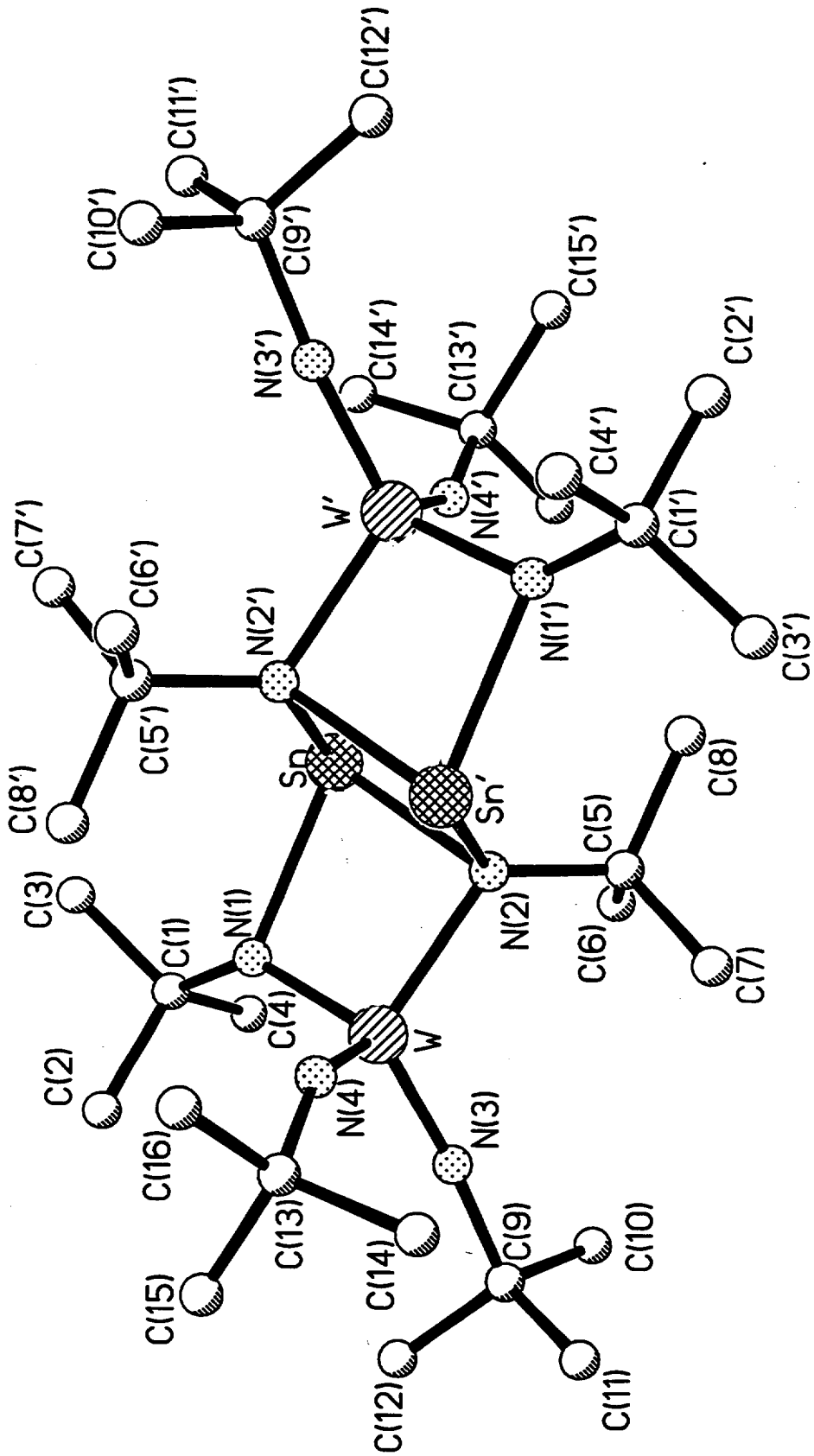

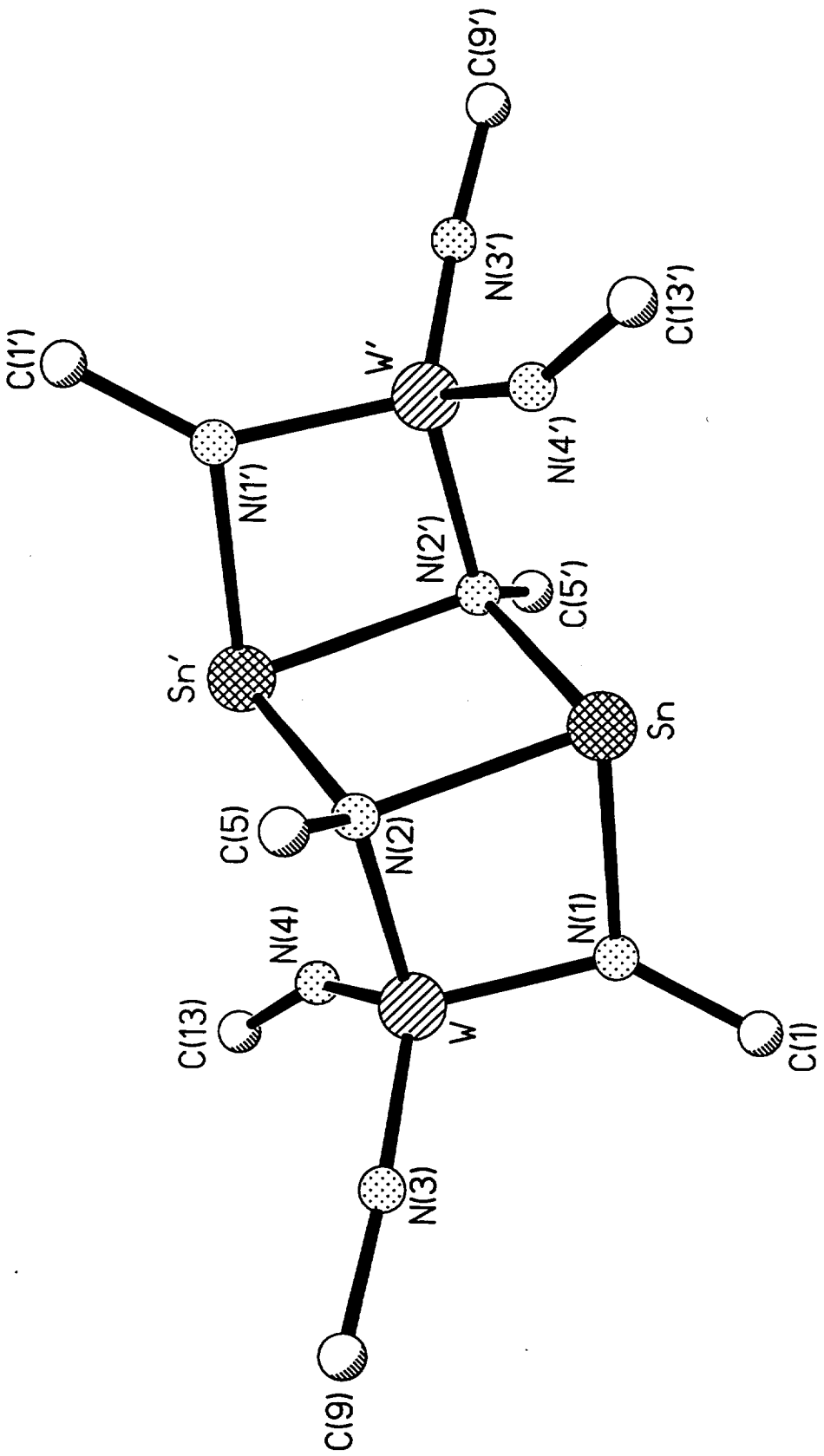

Table 1. Crystal data and structure refinement for 1(gwm).

Identification code	gwm
Empirical formula	$C_{16}H_{36}N_4SnW$
Formula weight	587.03
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 10.387(2) Å alpha = 90° b = 16.760(3) Å beta = 90° c = 24.957(5) Å gamma = 90°
Volume, Z	4345(2) $Å^3$, 8
Density (calculated)	1.795 Mg/m^3
Absorption coefficient	6.444 mm^{-1}
F(000)	2272
Crystal size	0.15 x 0.10 x 0.10 mm
θ range for data collection	1.63 to 28.73°
Limiting indices	$-13 \le h \le 12$, $-21 \le k \le 21$, $-26 \le l \le 33$
Reflections collected	24760
Independent reflections	5269 (R_{int} = 0.0631)
Absorption correction	SADABS
Max. and min. transmission	1.000 and 0.744
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5269 / 0 / 199
Goodness-of-fit on F^2	1.133
Final R indices [$I>2\sigma(I)$]	R1 = 0.0409, wR2 = 0.0747(for 3875reflections)
R indices (all data)	R1 = 0.0735, wR2 = 0.0846
Largest diff. peak and hole	0.844 and -1.435 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	9323.1(2)	532.5(1)	5989.0(1)	20(1)
Sn	11425.9(4)	-276.0(2)	5310.5(2)	24(1)
N(1)	10449(5)	-329(3)	6126.3(19)	24(1)
N(2)	10086(5)	806(3)	5254.1(19)	21(1)
N(3)	9396(5)	1282(3)	6478.4(19)	27(1)
N(4)	7706(5)	196(3)	5865.0(19)	26(1)
C(1)	11085(7)	-719(4)	6585(3)	35(2)
C(2)	10061(9)	-865(5)	7011(3)	53(2)
C(3)	11684(9)	-1510(5)	6430(3)	64(3)
C(4)	12118(9)	-164(5)	6818(3)	63(3)
C(5)	10683(6)	1615(4)	5155(2)	26(1)
C(6)	11784(7)	1762(4)	5552(3)	40(2)
C(7)	9639(8)	2245(4)	5214(3)	46(2)
C(8)	11242(7)	1667(4)	4584(2)	37(2)
C(9)	9227(7)	1873(4)	6902(3)	33(2)
C(10)	10412(9)	2421(5)	6896(4)	73(3)
C(11)	8032(9)	2364(5)	6804(3)	56(2)
C(12)	9108(10)	1448(5)	7436(3)	69(3)
C(13)	6350(6)	146(4)	5982(2)	28(1)
C(14)	5694(8)	939(5)	5838(4)	53(2)
C(15)	6203(8)	-6(5)	6587(3)	54(2)
C(16)	5702(7)	-530(4)	5677(3)	44(2)

Table 3. Bond lengths [Å] and angles [°] for 1.

W-N(3)	1.753(5)	W-N(4)	1.799(5)
W-N(1)	1.890(5)	W-N(2)	2.050(5)
W-Sn	3.0779(6)	Sn-N(1)	2.276(5)
Sn-N(2)#1	2.289(5)	Sn-N(2)	2.290(5)
N(1)-C(1)	1.474(8)	N(2)-C(5)	1.512(7)
N(2)-Sn#1	2.289(5)	N(3)-C(9)	1.460(7)
N(4)-C(13)	1.441(8)	C(1)-C(3)	1.515(9)
C(1)-C(2)	1.525(10)	C(1)-C(4)	1.534(10)
C(5)-C(7)	1.521(9)	C(5)-C(6)	1.533(9)
C(5)-C(8)	1.541(8)	C(9)-C(11)	1.509(10)
C(9)-C(12)	1.515(10)	C(9)-C(10)	1.536(11)
C(13)-C(16)	1.521(9)	C(13)-C(14)	1.537(10)
C(13)-C(15)	1.539(9)		

N(3)-W-N(4)	112.6(2)	N(3)-W-N(1)	113.2(2)
N(4)-W-N(1)	111.7(2)	N(3)-W-N(2)	116.5(2)
N(4)-W-N(2)	106.1(2)	N(1)-W-N(2)	95.4(2)
N(3)-W-Sn	131.9(2)	N(4)-W-Sn	115.5(2)
N(1)-W-Sn	47.5(2)	N(2)-W-Sn	48.07(13)
N(1)-Sn-N(2)#1	103.3(2)	N(1)-Sn-N(2)	79.3(2)
N(2)#1-Sn-N(2)	81.5(2)	N(1)-Sn-W	37.72(12)
N(2)#1-Sn-W	91.29(12)	N(2)-Sn-W	41.76(12)
C(1)-N(1)-W	139.2(4)	C(1)-N(1)-Sn	120.8(4)
W-N(1)-Sn	94.8(2)	C(5)-N(2)-W	120.3(3)
C(5)-N(2)-Sn#1	121.9(4)	W-N(2)-Sn#1	101.5(2)
C(5)-N(2)-Sn	118.1(4)	W-N(2)-Sn	90.2(2)
Sn#1-N(2)-Sn	98.5(2)	C(9)-N(3)-W	170.2(5)
C(13)-N(4)-W	153.7(4)	N(1)-C(1)-C(3)	112.0(5)
N(1)-C(1)-C(2)	107.5(6)	C(3)-C(1)-C(2)	108.9(6)
N(1)-C(1)-C(4)	109.8(6)	C(3)-C(1)-C(4)	109.9(7)
C(2)-C(1)-C(4)	108.7(6)	N(2)-C(5)-C(7)	108.3(5)
N(2)-C(5)-C(6)	110.1(5)	C(7)-C(5)-C(6)	111.1(6)
N(2)-C(5)-C(8)	110.8(5)	C(7)-C(5)-C(8)	108.6(6)
C(6)-C(5)-C(8)	107.9(6)	N(3)-C(9)-C(11)	110.6(6)
N(3)-C(9)-C(12)	109.1(5)	C(11)-C(9)-C(12)	109.4(7)
N(3)-C(9)-C(10)	107.6(6)	C(11)-C(9)-C(10)	109.3(7)
C(12)-C(9)-C(10)	110.8(7)	N(4)-C(13)-C(16)	112.0(5)
N(4)-C(13)-C(14)	109.6(6)	C(16)-C(13)-C(14)	109.4(6)
N(4)-C(13)-C(15)	107.7(5)	C(16)-C(13)-C(15)	108.9(6)
C(14)-C(13)-C(15)	109.2(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
W	19(1)	21(1)	18(1)	-1(1)	0(1)	0(1)
Sn	20(1)	28(1)	25(1)	-2(1)	-2(1)	4(1)
N(1)	28(3)	27(3)	18(3)	0(2)	-2(2)	5(2)
N(2)	18(3)	21(2)	24(3)	1(2)	1(2)	-1(2)
N(3)	31(3)	27(3)	23(3)	-4(2)	6(2)	-2(2)
N(4)	23(3)	35(3)	21(3)	5(2)	2(2)	-2(2)
C(1)	38(4)	42(4)	23(3)	7(3)	-4(3)	12(3)
C(2)	59(6)	65(5)	36(4)	28(4)	6(4)	11(5)
C(3)	87(7)	58(5)	47(5)	3(4)	-17(5)	47(5)
C(4)	47(6)	89(7)	52(5)	9(5)	-30(4)	-6(5)
C(5)	28(4)	23(3)	25(3)	-2(2)	8(3)	-7(3)
C(6)	42(5)	44(4)	33(4)	-2(3)	0(3)	-21(3)
C(7)	53(6)	28(4)	57(5)	0(3)	14(4)	9(3)
C(8)	50(5)	33(4)	29(4)	2(3)	9(3)	-14(3)
C(9)	37(4)	31(4)	29(4)	-11(3)	1(3)	-1(3)
C(10)	71(8)	75(7)	73(7)	-45(5)	17(5)	-24(5)
C(11)	54(6)	54(5)	59(5)	-17(4)	1(4)	20(4)
C(12)	124(9)	58(6)	26(4)	-12(4)	13(5)	12(6)
C(13)	23(3)	28(3)	32(4)	-2(3)	2(3)	-2(3)
C(14)	34(5)	48(5)	79(6)	2(4)	-8(4)	6(4)
C(15)	35(5)	84(6)	43(5)	5(4)	8(4)	-7(4)
C(16)	26(4)	49(4)	58(5)	-12(4)	0(4)	-12(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	9392	-1217	6867	80
H(2B)	9674	-355	7117	80
H(2C)	10458	-1116	7325	80
H(3A)	12342	-1423	6155	96
H(3B)	11017	-1866	6290	96
H(3C)	12082	-1754	6747	96
H(4B)	12784	-68	6547	94
H(4C)	12506	-414	7134	94
H(4A)	11722	344	6921	94
H(6A)	11454	1726	5919	59
H(6B)	12147	2294	5492	59
H(6C)	12456	1359	5499	59
H(7A)	9275	2219	5576	69
H(7B)	8958	2146	4950	69
H(7C)	10010	2775	5153	69
H(8A)	10556	1571	4322	56
H(8B)	11918	1264	4541	56
H(8C)	11608	2199	4526	56
H(10A)	10474	2687	6547	110
H(10B)	11189	2103	6958	110
H(10C)	10328	2823	7179	110
H(11A)	7274	2016	6811	83
H(11B)	8094	2624	6453	83
H(11C)	7953	2771	7084	83
H(12A)	8348	1101	7431	104
H(12B)	9019	1843	7723	104
H(12C)	9880	1125	7498	104
H(14A)	5789	1040	5453	80
H(14B)	6097	1374	6040	80
H(14C)	4777	910	5929	80
H(15A)	6624	-510	6681	81
H(15B)	5287	-35	6679	81
H(15C)	6606	431	6787	81
H(16A)	5794	-439	5291	66
H(16B)	4786	-548	5771	66
H(16C)	6109	-1038	5773	66