Crystal Structure of $[Sn(Bu)_3(O{=}PPh_3)_2][BPh_4]$

Nongnaphat Khosavithitkul[a], Kenneth J. Haller[a], Seik Weng Ng[b], [a]*School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.* [b]*Institute of Postgraduate Studies, University of Malaya, 50603 Kuala Lumpur, Malaysia.* E-mail: nkhosavithitkul@yahoo.com

The crystal structure of the title complex was determined by single crystal X-ray analysis. Data were collected on a Nonius KappaCCD diffractometer equipped with a fine focus molybdenum X-ray source, 0.3 mm *ifg* capilliary collimator, and an Oxford Cryosystems crystal cooler. Structure solution and refinement utilized SIR97, MaXus, and the SHELXTL system.

The cation consists of trigonal bipyramidal tin(IV), with three butyl groups coordinated in the three equatorial positions and triphenylphosphine oxide ligands in the axial positions. The supramolecular structure is dominated by extensive concerted phenyl-phenyl interactions [1] among the six phenyl groups of the cation triphenylphosphine moieties and the four phenyl groups of the anion tetraphenylborate moieties.

Crystal data: $C_{72}H_{77}BO_2P_2Sn$; M_r = 1165.78 Daltons; transparent colorless flat slabs; 0.17 x 0.20 x 0.23 mm; orthorhombic; $Pna2_1$; a = 19.2421(3), b = 14.9077(4), c = 21.9461(5) A, V = 6295.4 A^3; Z = 4; D_{calc} = 1.230 Mg/m^3; $\lambda_{MoK\alpha}$ = 0.71073 A; μ = 5.0 cm^{-1}; T = 200 K. Data collection: Bruker-Nonius KappaCCD, 0.3 mm *ifg* capillary collimator, 60,132 data collected, R_{int} = 0.0775, 8209 unique data, 6431 observed data ($I_o > 4\sigma(I_o)$).

[1] Dance I., Scudder M., *J. Chem. Soc., Chem. Commun.,* 1995, 1039.

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