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The Crystal and Molecular Structure of Dimethyltin Chloride *N,N*-Dimethyldithiocarbamate

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The molecular structure of dimethyltin chloride *N,N*-dimethyldithiocarbamate, $[(CH_3)_2SnCl(S_2CN(CH_3)_2)]$, has been determined from three-dimensional X-ray diffraction data. The unit-cell dimensions are $a=12.67$, $b=7.64$, $c=12.11$ Å, and $\beta=110.3°$. The space group is $P2_1/c$. Four formula units are contained in a unit-cell. The structure was established by the heavy-atom method. The coordination around the tin atom is a distorted trigonal bipyramid with the following bond distances: Sn–C, 2.17(5) and 2.20(5) Å; Sn–Cl, 2.46(1) Å, and Sn–S, 2.48(1) and 2.79(1) Å. Two methyl groups are both in equatorial positions.

Recently, numerous studies have been reported on transition metal complexes of dialkyldithiocarbamates. The crystal structures of several complexes have also been determined; however, few structures of non-transition metal complexes have yet been reported.

Tanaka and his co-workers[1] reported on the preparation and properties of some organotin *N,N*-dimethyldithiocarbamates. According to the spectroscopic studies, the three configurations shown in Fig. 1 were proposed for a penta-coordinated complex, dimethyltin chloride *N,N*-dimethyldithio-

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1) M. Honda, M. Komura, Y. Kawasaki, T. Tanaka and R. Okawara, *J. Inorg. Nucl. Chem.*, **30**, 3231 (1968).

carbamate, $[(CH_3)_2SnCl(S_2CN(CH_3)_2)]$ (to be abbreviated as $Me_2SnCl(dtc)$ hereafter). Among these configurations, (3) is considered to be most likely; in it the two methyl groups are both in equatorial positions.

To determine the exact configuration, the crystal structure analysis has now been undertaken by means of X-ray diffraction.

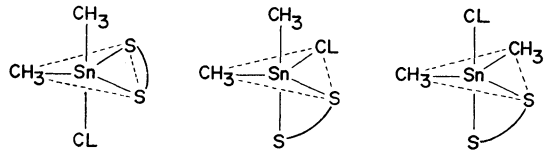

Fig. 1. Three possible configurations of Me_2SnCl-(dtc) molecule.

The purpose of this study is also to contribute to the understanding of the bonding nature of the tin atom in penta- and hexa-coordinated dimethyltin complexes, among which the crystal structures and molecular configurations of $[(CH_3)_2SnCl_2((CH_3)_2SO)_2]$,[2] $[(CH_3)_2Sn(C_9H_6NO)_2]$,[3] and $[((CH_3)_2$-SnCl, terpyridil)$^+\cdot((CH_3)_2SnCl_3)^-]$[4] have already been determined.

Experimental

The crystals of $Me_2SnCl(dtc)$ were recrystallized from a chloroform-ethanol solution. They belong to the monoclinic system, and the unit-cell dimensions are: $a=12.67\pm0.07$, $b=7.64\pm0.01$, $c=12.11\pm0.06$ Å, and $\beta=110.3\pm0.4°$. The unit-cell dimensions were determined from Weissenberg photographs taken around the b and c axes, on which Debye lines of aluminum were superposed for calibration. The observed density is 1.86 $g\cdot cm^{-3}$, while the calculated density, assuming four formula units per unit-cell, is 1.84 $g\cdot cm^{-3}$. From the systematic absences of reflections (l: odd for $h0l$ and k: odd for $0k0$), the space group was determined to be $P2_1/c$.

A set of three-dimensional intensity data was collected on multiple-film equi-inclination Weissenberg photographs with nickel-filtered Cu$K\alpha$ radiation. Layers from 0 through 5 were recorded around the b axis; layers from 0 through 5 around the c axis were also recorded, mainly for the purpose of inter-layer scaling. The intensities of 1968 independent reflections were estimated visually by using a calibrated standard scale. The intensities were corrected for the usual Lorentz and polarization factors. No absorption correction was made.

Determination and Refinement of the Structure

A three-dimensional Patterson function was computed; from it the location of the tin atom was easily determined. The chlorine and two sulfur atoms could also be located from the Patterson function, but the chlorine atom could not be distinguished from the sulfur atoms. Therefore, the first Fourier synthesis was computed with the phases based on the tin atom only, while the chlorine and two sulfur atoms were identified at the positions which had been suggested from the Patterson synthesis. The nitrogen and three carbon atoms were also found in the Fourier map. The remaining two carbon atoms were found in another Fourier map, with phases based on all the atoms which had already been located.

The structure factor calculation after a cycle of least-squares refinement gave a discrepancy factor, $R=\sum||F_o|-|F_c||/\sum|F_o|$, of 0.27. Successive block-diagonal least-squares refinement was carried out on a HITAC 5020E computer at the University of Tokyo. In the refinement, the weight was taken as unity for all reflections. After five cycles of

TABLE 1

(a) The final atomic coordinates along with their estimated standard deviations (in fraction of cell edges) in parentheses (each multiplied by 10^3)

Atom	x	y	z
Sn	0.1818(0.2)	0.1041(0.3)	0.1625(0.2)
Cl	0.1452(0.7)	−0.0682(1.8)	−0.0191(1.0)
S(1)	0.3851(0.6)	0.0557(1.2)	0.1995(0.8)
S(2)	0.3191(0.7)	0.2627(1.5)	0.3720(0.8)
N	0.528(2)	0.168(4)	0.400(3)
C(1)	0.421(2)	0.158(5)	0.330(3)
C(2)	0.621(3)	0.088(6)	0.365(4)
C(3)	0.596(3)	0.260(6)	0.524(3)
C(4)	0.113(4)	−0.075(7)	0.259(4)
C(5)	0.111(3)	0.355(5)	0.981(4)

(b) The anisotropic thermal parameters (each multiplied by 10^4) of the form: $\exp\{-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)\}$.

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Sn	16	66	44	3	17	20
Cl	27	228	70	13	12	−104
S(1)	21	85	41	13	15	−38
S(2)	25	151	48	17	27	−63
N	39	44	44	25	15	−45
C(1)	7	99	53	59	10	−12
C(2)	13	99	109	17	−1	11
C(3)	42	163	32	108	−4	92
C(4)	50	234	62	268	−60	125
C(5)	25	9	140	105	2	147

2) N. W. Isaacs, C. H. L. Kennard and W. Kitching, *Chem. Commun.*, **1968**, 820.

3) E. O. Schlemper, *Inorg. Chem.*, **6**, 2021 (1967).

4) F. W. B. Einshtein and B. R. Penfold, *J. Chem. Soc., A*, **1968**, 3019.

TABLE 2. THE OBSERVED AND CALCULATED STRUCTURE FACTORS

K	FO	FC
H,L= 0 0		
2	68	46
4	127	-107
6	105	-102
H,L= 0 1		
1	84	114
2	191	-185
3	18	11
4	67	-84
5	66	-64
6	63	42
7	43	-35
8	45	36
9	38	29
H,L= 0 2		
0	74	-69
1	44	-34
2	52	-42
3	131	-176
4	51	48
5	0	5
6	40	28
7	68	54
8	0	-6
H,L= 0 3		
1	82	-103
2	31	-22
3	40	38
4	0	-6
5	89	89
6	0	7
7	0	18
8	0	9
9	41	-46
H,L= 0 4		
0	104	-95
1	65	61
2	58	44
3	102	115
4	53	48
5	0	6
6	0	29
7	57	-48
H,L= 0 5		
1	119	113
2	124	124
3	28	-13
4	56	50
5	58	-51
6	73	-67
7	0	-12
8	50	-40
H,L= 0 6		
0	162	156
1	70	-57
2	48	39
3	0	5
4	83	-78
5	54	-46
H,L= 0 7		
1	68	54
2	110	-106
3	55	-39
4	63	-59
5	52	-46
H,L= 0 8		
0	0	-5
1	71	-59
2	44	-33
3	87	-69
4	43	35
5	0	6
H,L= 0 9		
1	63	-54
2	0	-8
3	0	31
4	0	-12
5	64	54
H,L= 0 10		
0	37	-28
1	50	38
2	0	0
3	37	20
4	36	31
5	0	-8
H,L= 0 11		
1	0	15
2	38	34
3	0	3
4	0	5
5	31	-26
H,L= 0 12		
0	43	32
1	0	-1
2	0	13
3	0	4
4	51	-58
5	0	-14
H,L= 0 13		
1	0	15
2	32	-34
3	0	-16
4	0	0
H,L= 1 0		
1	69	-142
2	47	62
3	59	-80
4	57	-67
5	0	2
6	35	-23
7	73	71
H,L= 1 1		
1	67	-76
2	43	-48
3	0	8

K	FO	FC
4	26	-22
5	65	62
6	69	58
7	0	7
8	57	62
H,L= 1 2		
0	126	-108
1	30	-22
2	59	-50
3	49	44
4	94	132
5	45	41
6	63	50
7	0	6
8	44	-33
H,L= 1 3		
1	40	27
2	137	177
3	59	51
4	55	51
5	44	39
6	59	-49
7	0	-19
8	49	-49
H,L= 1 4		
0	161	158
1	106	120
2	61	47
3	61	57
4	61	-46
5	0	0
6	66	-48
7	89	-86
H,L= 1 5		
1	100	97
2	0	2
3	54	-47
4	0	-13
5	98	-97
6	0	0
7	42	4
8	39	-12
H,L= 1 6		
0	47	33
1	41	-30
2	59	44
3	82	-77
4	80	-64
5	39	29
H,L= 1 7		
1	28	-1
2	85	-81
3	45	33
4	0	-15
5	40	20
H,L= 1 8		
0	60	-49
1	0	-6
2	0	12
3	0	11
4	62	57
5	0	-18
H,L= 1 9		
1	0	-16
2	55	40
3	0	13
4	0	15
5	38	37
H,L= 1 10		
0	42	37
1	42	36
2	0	-13
3	43	37
4	0	-10
5	0	-25
H,L= 1 11		
1	52	48
2	0	15
3	34	-33
4	0	6
5	37	-40
H,L= 1 12		
0	47	49
1	0	-7
2	8	13
3	33	-34
4	0	-18
5	21	28
H,L= 1 13		
1	0	4
2	29	-33
3	0	15
4	0	-25
H,L= 1 -1		
1	0	207
2	59	-62
3	40	-43
4	18	-15
5	93	-125
6	0	-6
7	0	-15
8	0	2
9	37	33
H,L= 1 -2		
0	122	142
1	129	178
2	120	126
3	88	128
4	84	-111
5	0	-1
6	44	-38
7	66	-54
8	0	-4
H,L= 1 -3		
1	75	-63

K	FO	FC
2	149	188
3	58	52
4	93	127
5	33	29
6	0	-18
7	0	-8
8	70	-62
9	0	-16
H,L= 1 -4		
0	131	-127
1	100	87
2	79	-71
3	57	44
4	80	80
5	52	38
6	69	68
7	0	-15
8	0	-24
H,L= 1 -5		
1	105	-99
2	87	-81
3	27	16
4	43	-34
5	73	62
6	46	37
7	0	11
8	41	27
H,L= 1 -6		
0	63	44
1	119	-104
2	0	-13
3	92	-86
4	0	-4
5	0	-5
H,L= 1 -7		
1	126	116
2	0	-8
3	51	-34
4	0	10
5	86	-84
H,L= 1 -8		
0	63	51
1	53	35
2	53	40
3	113	115
4	72	-64
5	0	2
H,L= 1 -9		
1	51	-39
2	102	98
3	0	-5
4	58	50
5	0	7
H,L= 1-10		
0	128	-118
1	0	20
2	0	-15
3	0	18
4	37	33
5	0	5
H,L= 1-11		
1	54	-40
2	38	-33
3	0	9
4	0	-20
5	46	47
H,L= 1-12		
0	0	22
1	0	-20
2	0	0
3	46	-47
4	0	0
5	0	10
H,L= 1-13		
1	31	31
H,L= 2 0		
0	100	-112
1	32	-24
2	29	-23
3	53	-58
4	52	51
5	73	72
6	82	64
7	69	68
H,L= 2 1		
1	109	-130
2	73	71
3	78	87
4	57	54
5	92	99
6	0	-4
7	0	9
8	0	-9
H,L= 2 2		
0	78	-70
1	53	52
2	42	32
3	119	146
4	29	29
5	50	-43
6	0	22
7	74	-66
8	43	-27
H,L= 2 3		
1	76	67
2	105	104
3	59	-51
4	69	58
5	61	-56
6	63	-64
7	0	10
8	41	-38
H,L= 2 4		
0	139	128
1	0	-10

K	FO	FC
2	0	-4
3	76	74
4	76	-70
5	0	12
6	74	-62
7	0	21
8	50	43
H,L= 2 5		
1	77	63
2	81	-74
3	31	-20
4	0	0
5	38	-29
6	78	74
7	0	-13
8	38	40
H,L= 2 6		
0	0	-12
1	31	-28
2	0	5
3	85	-68
4	69	67
5	0	14
H,L= 2 7		
1	54	-45
2	0	7
3	51	42
4	0	-9
5	62	63
H,L= 2 8		
0	88	-72
1	60	52
2	0	3
3	65	54
4	0	15
5	0	-8
H,L= 2 9		
1	0	10
2	81	81
3	0	-9
4	43	41
5	0	-27
H,L= 2 10		
0	86	78
1	0	-9
2	43	37
3	46	37
4	52	-60
5	0	13
H,L= 2 11		
1	50	49
2	35	-37
3	0	9
4	0	-6
5	29	-31
H,L= 2 12		
0	0	4
1	30	-31
2	0	0
3	30	-32
4	0	17
H,L= 2 13		
1	28	-32
2	21	-10
3	0	10
H,L= 2 -1		
1	12	-18
2	50	-62
3	18	-14
4	42	-40
5	44	-35
6	88	79
7	0	-2
8	51	53
9	42	36
H,L= 2 -2		
0	142	172
1	52	-41
2	75	-64
3	53	-54
4	80	-89
5	31	21
6	63	-53
7	0	-5
8	67	58
H,L= 2 -3		
1	88	92
2	104	119
3	51	-51
4	24	23
5	59	-55
6	66	-59
7	0	-19
8	43	-31
9	40	33
H,L= 2 -4		
0	24	4
1	92	85
2	23	-14
3	160	194
4	67	56
5	0	-11
6	0	-16
7	63	-63
8	0	-8
H,L= 2 -5		
1	119	-121
2	59	50
3	38	29
4	79	73
5	92	91
6	0	0
7	0	14
8	0	-16
H,L= 2 -6		

K	FO	FC
0	181	-176
1	44	-38
2	56	-50
3	42	-28
4	53	44
5	0	-1
H,L= 2 -7		
1	54	-40
2	113	-106
3	0	-15
4	54	-46
5	0	-6
H,L= 2 -8		
0	95	83
1	0	0
2	30	22
3	82	-64
4	71	-64
5	0	-6
H,L= 2 -9		
1	84	70
2	68	59
3	0	-22
4	0	14
5	56	-52
H,L= 2-10		
0	0	-1
1	75	66
2	39	-30
3	76	69
4	0	21
5	0	15
H,L= 2-11		
1	79	-74
2	39	34
3	0	10
4	35	25
5	52	53
H,L= 2-12		
0	63	-56
1	36	-32
2	45	-34
3	0	-20
4	40	41
5	0	-6
H,L= 2-13		
1	0	-4
2	51	-50
3	0	3
4	31	-36
5	17	2
H,L= 2-14		
0	30	28
1	0	-17
H,L= 3 0		
0	152	-173
1	55	49
2	72	-74
3	21	14
4	110	145
5	0	6
6	51	43
7	56	-39
H,L= 3 1		
1	95	-98
2	115	142
3	30	-27
4	26	20
5	53	47
6	67	-66
7	42	24
8	54	-54
H,L= 3 2		
0	18	-2
1	121	134
2	0	-9
3	84	78
4	69	-71
5	50	35
6	0	-20
7	69	-65
8	41	37
H,L= 3 3		
1	106	111
2	30	21
3	55	-53
4	46	33
5	94	-97
6	45	46
7	0	2
H,L= 3 4		
0	0	5
1	71	-65
2	66	49
3	76	-68
4	38	-30
5	37	29
6	0	-11
7	69	63
H,L= 3 5		
1	74	-64
2	86	-85
3	46	32
4	54	-39
5	64	58
6	0	26
7	0	0
8	35	35
H,L= 3 6		
0	109	-97
1	0	-12
2	68	-56
3	0	19
4	80	73
5	40	-22

K	FO	FC
H,L= 3 7		
1	75	-65
2	101	97
3	0	7
4	62	60
5	40	45
H,L= 3 8		
0	83	73
1	86	80
2	0	-17
3	79	84
4	0	-18
5	0	23
H,L= 3 9		
1	76	73
2	0	1
3	0	-13
4	0	17
5	49	-49
H,L= 3 10		
0	32	33
1	0	-15
2	0	24
3	52	-60
4	0	-14
5	0	12
H,L= 3 11		
1	0	-22
2	37	-38
3	0	6
4	25	-20
5	0	18
H,L= 3 12		
0	63	-67
1	0	-5
2	0	-12
H,L= 3 -1		
1	77	-88
2	65	-77
3	32	28
4	23	-17
5	99	98
6	44	40
7	0	3
8	50	41
9	50	-46
H,L= 3 -2		
0	0	0
1	101	-111
2	17	-17
3	83	-85
4	28	-22
5	0	14
6	0	-9
7	110	102
8	0	13
H,L= 3 -3		
1	19	4
2	59	-51
3	53	-51
4	0	7
5	87	-92
6	0	20
7	0	15
8	0	16
9	52	61
H,L= 3 -4		
0	29	25
1	63	53
2	21	14
3	64	53
4	104	-115
5	42	-35
6	0	7
7	53	-53
H,L= 3 -5		
1	32	-26
2	115	120
3	53	41
4	0	10
5	0	1
6	65	-66
7	0	-9
8	63	-58
H,L= 3 -6		
0	125	-126
1	67	56
2	25	-13
3	30	17
4	81	72
5	37	23
H,L= 3 -7		
1	102	-98
2	56	-45
3	0	12
4	0	-17
5	82	83
H,L= 3 -8		
0	46	-32
1	66	-52
2	52	-40
3	82	-80
4	0	14
5	0	12
H,L= 3 -9		
1	53	39
2	75	-65
3	46	-40
4	44	-32
5	46	-41
H,L= 3-10		
0	76	63
1	0	-6
2	34	25
3	0	18

K	FO	FC
4	49	-40
5	49	-45
H,L= 3-11		
1	0	10
2	62	57
3	0	15
4	36	28
5	0	-6
H,L= 3-12		
0	85	-73
1	0	20
2	0	5
3	0	37
4	31	26
5	0	5
H,L= 3-13		
1	53	-48
2	0	-19
3	0	9
4	0	-10
5	26	36
H,L= 3-14		
0	0	-16
1	0	-20
2	0	-7
3	43	-54
4	0	1
H,L= 4 0		
0	173	-160
1	40	30
2	80	-64
3	156	162
4	31	20
5	53	-36
6	56	40
7	60	-59
H,L= 4 1		
1	70	65
2	87	94
3	66	-61
4	71	64
5	73	-73
6	0	-27
7	0	5
8	0	-24
H,L= 4 2		
0	184	184
1	54	-48
2	0	13
3	39	-30
4	61	-62
5	0	-1
6	73	-73
7	41	32
H,L= 4 3		
1	0	4
2	133	-137
3	0	-1
4	71	-65
5	0	-9
6	56	50
7	0	-6
8	37	35
H,L= 4 4		
0	137	-140
1	29	-21
2	63	-51
3	103	-108
4	60	53
5	0	-8
6	63	50
7	38	36
H,L= 4 5		
1	139	-146
2	0	5
3	34	23
4	0	13
5	84	86
6	0	-2
7	38	32
H,L= 4 6		
0	96	-91
1	80	77
2	55	11
3	105	108
4	0	1
5	0	5
H,L= 4 7		
1	55	54
2	72	75
3	0	-19
4	49	47
5	39	-40
H,L= 4 8		
0	68	58
1	46	-43
2	0	22
3	0	-3
4	47	-52
5	0	-5
H,L= 4 9		
1	0	0
2	57	-56
3	0	-10
4	38	-39
5	0	-14
H,L= 4 10		
0	43	-39
1	30	-27
2	35	-33
3	36	-34
4	33	31
5	28	13
H,L= 4 11		
1	48	-51

K	FO	FC
2	25	23
3	0	22
H,L= 4 12		
0	0	-18
1	38	42
2	0	2
3	0	32
H,L= 4 -1		
1	124	-169
2	36	29
3	52	47
4	30	-17
5	114	93
6	59	-52
7	42	28
8	0	-16
9	50	-38
H,L= 4 -2		
0	134	-168
1	103	-109
2	0	10
3	98	-113
4	70	63
5	0	-8
6	79	68
7	0	24
8	42	-37
H,L= 4 -3		
1	0	7
2	114	-136
3	0	1
4	103	-97
5	0	2
6	71	62
7	0	0
8	63	65
9	0	-8
H,L= 4 -4		
0	112	109
1	35	-25
2	22	15
3	72	-73
4	77	-73
5	44	40
6	62	-57
7	0	32
8	40	36
H,L= 4 -5		
1	63	57
2	66	56
3	72	-68
4	31	26
5	59	-52
6	46	-37
7	0	0
8	0	-29
H,L= 4 -6		
0	23	16
1	60	54
2	52	-46
3	71	65
4	38	27
5	76	-65
H,L= 4 -7		
1	80	-69
2	0	0
3	60	54
4	0	9
5	72	67
H,L= 4 -8		
0	86	-64
1	66	-57
2	0	-12
3	0	-17
4	68	68
5	0	-12
H,L= 4 -9		
1	0	-9
2	90	-78
3	0	14
4	38	-34
5	0	-3
H,L= 4-10		
0	41	34
1	37	-30
2	0	16
3	62	-50
4	62	-58
5	0	-1
H,L= 4-11		
1	54	43
2	0	10
3	37	-25
4	36	-24
5	35	-35
H,L= 4-12		
0	37	31
1	41	39
2	0	10
3	0	17
4	0	9
5	34	-8
H,L= 4-13		
1	0	-9
2	29	27
3	0	19
H,L= 5 0		
0	143	120
1	85	69
2	98	77
3	27	15
4	101	-91
5	0	0
6	57	-53
7	50	-36

K	FO	FC
H,L= 5 1		
1	122	116
2	127	-122
3	50	-38
4	77	-62
5	103	-87
6	0	7
H,L= 5 2		
0	37	-26
1	120	-110
2	0	9
3	121	-123
4	0	-16
5	44	-39
6	0	-7
7	40	60
H,L= 5 3		
1	115	-120
2	98	-99
3	0	2
4	40	-39
5	94	87
6	0	28
7	0	18
8	33	38
H,L= 5 4		
0	116	-116
1	0	5
2	78	-77
3	56	46
4	87	97
5	0	0
6	0	44
7	0	-13
H,L= 5 5		
1	0	-3
2	103	99
3	0	10
4	37	29
5	0	14
6	38	-44
7	35	-12
H,L= 5 6		
0	101	109
1	48	40
2	0	-4
3	0	6
4	49	-45
5	0	-3
H,L= 5 7		
1	33	25
2	39	-38
3	0	-22
4	0	-22
5	60	-58
H,L= 5 8		
0	32	-24
1	38	-36
2	0	-9
3	73	-74
4	34	-23
5	0	9
H,L= 5 9		
1	54	-46
2	48	-46
3	0	12
4	0	-5
5	38	35
H,L= 5 10		
0	63	-58
1	0	-2
2	0	-6
3	28	28
4	42	44
5	0	-5
H,L= 5 11		
1	0	-11
2	0	34
3	0	-2
4	0	12
H,L= 5 12		
0	17	20
1	0	4
H,L= 5 -1		
1	0	-1
2	148	159
3	0	-11
4	78	67
5	0	6
6	45	-42
7	0	9
8	65	-56
9	0	-1
H,L= 5 -2		
0	133	-156
1	77	76
2	78	-77
3	0	-1
4	109	111
5	0	1
6	61	50
7	54	-47
8	0	-16
H,L= 5 -3		
1	89	-97
2	117	-122
3	44	29
4	73	-75
5	99	88
6	0	3
7	0	6
8	0	21
H,L= 5 -4		
0	74	65
1	114	-124

K	FO	FC
2	33	-16
3	126	-145
4	36	27
5	36	-18
6	0	0
7	66	66
H,L= 5 -5		
1	116	115
2	85	-77
3	30	5
4	50	-39
5	89	-80
6	40	27
7	42	-25
8	51	46
H,L= 5 -6		
0	134	129
1	0	0
2	62	60
3	71	68
4	96	-102
5	0	3
H,L= 5 -7		
1	0	-5
2	106	105
3	0	-5
4	0	18
5	0	-13
H,L= 5 -8		
0	125	-112
1	50	40
2	0	10
3	0	2
4	57	46
5	0	-8
H,L= 5 -9		
1	44	-30
2	53	-46
3	43	33
4	38	-25
5	69	65
H,L= 5-10		
0	41	25
1	32	-22
2	0	7
3	76	-80
4	0	20
5	0	16
H,L= 5-11		
1	60	47
2	55	-48
3	0	-20
4	0	-4
5	40	-42
H,L= 5-12		
0	67	60
1	0	1
2	0	0
3	0	20
4	37	-36
5	0	-8
H,L= 5-13		
1	0	11
2	37	35
H,L= 6 0		
0	175	138
1	78	-56
2	0	13
3	127	-107
4	79	-63
5	0	-18
6	67	-63
7	0	16
H,L= 6 1		
1	0	-2
2	154	-139
3	0	-5
4	100	-86
5	0	-9
6	56	61
7	0	1
H,L= 6 2		
0	128	-115
1	0	-10
2	0	-7
3	84	-63
4	58	52
5	39	25
6	56	64
7	38	33
H,L= 6 3		
1	76	-66
2	54	42
3	78	69
4	36	27
5	57	56
6	0	-20
H,L= 6 4		
0	0	7
1	49	41
2	44	37
3	67	54
4	37	-28
5	62	-55
6	0	12
7	46	-48
H,L= 6 5		
1	68	59
2	0	11
3	48	-35
4	0	2
5	60	-57
6	46	-46
H,L= 6 6		
0	67	61

TABLE 2. (continued)

K	FO	FC
1	50	-41
2	0	3
3	44	-25
4	57	-54
5	0	-6
H,L= 6 7		
1	0	2
2	70	-65
3	0	-15
4	40	-38
5	0	-1
H,L= 6 8		
0	52	-35
1	31	-23
2	0	-13
3	52	-54
4	48	48
5	0	14
H,L= 6 9		
1	41	-31
2	0	11
3	0	23
4	26	-21
5	28	32
H,L= 6 10		
0	35	-31
1	28	34
2	0	-5
3	0	15
H,L= 6 11		
1	0	5
2	0	20
H,L= 6 -1		
1	154	152
2	0	13
3	57	-37
4	0	-6
5	94	-79
6	46	-34
7	0	-19
8	37	-18
H,L= 6 -2		
0	88	97
1	54	46
2	58	49
3	146	149
4	0	3
5	0	-22
6	52	-41
7	53	-54
8	0	-14
H,L= 6 -3		
1	69	-63
2	94	94
3	48	37
4	59	54
5	71	61
6	39	-32
7	0	8
8	0	-17
H,L= 6 -4		
0	183	-187
1	78	-77
2	0	-4
3	55	-42
4	69	61
5	0	-1
6	63	62
7	39	38
H,L= 6 -5		
1	0	4
2	123	-126
3	0	5
4	81	-72
5	0	8
6	46	42
7	0	14
8	43	41
H,L= 6 -6		
0	131	121
1	34	-27
2	75	70
3	100	-96
4	68	-63
5	0	0
H,L= 6 -7		
1	122	130
2	34	22
3	0	-19
4	0	18
5	81	-84
H,L= 6 -8		
0	95	80
1	85	75
2	0	-15
3	99	96
4	0	-14
5	0	13
H,L= 6 -9		
1	77	-63
2	66	60
3	37	26
4	44	40
5	46	45
H,L= 6-10		
0	62	-52
1	53	-46
2	34	-24
3	0	-2
4	61	56
5	0	-11
H,L= 6-11		
1	0	4
2	62	-61
3	0	12

K	FO	FC
4	41	-33
5	0	6
H,L= 6-12		
0	41	39
1	45	-32
2	41	34
3	34	-24
4	41	-37
5	0	7
H,L= 6-13		
1	48	44
2	0	20
3	0	-23
4	0	14
5	34	-43
H,L= 7 0		
0	44	20
1	109	-84
2	0	-7
3	84	-63
4	0	10
5	0	0
6	0	-2
7	89	91
H,L= 7 1		
1	52	-30
2	61	-45
3	66	49
4	0	17
5	93	77
6	0	23
H,L= 7 2		
0	0	-9
1	66	44
2	0	-11
3	50	39
4	92	90
5	0	-22
6	0	3
7	35	-38
H,L= 7 3		
1	30	14
2	101	83
3	0	-12
4	0	8
5	0	2
6	51	-60
H,L= 7 4		
0	107	94
1	41	30
2	0	14
3	0	11
4	76	-72
5	0	14
6	39	-41
7	28	-40
H,L= 7 5		
1	83	71
2	34	-24
3	0	-9
4	0	-13
5	68	-73
6	32	26
H,L= 7 6		
0	0	20
1	66	-57
2	39	29
3	60	-55
4	0	-8
5	0	14
H,L= 7 7		
1	32	-24
2	53	-54
3	34	34
4	32	-28
5	29	30
H,L= 7 8		
0	49	-45
1	0	-10
2	0	-18
3	0	12
4	41	41
5	38	-40
H,L= 7 9		
1	0	-8
2	41	45
3	0	-12
4	0	19
H,L= 7 10		
0	0	46
1	19	18
2	0	-3
3	0	31
H,L= 7 -1		
1	88	75
2	104	-89
3	37	-34
4	35	-15
5	103	-83
6	39	37
7	0	1
8	34	31
H,L= 7 -2		
0	128	116
1	38	28
2	75	62
3	41	31
4	111	-96
5	0	-18
6	46	-42
7	39	-32
8	0	15
H,L= 7 -3		
1	83	86
2	110	112

K	FO	FC
3	0	7
4	40	30
5	50	-38
6	51	-50
7	0	-16
8	53	-52
H,L= 7 -4		
0	38	-31
1	95	101
2	0	7
3	75	68
4	70	60
5	45	34
6	0	14
7	49	-48
8	34	-38
H,L= 7 -5		
1	95	-92
2	0	7
3	33	28
4	35	20
5	89	87
H,L= 7 -6		
0	0	-3
1	75	-64
2	57	-49
3	83	-80
4	47	33
5	40	34
H,L= 7 -7		
1	69	63
2	72	-62
3	36	-30
4	53	-40
5	52	-50
H,L= 7 -8		
0	125	114
1	35	-16
2	53	42
3	0	22
4	66	-62
5	0	-14
H,L= 7 -9		
1	58	49
2	93	89
3	0	-4
4	58	54
5	45	-37
H,L= 7-10		
0	86	-71
1	76	64
2	0	5
3	79	78
4	0	14
5	0	16
H,L= 7-11		
1	76	-69
2	0	-1
3	0	14
4	0	7
5	47	45
H,L= 7-12		
0	0	-22
1	0	-12
2	0	-17
3	61	-62
4	0	10
H,L= 7-13		
1	33	27
2	46	-38
3	0	-7
H,L= 8 0		
0	120	-91
1	28	-12
2	61	37
3	35	-29
4	65	49
5	0	10
6	45	43
7	0	4
8	38	-45
H,L= 8 1		
1	80	-65
2	100	77
3	67	50
4	0	14
5	62	50
6	47	-46
H,L= 8 2		
0	0	13
1	59	50
2	0	-4
3	128	119
4	49	-36
5	0	-8
6	0	18
7	44	-49
H,L= 8 3		
1	92	76
2	61	45
3	38	-24
4	66	47
5	81	-73
H,L= 8 4		
0	153	129
1	33	-19
2	34	26
3	38	-27
4	48	-36
5	0	15
6	46	-50
7	28	40
H,L= 8 5		
1	46	37
2	78	-65

K	FO	FC
3	0	10
4	40	-34
5	0	2
H,L= 8 6		
0	67	-63
1	0	-5
2	0	-8
3	60	-58
4	52	55
5	0	3
H,L= 8 7		
1	51	-47
2	42	37
3	0	8
4	0	1
5	37	39
H,L= 8 8		
0	0	0
1	48	47
2	0	18
3	57	57
4	0	-15
H,L= 8 9		
1	48	55
2	0	28
H,L= 8 -1		
1	0	1
2	91	-74
3	0	11
4	36	-23
5	0	20
6	80	80
7	0	-2
8	33	41
H,L= 8 -2		
0	91	69
1	0	2
2	29	17
3	75	-52
4	67	-56
5	66	47
6	55	-43
7	52	52
H,L= 8 -3		
1	95	85
2	51	40
3	80	-64
4	51	36
5	93	-77
6	0	-6
7	0	-5
8	0	-22
H,L= 8 -4		
0	63	49
1	68	61
2	0	-14
3	99	96
4	0	-10
5	40	-32
6	38	-29
7	62	-63
H,L= 8 -5		
1	36	-31
2	80	78
3	41	28
4	57	46
5	52	38
6	51	-45
7	0	1
H,L= 8 -6		
0	113	-116
1	0	-17
2	0	-1
3	59	50
4	69	69
5	0	16
H,L= 8 -7		
1	58	-51
2	59	-55
3	0	7
4	0	-4
5	0	17
H,L= 8 -8		
0	0	7
1	31	-29
2	0	8
3	65	-57
4	70	-69
5	0	7
H,L= 8 -9		
1	50	45
2	0	9
3	38	-28
4	0	-15
5	58	-54
H,L= 8-10		
0	66	56
1	50	47
2	0	7
3	53	42
4	0	-19
5	0	4
H,L= 8-11		
1	0	-16
2	74	71
3	0	9
4	43	39
5	0	25
H,L= 8-12		
0	74	-65
1	0	-5
2	40	-35
3	0	27
4	45	48
5	0	12

K	FO	FC
H,L= 8-13		
1	42	-39
2	38	-40
3	0	-5
H,L= 9 0		
0	108	-77
1	98	90
2	82	-65
3	89	73
4	73	56
5	0	-4
6	46	37
7	43	-47
H,L= 9 1		
1	32	13
2	135	123
3	37	-20
4	91	82
5	0	-18
H,L= 9 2		
0	100	75
1	49	32
2	62	46
3	58	35
4	75	-67
5	44	33
6	37	-41
7	0	-3
H,L= 9 3		
1	87	72
2	52	-37
3	0	-11
4	36	-22
5	59	-57
6	0	22
H,L= 9 4		
0	32	-20
1	85	-77
2	33	12
3	59	-54
4	0	7
5	0	-2
H,L= 9 5		
1	80	-75
2	0	-9
3	0	23
4	0	-1
5	60	58
H,L= 9 6		
0	45	-47
1	34	25
2	34	-30
3	71	75
4	44	47
5	0	2
H,L= 9 7		
1	30	27
2	59	66
3	0	-1
4	36	37
H,L= 9 8		
0	68	75
1	21	23
H,L= 9 -1		
1	113	-108
2	49	-38
3	64	40
4	0	-10
5	93	84
6	0	-6
7	0	0
8	0	2
H,L= 9 -2		
0	41	9
1	86	-77
2	36	-32
3	76	-54
4	62	41
5	0	0
6	0	13
7	61	61
H,L= 9 -3		
1	54	45
2	63	-55
3	0	-11
4	0	-1
5	57	-46
6	52	50
7	0	-5
8	0	42
H,L= 9 -4		
0	89	65
1	0	-1
2	31	23
3	67	55
4	93	-91
5	0	4
6	47	-45
7	0	1
H,L= 9 -5		
1	0	-2
2	102	99
3	48	-38
4	49	37
5	40	-31
6	44	-41
7	0	18
H,L= 9 -6		
0	108	-102
1	67	67
2	0	-15
3	48	42
4	44	37
5	0	-9
H,L= 9 -7		

K	FO	FC
1	71	-63
2	0	6
3	37	31
4	0	-4
5	72	77
H,L= 9 -8		
0	32	-29
1	32	-24
2	39	-32
3	62	-59
4	48	47
5	38	34
H,L= 9 -9		
1	0	8
2	59	-54
3	37	-36
4	0	-14
5	0	-18
H,L= 9-10		
0	53	50
1	0	-10
2	0	-15
3	0	6
4	40	-38
5	0	-15
H,L= 9-11		
1	0	15
2	37	34
3	0	-5
4	0	12
5	29	-24
H,L= 9-12		
0	30	-22
1	0	24
2	0	9
3	40	41
4	0	10
5	23	-20
H,L= 9-13		
1	34	-40
H,L= 10 0		
0	67	49
1	46	32
2	0	1
3	109	103
4	37	-23
5	0	9
6	0	-17
7	34	-42
H,L= 10 1		
1	83	64
2	34	26
3	0	-20
4	0	6
5	63	-56
H,L= 10 2		
0	76	67
1	47	-36
2	0	-19
3	83	-80
4	35	-31
5	0	8
6	35	-23
H,L= 10 3		
1	59	-52
2	71	-71
3	0	-2
4	47	-40
5	31	27
6	22	38
H,L= 10 4		
0	123	-112
1	31	28
2	31	-25
3	0	1
4	49	57
5	27	29
H,L= 10 5		
1	41	-33
2	57	64
3	0	14
4	40	39
5	29	36
H,L= 10 6		
0	0	6
1	36	33
2	0	17
3	0	54
4	0	-14
H,L= 10 7		
1	36	41
2	0	9
3	34	-22
H,L= 10 -1		
1	87	-74
2	109	104
3	0	3
4	62	51
5	50	42
6	42	-36
7	0	15
H,L= 10 -2		
0	210	-200
1	0	-7
2	51	-34
3	0	-6
4	69	56
5	0	-12
6	68	74
7	0	3
H,L= 10 -3		
1	66	-60
2	113	-109
3	0	14
4	66	-54

K	FO	FC
5	56	46
6	34	36
7	0	14
H,L= 10 -4		
0	57	47
1	0	-13
2	38	28
3	102	-96
4	54	-40
5	0	4
6	0	-14
7	37	38
H,L= 10 -5		
1	78	70
2	0	-2
3	38	-33
4	0	2
5	71	-66
6	0	10
H,L= 10 -6		
0	49	44
1	65	59
2	33	-27
3	73	66
4	0	-24
5	0	4
H,L= 10 -7		
1	68	-63
2	62	68
3	0	2
4	37	30
5	48	41
H,L= 10 -8		
0	91	-97
1	33	-27
2	34	-25
3	0	2
4	63	69
5	36	-33
H,L= 10 -9		
1	38	-29
2	67	-67
3	0	27
4	40	-37
5	33	29
H,L= 10-10		
0	0	5
1	49	-44
2	0	25
3	49	-47
4	32	-32
5	0	8
H,L= 10-11		
1	40	33
2	0	1
3	0	-23
4	0	-11
5	33	-41
H,L= 10-12		
0	0	13
1	33	31
H,L= 11 0		
0	63	54
1	0	-7
2	39	36
3	0	-16
4	76	-73
5	0	-22
H,L= 11 1		
1	0	2
2	92	-86
3	35	-30
4	43	-43
5	31	-31
H,L= 11 2		
0	84	-85
1	71	-69
2	32	-29
3	39	-37
4	36	32
5	28	3
H,L= 11 3		
1	63	-55
2	0	7
3	0	21
4	0	5
5	54	54
H,L= 11 4		
0	28	-30
1	32	28
2	27	-19
3	43	45
4	39	46
5	0	-11
H,L= 11 5		
1	0	2
2	39	43
3	0	-18
4	0	11
H,L= 11 -1		
1	47	36
2	65	58
3	0	3
4	0	17
5	40	-37
6	40	-43
H,L= 11 -2		
0	0	-21
1	76	65
2	0	-19
3	69	48
4	36	21
5	0	7
6	30	27
H,L= 11 -3		

K	FO	FC
1	109	-109
2	0	18
3	0	31
4	0	7
5	82	81
6	0	2
H,L= 11 -4		
0	88	-63
1	78	-71
2	71	-57
3	87	-77
4	71	60
5	0	-5
6	0	30
H,L= 11 -5		
1	42	32
2	108	-108
3	0	-16
4	67	-64
5	36	-20
H,L= 11 -6		
0	99	92
1	47	-36
2	39	38
3	0	-8
4	56	-52
5	36	-32
H,L= 11 -7		
1	54	50
2	55	48
3	0	-8
4	35	32
5	53	-41
H,L= 11 -8		
0	60	-50
1	53	52
2	0	5
3	63	63
4	0	7
5	0	-3
H,L= 11 -9		
1	64	-68
2	0	6
3	0	19
4	0	-10
5	49	57
H,L= 11-10		
0	40	-37
1	31	-25
2	0	-14
3	68	-77
4	38	43
5	0	0
H,L= 11-11		
1	33	30
2	58	-64
3	0	-2
4	28	-31
5	20	-3
H,L= 11-12		
0	71	78
1	0	-10
H,L= 12 0		
0	31	23
1	41	-36
2	0	-16
3	78	-84
4	0	-12
5	32	32
H,L= 12 1		
1	39	-30
2	53	-55
3	0	16
4	33	-30
5	24	30
H,L= 12 2		
0	67	-71
1	0	2
2	0	6
3	29	-25
4	42	46
5	0	-11
H,L= 12 3		
1	30	-28
2	33	34
3	0	8
4	0	3
H,L= 12 4		
0	0	5
1	23	14
2	0	-4
3	36	46
4	0	-25
H,L= 12 -1		
1	62	61
2	0	-17
3	49	-41
4	32	-32
5	59	-57
6	0	-11
H,L= 12 -2		
0	75	74
1	0	15
2	0	4
3	35	29
4	0	-20
5	31	-29
6	33	-39
H,L= 12 -3		
1	0	0
2	54	48
3	0	18
4	34	24
5	0	25
H,L= 12 -4		

K	FO	FC
0	80	-72
1	0	4
2	0	4
3	36	30
4	56	52
5	0	-6
6	32	38
H,L= 12 -5		
1	68	-59
2	61	-60
3	36	30
4	0	-16
5	32	37
H,L= 12 -6		
0	0	7
1	46	-43
2	43	10
3	90	-100
4	39	-37
5	0	-3
H,L= 12 -7		
1	70	72
2	42	-33
3	0	-17
4	46	-41
5	49	-54
H,L= 12 -8		
0	82	88
1	48	38
2	32	27
3	0	18
4	31	-23
5	0	3
H,L= 12 -9		
1	30	13
2	56	61
3	0	5
4	37	36
5	0	8
H,L= 12-10		
0	53	-51
1	0	6
2	28	-24
3	29	31
4	47	47
5	0	3
H,L= 12-11		
1	37	-42
2	42	-41
3	0	14
4	0	-14
H,L= 12-12		
0	0	5
1	38	-46
2	22	17
3	37	-46
4	0	-9
H,L= 13 0		
0	0	-14
1	54	-56
2	0	4
3	40	-44
4	40	49
5	0	-7
H,L= 13 1		
1	43	-40
2	0	-12
3	0	20
H,L= 13 2		
0	0	-17
1	39	41
2	23	-17
3	25	33
H,L= 13 -1		
1	42	38
2	64	-62
3	0	2
4	0	-13
5	22	-26
H,L= 13 -2		
0	61	65
1	35	-25
2	35	31
3	0	-6
4	64	-74
5	0	-3
H,L= 13 -3		
1	44	41
2	50	47
3	0	-11
4	0	2
5	48	-56
H,L= 13 -4		
0	0	-7
1	40	43
2	0	17
3	33	36
4	0	6
5	0	-2
H,L= 13 -5		
1	31	-22
2	31	26
3	38	36
4	0	0
5	48	53
H,L= 13 -6		
0	31	-22
1	0	-17
2	0	-11
3	0	-32
4	48	48
5	26	24
H,L= 13 -7		
1	0	6
2	63	-69

K	FO	FC
3	0	-17
4	0	-10
5	0	-4
H,L= 13 -8		
0	68	72
1	29	-28
2	0	4
3	0	-13
4	37	-41
5	21	-18
H,L= 13 -9		
1	48	51
2	27	23
3	0	-2
4	0	13
5	26	-49
H,L= 13-10		
0	0	8
1	26	26
2	25	24
3	46	56
H,L= 13-11		
1	0	-26
2	31	35
3	0	19
H,L= 13-12		
0	45	-50
H,L= 14 0		
0	72	-81
1	0	9
2	0	-6
H,L= 14 2		
0	42	59
H,L= 14 -1		
1	0	-23
2	42	-48
3	0	26
4	0	-34
H,L= 14 -2		
0	44	46
1	0	-26
2	33	29
3	54	-68
4	0	-6
H,L= 14 -3		
1	65	73
2	0	-3
3	31	-33
4	0	3
H,L= 14 -4		
0	69	70
1	39	38
2	0	-8
3	42	44
4	27	-31
H,L= 14 -5		
1	0	-9
2	55	63
3	0	2
4	39	42
H,L= 14 -6		
0	32	-38
1	27	3
2	0	-13
3	27	33
4	41	44
H,L= 14 -7		
1	27	-28
2	26	-27
3	31	35
4	0	-10
H,L= 14 -8		
0	0	-3
1	30	-33
2	0	15
3	25	-32
4	0	-20
H,L= 14 -9		
1	34	32
2	0	-8
3	22	-29
H,L= 14-10		
0	36	35
1	31	34
H,L= 15 0		
0	16	-3
1	0	57
2	0	0
H,L= 15 -1		
1	37	-49
2	0	38
3	0	6
H,L= 15 -2		
0	44	-57
1	0	-20
2	0	-30
3	0	-19
H,L= 15 -3		
1	0	12
2	48	-67
3	0	1
H,L= 15 -4		
0	63	72
1	22	-31
2	28	29
3	0	-2
H,L= 15 -5		
1	40	40
2	44	59
3	45	-16
H,L= 15 -6		
0	27	-34
1	42	46
H,L= 15 -7		
1	40	-52
H,L= 15 -8		
0	41	-51
H,L= 15-10		
0	37	55

isotropic refinement for all the atoms except hydrogen, the R factor was reduced to 0.156 non-zero reflections. Anisotropic temperature factors for all atoms were introduced at this stage and the refinement was continued; four subsequent cycles of refinement gave $R=0.137$. The atomic scattering factors used in the refinement were taken from those of Hanson and his co-workers.[5]

The final positional and thermal parameters are given in Table 1. The observed and calculated structure factors are given in Table 2.

Result and Discussion

The Geometry around the Tin Atom. The molecular structure and the numbering system of $Me_2SnCl(dtc)$ are shown in Fig. 2. The bond distances and angles in the environment of the tin atom are listed in Table 3. As can be seen in Fig. 2 and Table 3, the configuration about the tin atom is a penta-coordinated distorted trigonal bipyramid. The four atoms, S(1), C(4), C(5), and Sn, lie on the same plane, the equatorial plane of the bipyramid. The Cl and S(2) are at the tops of the bipyramid; the Sn–Cl and the Sn–S(2) bonds cross the equatorial plane at angles of 81.8° and 72.7° respectively. The methyl groups attached to the tin atom are both in the equatorial positions. This configuration

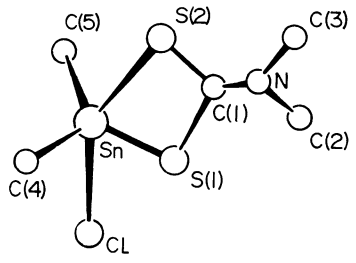

Fig. 2. The molecular structure and the numbering system of $Me_2SnCl(dtc)$.

Table 3. Geometry around the tin atom

(a) Bond distances and angles along with their estimated standard deviations in parentheses.

Bond distance (Å)		Bond angle (°)	
Sn-Cl	2.46 (1)	Cl-Sn-S(1)	86.4 (0.4)
Sn-S(1)	2.48 (1)	Cl-Sn-S(2)	154.5 (0.4)
Sn-S(2)	2.79 (1)	Cl-Sn-C(4)	99 (1)
Sn-C(4)	2.17 (5)	Cl-Sn-C(5)	98 (1)
Sn-C(5)	2.20 (5)	S(1)-Sn-S(2)	68.2 (0.3)
		S(1)-Sn-C(4)	113 (1)
		S(1)-Sn-C(5)	116 (1)
		S(2)-Sn-C(4)	91 (1)
		S(2)-Sn-C(5)	93 (1)
		C(4)-Sn-C(5)	128 (2)

b) The least-squares plane of four atoms, Sn, S(1), C(4), and C(5):

$-0.01339x - 0.52110y - 0.85339z + 2.15929\text{Å} = 0$,

Deviations from the least-squares plane(Å): Sn 0.15
S(1) −0.04
C(4) −0.05
C(5) −0.05

Angle between the least-squares plane and the Sn-Cl bond: 81.8°,

Angle between the least-squares plane and the Sn-S(2) bond: 72.7°.

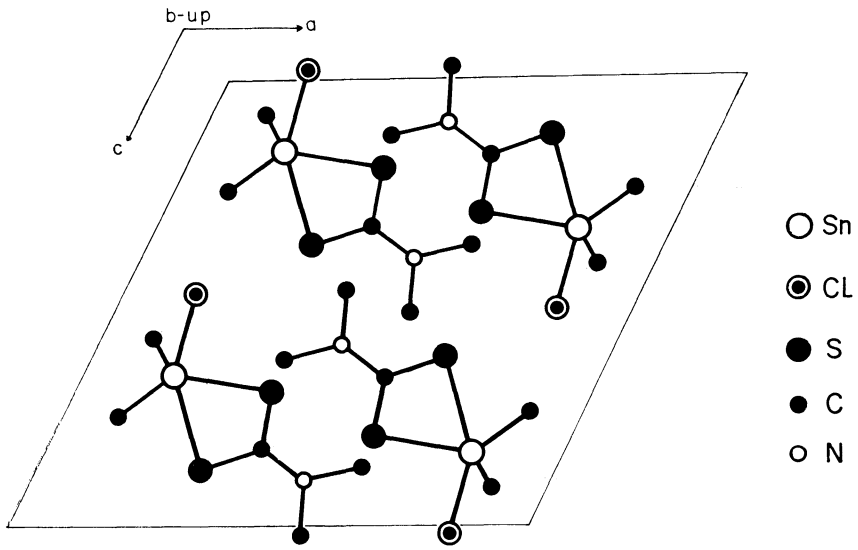

Fig. 3. The crystal structure of $Me_2SnCl(dtc)$ projected onto the (010) plane.

5) H. P. Hanson, F. Herman, J. D. Lea and S. S. Skillman, *Acta Crystallogr.*, **17**, 1040 (1964).

is in good agreement with the model (3) proposed in Fig. 1.

In tin compounds with coordination numbers greater than four, a qualitative MO approach to the bonding nature of the tin atom has been postulated in which no contribution of the 5*d*-orbital of a tin atom is considered.[6,7] In the case of the present complex, it may be assumed, in a way similar to that postulated by Schlemper,[3] that the bonding could also involve the sp^3 hybrid orbitals on the tin atom participating in normal covalent bonds with the two methyl groups and with the chlorine atom and in a three-centered bond with the ligand group. The M–Sn–C(4), M–Sn–C(5), and M–Sn–Cl angles, where M is the midpoint of the line connecting S(1) and S(2), are 104°, 107°, and 122° respectively. The C(4)–Sn–C(5) angle of 128(2°) is, however, considerably larger than the tetrahedral angle. Furthermore, as will be described later, the difference between the two Sn–S bond distances is significant (Table 3); it may be due to the difference in nature between the axial and equatorial bonds. From these facts and from the other angles around the tin atom listed in Table 3, it is better to consider that the configuration about the tin atom in the present complex is a distorted trigonal bipyramid similar to that of the $[(CH_3)_2SnCl_3]^-$ anion.[4]

The Sn–C bond distances, (2.17(5) and 2.20(5) Å), are in good agreement with the sum of the covalent radii of Sn and C, 2.17 Å. These observed values are, within the limits of experimental error, equal to those in $[(CH_3)_2SnCN]$,[8] $[CH_3SnH_3]$[9], and $[(CH_3)_2Sn(C_9H_6NO)_2]$;[3] in the first compound the tin atom takes a trigonal bipyramidal configuration, in the second, a tetrahedral one, and in the third, a hexa-coordination. On the other hand in $[(CH_3)_2SnF_2]$[10] a slightly shorter Sn–C distance (2.06 Å) is obtained.

The Sn–Cl distance, 2.46(1) Å, is slightly longer than the sum of the covalent radii, 2.39 Å. In the $[(CH_3)_2SnCl_3]^-$ ion,[3] the tin atom takes a penta-coordination, and the equatorial Sn–Cl bond distance, 2.32 Å, is shorter than the observed one, while the axial distance, 2.54 Å, is longer.

In the Sn–S distances, the equatorial one (Sn–S(1), 2.48(1) Å), is slightly longer than the sum of the covalent radii, 2.44 Å, but the axial one (Sn–S(2), 2.79(1) Å), is considerably longer. This may suggest that the Sn–S(2) is a weak coordination bond. Such a weak metal-sulfur bond as Sn–S(2) is also found in $[(C_6H_5)As(S_2CN(C_2H_5))_2]$[11] and in $[As(S_2CN(C_2H_5))_3]$.[12]

Table 4. Geometry of the ligand, *N,N*-dimethyldithiocarbamate group

a) Bond distances and angles along with their estimated standard deviations in parentheses.

Bond distance (Å)		Bond angle (°)	
S(1)–C(1)	1.68 (4)	Sn–S(1)–C(1)	91 (1)
S(2)–C(1)	1.74 (4)	Sn–S(2)–C(1)	80 (1)
C(1)–N	1.32 (5)	S(1)–C(1)–S(2)	120 (2)
N–C(2)	1.51 (6)	S(1)–C(1)–N	121 (3)
N–C(3)	1.57 (6)	S(2)–C(1)–N	119 (3)
		C(1)–N–C(2)	122 (3)
		C(1)–N–C(3)	124 (3)
		C(2)–N–C(3)	114 (3)

b) The lest-squares plane of the ligand $-0.27960x-0.85166y+0.4367z+0.5562=0$, Deviations from the least-squares plane (Å):

S(1)	0.02,
S(2)	−0.02,
N	0.00,
C(1)	0.02,
C(2)	−0.03,
C(3)	0.01,

Table 5. The short intermolecular atomic contacts less than 4.0 Å.

From the unit No. 1,			
To the unit No. 2			
Sn–Cl	3.90 Å	Cl–C(4)	3.69 Å
To the unit No. 3			
S(2)–C(3)	3.95		
To the unit No. 4			
N–S(1)	3.52	C(1)–S(1)	3.99
C(1)–C(2)	3.97	C(2)–Cl	3.90
C(2)–S(1)	3.96	C(3)–Cl	3.87
C(3)–S(1)	3.72	C(5)–C(2)	3.68
To the unit No. 5			
S(2)–Cl	3.76	C(3)–S(1)	3.94

Key			
No. 1	x,	y,	z
2	$-x$,	$-y$,	$-z$
3	$1-x$,	$1-y$,	$1-z$
4	$1-x$,	$1/2+y$,	$1/2-z$
5	x,	$1/2-y$,	$1/2+z$

The Geometry of the Ligand Group. The bond distances and angles in the ligand group, *N,N*-dimethyldithiocarbamate, are listed in Table 4(a). The S(1)–C(1) and S(2)–C(1) bond distances are

6) I. R. Beattie and G. P. McQuillan, *J. Chem. Soc.*, **1963**, 1519.

7) M. M. McGrady and R. S. Tobias, *J. Amer. Chem. Soc.*, **87**, 1909 (1965).

8) E. O. Schlemper and D. Britton, *Inorg. Chem.*, **5**, 507 (1966).

9) L. E. Sutton, Ed., "Tables of Interatomic Distances and Configuration in Molecules and Ions," The Chemical Society, London (1958).

10) E. O. Schlemper and W. C. Hamilton, *Inorg. Chem.*, **5**, 995 (1966).

11) R. Bally, *Acta Crystallogr.*, **23**, 295 (1967).

12) M. Colapietro, A. Domenicano, L. Scaramuzza and A. Vaciago, *Chem. Commun.*, **1968**, 302.

1.68(4) and 1.74(4) Å respectively, but the difference is not significant. The C(1)–N distance, 1.32(5) Å, is equal to those found *in other* dialkyldithiocarbamates;[11–19] this fact suggests that the carbon(sp^2)-nitrogen(sp^2) bond has a high double-bond character, as was to be expected on the basis of the IR studies. The N–C(2) and N–C(3) distances, 1.51(6) and 1.57(6) Å are equal; they are close to the N–C single bond distance (1.48 Å) within the limits of experimental error.

The ligand group is planar within ± 0.03 Å. Deviations from the least-squares plane are listed in Table 4(b).

Crystal Structure. The crystal structure projected along the *b* axis is shown in Fig. 3. The short intermolecular atomic contacts, less than 4.0 Å, are summarized in Table 5. None of them is short enough to suggest any significant deviation from the normal van der Waals interaction.

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16) M. Bonamico, G. Dessy, A. Mugnoli, A. Vaciago and L. Zambonelli, *ibid.*, **19**, 886 (1965).
17) M. Bonamico, G. Dessy, C. Mariani, A. Vaciago and L. Zambonelli, *ibid.*, **19**, 619 (1965).
18) K. Bowman and Z. Dori, *Chem. Commun.*, **1968**, 636.
19) A. Domenicano, L. Torelli, A. Vaciago and L. Zambonelli, *J. Chem. Soc., A*, **1968**, 1352.