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Crystallographic report

Ethyltriphenyltin(IV), $Et(Ph)_3Sn$

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The crystal lattice of the title compound comprises isolated molecules. The coordination polyhedron is a slightly distorted tetrahedron with C–Sn–C bond angles ranging from 106.62(17)° to 113.9(3)°.

KEYWORDS: ethyltriphenyltin(IV); X-ray diffraction; organotin(IV)

COMMENT

The crystal of ethyltriphenyltin, $Et(Ph)_3Sn$ (Fig. 1), comprises isolated molecules with the tin atom in a slightly distorted tetrahedral environment. The $Sn–C_{Ph}$ bond lengths (average value 2.133(5) Å) are similar to those found in other triphenyltin[1] and tetraphenyltin[2] compounds (average value 2.144(14) Å). There is evidence that the $Sn–C_{Et}$ bond is longer (2.172(7) Å) than the $Sn–C_{Ph}$ bond lengths, but the relatively high errors preclude a definitive statement on this matter. However, such a scenario is usually observed in $SnPh_3R$(R = alkyl) species.[1] The C–Sn–C angles involving the ethyl group (average value 111.1(2)°) are slightly wider than the ideal tetrahedral angle, whereas the $C_{Ph}–Sn–C_{Ph}$ angles (average value 107.6(1)°) are narrower. In the lattice, all the intermolecular $C–H\cdots\pi$ contacts have $H\cdots\pi$ distances longer than 3 Å and no $\pi–\pi$ stacking was detected.

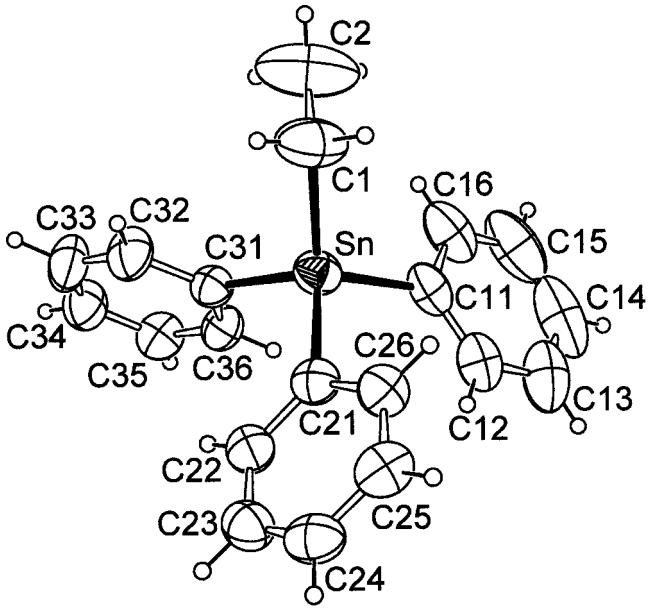

Figure 1. ORTEP plot showing the molecular structure of $Et(Ph)_3Sn$ (30% probability level). Selected bond lengths (Å) and angles (°): Sn–C1 2.172(7), Sn–C11 2.136(6), Sn–C21 2.131(5), Sn–C31 2.133(4), C1–Sn–C11 113.9(3), C1–Sn–C21 109.9(3), C1–Sn–C31 110.3(2), C11–Sn–C21 107.1(2), C11–Sn–C31 106.62(17), C21–Sn–C31 108.97(18).

EXPERIMENTAL

$Et(Ph)_3Sn$ was obtained by reaction of EtMgBr and Ph_3SnCl in dry diethyl ether following a published method.[3] Recrystallization of the crude product in ethanol afforded crystals suitable for X-ray diffractometry. Anal. Found: C, 63.1; H, 5.4. Calc. for $C_{20}H_{20}Sn$: C, 63.4; H, 5.3%. Intensity data were collected at 293(2) K for a crystal of dimensions $0.20 \times 0.20 \times 0.24$ mm^3 on an Enraf–Nonius Kappa-CCD diffractometer. Crystallographic data: $C_{20}H_{20}Sn$, $M = 379.05$, monoclinic, $C2/c$, $a = 16.6890(3)$, $b = 11.4410(3)$, $c = 19.4620(4)$ Å, $\beta = 102.932(1)°$, $V = 3621.80(14)$ Å^3, $Z = 8$, 3120 unique reflections and 2413 with $I > 2\sigma(I)$, $R = 0.045$, (obs. data) $wR = 0.128$, (all data), $\rho_{max} = 0.71$ e–Å^{-3}. Programs used: Multiscan, COLLECT, HKL Denzo and Scalepack, SHELXS-97, SHELXL-97, ORTEP.CCDC number: 169 905.

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