\text{-}5\text{-}NO_2)_2$ [Sn—S = 2.477 (3) Å; Domazetis, James, Mackay & Magee, 1979] or $Ph_2Sn(S_2COEt)_2$ [Sn—S = 2.482 (1) and 2.500 (1) Å; Donoghue & Tiekink, 1991]. The C—Sn—C axis is bent [125.5 (1)°] towards the coordinative Sn—N bonds. No intermolecular distances exist which are shorter than the sum of the van der Waals radii.