CRYSTAL STRUCTURE OF POLYMERIC [2-(DIMETHYLAMINOMETHYL)PHENYL]PHENYLTIN(IV) DIFLUORIDE

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ABSTRACT

The almost linear polymeric structure of $[L^{CN}PhSnF_2]_n$ (1) (where L^{CN} is 2-(dimethylaminomethyl)phenyl-) was determined by XRD techniques on the single crystalline material. The central tin atom is six-coordinated and reveals a distorted octahedral geometry.

COMMENT

We published previously the crystal structure of polymeric $[L^{CN}(n\text{-Bu})SnF_2]_n$ /1/. Now we report the molecular structure of analogous $[L^{CN}PhSnF_2]_n$ (1). Compound 1 was used as a part of selective and sensitive carriers for fluoride ion recognition /2/. It crystallizes as a linear polymer with "rod-like" F-Sn-F chains. The tin atom in the solid state structure is six-coordinated and tin atoms are interconnected by one bridging fluorine. This compound is almost insoluble in all common organic solvents,which was rather a limitation for the structural study in solution by multinuclear NMR spectroscopy. In contrast to $[L^{CN}(n\text{-Bu})SnF_2]_n$,which crystallizes as two different polymorphs (isotactic and syndiotactic polymers),compound 1 was isolated only as the syndiotactic polymer. The distances Sn1-F1 and Sn1-F2 are somewhat longer than in syndiotactic $[L^{CN}(n\text{-Bu})SnF_2]_n$, on the other hand the distance Sn1-N1 is much shorter in the case of 1. The interatomic angles of the F-Sn-F chain are essentially the same for both syndiotactic $[L^{CN}(n\text{-Bu})SnF_2]_n$ and 1.

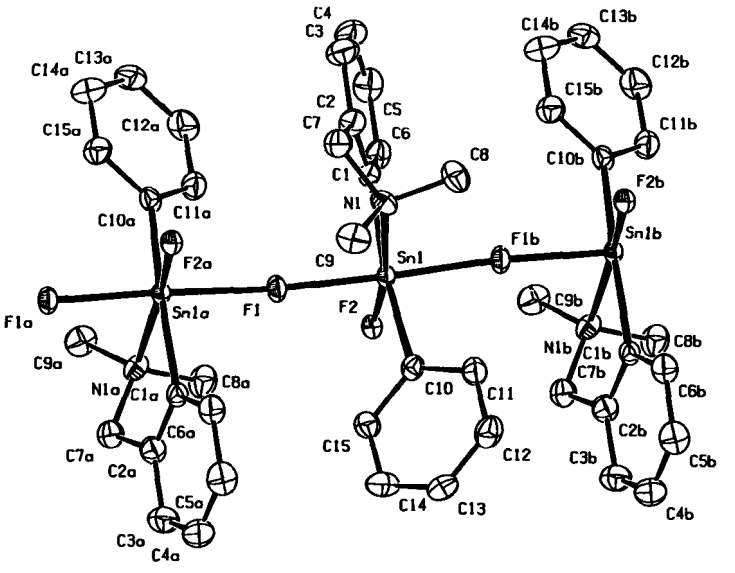

Fig. 1: The molecular structure of 1 (ORTEP 50% probability level), hydrogen atoms are omitted for clarity.

Selected interatomic distances [Å] and angles [°]: Sn1-F1 2.1415(18), Sn1-F2 2.081(3), Sn1-F1b 2.2070(18), Sn1-N1 2.438(4), Sn1-C1 2.099(4), Sn1-C10 2.115(4); F1-Sn1-F1b 176.96(9), Sn1-F1-Sn1a 175.50(13), F1-Sn1-F2 90.01(10), F1b-Sn1-F2 92.97(10), F1-Sn1-N1 83.41(11), F1b-N1-Sn1 93.56(10), N1-Sn1-C1 76.82(14), N1-Sn1-C10 92.62(14), C1-Sn1-C10 168.15(16).

EXPERIMENTAL

The synthesis and characterization of **1** has been published elsewhere /3/ (method D). Single crystalline material suitable for XRD analysis was obtained from a methanol solution by slow evaporation. M.p. = 208-210°C.

Formula	$C_{15}H_{17}F_2NSn$	D_{calcd} (g.cm^{-3})	1.787
Formula weight	367.99	F (000)	728
Crystal system	orthorhombic	θ_{max} (°)	27.5
Space group	$P\,2_12_12_1$	Reflns meas.	5834
Crystal size (mm)	0.22 x 0.22 x 0.20	Reflns unique (R_{int})	3015 (0.0351)
a (Å)	8.2061(7)	Reflns with $I \geq 2\sigma$ (I)	2530
b (Å)	8.6871(4)	Weighting scheme	0.025900 / 2.028700
c (Å)	19.1829(9)	Difractometer	Nonius KappaCCD
Volume (Å^3)	1367.47(15)	Temperature (K)	150(2)
Z	4	μ (mm^{-1})	1.877
Trans. factors T_{min}, T_{max}	0.665, 0.757	Programs used	SIR92 /4/, SHELXL97 /5/
ρ_{max}, ρ_{min} (eÅ^{-3})	0.737, -0.749	Deposition number	CCDC 733613

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