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The Crystal and Molecular Structure of Trichloroethoxytin(IV) ethanolate dimer, $[SnCl_3(OC_2H_5),C_2H_5OH]_2$

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The crystals are monoclinic, a = 9.69 ± 0.03, b = 7.67 ± 0.02, c = 15.08 ± 0.03 Å, *β = 111.16 ± 0.2°, space group $P2_1/c$ with four (monomeric) formula units per unit cell. The calculated density (2.01 g cm^{-3}) for Z = 4 agrees well with the measured density (2.03 g cm^{-3}). The structure consists of discrete centrosymmetric dimeric molecules with ethoxy groups bridging between the two tin atoms. Each tin atom is approximately octahedrally coordinated by three mutually cis chlorine atoms (Sn–Cl 2.347(6), 2.351(7), 2.400(7)* Å*) and three oxygen atoms (Sn–O 2.08(2), 2.11(2), 2.18(2)* Å).

Introduction

Many reactions of tin(IV) halides with oxygen containing compounds have been investigated and whilst innumerable compounds have been reported in the literature there is a comparative dearth of sound structural data. The reaction between $SnCl_4$ and ethanol has yielded the adduct $SnCl_4$,2EtOH[1] and the alcoholysis product $SnCl_3$(OEt),EtOH[2,3] depending upon the experimental conditions. The latter compound, first prepared in 1884,[4] was found to be dimeric in boiling benzene[3] and associated (dimers?) by cryoscopy in the same solvent.[2] A chlorine bridged structure has been tentatively suggested for the dimer[2] although subsequent structure determinations have firmly established the occurence of bridging alkoxy groupings. Reports of a number of ethanol adducts of $SnCl_4$ occur in the literature but the trisethanol complex[5] may be erroneous[1] since it has the same m.pt. (192° C) as the compound $SnCl_3$(OEt),EtOH. The two dimensional X-ray structure of $SnCl_3$(OMe),MeOH shows[6] a dimeric unit isomorphous with the bromo compound and containing methoxy bridges. As part of a study on the reaction of tin(IV) halides with oxygen donors we undertook a three dimensional X-ray analysis of a molecule of this type to establish more precise molecular parameters, and we report now the structure of $[SnCl_3(OEt),EtOH]_2$.

Experimental

Preparation

Tin tetrachloride and ethanol, dried by refluxing over Mg, were distilled prior to use. In a drybox, ethanol (10 ml) was added slowly to $SnCl_4$ (10 ml) when a vigorous exothermic reaction took place and some white solid formed. Benzene (30 ml) was added and the mixture heated to completely dissolve the solid. Slow cooling deposited well formed colourless crystals of $SnCl_3$(OEt),EtOH (m.pt. 191–193° (uncorr). Literature m.pt. 191–193°[1]). Found: Cl, 33.36%. Calc. for $SnCl_3(OC_2H_5),C_2H_5OH$: Cl, 33.64%. Crystals were removed from the supernatant liquid and mounted for crystallographic examination in Lindemann glass capillaries which were sealed off.

Crystal data

Lattice parameters and diffraction symmetry were determined from Weissenberg and precession photographs at room temperature. The crystals are monoclinic, a = 9.69 ± 0.03, b = 7.67 ± 0.02, c = 15.08 ± 0.03 Å, β = 111.16 ± 0.2°, V = 1045.2 Å.[3] The systematic absences h0l for l odd and 0k0 for k odd uniquely determined the space group as $P2_1/c$ (No. 14). The calculated density ($C_4H_{11}Cl_3O_2Sn$, M.W. 316.18) of 2.01 g cm^{-3} for Z = 4, agrees well with the value of 2.03 g cm^{-3} obtained by flotation in ethylene dibromide/carbon tetrachloride mixtures. The linear absorption coefficient was calculated as μ(MoKα) 32.0 cm^{-1}.

A crystal of approximate dimensions 0.20 × 0.52 × 0.25 mm, mounted about the b axis was used to record multiple film equi-inclination Weissenberg photographs (h0l–h6l) using zirconium filtered MoKα radiation (0.7107 Å). Intensities were estimated visually by comparison with a calibrated wedge, and no spot shape correction was applied. 1159 reflections were measured from two octants of reciprocal space of which 946 were observed reflections, and 213 which were too weak to be measured were classed as "less thans". These were given an intensity of half the minimum observed value. Approximate level to level scale fac-

TABLE I. Atomic Positional and Thermal Parameters[a] with Standard Deviations in Parenthesis.

Atom	x/a	y/b	z/c	U(Å^2)
Sn	0.1455(2)	0.0515(2)	0.0996(1)	–
Cl(1)	0.8072(7)	0.4831(10)	0.2403(4)	–
Cl(2)	0.3864(6)	0.1412(11)	0.1180(5)	–
Cl(3)	0.0499(7)	0.3396(9)	0.1015(4)	–
O(1)	0.0641(14)	0.4398(23)	0.4498(9)	0.045(4)
O(2)	0.7924(18)	0.2856(25)	0.4209(11)	0.058(5)
C(1)	0.1341(23)	0.3500(34)	0.3936(14)	0.043(6)
C(2)	0.6574(28)	0.1903(40)	0.3653(17)	0.059(7)
C(3)	0.5830(38)	0.1343(56)	0.4359(24)	0.095(10)
C(4)	0.7739(30)	−0.0360(46)	0.1417(19)	0.071(7)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.043(1)	0.039(8)	0.037(1)	−0.001(1)	0.008(1)	−0.002(1)
Cl(1)	0.069(4)	0.064(10)	0.041(3)	−0.001(3)	0.010(3)	−0.005(3)
Cl(2)	0.047(3)	0.077(10)	0.069(4)	−0.016(3)	0.010(3)	−0.004(4)
Cl(3)	0.065(4)	0.041(10)	0.060(3)	0.002(3)	0.009(3)	−0.011(3)

[a] The anisotropic temperature factor is of the form $T = \exp\{-2\pi^2(U_{11}h^2(a^*)^2 + U_{22}k^2(b^*)^2 + U_{33}l^2(c^*)^2 + 2U_{12}Hka^*b^*\cos\gamma^* + 2U_{13}hla^*c^*\cos\beta^* + 2U_{23}klb^*c^*\cos\alpha^*)\}$.

tors were obtained intially and treated as variables in the refinement. The crystal showed no evidence of deterioration in the X-ray beam in the period of the experiment. The data were corrected for Lorentz and polarisation factors but no absorption or extinction correction was applied ($0.30 < \mu R < 1.00$). Scattering factors for neutral atoms were taken from International Tables[7] and anomalous dispersion corrections used for Sn and Cl.[7]

Structure Solution

Conventional heavy atom procedures were used to find the tin atom position from the unsharpened three dimensional Patterson function. The tin atom occupies a 4-fold general position and an electron density synthesis phased on this atom located the three chlorine atoms which were subsequently introduced into the model. Electron density syntheses and least squares techniques located the remaining two oxygen atoms and four carbon atom positions demanded by the formula. Full matrix least squares refinement of the atom positional and isotropic thermal parameters and scale factors (unit weights) reduced R_1 to 9.9%. An empirical weighting scheme was derived from the plot of $|\overline{\Delta F}|$ versus $\overline{F}_0$ for various ranges of F_0. (The weight(w) = $1/(A+BF_0)$ where $A = 2.35$ and $B = 0.044$. w(less than) = 0.594 w (observed)). The resulting $\Sigma w\Delta^2$ values showed an acceptable dependence on F_0 and $\mathrm{Sin}\Theta/\lambda$. The introduction of anisotropic temperature factors for the tin and chlorine atoms into the least squares refinement (67 parameters, calculated weights, positional parameters, scale factors, isotropic O and C atoms and anisotropic Sn and Cl thermal parameters) reduced R_1 to 7.9% (excluding less thans) with no unreasonable temperature factors. A difference electron density synthesis phased on the final parameters showed no anomalies except for some small regions very close to the tin atom. At this stage refinement was terminated. In Table I we detail the final structure parameters and the standard deviations derived from the least squares matrix, and in Table II are presented our observed and calculated structure factors.

All calculations were performed on the ICL 1906A computer, Harwell, England using the X-ray system of crystallographic programs devised by J.M. Stewart.

Description of the Structure and Discussion

The structure which is shown in Figures 1 and 2 consists of discrete centrosymmetric dimeric mole-

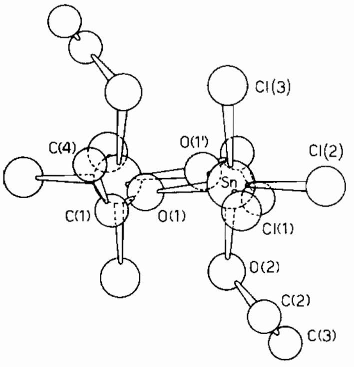

Figure 1. An isolated dimeric molecule $[SnCl_3(OEt),EtOH]_2$ looking in the positive z direction.

TABLE II. Observed and Calculated Structure Factors (× 10)

H,0,0		
3	1486	1389
4	1467	1407
5	546	487
6	517	505
7	382	369
8	122*	163
9	317	341
10	290	308
11	262	259
H,0,2		
-9	338	330
-8	776	736
-7	310	296
-6	171	183
-5	1312	1249
-4	1043	937
-3	1273	1286
3	1076	1112
4	88*	56
5	665	635
6	108*	145
7	117*	163
8	428	411
9	428	465
10	215	176
H,0,4		
-11	251	223
-10	478	427
-9	373	487
-8	117*	129
-7	514	446
-6	330	472
-5	311	474
-4	579	537
-3	650	627
-2	734	771
-1	575	588
0	1932	2199
1	1506	1705
2	840	855
3	88*	139
4	1675	1492
5	483	481
6	204	122
7	496	501
8	609	587
9	143*	20
10	224	199
11	238	232
H,0,6		
-12	224	220
-11	249	278
-10	384	325
-9	126*	8
-8	512	441
-7	569	513
-6	582	571
-5	298	265
-4	908	853
-3	436	396
-2	315	272
-1	1939	2177
0	2006	2148
1	85*	96
2	825	798
3	1505	1546
4	554	530
5	526	521
6	328	317
7	272	245
8	208	184
9	282	301
H,0,8		
-9	533	512
-8	342	325
-7	112*	25
-6	553	532
-5	774	751
-4	229	243
-3	993	953
-2	1328	1386
-1	836	817
0	886	864
1	926	994
2	701	680
3	268	263
4	451	466
5	183	196
6	133*	51
7	142*	110
8	364	362
H,0,10		
-10	468	401
-9	192	139
-8	479	422
-7	557	533
-6	511	443
-5	285	255
-4	583	560
-3	346	360
-2	328	323
-1	689	669
0	851	843
1	613	641
2	306	298
3	682	605
4	665	659
5	136*	97
6	249	201
7	434	413
H,0,12		
-10	163*	45
-9	305	274
-8	315	313
-7	280	276
-6	121*	105
-5	394	348
-4	347	290
-3	114*	120
-2	567	552
-1	1014	952
0	442	242
1	384	349
2	711	770
3	494	546
4	205	155
5	300	276
H,0,14		
-10	258	234
-9	408	339
-8	138*	56
-7	195	228
-6	517	471
-5	127*	142
-4	444	421
-3	326	567
-2	447	459
-1	188	223
0	817	586
1	456	458
2	286	260
3	146*	167
4	423	242
H,0,16		
-8	253	282
-7	247	230
-6	140*	42
-5	439	273
-4	401	249
-3	137*	123
-2	139*	93
-1	266	336
0	472	244
H,1,0		
3	908	934
4	428	200
5	184	194
6	99*	6
7	108*	39
8	340	327
9	420	216
H,1,1		
-11	411	191
-10	197	232
-9	125*	23
-8	624	591
-7	394	566
-6	400	201
-5	872	870
-4	1716	1888
-3	982	1008
2	1111	1286
3	1126	1175
4	120	137
5	736	726
6	546	548
7	426	425
8	120*	25
9	293	289
10	440	199
H,1,2		
-9	302	313
-8	116*	47
-7	105*	116
-6	96*	77
-5	149	163
-4	621	594
-3	113	167
2	735	697
3	490	269
4	312	278
5	95*	9
6	104*	27
7	166	166
8	180	180
9	193	155
H,1,3		
-10	192	143
-9	360	513
-8	503	282
-7	475	463
-6	902	898
-5	1480	1294
-4	173	137
-3	895	897
1	480	481
2	380	331
3	80*	64
4	819	839
5	903	914
6	550	521
7	117*	64
8	542	573
9	563	323
H,1,4		
-8	423	367
-7	104*	68
-6	195	188
-5	350	309
-4	536	306
-3	825	719
-2	621	594
-1	901	875
1	387	332
2	236	232
3	483	493
H,1,5		
-11	241	227
-10	377	296
-9	121*	141
-8	542	488
-7	362	347
-6	544	537
-5	199	206
-4	816	771
-3	755	796
-2	1051	1035
-1	196	219
0	1631	1580
1	966	921
2	301	254
3	1349	1307
4	1004	1407
5	107*	40
6	527	492
7	634	615
8	195	213
H,1,6		
-9	386	383
-8	166	173
-7	103*	17
-6	97*	53
-5	460	406
-4	674	685
-3	526	478
-2	130	123
-1	75*	82
0	606	639
1	624	585
2	505	496
3	388	371
H,1,7		
-9	212	224
-8	463	484
-7	308	272
-6	99*	98
-5	1357	1173
-4	1116	1075
-3	170	160
-2	1085	1060
-1	1637	1539
0	84*	113
1	841	847
2	865	867
3	480	437
4	396	381
5	471	492
6	334	335
H,1,8		
-8	200	156
-7	108*	9
-6	177	202
-5	96*	88
-4	371	442
-3	237	206
-2	167	179
-1	390	386
0	576	540
1	95*	52
2	100*	106
3	218	208
4	186	109
H,1,9		
-10	300	285
-9	408	369
-8	226	192
-7	762	633
-6	823	755
-5	405	356
-4	696	690
-3	771	780
-2	673	644
-1	94*	161
0	549	567
1	368	374
2	204	204
3	356	321
4	570	604
5	337	325
6	196	50
7	344	308
8	260	314
H,1,10		
-9	219	218
-8	176	186
-7	114*	114
-6	108*	40
-5	390	419
-4	101*	15
-3	287	304
-2	339	296
-1	405	422
0	150	167
1	279	256
2	253	265
3	241	238
H,1,11		
-8	421	406
-7	372	336
-6	233	207
-5	372	330
-4	841	634
-3	452	438
-2	214	178
-1	310	530
0	524	559
1	113*	79
2	456	408
3	701	726
4	190	255
5	237	224
6	349	396
7	263	278
H,1,12		
-1	232	208
0	355	375
H,1,13		
-9	276	272
-8	265	196
-7	125*	5
-6	384	347
-5	566	565
-4	116*	147
-3	378	341
-2	860	679
-1	405	444
0	334	324
1	540	565
2	376	387
3	155*	71
4	377	370
5	256	240
H,1,14		
-2	179	158
-1	343	320
0	127*	107
H,1,15		
-7	388	372
-6	318	304
-5	128*	178
-4	515	514
-3	415	392
-2	128*	104
-1	295	255
0	275	280
H,1,16		
8	139*	134
H,1,17		
-1	246	238
0	213	132
H,2,0		
3	1369	1397
4	710	679
5	89*	7
6	493	469
7	481	504
8	118*	111
9	186	126
10	200	198
H,2,1		
-9	278	284
-8	116*	24
-7	497	457
-6	502	482
-5	736	796
-4	184	171
-3	773	772
3	362	307
4	1062	1074
5	665	626
6	101*	121
7	111*	91
8	451	457
H,2,2		
-9	253	255
-8	563	588
-7	251	249
-6	750	735
-5	1195	1271
-4	835	868
-3	338	455
2	684	601
3	180	229
4	85*	161
5	500	493
6	849	677
7	230	216
8	249	222
9	294	310
10	245	192
H,2,3		
-8	403	409
-7	349	366
-6	269	289
-5	205	227
-4	1120	1213
-3	621	579
1	1008	819
2	391	350
3	720	678
4	370	531
5	461	480
6	360	350
7	463	474
8	236	177
H,2,4		
-10	317	289
-9	349	269
-8	113*	67
-7	375	395
-6	632	662
-5	362	318
-4	78*	153
-3	707	732
-2	387	395
-1	221	143
0	177	141
1	789	722
2	358	384
3	472	485
4	864	807
5	756	733
6	111*	85
7	477	477
8	411	389
H,2,5		
-9	376	351
-8	349	332
-7	104*	71
-6	405	436
-5	964	1029
-4	558	486
-3	292	263
-2	385	302
-1	813	787
0	334	319
1	797	734
2	302	277
3	429	406
4	532	565
5	601	609
6	387	334
7	182	233
H,2,6		
-8	379	332
-7	491	499
-6	87*	172
-5	449	430
-4	997	1001
-3	591	652
-2	661	442
-1	897	958
0	784	837
1	82*	18
2	984	947
3	834	850
4	248	203
5	316	318
6	532	541
7	262	230
H,2,7		
-9	179	184
-8	198	169
-7	259	284
-6	465	470
-5	136	148
-4	536	582
-3	467	502
-2	539	531
-1	81*	53
0	536	522
1	89*	29
2	94*	78
3	313	303
4	601	591
5	116*	82
6	184*	7
7	230	258
8	245	224
H,2,8		
-9	296	309
-8	303	330
-7	203	144
-6	678	713
-5	794	852
-4	185	175
-3	971	920
-2	1131	1050
-1	312	306
0	359	358
1	581	606
2	260	239
3	126	174
4	213	241
5	290	322
H,2,9		
-8	283	275
-7	111*	114
-6	105*	95
-5	696	708
-4	639	636
-3	334	328
-2	93*	48
-1	623	629
0	181	184
1	283	226
2	301	315
3	376	433
4	119*	146
5	330	339
6	274	276
7	246	224
H,2,10		
-8	288	282
-7	452	505
-6	260	291
-5	152	163
-4	531	563
-3	463	485
-2	99*	117
-1	100*	81
0	247	290
1	331	291
2	164	75
3	334	361
4	385	418
5	192	158
6	241	247
7	254	312
H,2,11		
-9	265	251
-8	123*	39
-7	117*	115
-6	446	493
-5	541	533
-4	106*	4
-3	251	226
-2	460	491
-1	220	165
0	286	282
1	113*	144
2	118*	145
3	123*	140
4	368	368
H,2,12		
-5	415	414
-4	521	542
-3	110*	109
-2	438	439
-1	621	608
0	256	232
1	368	390
2	537	544
3	265	219
4	135*	131
5	345	319
H,2,13		
-5	239	225
-4	329	313
-3	237	230
-2	116*	104
-1	285	281
0	210	166
1	125*	17
2	130*	109
3	299	310
H,2,14		
-7	264	216
-6	426	412
-5	215	224
-4	295	271
-3	576	530
-2	350	329
-1	124*	80
0	360	365
1	314	262
H,2,15		
-5	368	367
-4	186	180
-3	127*	14
-2	311	273
-1	316	281
0	135*	7
H,2,16		
-4	322	294
-3	133*	133
-2	134*	64
-1	236	178
0	139*	187
H,3,0		
3	554	571
4	329	315
5	548	634
6	239	293
7	101*	9
8	309	355
9	242	291
10	186	61
H,3,1		
-7	467	490
-6	90*	69
-5	409	449
-4	338	360
-3	106	136
2	729	694
3	517	410
4	76*	8
5	85*	67
6	287	300
7	103*	43
8	229	178
9	120*	146
10	264	252
H,3,2		
-10	214	188
-9	235	208
-8	155	133
-7	389	395
-6	447	456
-5	247	229
-4	654	672
-3	806	755
2	336	222
3	705	609
4	945	855
5	88*	125
6	299	335
7	450	475
8	277	289
H,3,3		
-10	251	233
-9	276	276
-8	324	340
-7	97*	52
-6	544	620
-5	194	163
-4	146	190
-3	760	708
-2	714	827
1	623	471
2	781	651
3	417	380
4	202	209
5	334	363
6	261	292
7	168	186
8	240	233
9	257	259
H,3,4		
-8	413	669
-7	298	310
-6	88*	69
-5	597	604
-4	790	872
-3	325	300
-2	389	392
0	635	579
1	697	605
2	1089	931
3	864	772
4	87*	91
5	534	523
6	413	414
7	271	231
H,3,5		
-8	181	84
-7	278	301
-6	89*	148
-5	82*	98
-4	143	142
-3	323	377
-2	66*	58
-1	563	300
0	864	776
1	1101	991
2	77*	13
3	470	455
4	433	424
5	204	146
6	331	349
7	200	188
H,3,6		
-9	384	400
-8	182	190
-7	200	208
-6	406	449
-5	468	470
-4	219	268
-3	569	610
-2	765	724
-1	328	338
0	664	690
1	835	814
2	686	671
3	89*	32
4	636	572
5	413	396
H,3,7		
-8	258	310
-7	391	431
-6	135	203
-5	328	337
-4	383	371
-3	261	260
-2	1397	1292
-1	701	710
0	114	117
1	545	540
2	616	695
H,3,8		
-8	261	279
-7	263	256
-6	164	143
-5	276	231
-4	666	644
-3	316	310
-2	197	221
-1	756	664
0	919	880
1	376	352
2	191	138
3	656	631
4	301	310
5	210	135
6	264	292
7	261	254
H,3,9		
-8	160	190
-7	296	288
-6	356	353
-5	93*	88
-4	183	169
-3	464	521
-2	150	140
-1	332	303
0	215	218
1	407	461
2	202	211
3	104*	70
4	111*	31
5	240	201
H,3,10		
-9	242	281
-8	271	301
-7	100*	30
-6	290	300
-5	544	600
-4	319	324
-3	92*	137
-2	565	568
-1	816	634
0	96*	6
1	392	396
2	450	518
3	224	208
4	280	296
5	296	323
H,3,11		
-2	275	327
-1	330	355
0	369	402
1	215	172
2	261	316
3	254	305
H,3,12		
-4	291	294
-3	342	373
-2	245	267
-1	214	197
0	422	459
1	341	320
2	115*	96
3	246	256
4	258	286
H,3,13		
-3	305	316
-2	470	489
-1	110*	155
0	112*	149
1	458	465
2	292	278
H,3,14		
-2	197	201
-1	385	407
0	286	271
1	122*	18
2	258	248
3	268	287
H,3,15		
-2	174	163
-1	209	217
0	181	171
H,3,16		
-3	255	223
-2	357	319
H,4,0		
3	386	642
4	77*	60
5	87*	24
6	275	286
H,4,1		
-9	296	290
-8	196	200
-7	213	209
-6	377	444
-5	207	168
-4	130	155
-3	775	878
3	120	117
4	509	539
5	455	435
6	99*	18
7	413	480
8	337	386
H,4,2		
-7	178	185
-6	291	347
-5	400	471
-4	231	227
-3	131	130
2	498	390
3	296	244
4	85*	113
5	93*	143
6	400	314
H,4,3		
-8	291	264
-7	445	553
-6	264	320
-5	145	134
-4	896	753
-3	855	788
0	1163	1209
1	926	878
2	831	816
3	1110	923
4	415	359
5	96*	81
6	532	506
7	324	381
H,4,4		
-6	225	214
-5	84*	38
-4	218	222
-3	68*	21
-2	348	358
-1	59*	131
0	406	324
1	267	247
2	182	141
3	306	287
4	223	177
5	312	369
H,4,5		
-9	312	345
-8	438	486
-7	102*	164
-6	266	295
-5	408	441
-4	355	321
-3	406	418
-2	1063	965
-1	618	580
0	69*	48
1	1054	890
2	1270	1081
3	297	278
4	234	197
5	386	394
6	296	297
H,4,6		
-4	198	213
-3	484	503
-2	73*	13
-1	248	197
0	184	190
1	80*	30
2	376	368
3	268	244
4	101*	50
5	264	204
6	240	294
H,4,7		
-10	261	295
-9	245	242
-8	112*	34
-7	324	376
-6	276	319
-5	91*	31
-4	457	460
-3	758	769
-2	226	260
-1	406	405
0	906	893
1	1043	1002
2	265	267
3	379	358
4	426	456
5	323	299
6	178	169
7	314	334
H,4,8		
-6	286	339
-5	228	239
-4	183	204
-3	210	197
-2	325	324
-1	86*	33
0	88*	63
1	225	193
2	98*	9
3	253	212
H,4,9		
-8	358	354
-7	309	271
-6	103*	32
-5	329	325
-4	504	545
-3	222	206
-2	432	408
-1	724	740
0	629	659
1	99*	55
2	584	642
3	418	458
4	116*	80
5	252	251
6	317	311
H,4,10		
0	101*	92
H,4,11		
-9	306	299
-8	208	195
-7	116*	146
-6	370	384
-5	357	355
-4	104*	44
-3	411	500
-2	369	426
-1	104*	43
0	362	406
1	589	625
2	330	305
3	121*	80
4	260	255
5	273	270
H,4,12		
-4	311	263
-3	108*	134
-2	108*	102
-1	160	148
0	112*	150
H,4,13		
-4	476	309
-3	196	198
-2	114*	105
-1	400	358
0	475	489
1	450	248
2	126*	138
3	270	290
4	482	249
H,4,15		
-2	329	312
-1	334	300
0	130*	63
1	431	243
2	482	289
H,5,0		
3	72*	127
4	293	344
5	492	602
6	516	574
7	115*	42
8	215	230
9	196	235
H,5,1		
-4	141	90
-3	400	237
2	457	250
3	75*	69
4	299	232
H,5,2		
-7	518	555
-6	557	597
-5	91*	18
-4	394	445
-3	876	1027
-2	665	696
2	69*	66
3	1092	801
4	869	753
5	416	390
6	349	340
7	527	562
8	425	255
H,5,3		
-5	91*	90
-4	81*	22
-3	71*	12
1	187	146
2	75*	91
3	85*	63
4	95*	96
H,5,4		
-9	423	166
-8	548	556
-7	455	480
-6	101*	160
-5	628	626
-4	793	872
-3	570	629
-2	413	441
-1	615	587
1	423	323
2	1110	855
3	524	587
4	99*	52
5	429	411
6	579	570
7	420	211
H,5,5		
-2	197	199
-1	468	271
0	74*	44
1	430	206
H,5,6		
-7	319	320
-6	637	698
-5	329	315
-4	88*	38
-3	875	860
-2	947	593
-1	79*	52
0	323	250
1	795	601
2	499	268
3	491	268
4	481	454
5	579	555
H,5,7		
0	89*	3
1	94*	127
2	146	25
3	186	203
H,5,8		
-8	412	229
-7	397	463
-6	108*	127
H,5,8		
-5	252	264
-4	563	598
-3	762	799
-2	92*	105
-1	321	340
0	557	527
1	347	311
2	367	389
3	601	480
4	385	326
5	128*	36
6	336	379
7	296	259
H,5,9		
0	102*	150
H,5,10		
-8	308	266
-7	121*	41
-6	431	418
-5	486	521
-4	443	464
-3	105*	80
-2	460	511
-1	309	289
0	109*	41
1	397	393
2	519	368
3	125*	33
4	192	260
5	398	389
H,5,11		
0	115*	69
H,5,12		
-7	372	379
-6	359	350
-5	120*	78
-4	285	261
-3	476	526
-2	117*	196
-1	119*	134
0	295	308
1	257	274
2	131*	104
3	279	262
4	293	286
H,5,14		
-5	225	244
-4	369	336
-1	192	233
0	275	227
H,5,16		
-3	263	250
-2	290	275
H,6,0		
3	249	250
4	158	141
5	103*	162
6	114*	73
7	256	205
H,6,1		
-6	385	444
-5	101*	165
-4	182	199
-3	374	442
3	82*	69
4	392	346
5	521	485
6	117*	42
7	310	321
8	239	248
H,6,2		
-6	191	215
-5	204	226
-4	292	333
-3	240	490
2	371	377
3	87*	67
4	283	417
5	350	300
6	296	311
H,6,3		
-7	369	402
-6	266	268
-5	267	270
-4	460	524
-3	503	607
1	315	310
2	449	379
3	602	516
4	362	296
5	114*	29
6	427	409
7	233	244
H,6,4		
-6	295	299
-5	242	234
-4	90*	68
-3	329	325
-2	325	317
-1	70*	20
0	74*	25
1	110	101
2	89*	135
3	401	357
4	188	186
5	173	154
H,6,5		
-9	204	215
-8	225	293
-7	176	140
-6	322	362
-5	413	425
-4	161	156
-3	247	265
-2	650	664
-1	319	322
0	81*	109
1	539	444
2	637	515
3	104*	108
4	114*	114
5	358	328
6	230	213
H,6,6		
-5	180	190
-4	220	233
-3	174	153
-2	87*	86
-1	87*	5
0	89*	27
1	139	12
2	210	187
H,6,7		
-7	298	306
-6	308	307
-5	107*	69
-4	347	331
-3	530	549
-2	252	221
-1	275	279
0	482	448
1	334	477
2	109*	110
3	802	212
4	306	319
5	196	217
H,6,8		
-5	163	173
-4	217	197
-3	102*	18
-2	176	191
-1	249	250
0	216	182
H,6,9		
-5	284	290
-4	582	400
-3	188	197
-2	312	322
-1	479	490
0	354	356
1	116*	55
2	355	383
3	265	258
H,6,10		
-3	332	295
-2	116*	137
-1	116*	7
0	119*	71
H,6,11		
-6	316	327
-5	257	230
-4	122*	34
-3	415	430
-2	351	368
-1	122*	7
0	442	239
1	319	368
H,6,13		
-4	432	239
-3	273	213
-2	136*	79
-1	279	233
0	485	286

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* experimentally unobserved reflections.

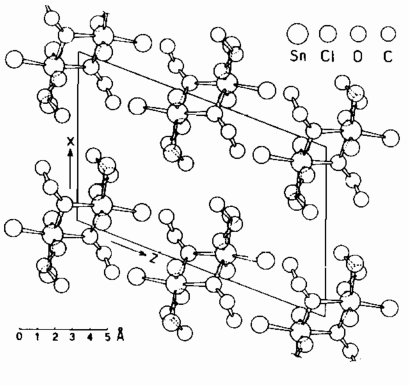

Figure 2. Projection of the unit cell and surroundings onto the (010) plane showing the molecular packing arrangement.

cules. The tin atoms are linked through bridging ethoxy groups and each tin atom is six coordinate (3 mutually *cis* Sn–Cl bonds and 3 Sn–O bonds) in an approximately octahedral arrangement. Pertinent intramolecular distances and angles are listed in Table III.

TABLE III. Intramolecular Distances (Å) and Angles (deg.) with Standard Deviations in Parenthesis.[a]

Sn–Cl(1)	2.347(6)	Cl(1)–Sn–Cl(2)	97.3(2)
Sn–Cl(2)	2.351(7)	Cl(1)–Sn–Cl(3)	97.3(2)
Sn–Cl(3)	2.400(7)	Cl(2)–Sn–Cl(3)	95.7(3)
Sn–O(1)	2.08(1)	Cl(1)–Sn–O(1)	94.6(4)
Sn–O(2)	2.18(2)	Cl(1)–Sn–O(1′)	165.3(5)
Sn–O(1′)	2.11(1)	Cl(1)–Sn–O(2)	88.6(5)
O(1)–C(1)	1.44(3)	Cl(2)–Sn–O(1)	164.2(5)
O(2)–C(2)	1.47(3)	Cl(2)–Sn–O(1′)	95.1(4)
C(1)–C(4)	1.48(4)	Cl(2)–Sn–O(2)	88.7(5)
C(2)–C(3)	1.55(5)	Cl(3)–Sn–O(1)	93.0(5)
Sn–Sn′	3.390(2)	Cl(3)–Sn–O(1′)	89.2(5)
O(1)–O(1′)	2.46(2)	Cl(3)–Sn–O(2)	172.1(4)
O(1)–Sn–O(1′)		71.9(6)	
O(1)–Sn–O(2)		81.2(7)	
O(1′)–Sn–O(2)		83.9(6)	
Sn–O(1)–Sn′		108.1(7)	
Sn–O(1)–C(1)		125.0(1.1)	
Sn–O(2)–C(2)		128.2(1.4)	
Sn–O(1′)–C(1′)		126.4(1.0)	
O(1)–C(1)–C(4)		113.8(2.3)	
O(2)–C(2)–C(3)		106.6(2.1)	

[a] Primed(′) atoms refer to the centrosymmetrically related atom at $\bar{x}, \bar{y}, \bar{z}$.

Other compounds with bridging ethoxy groups include $TiCl_2(OEt)_2$[8] and $SbCl_4(OEt)$[9] both of which are dimeric molecules. The tin–tin distance (3.390(2) Å) in the present compound may be compared with the Ti–Ti distance (3.30 Å) and Sb–Sb distance (3.50 Å) in the above compounds and the obtuse Sn–O(1)–Sn′ angle (108.1°) confirms the view that metal–metal bonding is unimportant in these structures. In general the bond lengths and angles are as expected. The short nonbonded intermolecular chlorine–chlorine distances (shortest 3.77 Å) are comparable with the intramolecular chlorine–chlorine distances of adjacent chlorine atoms (3.52–3.56 Å) indicating that the origin of the observed distortions from the 90° angles of a regular octahedron is the steric requirements of the ligands. There is clearly the possibility of O–H.....O hydrogen bonding between the oxygen atoms of the terminal and bridging OC_2H_5 groups. Since no hydrogen atoms were located in the structure, the exact nature of any hydrogen bonding is not established (O(1)–O(2) 2.77(2), O(1′)–O(2) 2.87(2), O(1)–O(1′) 2.46(2) Å).

Recently compounds with the composition $SnCl_3$ (OEt), L have been reported[10] for a variety of monodentate ligands (L). The present structure supports the proposed dimeric structure with bridging alkoxy groups.

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