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Hydrogen Bonds in Molecular Complexes: Crystal Structure of the Adduct (1:4) of Tin(IV) Chloride with Cyclohexanol

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The mononuclear complex $SnCl_4 \cdot 4C_6H_{11}OH$ *has been prepared by reaction of solutions of* $SnCl_4$ *and cyclohexanol. The structure has been solved by the heavy atom method and refined to a conventional R-factor of 0.0338, using 5697 reflections with* $F_{obs} > 10\sigma(F)_{obs}$. *The crystals are triclinic, with* $a = 12.693(2)$, $b = 9.857(3)$, $c = 6.5147(6)$ Å, $\alpha = 100.290(1)$, $\beta = 92.692(9)$, $\gamma = 105.907(14)^\circ$, $Z = 1$, $d_{obs} = 1.46(5)$ g cm^{-3}, $d_{calc} = 1.430$ g cm^{-3}, *centrosymmetric space group* $P\bar{1}$. *The centre of symmetry is at the tin atom site. The tin atom is octahedrally coordinated by four chlorine atoms in a plane (containing the tin atoms) and two oxygen atoms in* trans *positions* ($Sn-Cl(1) = 2.367(1)$, $Sn-Cl(2) = 2.387(1)$, $Sn-O(1) = 2.137(2)$ Å, $Cl(1)-Sn-Cl(2) = 89.80(5)$, $Cl(1)-Sn-O(1) = 89.20(5)$, $Cl(2)-Sn-O(1) = 90.1(1)^\circ$). *The coordination symmetry is close to* D_{4h}. *The structure consists of an adduct* $SnCl_4 \cdot 2C_6H_{11}OH$ *with two other cyclohexanol molecules linked by hydrogen bonds. Furthermore a second type of hydrogen binding is displayed by the structure. These* $O-H \cdots Cl$ *bonds hold the* $SnCl_4 \cdot 4C_6H_{11}OH$ *molecules together. We have studied both types of hydrogen bonds by infrared spectrometry.*

Introduction

Many reactions of tin(IV) halides with compounds containing oxygen have been investigated and whilst a lot of compounds have been reported in the literature, there are only few structural data. The reaction between $SnCl_4$ and cyclohexanol has yielded the adducts $SnCl_4 \cdot 2C_6H_{11}OH$ or $SnCl_4 \cdot 4C_6H_{11}OH$ depending on the experimental conditions. The latter compound is the most interesting adduct, with regards to the coordination number of tin. In $SnCl_4 \cdot 4C_6H_{11}OH$, the tin atom has been reported to be octacoordinated [1]. In this paper we show that tin is hexacoordinated, with a formula like $SnCl_4 \cdot 2L$ ($L = (C_6H_{11}OH)_2$), and that the two other molecules of cyclohexanol are bonded by hydrogen bonds.

Experimental

Preparation

Tin tetrachloride and dry cyclohexanol in excess were mixed under nitrogen pressure, in order to form the white adduct $SnCl_4 \cdot 4C_6H_{11}OH$. This adduct was isolated, diethyl ether added and the mixture heated in order to completely dissolve the solid. Slow cooling deposited well formed colourless crystals of $SnCl_4 \cdot 4C_6H_{11}OH$ (m.p. 101–2 °C). Found: Sn, 18.40%; Cl, 21.47%; C, 43.59%; H, 9.32%. Calculated for $SnCl_4 \cdot 4C_6H_{11}OH$: Sn, 17.97%; Cl, 21.47%; C, 43.60%; H, 9.69%. 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 20 °C. The crystals are triclinic, $a = 12.693(2)$, $b = 9.857(3)$, $c = 6.5147(6)$ Å, $\alpha = 100.290(1)$, $\beta = 92.692(9)$, $\gamma = 105.907(14)^\circ$. Estimated standard deviations were calculated with the 4-circles diffractometer (NONIUS CAD 4). Space group proved to be $P\bar{1}$. The calculated density ($C_{24}H_{48}O_4Cl_4Sn$, M.W. 661.1) of 1.430 g cm^{-3} for $Z = 1$, agrees well with the value of 1.46(5) g cm^{-3}

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TABLE I. Atomic Positional with Standard Deviation in Parenthesis.

Atom	x	y	z	Atom	x	y	z
Sn	0.5000(0)	0.5000(0)	0.5000(0)	H(1)	0.3467(27)	0.5460(36)	0.7302(53)
Cl(1)	0.5873(1)	0.6167(1)	0.8395(1)	H(2)	0.3804(36)	0.6522(47)	1.0763(69)
Cl(2)	0.5108(1)	0.7286(1)	0.4140(1)	H(11)	0.2605(20)	0.3025(27)	0.4510(39)
O(1)	0.3440(1)	0.4922(2)	0.6153(3)	H(21)	0.1997(29)	0.4686(39)	0.3096(57)
O(2)	0.3353(2)	0.6484(2)	0.9716(3)	H(22)	0.1524(27)	0.5215(37)	0.5198(54)
C(1)	0.2406(2)	0.3800(3)	0.5434(4)	H(31)	0.0674(32)	0.2451(43)	0.2540(62)
C(2)	0.1663(2)	0.4378(4)	0.4181(6)	H(32)	0.0074(34)	0.3534(43)	0.2612(64)
C(3)	0.0582(3)	0.3216(5)	0.3405(6)	H(41)	−0.0643(31)	0.1859(39)	0.4683(56)
C(4)	0.0024(2)	0.2622(4)	0.5200(7)	H(42)	−0.0142(29)	0.3384(39)	0.6171(57)
C(5)	0.0795(3)	0.2085(4)	0.6474(7)	H(51)	0.0907(31)	0.1260(42)	0.5646(61)
C(6)	0.1874(2)	0.3244(4)	0.7257(5)	H(52)	0.0462(34)	0.1715(44)	0.7592(65)
C(7)	0.3338(2)	0.7965(3)	1.0168(4)	H(61)	0.2339(31)	0.2930(40)	0.8002(59)
C(8)	0.3010(4)	0.8354(4)	0.8142(5)	H(62)	0.1756(25)	0.4014(34)	0.8093(48)
C(9)	0.2901(4)	0.9888(4)	0.8543(7)	H(71)	0.4095(24)	0.8615(31)	1.0763(45)
C(10)	0.2117(3)	1.0079(4)	1.0141(6)	H(81)	0.2223(44)	0.7617(56)	0.7462(81)
C(11)	0.2433(4)	0.9675(4)	1.2138(6)	H(82)	0.3504(32)	0.8230(41)	0.7164(61)
C(12)	0.2534(2)	0.8146(4)	1.1746(6)	H(91)	0.2690(34)	1.0098(45)	0.7212(68)
				H(92)	0.3609(29)	1.0508(37)	0.9238(54)
				H(101)	0.1331(32)	0.9437(41)	0.9611(59)
				H(102)	0.2099(30)	1.1114(41)	1.0427(56)
				H(111)	0.1981(33)	0.9777(42)	1.3141(63)
				H(112)	0.3267(37)	1.0424(47)	1.2730(67)
				H(121)	0.1765(32)	0.7423(41)	1.0957(59)
				H(122)	0.2810(36)	0.7959(46)	1.2950(68)

obtained by flotation techniques. Reflection intensities were measured with a NONIUS CAD 4 automated diffractometer and graphite monochromatized Mo-Kα radiation (λ = 0.7107 Å; $1 < \theta < 35°$).

A crystal with approximate dimensions 0.20 × 0.20 × 0.30 mm was studied and showed no evidence of deterioration in the X-ray beam in the period of the experiment. 6994 independent reflections were measured. 5697 independent reflections were kept with $F_{obs} > 10\ \sigma\ (F_{obs})$ and corrected for Lorentz and polarization factors. Scattering factors were taken from International Tables [2].

Structure Solution

The structure was solved by the heavy atom method and for calculations the SHELX program [3] was used.

At first, the structure was assumed to be non centrosymmetric. With the tin atom at the center of the cell the conventional R-factor was 0.48. The Fourier synthesis located four chlorine atoms around tin atom (recognizable with the Sn–Cl bonds, near 2.37 Å), an oxygen atom above and below the Sn–Cl plane (Sn–O: 2.14 Å), and seven carbon atoms: conventional R-factor 0.33. A second Fourier synthesis located all oxygen and carbon atoms. The structure appeared to be centrosymmetric with an inversion center at tin atom site; all calculations were resumed on this basis. After three cycles of refinement, considering anisotropic thermal parameters for tin, chlorine and oxygen atoms, the conventional R-factor dropped to 0.0506. A third Fourier synthesis located the positions of twenty hydrogen atoms (24 hydrogen atoms are required by the asymmetric unit). Geometrical considerations were used to locate the other hydrogen atoms when this could be made without ambiguity.

Anisotropic thermal parameters were considered for Sn, Cl, C and O atoms and isotropic thermal parameters were considered for hydrogen atoms. After five cycles, the conventional R-factor was 0.0338. At this stage, refinement was terminated. The final difference Fourier map, multiplied by 457, showed the strongest peak was 157 high. This peak was near the tin atom.

Final structure parameters (atomic positional U and B factors) and standard deviations are given in Tables I, II and II bis.

Results and Discussion

Description of the Structure

The structure is shown in Fig. 1. The tin atom is octahedrally coordinated by four chlorine atoms

TABLE II. Thermal Parameters[a] with Standard Deviation in Parenthesis.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{12}	U_{12}	B ($Å^2$)
Sn	0.0271(1)	0.0350(1)	0.0315(1)	0.0070(1)	0.0013(1)	0.0063(1)	2.463(8)
Cl(1)	0.0438(3)	0.0533(3)	0.0339(3)	0.0024(2)	−0.0022(2)	0.0068(3)	3.448(28)
Cl(2)	0.0556(4)	0.0404(3)	0.0552(4)	0.0163(3)	0.0011(3)	0.0124(3)	3.979(29)
O(1)	0.0303(7)	0.0461(9)	0.0489(10)	−0.0011(8)	0.0071(7)	0.0061(7)	2.298(48)
O(2)	0.0670(13)	0.0575(12)	0.485(11)	0.0059(9)	0.0035(10)	0.0340(11)	4.553(95)
C(1)	0.0274(9)	0.0411(11)	0.0472(13)	0.0071(10)	0.0037(8)	0.0086(8)	3.045(87)
C(2)	0.0411(13)	0.0607(18)	0.0628(15)	0.0241(12)	0.0007(12)	0.0118(12)	4.31(12)
C(3)	0.0420(14)	0.0850(26)	0.0685(22)	0.0211(19)	−0.0093(14)	0.0122(15)	5.15(16)
C(4)	0.0325(12)	0.0745(22)	0.0857(25)	0.0188(19)	0.0035(14)	0.0078(13)	5.07(16)
C(5)	0.0451(15)	0.0636(21)	0.0837(19)	0.0317(15)	0.0047(15)	−0.0006(14)	5.06(15)
C(6)	0.0423(14)	0.0655(19)	0.0587(18)	0.0255(16)	0.0021(12)	0.0051(13)	4.38(13)
C(7)	0.0445(13)	0.0496(14)	0.0460(14)	0.0062(11)	0.0041(10)	0.0167(11)	3.69(11)
C(8)	0.0988(28)	0.0692(21)	0.0446(16)	0.0166(15)	0.0181(17)	0.0430(21)	5.59(17)
C(9)	0.1078(33)	0.0608(21)	0.0641(22)	0.0264(18)	0.0196(22)	0.0315(22)	6.12(20)
C(10)	0.0731(22)	0.0471(16)	0.0786(24)	0.0112(16)	0.0075(18)	0.0253(16)	5.23(16)
C(11)	0.0952(29)	0.0637(21)	0.0605(20)	0.0090(16)	0.0277(20)	0.0376(20)	5.77(18)
C(12)	0.0797(23)	0.0588(18)	0.0545(18)	0.0202(15)	0.0261(16)	0.0329(17)	5.08(16)

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

TABLE II bis. Thermal Parameters with Standard Deviation in Parenthesis.

Atom	U	B
H(1)	0.065(10)	5.1(0.8)
H(2)	0.106(16)	8.4(1.3)
H(11)	0.033(6)	2.6(0.5)
H(21)	0.066(10)	5.2(0.8)
H(22)	0.075(11)	5.9(0.9)
H(31)	0.076(14)	6.0(1.1)
H(32)	0.090(14)	7.1(1.1)
H(41)	0.077(11)	6.0(0.9)
H(42)	0.074(11)	5.8(0.9)
H(51)	0.070(13)	5.6(1.0)
H(52)	0.087(14)	6.8(1.1)
H(61)	0.081(12)	6.4(1.0)
H(62)	0.050(9)	4.0(0.7)
H(71)	0.048(8)	3.8(0.6)
H(81)	0.150(21)	11.8(1.6)
H(82)	0.082(12)	6.5(1.0)
H(91)	0.097(14)	7.7(1.1)
H(92)	0.064(11)	5.1(0.8)
H(101)	0.083(12)	6.6(1.0)
H(102)	0.079(11)	6.2(0.9)
H(111)	0.086(13)	6.8(1.0)
H(112)	0.107(15)	8.4(1.2)
H(121)	0.082(12)	6.5(1.0)
H(122)	0.103(15)	8.1(1.2)

in a plane and two oxygen atoms *trans* to each other. Only two cyclohexanol molecules are directly coordinated to tin and each of these is linked, via a hydrogen bond, to an additional cyclohexanol molecule. The hydrogen bonds (Fig. 2) are strong (O(1)–O(2) = 2.572 Å; O(1)–H(1)···O(2) = 173°). Another interesting feature of this structure is a second hydrogen bond between the functional hydrogen of the second type of cyclohexanol molecule and the chlorine atom Cl(2^i) (x = 0.51; y = 0.73; z = 1.41) of an adjacent molecule. This hydrogen bond is weak, with O(2)–H(2)···Cl(2^i) = 165° and O(2)–Cl(2^i) = 3.39 Å. In fact, the structure may be described as a collection of $SnCl_4 \cdot 2C_6H_{11}OH$ adducts, connected together by cyclohexanol molecules linked via hydrogen bonds: strong O–H···O bond, weak O–H···Cl bond.

With regards to the cyclohexanol molecules, the structure shows that the C_6H_{11} groups are staggered (chair form). Distances and angles are listed in Tables III, IV and V.

Relation of the Structure with the Infrared Spectrum (Hydrogen Bonds)

The infrared spectrum of the adduct $SnCl_4 \cdot 4C_6H_{11}OH$ contains two interesting bands in the 2000–4000 cm^{-1} region: a very broad band at 2450 cm^{-1} (band width: 800 cm^{-1}) and a narrow band at 3495 cm^{-1}. Novak [4] has studied the OH···O infrared bands by plotting νOH frequencies *versus* the R(O···O) distances for fifty-five O–H···O hydrogen bonds of compounds studied by single crystal structures and neutron diffraction. He found a relationship between the broadness and position of the bands and the O–H···O distances.

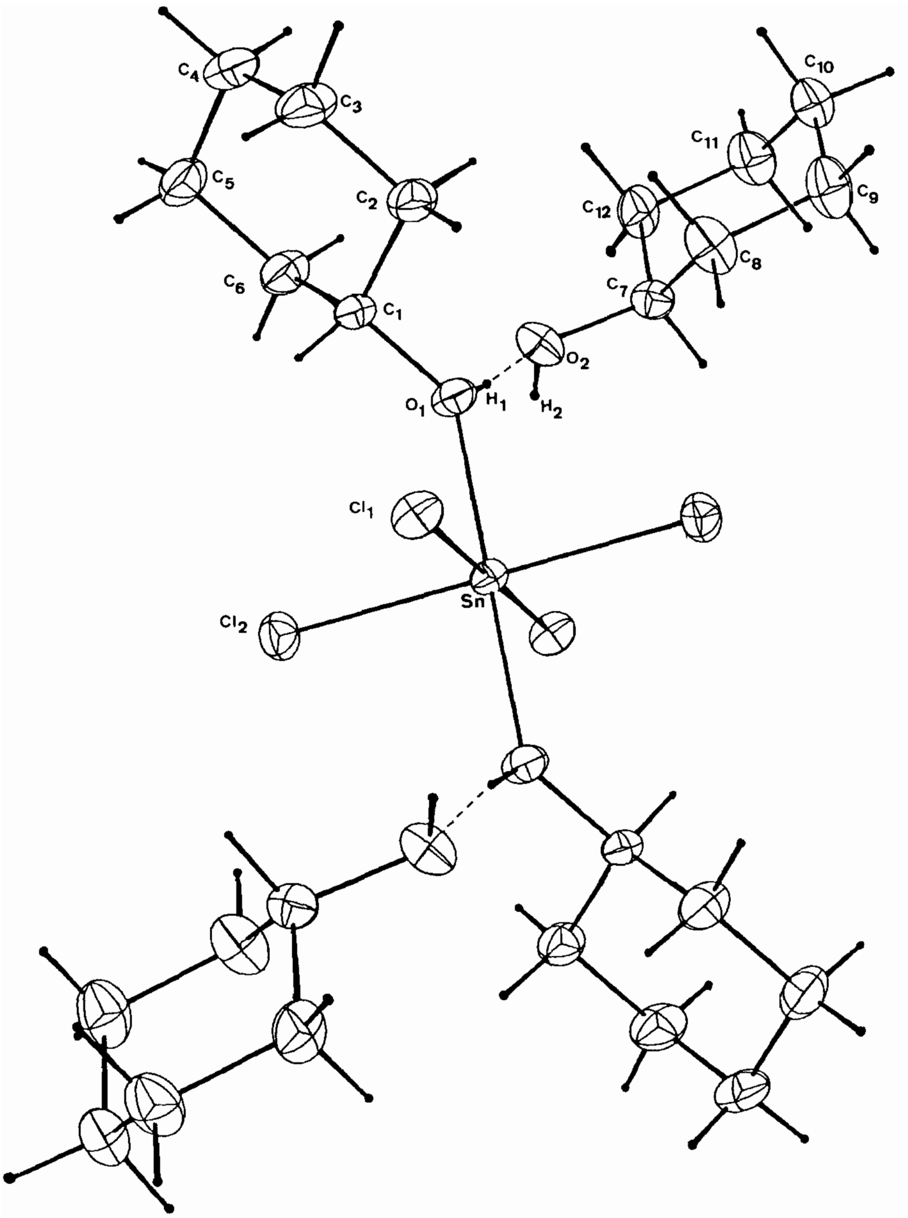

Fig. 1. An isolated molecule of $SnCl_4 \cdot 4C_6H_{11}OH$.

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

Sn–Cl(1)	2.367(1)	Cl(1)–Sn–Cl(2)	89.80(5)
Sn–Cl(2)	2.387(1)	Cl(1)–Sn–O(1)	89.20(5)
Sn–O(1)	2.137(1)	Cl(2)–Sn–O(1)	90.10(10)
O(1)–H(1)	0.830(32)	Cl(1)–Sn–Cl(2′)	90.20(5)
O(1)–O(2)	2.572(3)	Cl(1)–Sn–O(1′)	90.80(5)
H(1)–O(2)	1.743(34)	Cl(2)–Sn–O(1′)	89.90(10)
O(2)–H(2)	0.859(46)	Sn–O(1)–C(1)	126.40(20)
O(1)–C(1)	1.458(2)		
O(2)–C(7)	1.442(4)	Sn–O(1)–H(1)	115.0(2.3)
		C(1)–O(1)–H(1)	116.6(2.2)
		O(1)–H(1)–O(2)	173.3(1.0)
		H(1)–O(2)–H(2)	117.8(3.5)
		H(1)–O(2)–C(7)	127.8(2.0)
		H(2)–O(2)–C(7)	98.0(2.0)

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

TABLE IV. Intramolecular Distances (A) and Angles (deg.) in the First Cyclohexanol Molecule with Standard Deviations in Parenthesis.

C(1)–C(2)	1.506(5)	H(11)–C(1)–O(1)	105.4(1.3)
C(2)–C(3)	1.522(4)		
C(3)–C(4)	1.519(6)	C(2)–C(1)–O(1)	109.3(0.2)
C(4)–C(5)	1.514(6)	C(6)–C(1)–O(1)	110.8(0.2)
C(5)–C(6)	1.520(4)		
C(6)–C(1)	1.509(5)	H(21)–C(2)–H(22)	110.7(3.2)
		H(31)–C(3)–H(32)	104.6(3.6)
C(1)–H(11)	0.975(26)	H(41)–C(4)–H(42)	109.8(3.1)
C(2)–H(21)	0.897(39)	H(51)–C(5)–H(52)	101.9(3.7)
C(2)–H(22)	1.024(36)	H(61)–C(6)–H(62)	107.3(3.2)
C(3)–H(31)	0.895(41)		
C(3)–H(32)	0.958(48)	C(1)–C(2)–H(21)	110.1(2.7)
C(4)–H(41)	0.964(32)	C(1)–C(2)–H(22)	105.5(2.1)
C(4)–H(42)	0.969(38)	C(3)–C(2)–H(21)	110.5(2.0)
C(5)–H(51)	0.941(41)	C(3)–C(2)–H(22)	110.2(2.0)
C(5)–H(52)	0.938(44)	C(2)–C(3)–H(31)	112.6(2.4)
C(6)–H(61)	0.898(44)	C(2)–C(3)–H(32)	113.3(2.2)
C(6)–H(62)	0.904(33)	C(4)–C(3)–H(31)	105.1(2.7)
		C(4)–C(3)–H(32)	109.0(2.6)
C(1)–C(2)–C(3)	109.9(0.3)	C(3)–C(4)–H(41)	110.9(2.3)
C(2)–C(3)–C(4)	111.7(0.3)	C(3)–C(4)–H(42)	110.0(2.3)
C(3)–C(4)–C(5)	110.7(0.3)	C(5)–C(4)–H(41)	110.1(2.6)
C(4)–C(5)–C(6)	111.7(0.3)	C(5)–C(4)–H(42)	105.1(2.4)
C(5)–C(6)–C(1)	109.9(0.3)	C(4)–C(5)–H(51)	108.3(2.6)
C(6)–C(1)–C(2)	112.1(0.2)	C(4)–C(5)–H(52)	111.8(2.9)
		C(6)–C(5)–H(51)	111.9(2.2)
		C(6)–C(5)–H(52)	110.8(2.2)
		C(5)–C(6)–H(61)	112.3(2.2)
		C(5)–C(6)–H(62)	110.9(1.8)
		C(1)–C(6)–H(61)	110.5(2.5)
		C(1)–C(6)–H(62)	105.7(2.1)
		C(6)–C(1)–H(11)	110.1(1.6)
		C(2)–C(1)–H(11)	108.9(1.6)

TABLE V. Intramolecular Distances (A) and Angles (deg) in the Second Cyclohexanol Molecule with Standard Deviation in Parenthesis.

C(7)–C(8)	1.510(5)	H(71)–C(7)–O(2)	110.2(1.9)
C(8)–C(9)	1.533(6)		
C(9)–C(10)	1.497(7)	C(8)–C(7)–O(2)	108.1(0.2)
C(10)–C(11)	1.495(5)	C(12)–C(7)–O(2)	109.6(0.2)
C(11)–C(12)	1.524(6)		
C(12)–C(7)	1.504(5)	H(81)–C(8)–H(82)	105.7(3.5)
		H(91)–C(9)–H(92)	114.6(3.2)
		H(101)–C(10)–H(102)	107.9(3.2)
C(7)–H(71)	1.011(26)	H(111)–C(11)–H(112)	108.0(3.2)
C(8)–H(81)	1.081(47)	H(121)–C(12)–H(122)	118.2(3.3)
C(8)–H(82)	0.931(42)		
C(9)–H(91)	0.969(47)	C(7)–C(8)–H(81)	109.1(3.1)
C(9)–H(92)	0.973(31)	C(7)–C(8)–H(82)	110.6(2.8)
C(10)–H(101)	1.029(35)	C(9)–C(8)–H(81)	108.5(3.3)
C(10–H(102)	1.011(42)	C(9)–C(8)–H(82)	112.1(2.5)
C(11)–H(111)	0.900(43)	C(8)–C(9)–H(91)	108.2(2.6)
C(11)–H(112)	1.116(39)	C(8)–C(9)–H(92)	105.9(2.5)
C(12)–H(122)	0.913(48)	C(10)–C(9)–H(91)	112.9(2.8)
		C(10)–C(9)–H(92)	103.5(2.2)

(continued overleaf)

TABLE V. *(continued)*

C(7)–C(8)–C(9)	110.6(0.3)	C(9)–C(10)–H(101)	111.2(2.2)
C(8)–C(9)–C(10)	111.5(0.3)	C(9)–C(10)–H(102)	109.4(2.2)
C(9)–C(10)–C(11)	111.5(0.4)	C(11)–C(10)–H(101)	106.9(2.4)
C(10)–C(11)–C(12)	111.3(0.3)	C(11)–C(10)–H(102)	109.9(2.1)
C(11)–C(12)–C(7)	111.1(0.3)	C(10)–C(11)–H(111)	114.2(2.9)
C(12)–C(7)–C(8)	110.8(0.3)	C(10)–C(11)–H(112)	105.7(2.5)
		C(12)–C(11)–H(111)	109.7(2.7)
		C(12)–C(11)–H(112)	107.7(2.7)
		C(11)–C(12)–H(121)	107.7(2.7)
		C(11)–C(12)–H(121)	108.5(2.4)
		C(11)–C(12)–H(122)	110.0(2.8)
		C(7)–C(12)–H(121)	102.8(2.2)
		C(7)–C(12)–H(122)	105.9(3.0)
		C(12)–C(7)–H(71)	108.9(1.7)
		C(8)–C(7)–H(71)	109.2(1.8)

If we plot our result (2.57 Å for the O(1)–H(1)$\cdots$O(2) distance), we obtain a νOH value near 2450 cm^{-1}. So the broad band at 2450 cm^{-1} may be attributed to the O(1)–H(1) stretching frequency. On the other hand, Novak [4] has pointed out that the band width increases in order of magnitude in going from weak (half band width $\cong$ 10 cm^{-1}) to medium-strong (10^2 cm^{-1}) hydrogen bonds and can reach 10^3 cm^{-1} for strong OH$\cdots$O bonds. Our result (band width: 800 cm^{-1} for the broad band at 2450 cm^{-1}) correlates well with this observation.

The second band, at 3495 cm^{-1}, is very narrow. It may be attributed to the OH stretching frequency of the second type of hydrogen bond O(2)–H(2)$\cdots$Cl (2^i). Thus the hydrogen bond should be very weak.

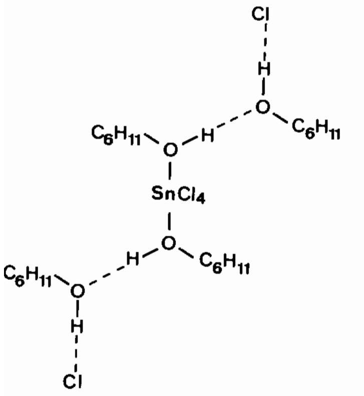

Fig. 2. Hydrogen bonds in the crystal.

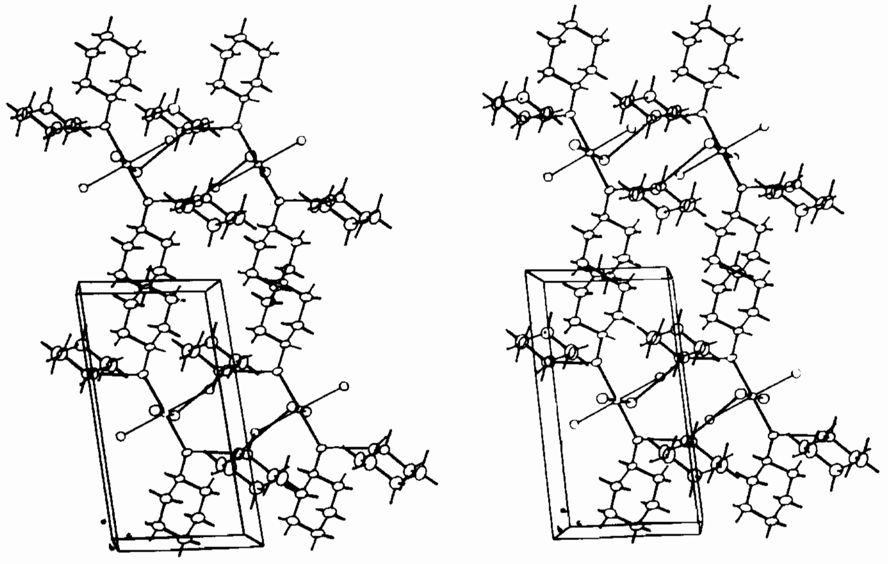

Fig. 3. ORTEP view of 4 cells showing H-bonds.

Conclusions

The adduct $SnCl_4 \cdot 4C_6H_{11}OH$ may be described as $SnCl_4 \cdot L_2$ with two additional L molecules of crystallization: $SnCl_4L_2 \cdot L_2$. The tin atom is hexacoordinated (octahedrally). Cyclohexanol molecules are bonded by three types of bonds (Fig. 2):

- between the oxygen atom and the tin atom.
- between the hydrogen atom of the first and the oxygen atom of the second cyclohexanol molecule (strong hydrogen bond).
- between the hydrogen atom of the second cyclohexanol molecule and a chlorine atom of an adjacent molecule of tin tetrachloride (weak hydrogen bond).

In catalysis cyclohexanol may be expected to be adsorbed or fixed on Sn ions in two ways: either directly via coordination of the oxygen atom or indirectly via hydrogen bonding to a cyclohexanol molecule already fixed on the tin atom.

The strong hydrogen bond between the first and the second cyclohexanol molecule agrees well with the electrochemical behaviour in benzene solution. According to several authors [1, 5–8] and cryoscopic measurements $SnCl_4 \cdot 4ROH$ dissociates into 3 ions:

$$SnCl_4 \cdot 4ROH \rightarrow SnCl_4(OR)_2^{2-} + 2ROH_2^+$$

The most probable explanation is that the bond between H(1) and O(1) is broken during this process whilst O(2) retains H(1).

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