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Crystallographic report

Crystal and molecular structure of tetramethylammoniumdiisothiocyanato-triphenyltin(IV), [$NMe_4SnPh_3(NCS)_2$]

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The structure of $NMe_4SnPh_3(NCS)_2$ is molecular, without any significant intermolecular contacts in the lattice. The trigonal plane around the tin atom is defined by three carbon atoms from the phenyl groups and the axial positions occupied by the NCS groups. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: organotin(IV); X-ray diffraction; spectroscopic techniques

COMMENT

The structure consists of discrete $NMe_4SnPh_3(NCS)_2$ molecules (**I**) with no significant intermolecular interactions. In Fig. 1, the tin(IV) atom is coordinated in an almost regular trigonal bipyramidal environment, with three phenyl groups in an equatorial position and two thiocyanates in an axial position. The slight distortion from the ideal trigonal bipyramidal geometry in the molecule is evident from the magnitude of the N–Sn–N (177.4(1)°) and N–Sn–C bonds angles (which range from 89.0(2) to 91.7(1)°), whereas the three phenyl groups exhibit perfectly planar Sn–C_3 units ($\sum$ C–Sn–C: 360°) in the basal plane. The bond lengths of Sn–C (2.131(4), 2.132(4) and 2.142(4) Å) and Sn–N (2.268(4) and 2.282(4) Å) fall within the range of corresponding bond lengths reported for other organotin compounds. The NCS groups are almost linear, with N–C–S angles being 179.0(4)° and 179.1(4)°. The short N–C (1.140(5) and 1.148(5) Å) and long C–S (1.604(4) and 1.620(5) Å) distances are also similar to those found in isothiocyanatotriphenyltin(IV) and other metal isothiocyanate complexes.[1]

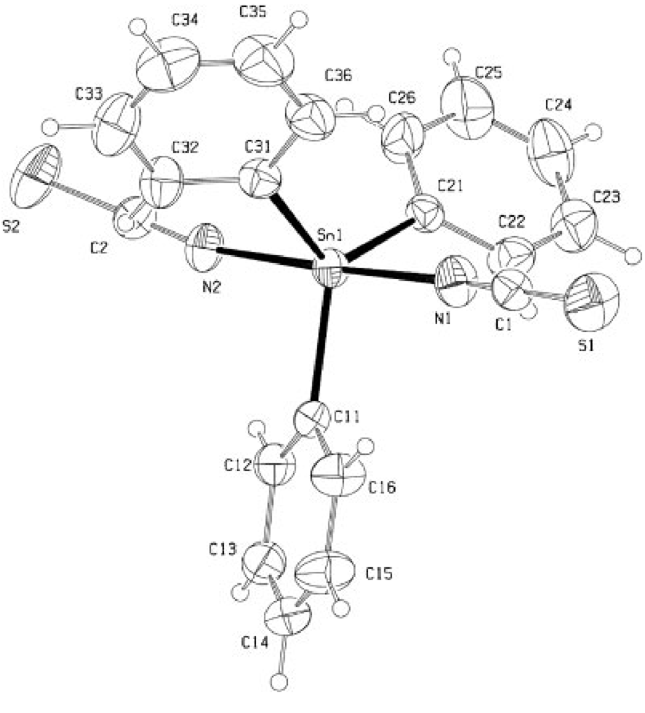

Figure 1. Molecular structure of **I**.

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EXPERIMENTAL

Synthesis

The adduct was prepared according to

$$(NMe_4)_2SO_4{\cdot}2H_2O + 2SnPh_3SCN \longrightarrow Me_4NSO_4SnPh_3 + NMe_4SnPh_3(NCS)_2 + 2H_2O$$

with a yield of 56%; m.p. 207–209 °C. Anal. Found: C, 53.4; H, 4.9; N, 7.6; Sn, 21.9. Calc. for $C_{24}H_{27}N_3S_2Sn$: C, 53.3; H, 5.0; N, 7.8; Sn, 22.0%. IR (cm^{-1}): 2060vs (ν(CN)); 274vs ($\nu_{as}(SnC_3)$); 209vs (ν(SnN)). ^{1}H NMR: δ (ppm) 3.1 (s, 12H, CH_3); 7–8 (m, 15H, Ar). ^{13}C NMR: δ (ppm) 142.2 (C_i), 137.1 (C_o), 130.3 (C_p), 129.4 (C_m); $^nJ(^{119}Sn{-}^{13}C)$ (Hz): 760 (^1J), 46.6 (^2J), 70.2 (^3J), 15 (^4J). ^{119}Sn NMR: δ (ppm) −250. Mössbauer data (mm s^{-1}): IS = 1.53, QS = 3.54; $\Gamma = 0.89$.

Crystallography

Intensity data for **I** were collected at 293 K on an Enraf Nonius CAD4 diffractometer for a colourless crystal 0.72 × 0.36 × 0.43 mm^3, $C_{24}H_{27}N_3S_2Sn$, $M = 540.3$, monoclinic, $P2_1/n$, $a = 10.190(8)$, $b = 15.716(8)$, $c = 16.638(8)$ Å, $\beta = 101.95(3)°$, $V = 2607(2)$ Å^3, $Z = 4$, 4566 unique data ($\theta_{max} = 25.0°$), 3645 data with $I > 2\sigma(I)$, $R = 0.034$(obs.), $wR = 0.086$(obs.), $\rho_{max} = 0.50$ e$^-$ Å^{-3}. Programs used: SHELXS, SHELXL and ORTEP. CCDC deposition number: 189258.

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REFERENCE

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