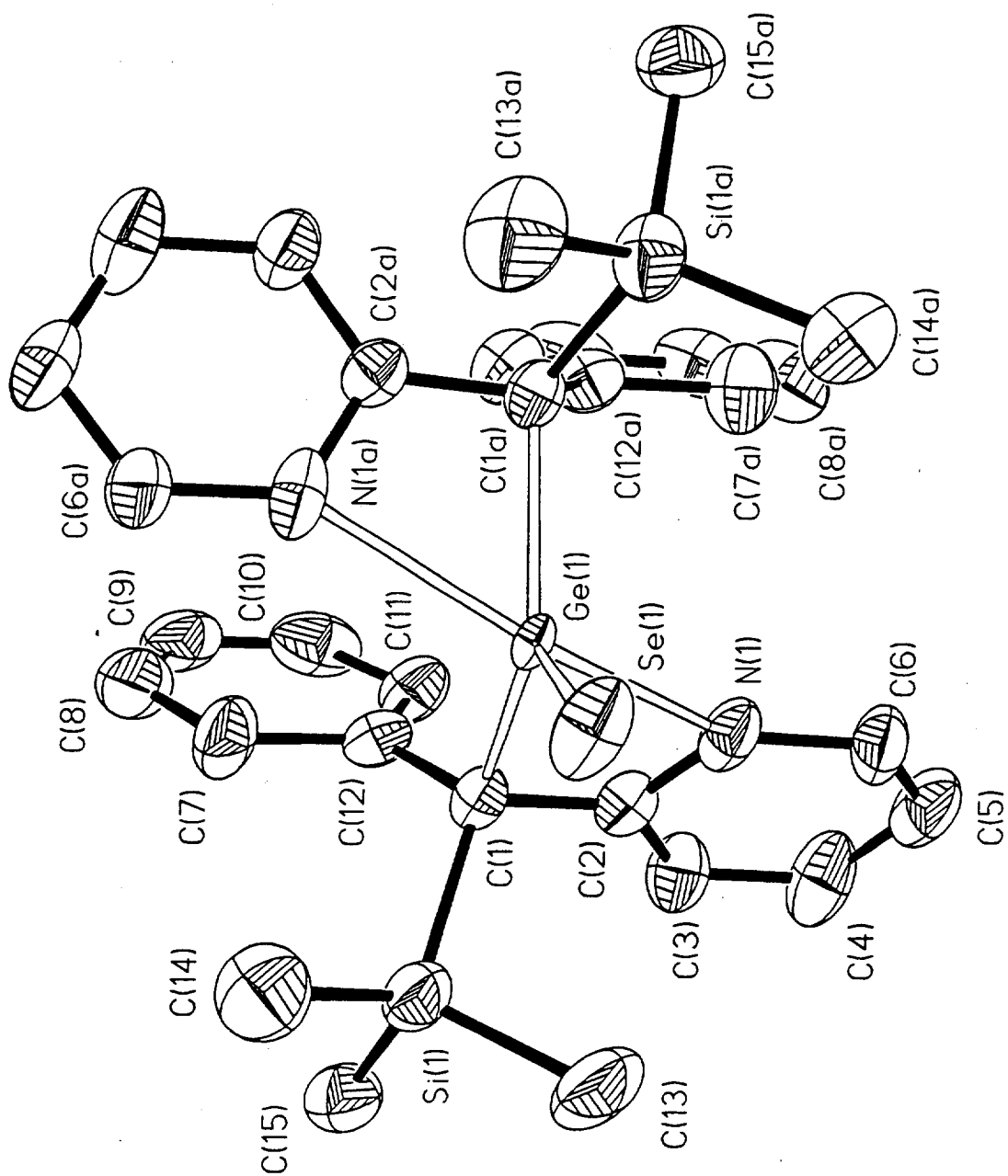




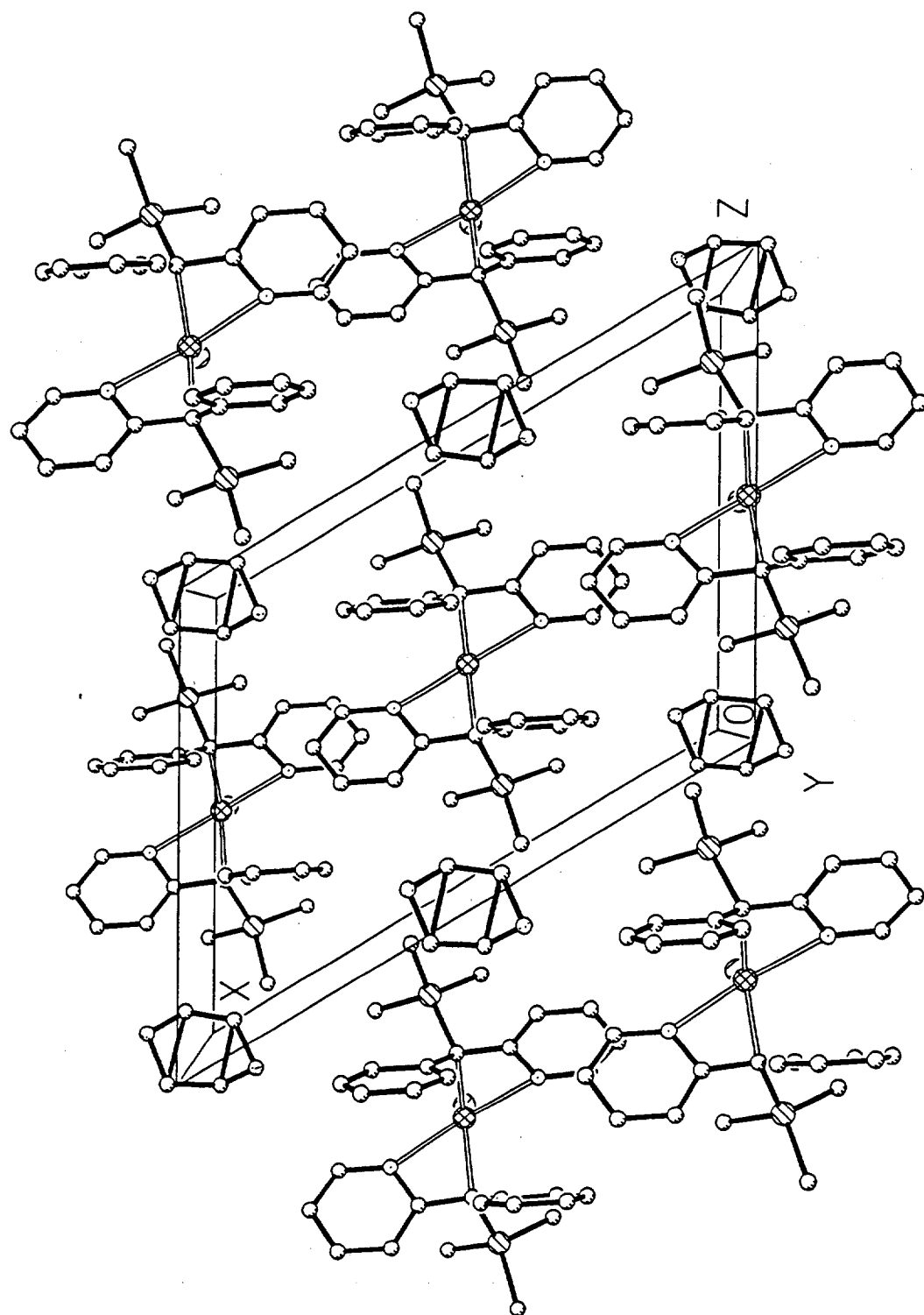


Table 1. Data collection and processing parameters.

Directory	ZZY\leu114	The sample from W.B.Leung	4 Sep. 1995
Molecular formula	$C_{30}H_{36}N_2Si_2GeSe.C_4H_8O$		
Molecular weight	704.44		
Color and habit	colorless prism		
Crystal size	0.20 x 0.18 x 0.28 mm ³		
Crystal system	monoclinic		
Space group	C2 (No. 5)		
Unit cell parameters	$a = 16.296(3)$ $\alpha = 90^\circ$ $b = 10.724(2)$ $\beta = 121.27(1)^\circ$ $V = 1803.05(.71)\text{\AA}^3$ $c = 12.071(2)$ $\gamma = 90^\circ$ $Z = 2$ $F(000) = 728$		
Density (calcd)	1.298 gcm ⁻³		
Radiation	graphite-monochromatized MoK α , $\lambda = 0.71073 \text{\AA}$		
R_{int} (from merging of equiv. reflections)	0.054		
Scan type and rate	taking oscillation IP photos; 30 frames in total, $\phi = -30 - 150^\circ$, $\Delta\phi = 6^\circ$. 8 mins per frame.		
Crystal to detector distance	69.52 mm		
Background level	-70		
Collection range	$0 \leq h \leq 19$, $0 \leq k \leq 12$, $-14 \leq l \leq 12$;		
Reflections Collected	1745		
Independent Reflections	1682 ($R_{int} = 2.28\%$)		
Obs. data with $ F_o \geq 6\sigma(F_o)$, n	1324		
No. of variables, p	186		
Extinction Correction	$\chi = 0.0043$, where $F^* = F [1 + 0.002\chi F^2 / \sin(2\theta)]^{-1/4}$		
Weighting scheme	$w = [\sigma^2 F_o + 0.0008 F_o ^2]^{-1}$		
$R_F = \sum F_o - F_c / \sum F_o $	0.056		
$wR = [\sum w(F_o - F_c)^2 / \sum w F_o ^2]^{1/2}$	0.076		
$S = [\sum w(F_o - F_c)^2 / (n - p)]^{1/2}$	1.61		
Largest and mean Δ/σ	0.012, 0.006		
Residual extrema in final difference map	+0.50 to -0.57 e $\text{\AA}^{-3}$		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic temperature factors* ($\text{\AA}^2 \times 10^3$)

Atom	x	y	z	U_{eq}
Ge(1)	5000	3183	5000	41(1)
Se(1)	5000	921(2)	5000	113(1)
Si(1)	4317(2)	3334(3)	1822(3)	105(1)
N(1)	6391(3)	3872(3)	5008(3)	98(1)
C(1)	4845(3)	4388(4)	3342(4)	77(1)
C(2)	5847(3)	4547(3)	3897(3)	83(1)
C(3)	6338(3)	5231(4)	3444(3)	107(1)
C(4)	7335(3)	5156(4)	4051(3)	135(1)
C(5)	7884(3)	4489(3)	5198(3)	125(1)
C(6)	7369(3)	3790(4)	5606(3)	116(1)
C(7)	3270(3)	5502(3)	2472(4)	124(1)
C(8)	2714(3)	6570(3)	2230(4)	144(1)
C(9)	3171(3)	7721(3)	2617(4)	143(1)
C(10)	4166(3)	7786(3)	3220(4)	142(1)
C(11)	4710(3)	6705(3)	3495(4)	111(1)
C(12)	4269(3)	5547(3)	3096(4)	87(1)
C(13)	5300(4)	2155(4)	2158(4)	160(1)
C(14)	3275(4)	2451(4)	1512(4)	158(1)
C(15)	3972(4)	4434(4)	368(4)	127(1)
C(16)	4388(4)	8861(4)	275(4)	306(1)
C(17)	5338(4)	8190(4)	1035(4)	337(1)
O(1)	6011(4)	8653(4)	1091(4)	175(1)

* U_{eq} defined as one third of the trace of the orthogonalized U tensor.

Table 3. Bond lengths (Å) and bond angles (°).

Ge(1)-Se(1)	2.426 (2)	Ge(1)-N(1)	2.379 (5)
Ge(1)-C(1)	2.283 (5)	Ge(1)-N(1A)	2.379 (5)
Ge(1)-C(1A)	2.283 (5)	Si(1)-C(1)	1.936 (5)
Si(1)-C(13)	1.911 (6)	Si(1)-C(14)	1.805 (7)
Si(1)-C(15)	1.939 (5)	N(1)-C(2)	1.369 (5)
N(1)-C(6)	1.369 (5)	C(1)-C(2)	1.417 (7)
C(1)-C(12)	1.491 (6)	C(2)-C(3)	1.391 (7)
C(3)-C(4)	1.394 (6)	C(4)-C(5)	1.395 (5)
C(5)-C(6)	1.392 (7)	C(7)-C(8)	1.394 (6)
C(7)-C(12)	1.396 (6)	C(8)-C(9)	1.391 (5)
C(9)-C(10)	1.393 (6)	C(10)-C(11)	1.390 (5)
C(11)-C(12)	1.390 (5)	C(16)-C(17)	1.510 (7)
C(16)-O(1a)	1.441 (6)	C(17)-O(1)	1.173 (9)
Se(1)-Ge(1)-N(1)	108.1(1)	Se(1)-Ge(1)-C(1)	124.5(1)
N(1)-Ge(1)-C(1)	60.0(2)	N(1)-Ge(1)-N(1A)	143.8(2)
C(1)-Ge(1)-N(1A)	98.5(2)	Se(1)-Ge(1)-C(1A)	124.5(1)
C(1)-Ge(1)-C(1A)	111.1(2)	C(1)-Si(1)-C(13)	105.9(2)
C(1)-Si(1)-C(14)	114.1(3)	C(13)-Si(1)-C(14)	107.0(3)
C(1)-Si(1)-C(15)	106.3(2)	C(13)-Si(1)-C(15)	114.3(3)
C(14)-Si(1)-C(15)	109.4(2)	Ge(1)-N(1)-C(2)	91.6(3)
Ge(1)-N(1)-C(6)	145.9(3)	C(2)-N(1)-C(6)	122.4(5)
Ge(1)-C(1)-Si(1)	107.1(2)	Ge(1)-C(1)-C(2)	94.4(2)
Si(1)-C(1)-C(2)	110.7(4)	Ge(1)-C(1)-C(12)	114.7(4)
Si(1)-C(1)-C(12)	112.0(2)	C(2)-C(1)-C(12)	116.4(3)
N(1)-C(2)-C(1)	113.7(4)	N(1)-C(2)-C(3)	116.8(4)
C(1)-C(2)-C(3)	129.4(3)	C(2)-C(3)-C(4)	121.0(3)
C(3)-C(4)-C(5)	121.5(5)	C(4)-C(5)-C(6)	115.7(4)
N(1)-C(6)-C(5)	122.0(3)	C(8)-C(7)-C(12)	122.3(3)
C(7)-C(8)-C(9)	118.8(4)	C(8)-C(9)-C(10)	119.7(4)
C(9)-C(10)-C(11)	120.6(3)	C(10)-C(11)-C(12)	120.7(4)
C(1)-C(12)-C(7)	121.0(3)	C(1)-C(12)-C(11)	121.1(4)
C(7)-C(12)-C(11)	117.8(4)	C(17)-C(16)-O(1a)	109.4(5)
C(16)-C(17)-O(1)	117.8(4)	C(17)-O(1)-C(16a)	98.4(4)

Symmetry transformation a (-x, y, -z)

Table 4. Anisotropic thermal parameters* ($\text{\AA}^2 \times 10^3$).

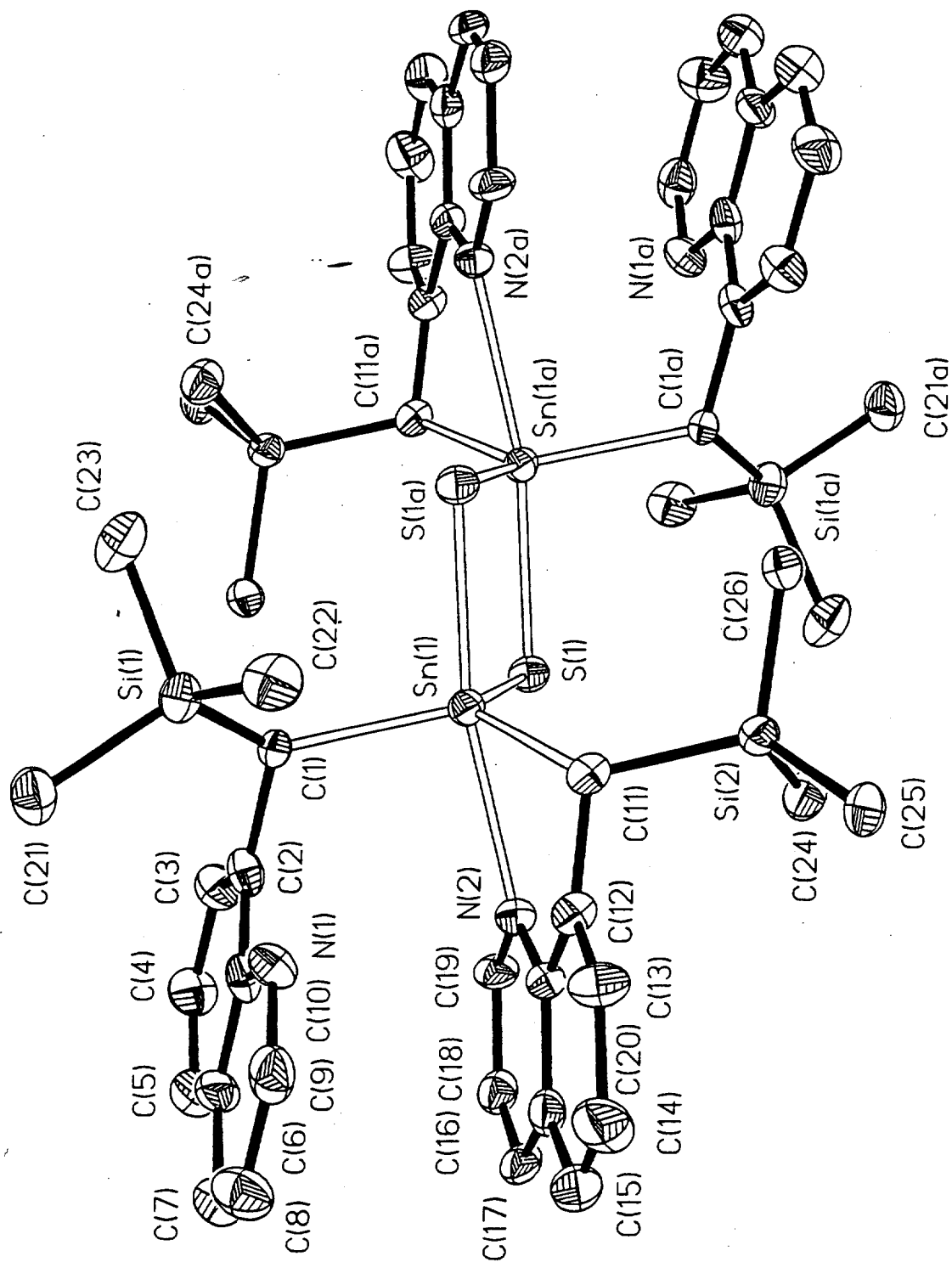
Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge(1)	36(1)	30(1)	66(1)	0	32(1)	0
Se(1)	105(1)	62(1)	199(1)	0	97(1)	0
Si(1)	91(1)	107(1)	126(1)	-3(1)	62(1)	-31(1)
N(1)	65(1)	95(1)	142(1)	-15(1)	58(1)	-40(1)
C(1)	69(1)	76(1)	96(1)	5(1)	49(1)	-2(1)
C(2)	83(1)	79(1)	101(1)	4(1)	58(1)	3(1)
C(3)	86(1)	107(1)	135(1)	-3(1)	61(1)	15(1)
C(4)	99(1)	97(1)	229(1)	-10(1)	99(1)	0(1)
C(5)	92(1)	146(1)	170(1)	-16(1)	91(1)	-21(1)
C(6)	72(1)	160(1)	120(1)	29(1)	53(1)	25(1)
C(7)	92(1)	114(1)	159(1)	33(1)	62(1)	1(1)
C(8)	141(1)	157(1)	119(1)	66(1)	56(1)	1(1)
C(9)	173(1)	154(1)	112(1)	85(1)	81(1)	13(1)
C(10)	217(1)	89(1)	113(1)	27(1)	80(1)	-9(1)
C(11)	120(1)	93(1)	141(1)	9(1)	83(1)	-10(1)
C(12)	106(1)	75(1)	99(1)	3(1)	68(1)	-8(1)
C(13)	160(1)	145(1)	210(1)	21(1)	119(1)	-51(1)
C(14)	154(1)	173(1)	167(1)	-22(1)	98(1)	10(1)
C(15)	135(1)	154(1)	109(1)	14(1)	75(1)	4(1)
C(16)	146(1)	344(1)	362(1)	158(1)	86(1)	37(1)
C(17)	138(1)	638(1)	165(1)	-19(1)	31(1)	269(1)

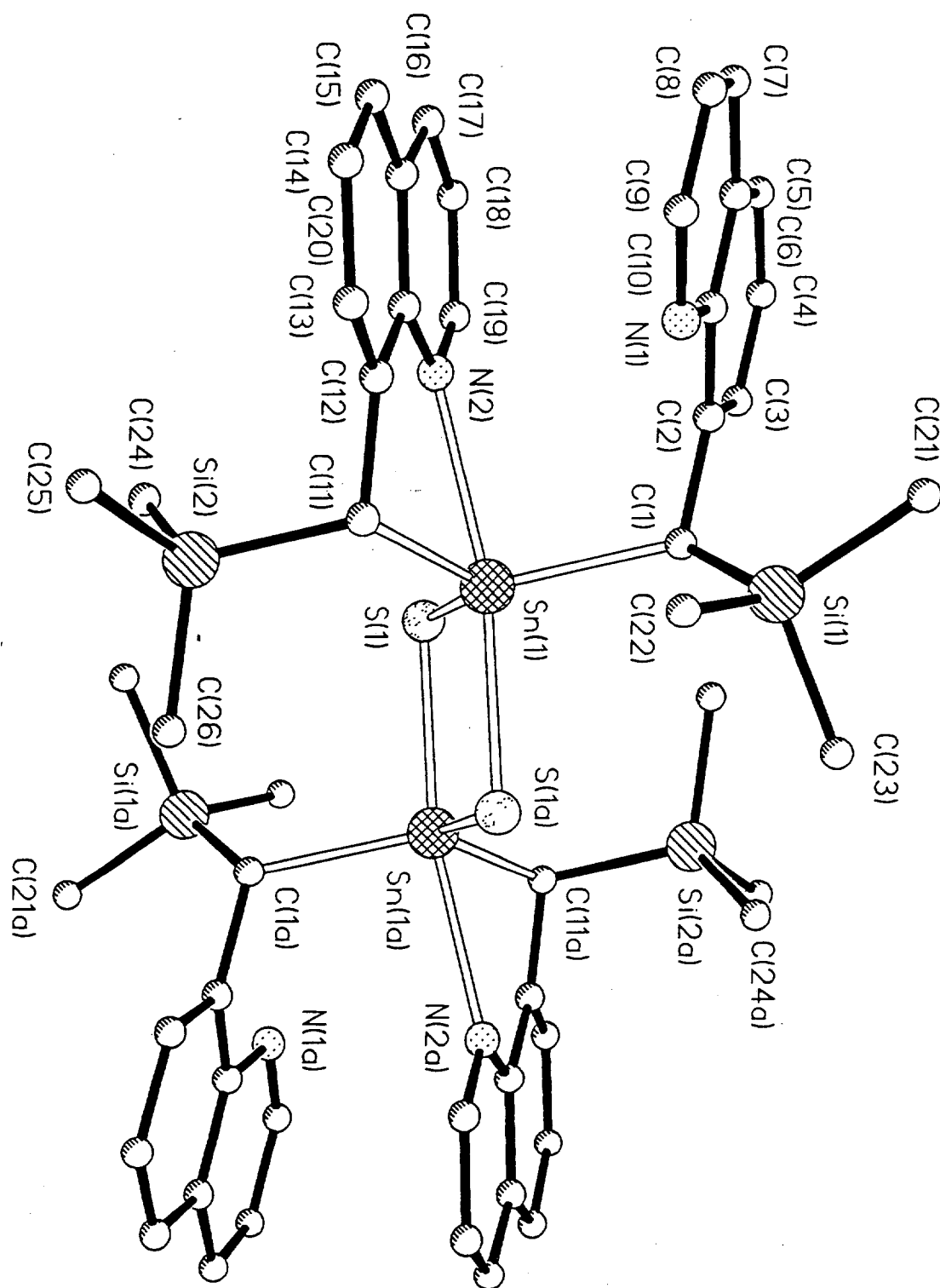
* The exponent takes the form: $-2\pi^2 \sum_{ij} U_{ij} h_i h_j a_i^* \cdot a_j^*$.

Table 5. Hydrogen atom coordinates ($\times 10^4$) and assigned isotropic temperature factors* ($\text{\AA}^2 \times 10^3$).

Atom	x	y	z	U
H(3A)	5952	5650	2631	80
H(4A)	7650	5583	3674	80
H(5A)	8572	4443	5653	80
H(6A)	7746	3330	6395	80
H(7)	2955	4708	2202	150
H(8)	2027	6521	1800	150
H(9)	2799	8467	2457	150
H(10)	4481	8580	3490	150
H(11)	5403	6759	3909	100
H(13A)	5069	1647	1398	200
H(13B)	5846	2627	2295	200
H(13C)	5484	1632	2896	200
H(14A)	3060	1954	748	200
H(14B)	3458	1916	2242	200
H(14C)	2766	2993	1391	200
H(15A)	3725	3942	-405	150
H(15B)	3489	5009	274	150
H(15C)	4526	4888	510	150

*The exponent takes the form: $-8\pi^2 U \sin^2 \theta / \lambda^2$.





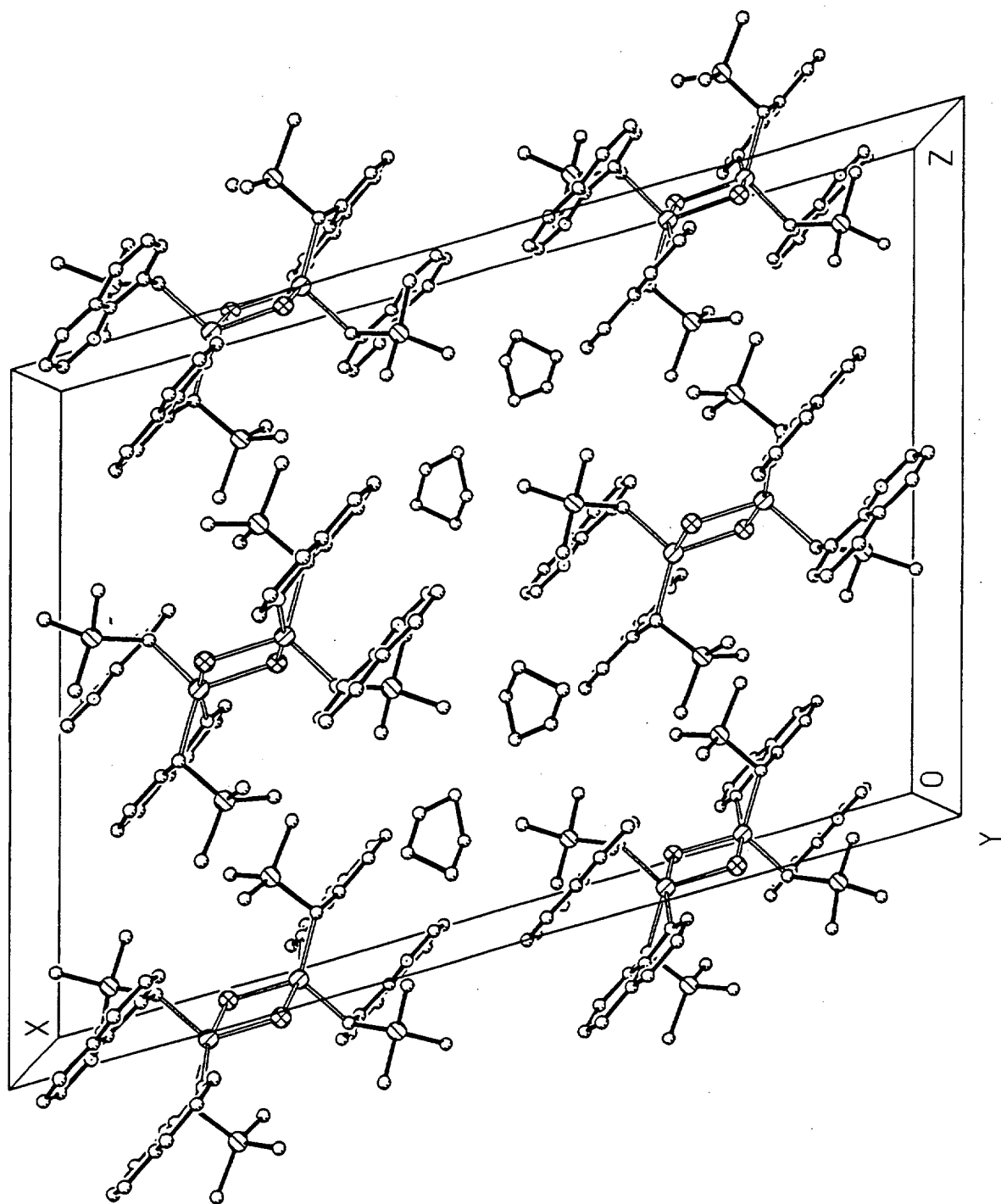


Table 1. Data collection and processing parameters.

Directory	ZZY\LEUHK16	The sample from Dr. W.B.Leung	8 Sep. 1995
Molecular formula	$[\text{C}_{26}\text{H}_{32}\text{N}_2\text{Si}_2\text{S}_2\text{S}]_2 \cdot \text{C}_4\text{H}_8\text{O}$		
Molecular weight	1231.04		
Color and habit	colorless prism		
Crystal size	0.16 x 0.28 x 0.30 mm ³		
Crystal system	monoclinic		
Space group	C2/c (No. 15)		
Unit cell parameters	$a = 29.659(3)$ $\alpha = 90^\circ$ $b = 10.444(1)$ $\beta = 106.0043(1)^\circ$ $V = 6453.2(8)\text{\AA}^3$ $c = 21.673(2)$ $\gamma = 90^\circ$ $Z = 4$ $F(000) = 2528$		
Density (calcd)	1.267 gcm ⁻³		
Radiation	graphite-monochromatized MoK α , $\lambda = 0.71073 \text{ \AA}$		
R_{int} (from merging of equiv. reflections)	0.038		
Absorption coefficient	0.95 mm ⁻¹		
Mean μ_r	0.122		
Scan type and rate	taking oscillation IP photos; 50 frames in total, $\phi = -30 - 120^\circ$, $\Delta\phi = 3^\circ$. 8 mins per frame.		
Crystal to detector distance	69.61 mm		
Background level	-50		
Collection range	$-36 \leq h \leq 37$, $-12 \leq k \leq 12$, $-27 \leq l \leq 0$;		
Reflections Collected	7185		
Independent Reflections	4829 ($R_{\text{int}} = 4.12\%$)		
Obs. data with $ F_o \geq 6\sigma(F_o)$, n	3271		
No. of variables, p	309		
Extinction Correction	$\chi = 0.00031$, where $F^* = F [1 + 0.002\chi F^2 / \sin(2\theta)]^{-1/4}$		
Weighting scheme	$w = [\sigma^2 F_o + 0.0012 F_o ^2]^{-1}$		
$R_F = \sum F_o - F_c / \sum F_o $	0.059		
$wR = [\sum w(F_o - F_c)^2 / \sum w F_o ^2]^{1/2}$	0.088		
$S = [\sum w(F_o - F_c)^2 / (n - p)]^{1/2}$	1.97		
Largest and mean Δ/σ	0.019, 0.001		
Residual extrema in final			

difference map

+0.74 to -0.91 eÅ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic temperature factors* ($\text{\AA}^2 \times 10^3$)

Atom	x	y	z	U_{eq}
Sn(1)	2042(1)	1660(1)	194(1)	43(1)
Si(1)	962(1)	2107(2)	-921(1)	63(1)
Si(2)	2333(1)	2430(2)	1812(1)	51(1)
S(1)	2822(1)	1089(2)	143(1)	50(1)
N(1)	876(2)	-141(3)	-81(2)	60(1)
N(2)	2053(2)	-477(2)	701(2)	47(1)
C(1)	1498(2)	1053(3)	-667(2)	47(1)
C(2)	1408(2)	-379(3)	-695(2)	50(1)
C(3)	1614(2)	-1208(3)	-1046(2)	67(1)
C(4)	1538(2)	-2548(3)	-1068(2)	79(1)
C(5)	1241(2)	-3049(3)	-751(2)	82(1)
C(6)	1002(2)	-2250(3)	-428(2)	66(1)
C(7)	679(2)	-2756(3)	-114(2)	84(1)
C(8)	472(2)	-1928(3)	189(2)	84(1)
C(9)	576(2)	-640(3)	203(2)	72(1)
C(10)	1085(2)	-934(3)	-396(2)	53(1)
C(11)	1839(2)	1947(3)	1089(2)	45(1)
C(12)	1620(2)	787(3)	1256(2)	54(1)
C(13)	1291(2)	786(3)	1612(2)	64(1)
C(14)	1121(2)	-354(3)	1842(2)	85(1)
C(15)	1283(2)	-1562(3)	1691(2)	69(1)
C(16)	1606(2)	-1617(3)	1305(2)	59(1)
C(17)	1761(2)	-2759(3)	1121(2)	65(1)
C(18)	2072(2)	-2745(3)	753(2)	63(1)
C(19)	2204(2)	-1594(3)	552(2)	59(1)
C(20)	1766(2)	-470(3)	1084(2)	47(1)
C(21)	433(2)	1250(3)	-1384(2)	71(1)
C(22)	842(2)	3030(3)	-256(2)	81(1)
C(23)	1084(2)	3294(3)	-1501(2)	80(1)
C(24)	2808(2)	1232(3)	1981(2)	71(1)
C(25)	2097(2)	2573(3)	2527(2)	69(1)
C(26)	2569(2)	4004(3)	1677(2)	66(1)
O(1)	469(2)	3241(3)	2065(2)	284(1)
C(27)	194(3)	3495(3)	1412(2)	205(1)
C(28)	315(2)	4872(3)	1349(3)	196(1)
C(29)	839(2)	4710(3)	1555(2)	177(1)
C(30)	873(2)	4080(3)	2186(2)	172(1)

* U_{eq} defined as one third of the trace of the orthogonalized U tensor.

Table 3. Bond lengths (Å) and bond angles (°).

Sn(1)-S(1)	2.420 (3)	Sn(1)-N(2)	2.483 (3)
Sn(1)-C(1)	2.198 (4)	Sn(1)-C(11)	2.203 (6)
Sn(1)-S(1a)	2.528 (2)	Si(1)-C(1)	1.886 (5)
Si(1)-C(21)	1.846 (5)	Si(1)-C(22)	1.848 (6)
Si(1)-C(23)	1.870 (6)	Si(2)-C(11)	1.895 (5)
Si(2)-C(24)	1.843 (5)	Si(2)-C(25)	1.874 (7)
Si(2)-C(26)	1.840 (4)	S(1)-Sn(1a)	2.528 (2)
N(1)-C(9)	1.320 (8)	N(1)-C(10)	1.330 (7)
N(2)-C(19)	1.320 (5)	N(2)-C(20)	1.343 (8)
C(1)-C(2)	1.518 (4)	C(2)-C(3)	1.400 (7)
C(2)-C(10)	1.418 (8)	C(3)-C(4)	1.416 (4)
C(4)-C(5)	1.362 (9)	C(5)-C(6)	1.402 (8)
C(6)-C(7)	1.421 (9)	C(6)-C(10)	1.395 (4)
C(7)-C(8)	1.334 (7)	C(8)-C(9)	1.378 (4)
C(11)-C(12)	1.467 (6)	C(12)-C(13)	1.400 (9)
C(12)-C(20)	1.464 (5)	C(13)-C(14)	1.435 (6)
C(14)-C(15)	1.421 (5)	C(15)-C(16)	1.436 (9)
C(16)-C(17)	1.377 (6)	C(16)-C(20)	1.420 (6)
C(17)-C(18)	1.376 (9)	C(18)-C(19)	1.372 (5)
O(1)-C(27)	1.448 (7)	O(1)-C(30)	1.450 (8)
C(27)-C(28)	1.497 (5)	C(28)-C(29)	1.504 (9)
C(29)-C(30)	1.495 (7)		

S(1)-Sn(1)-N(2)	84.4(1)	S(1)-Sn(1)-C(1)	112.2(2)
N(2)-Sn(1)-C(1)	91.9(1)	S(1)-Sn(1)-C(11)	124.8(1)
N(2)-Sn(1)-C(11)	73.0(1)	C(1)-Sn(1)-C(11)	118.2(2)
S(1)-Sn(1)-S(1a)	89.2(1)	N(2)-Sn(1)-S(1a)	168.6(1)
C(1)-Sn(1)-S(1a)	99.2(1)	C(11)-Sn(1)-S(1a)	103.4(1)
C(1)-Si(1)-C(21)	113.4(2)	C(1)-Si(1)-C(22)	113.9(2)
C(21)-Si(1)-C(22)	111.1(3)	C(1)-Si(1)-C(23)	106.2(3)
C(21)-Si(1)-C(23)	104.4(2)	C(22)-Si(1)-C(23)	107.0(2)
C(11)-Si(2)-C(24)	111.0(2)	C(11)-Si(2)-C(25)	109.0(3)
C(24)-Si(2)-C(25)	109.1(2)	C(11)-Si(2)-C(26)	110.3(2)
C(24)-Si(2)-C(26)	109.6(3)	C(25)-Si(2)-C(26)	107.7(2)
Sn(1)-S(1)-Sn(1a)	90.8(1)	C(9)-N(1)-C(10)	117.6(3)
Sn(1)-N(2)-C(19)	130.5(4)	Sn(1)-N(2)-C(20)	109.6(2)
C(19)-N(2)-C(20)	118.1(4)	Sn(1)-C(1)-Si(1)	116.2(2)
Sn(1)-C(1)-C(2)	113.4(3)	Si(1)-C(1)-C(2)	116.0(4)
C(1)-C(2)-C(3)	122.1(5)	C(1)-C(2)-C(10)	121.2(4)
C(3)-C(2)-C(10)	116.6(3)	C(2)-C(3)-C(4)	122.6(5)
C(3)-C(4)-C(5)	118.9(5)	C(4)-C(5)-C(6)	120.6(3)
C(5)-C(6)-C(7)	121.2(3)	C(5)-C(6)-C(10)	120.3(5)
C(7)-C(6)-C(10)	118.5(5)	C(6)-C(7)-C(8)	117.2(3)
C(7)-C(8)-C(9)	120.8(6)	N(1)-C(9)-C(8)	123.4(5)
N(1)-C(10)-C(2)	116.7(3)	N(1)-C(10)-C(6)	122.5(5)
C(2)-C(10)-C(6)	120.8(5)	Sn(1)-C(11)-Si(2)	115.3(3)
Sn(1)-C(11)-C(12)	110.6(3)	Si(2)-C(11)-C(12)	108.0(3)
C(11)-C(12)-C(13)	124.1(3)	C(11)-C(12)-C(20)	119.6(5)
C(13)-C(12)-C(20)	116.1(4)	C(12)-C(13)-C(14)	123.9(4)
C(13)-C(14)-C(15)	118.9(6)	C(14)-C(15)-C(16)	119.5(4)
C(15)-C(16)-C(17)	122.2(4)	C(15)-C(16)-C(20)	120.2(4)
C(17)-C(16)-C(20)	117.6(5)	C(16)-C(17)-C(18)	119.3(4)
C(17)-C(18)-C(19)	119.3(4)	N(2)-C(19)-C(18)	123.5(6)

N(2)-C(20)-C(12)	116.5(4)	N(2)-C(20)-C(16)	122.2(4)
C(12)-C(20)-C(16)	121.3(5)	C(27)-O(1)-C(30)	106.3(4)
O(1)-C(27)-C(28)	100.4(4)	C(27)-C(28)-C(29)	96.9(4)
C(28)-C(29)-C(30)	97.1(5)	O(1)-C(30)-C(29)	104.8(4)

*Symmetry transformation a (0.5-x, 0.5-y, -z)

Table 4. Anisotropic thermal parameters* ($\text{\AA}^2 \times 10^3$).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	47(1)	41(1)	41(1)	1(1)	12(1)	-1(1)
Si(1)	50(1)	72(1)	62(1)	7(1)	6(1)	5(1)
Si(2)	62(1)	47(1)	44(1)	-3(1)	16(1)	0(1)
S(1)	50(1)	44(1)	57(1)	5(1)	18(1)	3(1)
N(1)	44(1)	67(1)	70(1)	-4(1)	17(1)	-8(1)
N(2)	47(1)	49(1)	46(1)	0(1)	15(1)	3(1)
C(1)	57(1)	50(1)	31(1)	-5(1)	9(1)	3(1)
C(2)	49(1)	46(1)	50(1)	1(1)	6(1)	-17(1)
C(3)	66(1)	64(1)	70(1)	2(1)	16(1)	-12(1)
C(4)	91(1)	68(1)	86(1)	-13(1)	39(1)	-24(1)
C(5)	106(1)	33(1)	101(1)	-18(1)	18(1)	-22(1)
C(6)	90(1)	50(1)	58(1)	-21(1)	23(1)	-14(1)
C(7)	75(1)	82(1)	89(1)	-22(1)	15(1)	3(1)
C(8)	57(1)	72(1)	127(1)	-8(1)	29(1)	4(1)
C(9)	45(1)	106(1)	61(1)	-1(1)	6(1)	4(1)
C(10)	38(1)	72(1)	46(1)	-8(1)	5(1)	-14(1)
C(11)	47(1)	41(1)	49(1)	5(1)	18(1)	4(1)
C(12)	55(1)	55(1)	54(1)	13(1)	20(1)	6(1)
C(13)	59(1)	64(1)	82(1)	10(1)	38(1)	9(1)
C(14)	79(1)	102(1)	87(1)	-30(1)	41(1)	7(1)
C(15)	70(1)	79(1)	69(1)	-25(1)	35(1)	-4(1)
C(16)	55(1)	75(1)	44(1)	-12(1)	9(1)	-5(1)
C(17)	97(1)	40(1)	54(1)	0(1)	12(1)	14(1)
C(18)	74(1)	65(1)	46(1)	6(1)	14(1)	-1(1)
C(19)	55(1)	44(1)	75(1)	6(1)	16(1)	5(1)
C(20)	50(1)	48(1)	42(1)	-1(1)	14(1)	3(1)
C(21)	66(1)	69(1)	69(1)	2(1)	7(1)	-3(1)
C(22)	66(1)	77(1)	95(1)	25(1)	17(1)	2(1)
C(23)	76(1)	87(1)	77(1)	22(1)	21(1)	18(1)
C(24)	81(1)	80(1)	52(1)	16(1)	17(1)	5(1)
C(25)	90(1)	82(1)	33(1)	-6(1)	15(1)	-12(1)
C(26)	90(1)	51(1)	53(1)	-8(1)	15(1)	-9(1)

* The exponent takes the form: $-2\pi^2 \sum \sum U_{ij} h_i h_j a_i^* a_j^*$.

Table 5. Hydrogen atom coordinates ($\times 10^4$) and assigned isotropic temperature factors* ($\text{\AA}^2 \times 10^3$).

Atom	x	y	z	U
H(1A)	947	698	-58	120
H(1B)	1646	1177	-1005	80
H(3A)	1814	-853	-1283	100
H(4A)	1692	-3075	-1311	150
H(5A)	1194	-3959	-758	80
H(7A)	612	-3656	-123	150
H(8A)	258	-2219	419	80
H(9A)	415	-65	415	120
H(11A)	1606	2611	1015	80
H(13A)	1189	1606	1722	80
H(14A)	878	-270	2056	180
H(15A)	1189	-2323	1871	150
H(17A)	1664	-3556	1264	120
H(18A)	2190	-3523	619	80
H(19A)	2422	-1577	297	80
H(21A)	516	779	-1717	120
H(21B)	335	665	-1104	120
H(21C)	180	1827	-1573	120
H(22A)	774	2466	57	120
H(22B)	1114	3535	-57	120
H(22C)	579	3585	-425	120
H(23A)	1148	2881	-1863	100
H(23B)	816	3844	-1646	100
H(23C)	1351	3794	-1278	100
H(24A)	2675	426	2054	150
H(24B)	2940	1152	1626	150
H(24C)	3049	1474	2359	150
H(25A)	1970	1772	2617	100
H(25B)	2343	2837	2894	100
H(25C)	1854	3209	2432	100
H(26A)	2697	3943	1316	100
H(26B)	2322	4629	1588	100
H(26C)	2811	4257	2051	100

* The exponent takes the form: $-8\pi^2 U \sin^2 \theta / \lambda^2$.

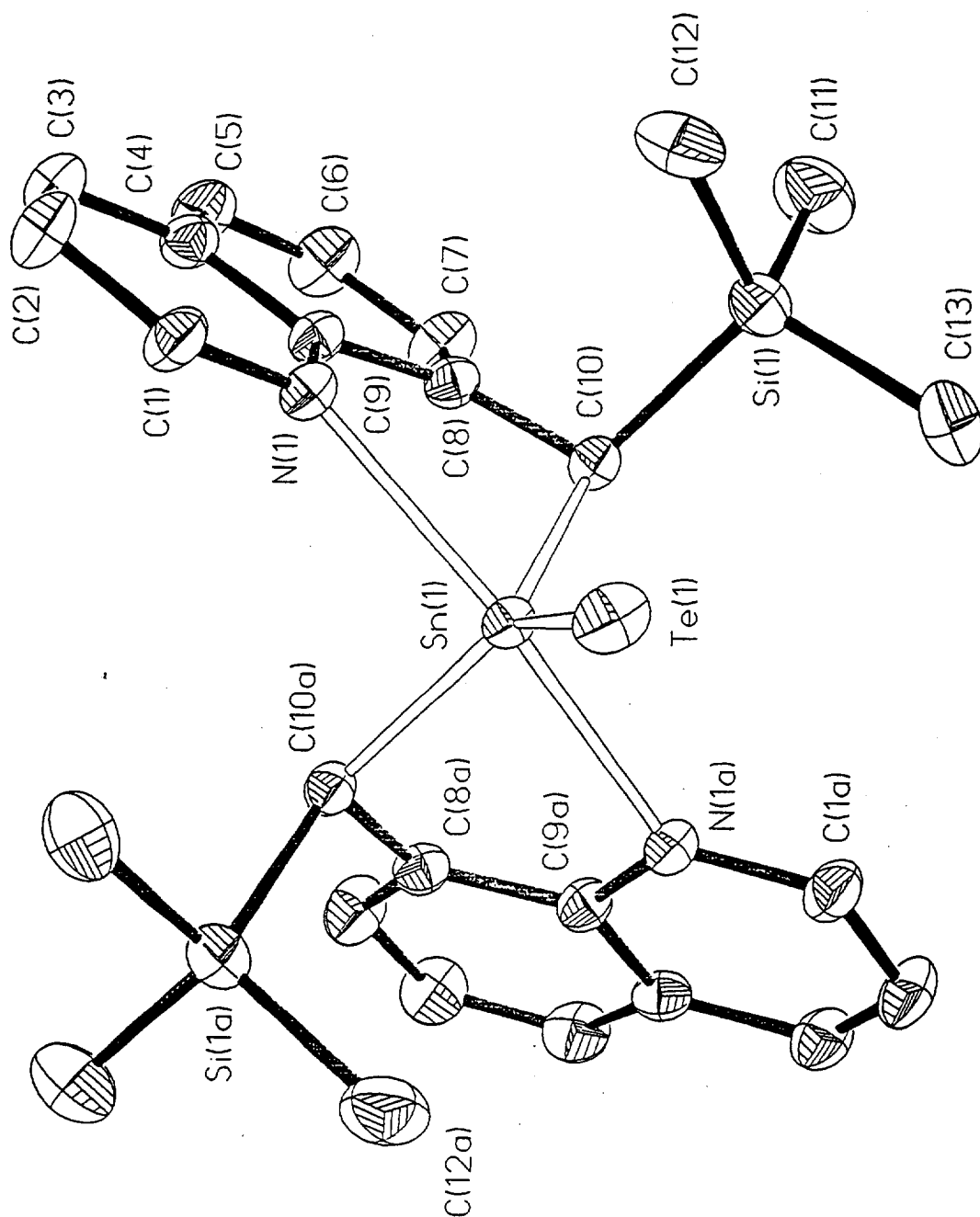


Table 2. Bond lengths (Å)

Sn(1)-Te(1)	2.618 (1)	Sn(1)-N(1)	2.382 (4)
Sn(1)-C(10)	2.174 (5)	Sn(1)-N(1a)	2.382 (4)
Sn(1)-C(10a)	2.174 (5)	N(1)-C(1)	1.331 (7)
N(1)-C(9)	1.379 (6)	C(1)-C(2)	1.417 (7)
C(2)-C(3)	1.345 (8)	C(3)-C(4)	1.417 (8)
C(4)-C(5)	1.404 (8)	C(4)-C(9)	1.430 (7)
C(5)-C(6)	1.342 (8)	C(6)-C(7)	1.395 (8)
C(7)-C(8)	1.384 (7)	C(8)-C(9)	1.407 (7)
C(8)-C(10)	1.502 (6)	C(10)-Si(1)	1.896 (5)
Si(1)-C(11)	1.866 (7)	Si(1)-C(12)	1.862 (6)
Si(1)-C(13)	1.860 (6)	C(21)-C(22)	0.924 (27)
C(21)-C(23)	1.256 (26)	C(21)-C(24)	1.474 (23)
C(21)-C(25)	1.450 (28)	C(21)-C(26)	1.651 (24)
C(21)-C(25a)	1.978 (28)	C(22)-C(23)	1.878 (29)
C(22)-C(24)	1.599 (27)	C(22)-C(25)	0.782 (31)
C(22)-C(26)	1.958 (33)	C(22)-C(22a)	1.718 (43)
C(22)-C(25a)	1.614 (32)	C(23)-C(26)	1.308 (17)
C(23)-C(24a)	1.496 (22)	C(23)-C(25a)	1.830 (29)
C(24)-C(25)	1.263 (28)	C(24)-C(26)	1.416 (18)
C(24)-C(23a)	1.496 (22)	C(25)-C(26)	1.917 (33)
C(25)-C(21a)	1.978 (28)	C(25)-C(22a)	1.614 (32)
C(25)-C(23a)	1.830 (29)	C(25)-C(25a)	1.858 (43)
C(26)-C(21a)	1.651 (24)	C(26)-C(22a)	1.958 (33)
C(26)-C(23a)	1.308 (17)	C(26)-C(24a)	1.416 (18)
C(26)-C(25a)	1.917 (33)		

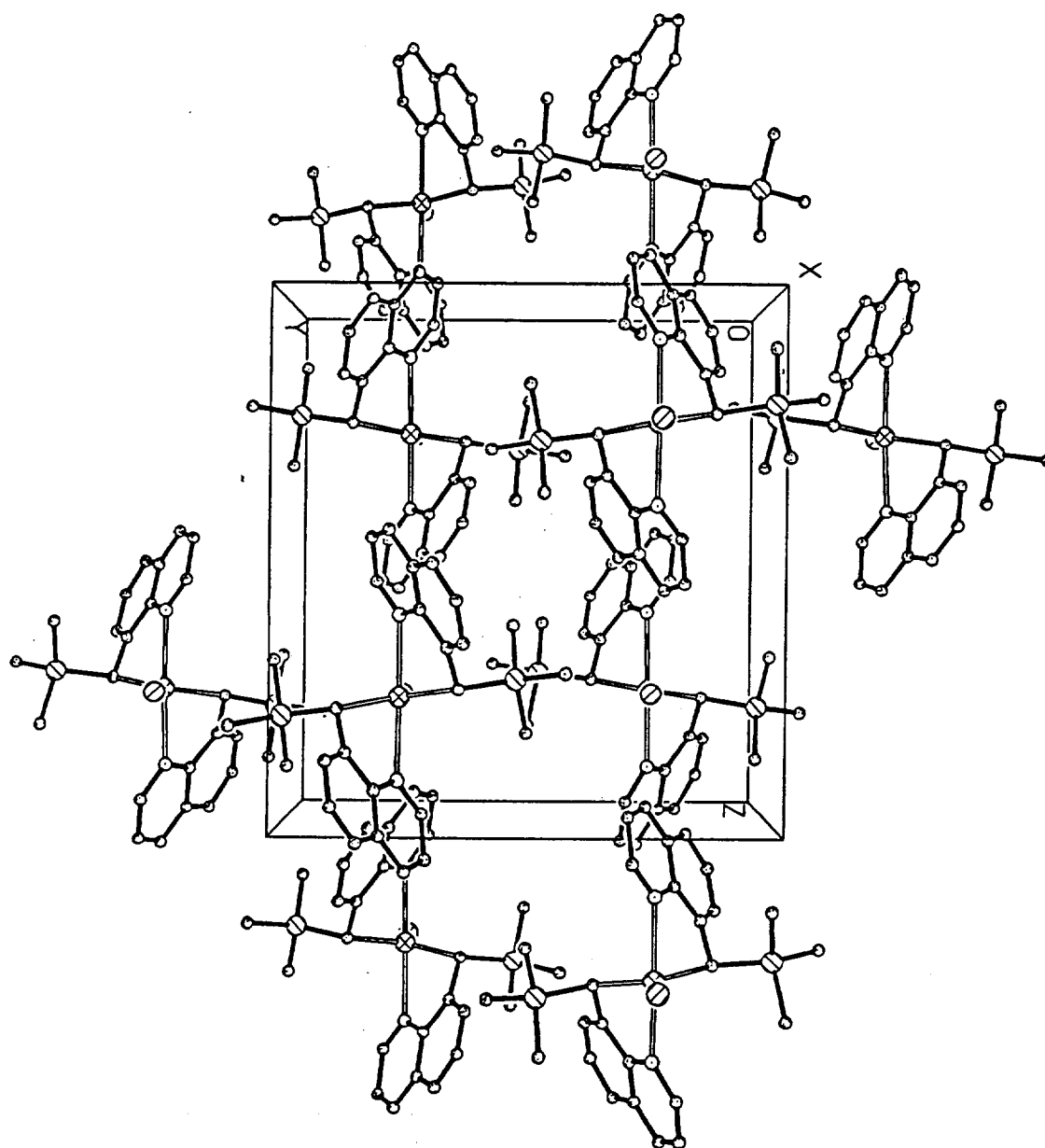


Table 3. Bond angles ($^{\circ}$)

Te(1)-Sn(1)-N(1)	101.5(1)	Te(1)-Sn(1)-C(10)	127.3(1)
N(1)-Sn(1)-C(10)	75.2(1)	Te(1)-Sn(1)-N(1a)	101.5(1)
N(1)-Sn(1)-N(1a)	157.1(2)	C(10)-Sn(1)-N(1a)	90.8(1)
C(10)-Sn(1)-C(10a)	105.5(3)	N(1a)-Sn(1)-C(10a)	75.2(1)
Sn(1)-N(1)-C(1)	129.7(3)	Sn(1)-N(1)-C(9)	108.2(3)
C(1)-N(1)-C(9)	120.6(4)	N(1)-C(1)-C(2)	120.2(5)
C(1)-C(2)-C(3)	121.2(5)	C(2)-C(3)-C(4)	120.0(5)
C(3)-C(4)-C(5)	125.0(5)	C(3)-C(4)-C(9)	117.3(5)
C(5)-C(4)-C(9)	117.7(5)	C(4)-C(5)-C(6)	120.3(5)
C(5)-C(6)-C(7)	121.4(5)	C(6)-C(7)-C(8)	122.3(5)
C(7)-C(8)-C(9)	115.9(4)	C(7)-C(8)-C(10)	124.6(4)
C(9)-C(8)-C(10)	119.4(4)	N(1)-C(9)-C(4)	120.6(4)
N(1)-C(9)-C(8)	117.3(4)	C(4)-C(9)-C(8)	122.1(4)
Sn(1)-C(10)-C(8)	107.7(3)	Sn(1)-C(10)-Si(1)	113.0(2)
C(8)-C(10)-Si(1)	111.3(3)	C(10)-Si(1)-C(11)	109.9(3)
C(10)-Si(1)-C(12)	110.2(2)	C(11)-Si(1)-C(12)	109.1(3)
C(10)-Si(1)-C(13)	107.9(2)	C(11)-Si(1)-C(13)	108.7(3)
C(12)-Si(1)-C(13)	111.0(3)	C(22)-C(21)-C(23)	118.2(23)
C(23)-C(21)-C(24)	103.3(15)	C(23)-C(21)-C(25)	118.0(16)
C(22)-C(21)-C(26)	94.9(19)	C(24)-C(21)-C(25a)	94.3(12)
C(21)-C(22)-C(25)	116.2(32)	C(23)-C(22)-C(25)	115.2(26)
C(21)-C(22)-C(22a)	115.0(21)	C(24)-C(22)-C(22a)	92.2(13)
C(21)-C(22)-C(25a)	98.8(23)	C(24)-C(22)-C(25a)	105.3(15)
C(21)-C(23)-C(24a)	113.7(15)	C(21)-C(24)-C(23a)	112.0(14)
C(22)-C(24)-C(23a)	97.6(14)	C(22)-C(25)-C(24)	100.2(27)
C(24)-C(25)-C(22a)	111.9(18)	C(21)-C(25)-C(23a)	96.6(15)
C(22)-C(25)-C(23a)	120.9(27)	C(24)-C(25)-C(25a)	108.3(12)
C(23)-C(26)-C(24)	103.9(13)	C(21)-C(26)-C(21a)	104.4(20)
C(23)-C(26)-C(21a)	112.2(17)	C(21)-C(26)-C(23a)	112.2(17)
C(22)-C(26)-C(23a)	88.7(16)	C(23)-C(26)-C(23a)	153.2(29)
C(24)-C(26)-C(24a)	140.0(25)	C(25)-C(26)-C(24a)	98.9(17)
C(23a)-C(26)-C(24a)	103.9(13)	C(24)-C(26)-C(25a)	98.9(17)

* Symmetry transformation: a (x, 0.5-y, 0.5-z)

STRUCTURE DETERMINATION SUMMARYCrystal Data

Empirical Formula	$C_{32} H_{30} N_2 Si_2 Sn Te$
Color; Habit	golden prism
Crystal size (mm)	0.26 x 0.12 x 0.22
Crystal System	Orthorhombic
Space Group	Pnna
Unit Cell Dimensions	$a = 14.5840(10) \text{ \AA}$ $b = 14.6490(10) \text{ \AA}$ $c = 15.7260(10) \text{ \AA}$
Volume	$3359.8(17) \text{ \AA}^3$
Z	4
Formula weight	745.0
Density(calc.)	1.473 g/cm^3
Absorption Coefficient	1.704 mm^{-1}
F(000)	1464

Data Collection

Diffractometer Used	Siemens P4
Radiation	MoK α (λ = 0.71073 Å)
Temperature (K)	295
Monochromator	Highly oriented graphite crystal
2 θ Range	4.0 to 50.0°
Scan Type	ω
Scan Speed	Variable; 32.00°/min. in ω
Scan Range (ω)	0.60°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 0.5% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$0 \leq h \leq 17$, $0 \leq k \leq 17$ $0 \leq l \leq 18$
Reflections Collected	2964
Independent Reflections	2964 ($R_{\text{int}} = 0.00\%$)
Observed Reflections	1944 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement

System Used	Siemens SHELXTL P4/PC
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	$\chi = 0.000129(16)$, where $F^* = F [1 + 0.002\chi F^2 / \sin(2\theta)]^{-1/4}$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0001F^2$
Number of Parameters Refined	197
Final R Indices (obs. data)	R = 2.94 %, wR = 3.90 %
R Indices (all data)	R = 5.01 %, wR = 4.12 %
Goodness-of-Fit	1.57
Largest and Mean Δ/σ	0.409, 0.027
Data-to-Parameter Ratio	9.9:1
Largest Difference Peak	0.41 eÅ ⁻³
Largest Difference Hole	-0.39 eÅ ⁻³

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
Sn(1)	620(1)	2500	2500	41(1)
Te(1)	2416(1)	2500	2500	60(1)
N(1)	296(3)	2513(3)	3984(2)	48(1)
C(1)	693(4)	2052(4)	4614(3)	62(1)
C(2)	248(4)	1966(4)	5411(3)	73(1)
C(3)	-588(4)	2327(4)	5544(4)	72(1)
C(4)	-1033(3)	2814(4)	4884(3)	54(1)
C(5)	-1913(4)	3198(4)	4941(4)	72(1)
C(6)	-2266(4)	3661(4)	4282(4)	80(1)
C(7)	-1771(4)	3786(4)	3532(4)	73(1)
C(8)	-886(3)	3463(3)	3433(3)	48(1)
C(9)	-545(3)	2925(3)	4103(3)	47(1)
C(10)	-282(3)	3665(3)	2682(3)	47(1)
Si(1)	363(1)	4777(1)	2829(1)	62(1)
C(11)	-466(5)	5737(4)	2966(5)	107(2)
C(12)	1112(4)	4711(4)	3786(4)	94(1)
C(13)	1051(4)	4985(4)	1853(4)	-90(1)
C(21)	3346(11)	289(13)	5681(11)	121(2)
C(22)	2979(14)	342(17)	5205(13)	155(2)
C(23)	3266(11)	-415(12)	6131(12)	134(2)
C(24)	2629(11)	899(10)	6016(10)	112(2)
C(25)	2533(16)	633(15)	5258(15)	160(2)
C(26)	2500	0	6324(18)	392(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 4. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

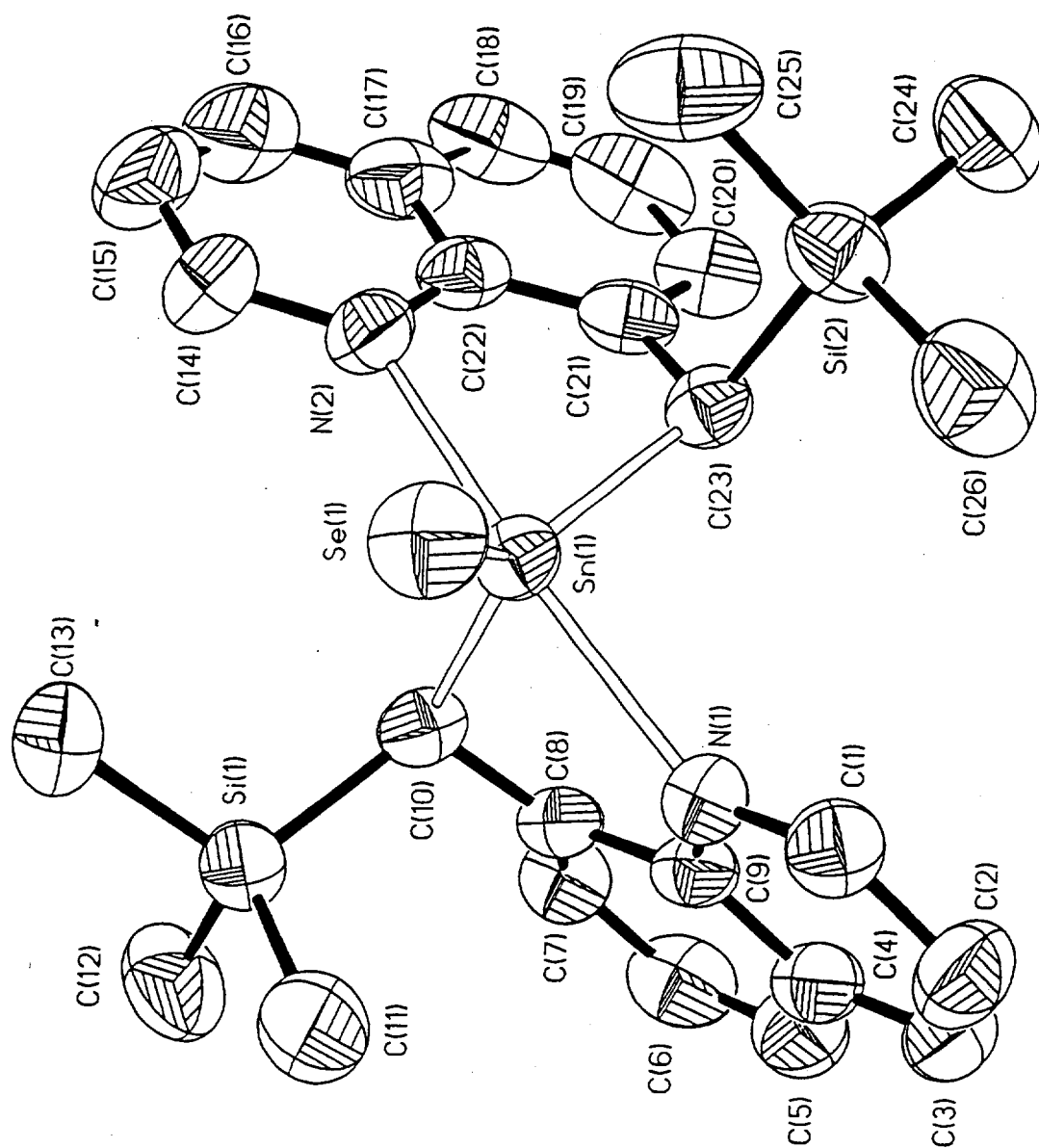
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	38(1)	48(1)	37(1)	0	0	-1(1)
Te(1)	39(1)	84(1)	56(1)	0	0	-6(1)
N(1)	47(2)	58(2)	39(2)	1(2)	-2(2)	2(2)
C(1)	74(2)	74(2)	39(2)	5(2)	-3(2)	5(2)
C(2)	77(2)	97(3)	44(2)	7(2)	0(2)	18(2)
C(3)	86(3)	84(3)	45(2)	-2(2)	8(2)	6(2)
C(4)	54(2)	59(2)	48(2)	-2(2)	8(2)	-7(2)
C(5)	66(2)	89(3)	62(2)	4(2)	28(2)	-6(2)
C(6)	54(2)	106(3)	80(2)	24(2)	15(2)	-3(2)
C(7)	54(2)	102(3)	64(2)	22(2)	2(2)	5(2)
C(8)	43(2)	56(2)	45(2)	1(2)	2(2)	-5(2)
C(9)	42(2)	59(2)	41(2)	0(2)	2(2)	-1(2)
C(10)	48(2)	52(2)	41(2)	4(2)	1(2)	3(2)
Si(1)	67(1)	51(1)	69(1)	3(1)	0(1)	-2(1)
C(11)	111(3)	74(3)	137(3)	13(3)	11(3)	-12(3)
C(12)	95(3)	81(3)	106(3)	-10(2)	-22(3)	-26(2)
C(13)	90(3)	68(2)	112(3)	-18(2)	8(3)	14(2)
C(21)	97(3)	139(3)	127(3)	-8(3)	-20(3)	24(3)
C(22)	149(3)	180(3)	136(3)	-18(3)	51(3)	0(3)
C(23)	105(3)	144(3)	154(3)	39(3)	-34(3)	31(3)
C(24)	121(3)	108(3)	107(3)	-26(3)	0(3)	-28(3)
C(25)	172(3)	138(3)	168(3)	29(3)	-22(3)	40(3)
C(26)	403(3)	411(3)	363(3)	9(3)	0	0

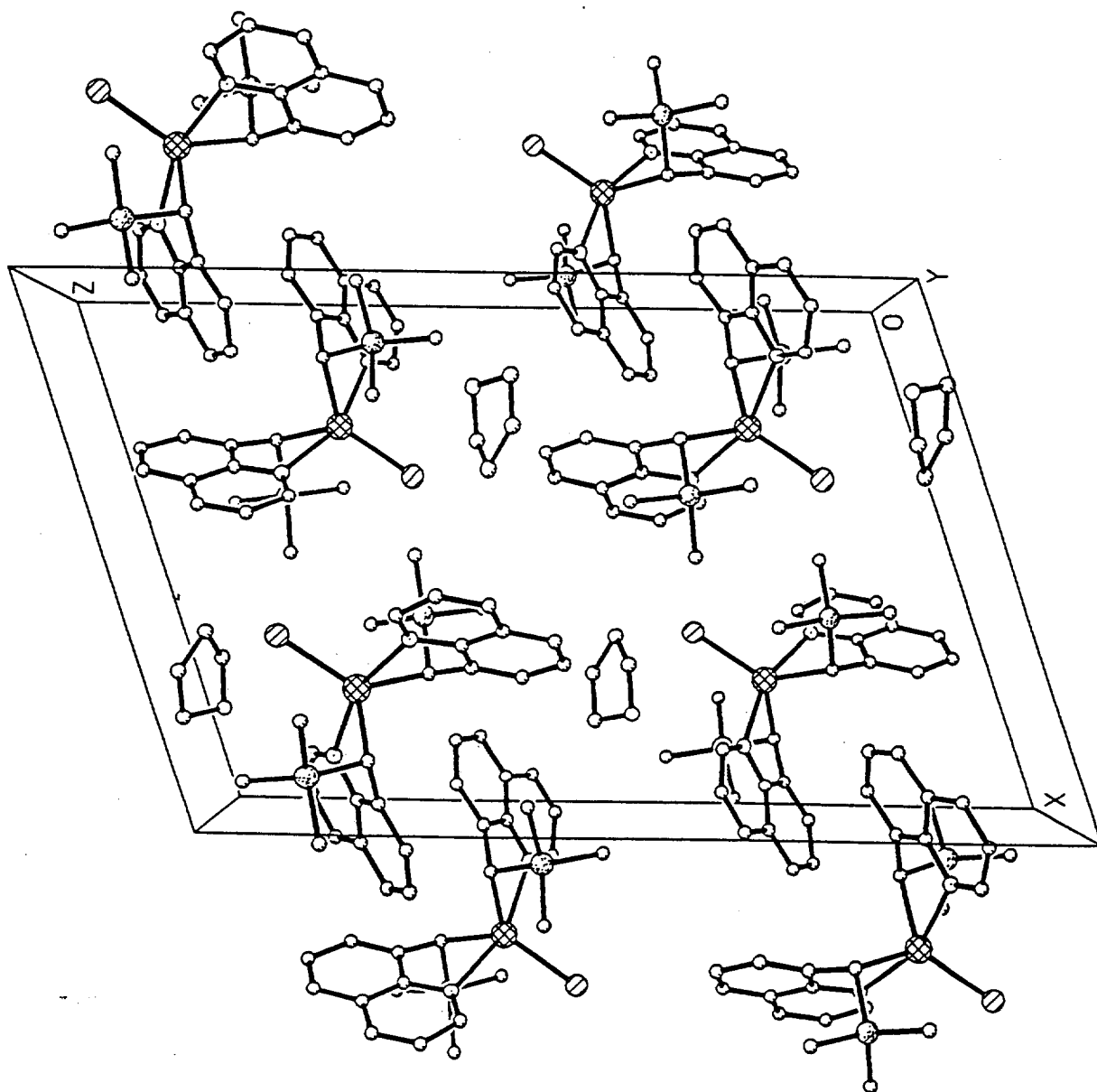
The anisotropic displacement exponent takes the form:

$$-2\pi^2(h^2a^2U_{11} + \dots + 2hka*b*U_{12})$$

Table 5. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
H(2)	544	1634	5859	90
H(3)	-889	2276	6084	80
H(5)	-2242	3179	5470	80
H(6)	-2901	3833	4299	90
H(7)	-2045	4142	3087	90
H(10)	-637	3761	2176	60
H(11A)	-836	5656	3465	120
H(11B)	-855	5768	2474	120
H(11C)	-121	6292	3014	120
H(12A)	735	4598	4275	120
H(12B)	1440	5273	3862	120
H(12C)	1541	4219	3718	120
H(13A)	1478	4495	1767	120
H(13B)	1381	5549	1913	120
H(13C)	647	5025	1373	120





STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{30} H_{40} N_2 O Se Si_2 Sn$
Color; Habit	yellow prism
Crystal size (mm)	0.25 x 0.25 x 0.20
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a} = 14.456(3) \text{ \AA}$ $\underline{b} = 10.700(2) \text{ \AA}$ $\underline{c} = 21.915(4) \text{ \AA}$ $\beta = 109.26(3)^\circ$
Volume	$3200.2(16) \text{ \AA}^3$
Z	4
Formula weight	698.5
Density(calc.)	1.450 Mg/m^3
Absorption Coefficient	2.035 mm^{-1}
F(000)	1416

Data Collection

Diffractometer Used	Rigaku Raxis II c system
Radiation	MoK α (λ = 0.71073 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
Crystal to Detector Distance	69.65 mm
Simulation Range	-40.0 to 80.0°
Scillation Range	2.0°
Frame Number	60
Exposure time	12 mins
Background Level	-40
Index Ranges	-17 $\leq$ h $\leq$ 0, -12 $\leq$ k $\leq$ 13 -25 $\leq$ l $\leq$ 27
Reflections Collected	7778
Independent Reflections	5205 (R_{int} = 7.64%)
Observed Reflections	3813 ($F > 8.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	$\chi = 0.00078(10)$, where $F^* = F [1 + 0.002\chi F^2 / \sin(2\theta)]^{-1/4}$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0004F^2$
Number of Parameters Refined	335
Final R Indices (obs. data)	R = 4.58 %, wR = 5.94 %
R Indices (all data)	R = 6.87 %, wR = 8.57 %
Goodness-of-Fit	1.80
Largest and Mean Δ/σ	0.000, 0.000
Data-to-Parameter Ratio	11.4:1
Largest Difference Peak	0.77 eÅ ⁻³
Largest Difference Hole	-1.22 eÅ ⁻³

Table 1. Data collection and processing parameters.

Molecular formula	$\text{SnSe}(\text{C}_{13}\text{H}_{16}\text{NSi})_2 \cdot \text{thf}$		
Molecular weight	698.5		
Color and habit	yellow prism		
Crystal size	0.25 x 0.25 x 0.20 mm ³		
Crystal system	monoclinic		
Space group	$P2_1/c$ (No. 14)		
Unit cell parameters	$a = 14.456(3)\text{\AA}$	$\beta = 109.26(3)^\circ$	
	$b = 10.700(2)$	$V = 3200.2(2)\text{\AA}^3$	
	$c = 21.915(4)$	$Z = 4$	$F(000) = 1416$
Density (calcd)	1.450 g cm ⁻³		
Radiation	graphite-monochromatized MoK α , $\lambda = 0.71073\text{\AA}$		
R_{int} (from merging of equiv. reflections)	0.076		
Absorption coefficient	2.04 mm ⁻¹		
Rigaku R-Axis II	Imaging plate size	200 x 200 mm	
Camera length	69.65 mm	Start angle	-40.0°
Frame number	60	Oscillation angle	2.0°
Exposure time	12 mins		
Background level	-40		
Collection range	$-17 \leq h \leq 0, -12 \leq k \leq 13, -25 \leq l \leq 27$		
Unique data measured	5205		
Obs. data with $ F_o \geq 8\sigma(F_o)$, n	3813		
No. of variables, p	335		
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0004F^2$		
Extinction Correction	$\chi = 0.00078(10)$, where		
	$F^* = F [1 + 0.002\chi F^2 / \sin(2\theta)]^{-1/4}$		
$R_F = \sum F_o - F_c / \sum F_o $	0.046		
$wR = [\sum w(F_o - F_c)^2 / \sum w F_o ^2]^{1/2}$	0.059		
$S = [\sum w(F_o - F_c)^2 / (n - p)]^{1/2}$	1.80		
Largest and mean Δ/σ	0.00, 0.00		
Residual extrema in final difference map	+0.77 to -1.22 eÅ ⁻³		

Table 3. Bond lengths (Å) and bond angles (°).

Sn(1)-Se(1)	2.398 (1)	Sn(1)-N(1)	2.361 (4)
Sn(1)-C(10)	2.190 (6)	Sn(1)-N(2)	2.390 (4)
Sn(1)-C(23)	2.183 (6)	N(1)-C(1)	1.321 (7)
N(1)-C(9)	1.372 (9)	C(1)-C(2)	1.407 (10)
C(2)-C(3)	1.362 (13)	C(3)-C(4)	1.390 (9)
C(4)-C(5)	1.395 (11)	C(4)-C(9)	1.411 (8)
C(5)-C(6)	1.341 (10)	C(6)-C(7)	1.420 (10)
C(7)-C(8)	1.368 (10)	C(8)-C(9)	1.436 (8)
C(8)-C(10)	1.487 (8)	C(10)-Si(1)	1.897 (6)
Si(1)-C(11)	1.859 (7)	Si(1)-C(12)	1.850 (8)
Si(1)-C(13)	1.879 (9)	N(2)-C(14)	1.322 (8)
N(2)-C(22)	1.371 (9)	C(14)-C(15)	1.387 (11)
C(15)-C(16)	1.335 (15)	C(16)-C(17)	1.419 (11)
C(17)-C(18)	1.406 (12)	C(17)-C(22)	1.402 (9)
C(18)-C(19)	1.346 (12)	C(19)-C(20)	1.426 (11)
C(20)-C(21)	1.385 (10)	C(21)-C(22)	1.430 (8)
C(21)-C(23)	1.493 (8)	C(23)-Si(2)	1.894 (6)
Si(2)-C(24)	1.865 (8)	Si(2)-C(25)	1.861 (9)
Si(2)-C(26)	1.870 (7)	O(1)-C(27)	1.387 (12)
O(1)-C(30)	1.383 (15)	C(27)-C(28)	1.461 (16)
C(28)-C(29)	1.466 (14)	C(29)-C(30)	1.459 (15)

Se(1)-Sn(1)-N(1)	99.5(1)	Se(1)-Sn(1)-C(10)	127.3(2)
N(1)-Sn(1)-C(10)	75.9(2)	Se(1)-Sn(1)-N(2)	102.5(1)
N(1)-Sn(1)-N(2)	158.0(2)	C(10)-Sn(1)-N(2)	91.0(2)
Se(1)-Sn(1)-C(23)	125.4(2)	N(1)-Sn(1)-C(23)	91.7(2)
C(10)-Sn(1)-C(23)	107.3(2)	N(2)-Sn(1)-C(23)	75.1(2)
Sn(1)-N(1)-C(1)	129.1(4)	Sn(1)-N(1)-C(9)	109.5(3)
C(1)-N(1)-C(9)	120.2(5)	N(1)-C(1)-C(2)	121.2(7)
C(1)-C(2)-C(3)	119.4(6)	C(2)-C(3)-C(4)	120.4(6)
C(3)-C(4)-C(5)	124.7(6)	C(3)-C(4)-C(9)	117.9(7)
C(5)-C(4)-C(9)	117.4(6)	C(4)-C(5)-C(6)	121.2(7)
C(5)-C(6)-C(7)	120.8(7)	C(6)-C(7)-C(8)	122.2(6)
C(7)-C(8)-C(9)	115.4(5)	C(7)-C(8)-C(10)	124.1(5)
C(9)-C(8)-C(10)	120.2(6)	N(1)-C(9)-C(4)	120.7(5)
N(1)-C(9)-C(8)	116.4(5)	C(4)-C(9)-C(8)	123.0(6)
Sn(1)-C(10)-C(8)	107.0(3)	Sn(1)-C(10)-Si(1)	112.1(3)
C(8)-C(10)-Si(1)	111.9(4)	C(10)-Si(1)-C(11)	109.5(3)
C(10)-Si(1)-C(12)	110.8(3)	C(11)-Si(1)-C(12)	110.5(4)
C(10)-Si(1)-C(13)	109.8(4)	C(11)-Si(1)-C(13)	108.0(4)
C(12)-Si(1)-C(13)	108.1(3)	Sn(1)-N(2)-C(14)	130.8(5)
Sn(1)-N(2)-C(22)	109.7(3)	C(14)-N(2)-C(22)	118.2(5)
N(2)-C(14)-C(15)	122.9(8)	C(14)-C(15)-C(16)	119.7(7)
C(15)-C(16)-C(17)	120.2(7)	C(16)-C(17)-C(18)	123.2(7)
C(16)-C(17)-C(22)	116.8(7)	C(18)-C(17)-C(22)	120.0(6)
C(17)-C(18)-C(19)	119.2(7)	C(18)-C(19)-C(20)	122.1(8)
C(19)-C(20)-C(21)	120.2(7)	C(20)-C(21)-C(22)	117.5(6)
C(20)-C(21)-C(23)	123.4(5)	C(22)-C(21)-C(23)	119.0(6)
N(2)-C(22)-C(17)	121.9(6)	N(2)-C(22)-C(21)	117.3(5)
C(17)-C(22)-C(21)	120.8(6)	Sn(1)-C(23)-C(21)	109.7(4)
Sn(1)-C(23)-Si(2)	112.6(3)	C(21)-C(23)-Si(2)	111.6(4)
C(23)-Si(2)-C(24)	109.2(4)	C(23)-Si(2)-C(25)	110.6(3)
C(24)-Si(2)-C(25)	109.6(4)	C(23)-Si(2)-C(26)	108.1(3)

Table 2. Atomic coordinates ($\times 10^5$ for Sn and Se atoms; $\times 10^4$ for others) and equivalent isotropic temperature factors* ($\times 10^4$ for Sn and Se atoms; $\times 10^3$ for others)

Atom	x	y	z	U_{eq}
Sn(1)	25081(3)	34109(3)	21729(2)	441(2)
Se(1)	34737(5)	33478(6)	14693(4)	657(3)
N(1)	3476(3)	2119(4)	3016(2)	47(2)
C(1)	3926(4)	1060(5)	2979(3)	56(3)
C(2)	4273(5)	258(6)	3516(4)	71(3)
C(3)	4121(5)	563(6)	4079(4)	67(3)
C(4)	3654(4)	1674(5)	4130(3)	55(2)
C(5)	3461(5)	2065(7)	4684(4)	69(3)
C(6)	3014(5)	3158(7)	4698(3)	71(3)
C(7)	2744(5)	3966(6)	4153(3)	59(3)
C(8)	2919(4)	3672(5)	3594(3)	46(2)
C(9)	3363(4)	2474(5)	3588(3)	46(2)
C(10)	2769(4)	4550(5)	3044(3)	47(2)
Si(1)	3849(1)	5646(2)	3178(1)	55(1)
C(11)	4990(5)	4718(6)	3329(4)	83(4)
C(12)	3658(6)	6691(5)	2475(4)	76(3)
C(13)	3995(7)	6646(6)	3909(4)	91(4)
N(2)	1164(4)	4713(4)	1590(3)	53(2)
C(14)	1146(6)	5798(6)	1297(4)	73(3)
C(15)	318(7)	6547(6)	1089(4)	88(4)
C(16)	-488(6)	6216(7)	1219(5)	87(4)
C(17)	-512(5)	5077(6)	1545(4)	71(3)
C(18)	-1333(5)	4677(8)	1702(4)	82(4)
C(19)	-1299(5)	3571(8)	2001(4)	84(4)
C(20)	-464(5)	2771(7)	2150(4)	66(3)
C(21)	345(4)	3120(5)	1985(3)	51(2)
C(22)	329(4)	4328(5)	1701(3)	52(2)
C(23)	1205(4)	2284(5)	2064(3)	48(2)
Si(2)	953(1)	1117(2)	1379(1)	61(1)
C(24)	-183(5)	226(6)	1318(4)	85(4)
C(25)	796(6)	1930(8)	600(4)	93(4)
C(26)	2011(5)	8(6)	1570(5)	90(4)
O(1)	1936(5)	7699(8)	320(4)	156(5)
C(27)	2910(7)	8049(10)	477(8)	162(9)
C(28)	3451(8)	6913(11)	441(6)	146(7)
C(29)	2682(8)	6133(9)	3(6)	144(7)
C(30)	1757(7)	6813(11)	-164(5)	163(8)

* U_{eq} defined as one third of the trace of the orthogonalized U tensor.

C(24)-Si(2)-C(26)	109.1(3)	C(25)-Si(2)-C(26)	110.2(4)
C(27)-O(1)-C(30)	107.0(10)	O(1)-C(27)-C(28)	106.3(9)
C(27)-C(28)-C(29)	101.8(8)	C(28)-C(29)-C(30)	108.4(9)
O(1)-C(30)-C(29)	103.0(8)		

Table 4. Anisotropic thermal parameters* ($\text{\AA}^2 \times 10^4$ for Sn and Se atoms; $\times 10^3$ for others).

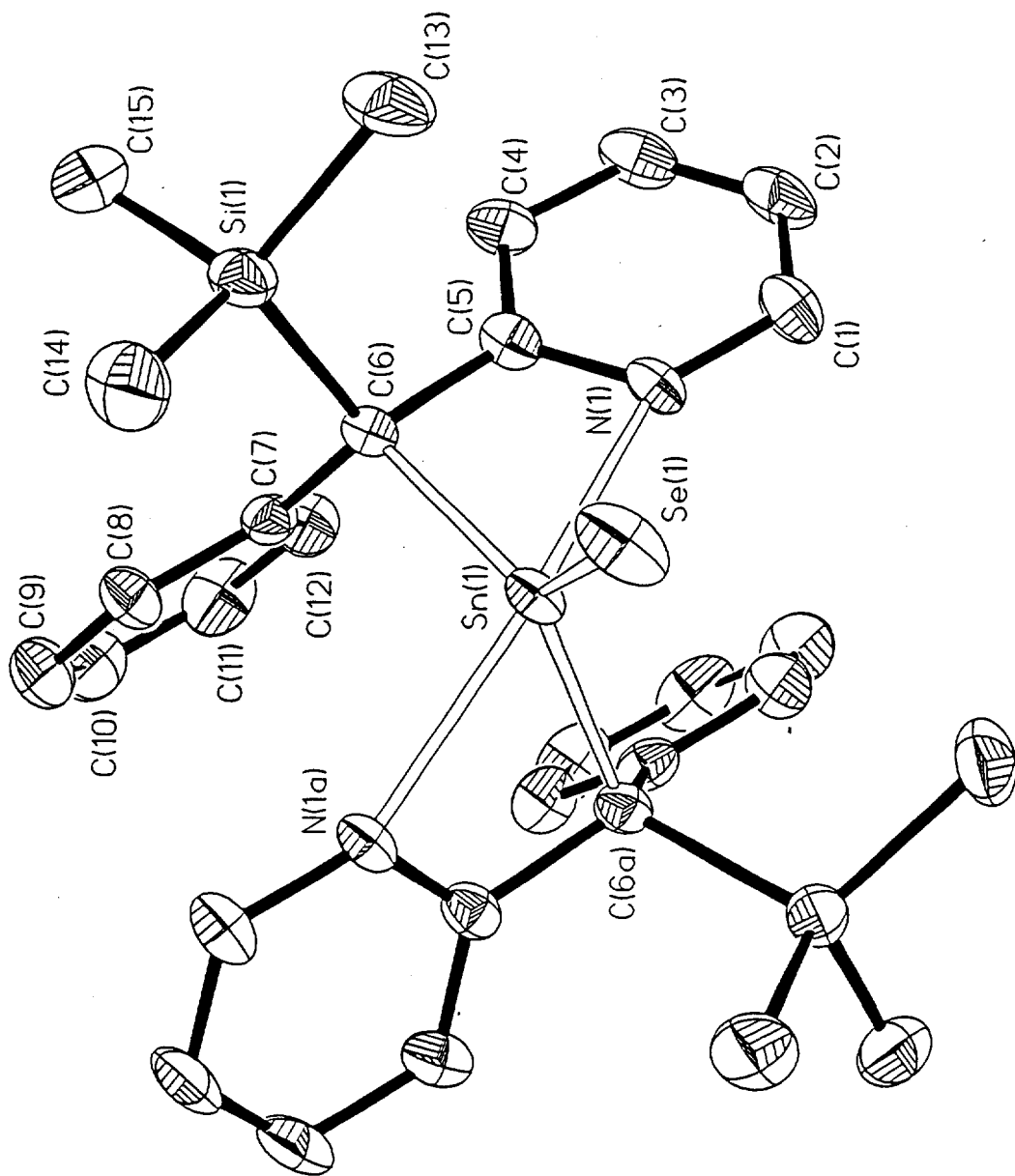
Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	46(1)	50(1)	39(1)	2(1)	18(1)	4(1)
Se(1)	68(1)	85(1)	57(1)	-2(1)	37(1)	3(1)
N(1)	50(3)	48(2)	46(3)	2(2)	21(3)	2(2)
C(1)	49(4)	55(3)	68(5)	5(3)	22(3)	1(3)
C(2)	62(4)	63(4)	85(6)	14(3)	21(4)	17(4)
C(3)	59(4)	63(4)	69(5)	1(3)	8(4)	17(3)
C(4)	47(3)	69(4)	47(4)	-11(3)	13(3)	14(3)
C(5)	77(5)	78(4)	49(4)	-10(4)	16(4)	6(3)
C(6)	75(5)	104(5)	40(4)	-15(4)	28(4)	-8(4)
C(7)	62(4)	69(4)	51(4)	-2(3)	26(4)	-4(3)
C(8)	38(3)	61(3)	38(3)	-2(2)	12(3)	3(2)
C(9)	38(3)	58(3)	39(3)	-4(2)	11(3)	5(2)
C(10)	49(3)	49(3)	41(3)	12(2)	12(3)	-4(2)
Si(1)	59(1)	51(1)	55(1)	-5(1)	17(1)	1(1)
C(11)	50(4)	89(5)	111(7)	-4(3)	27(5)	18(5)
C(12)	87(5)	62(4)	79(6)	-8(3)	27(5)	13(4)
C(13)	117(7)	78(5)	75(6)	-30(4)	29(6)	-22(4)
N(2)	56(3)	55(3)	44(3)	3(2)	12(3)	7(2)
C(14)	84(5)	65(4)	61(5)	4(3)	13(4)	18(3)
C(15)	105(7)	62(4)	81(6)	27(4)	8(5)	12(4)
C(16)	78(6)	75(5)	93(7)	30(4)	7(5)	-8(4)
C(17)	67(5)	70(4)	62(5)	19(3)	3(4)	-18(4)
C(18)	48(4)	102(6)	90(6)	16(4)	13(4)	-40(5)
C(19)	56(5)	117(6)	88(6)	-6(4)	37(5)	-39(5)
C(20)	55(4)	86(4)	59(5)	-1(3)	22(4)	-9(3)
C(21)	42(3)	71(4)	38(3)	-2(3)	12(3)	-10(3)
C(22)	53(4)	58(3)	39(3)	8(3)	7(3)	-8(3)
C(23)	49(3)	54(3)	43(3)	1(2)	18(3)	6(2)
Si(2)	59(1)	62(1)	61(1)	-2(1)	20(1)	-11(1)
C(24)	75(5)	74(4)	102(7)	-10(4)	24(5)	-16(4)
C(25)	82(6)	140(7)	57(5)	3(5)	23(5)	-5(5)
C(26)	85(5)	75(4)	113(8)	9(4)	39(6)	-26(5)
O(1)	120(6)	189(7)	146(9)	22(5)	27(6)	-70(7)
C(27)	88(8)	189(12)	218(19)	-30(8)	63(11)	-75(11)
C(28)	111(9)	233(15)	100(10)	45(9)	42(9)	14(10)
C(29)	194(13)	103(7)	124(12)	60(8)	36(11)	-7(7)
C(30)	122(9)	196(12)	141(13)	37(8)	2(9)	-92(10)

The exponent takes the form: $-2\pi^2 \sum U_{ij} h_i h_j a_i^ a_j^*$.

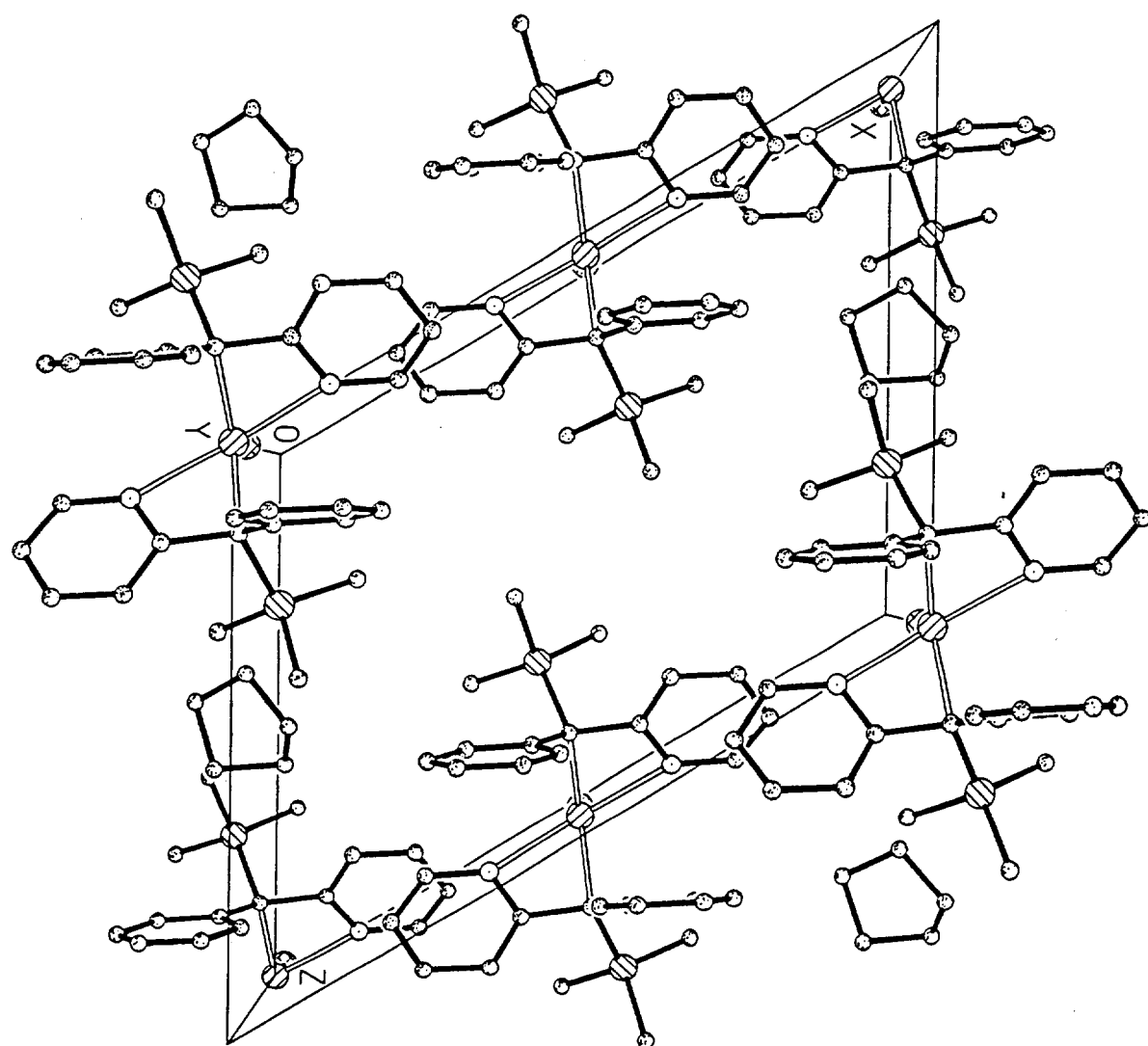
Table 5. Hydrogen atom coordinates ($\times 10^4$) and assigned isotropic temperature factors* ($\text{\AA}^2 \times 10^3$).

Atom	x	y	z	U
H(1)	4020	834	2580	90
H(2)	4616	-495	3487	90
H(3)	4336	5	4441	90
H(5)	3649	1541	5061	90
H(6)	2873	3396	5080	90
H(7)	2433	4746	4181	90
H(10)	2217	5084	2999	70
H(11A)	4930	4196	2961	120
H(11B)	5098	4206	3706	120
H(11C)	5533	5278	3395	120
H(12A)	3578	6199	2095	120
H(12B)	4215	7231	2550	120
H(12C)	3081	7185	2415	120
H(13A)	3411	7131	3845	120
H(13B)	4543	7196	3972	120
H(13C)	4108	6124	4283	120
H(14)	1732	6078	1225	90
H(15)	329	7300	854	90
H(16)	-1050	6756	1093	90
H(18)	-1911	5187	1596	90
H(19)	-1849	3314	2124	90
H(20)	-465	1988	2363	90
H(23)	1320	1798	2450	70
H(24A)	-98	-195	1720	120
H(24B)	-308	-378	976	120
H(24C)	-727	792	1228	120
H(25A)	1380	2388	631	120
H(25B)	252	2496	510	120
H(25C)	671	1326	258	120
H(26A)	2596	465	1601	120
H(26B)	1893	-608	1235	120
H(26C)	2089	-397	1975	120
H(27A)	2984	8656	174	200
H(27B)	3142	8393	905	200
H(28A)	3967	7081	268	200
H(28B)	3720	6531	859	200
H(29A)	2627	5363	214	200
H(29B)	2842	5956	-379	200
H(30A)	1228	6269	-165	200
H(30B)	1609	7202	-580	200

*The exponent takes the form: $-8\pi^2 U \sin^2 \theta / \lambda^2$.



LEUNG



STRUCTURE DETERMINATION SUMMARYCrystal Data

Empirical Formula	$C_{35} H_{36} N_2 Se Si_2 Sn$
Color; Habit	Yellow Prism
Crystal size (mm)	0.14 x 0.16 x 0.20
Crystal System	Monoclinic
Space Group	C2
Unit Cell Dimensions	$a = 16.302(2) \text{ \AA}$ $b = 10.7300(10) \text{ \AA}$ $c = 12.0670(10) \text{ \AA}$ $\beta = 121.310(10)^\circ$
Volume	$1803.3(9) \text{ \AA}^3$
Z	2
Formula weight	738.5
Density(calc.)	1.360 Mg/m^3
Absorption Coefficient	1.808 mm^{-1}
F(000)	744