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Crystallographic report

Crystal and molecular structure of $Ph_3GeO_2CC_4H_3O$

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The germanium atom in the title compound is in a distorted tetrahedral geometry defined by an oxygen donor, derived from an effectively monodentate carboxylate ligand, and three *ipso*-carbon atoms from the phenyl substituents. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; triphenylgermanium; furanylcarboxylate

COMMENT

The structure of $Ph_3GeO_2CC_4H_3O$, Fig. 1, reveals a monomeric structure with two significantly different Ge–O distances: Ge–O1 is 1.8425(13) Å and Ge···O(2) is 2.9335(16) Å. Thus, the carboxylate ligand is binding in the monodentate mode and the germanium atom geometry is distorted tetrahedral. The structure reported here resembles closely those found for triorganotin carboxylates.[1–3]

EXPERIMENTAL

The $OC_4H_3CO_2Na$ ligand (1.0 mmol) was added to a CH_2Cl_2 (20 ml) solution of Ph_3GeCl (1.0 mmol) and stirred for 8 h at 30 °C. After filtration, the clear solution was evaporated under vacuum to leave a white solid. The product was recrystallized from CH_2Cl_2–hexane to give colorless crystals; m.p. 118–119 °C. IR (KBr), ν: 3045, 3021, 1613, 1347, 1095, 992 cm^{-1}. Intensity data were collected at 293 K on a Bruker Smart 1000 CCD for a colorless block 0.40 × 0.50 × 0.60 mm^3. $C_{23}H_{18}GeO_3$, $M = 414.96$, monoclinic, $P2_1/c$, $a = 11.945(4)$, $b = 9.934(3)$, $c = 16.284(5)$ Å, $\beta = 91.590(5)°$, $V = 1931.7(11)$ $Å^3$, $Z = 4$, 3937 unique data ($\theta_{max} = 26.4°$), 3256 data with $I \geq 2\sigma(I)$. $R = 0.024$, $wR = 0.066$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 237627.

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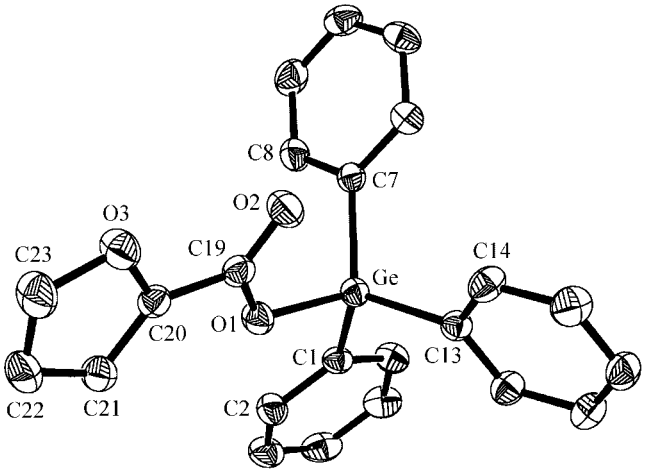

Figure 1. The molecular structure of $Ph_3GeO_2CC_4H_3O$; hydrogen atoms have been omitted for clarity. Key geometric parametric parameters: Ge–O1 1.8425(13), Ge–C1 1.9406(16), Ge–C7 1.9437(17), Ge–C13 1.9446(17) Å; O1–Ge–C1 100.33(7), O1–Ge–C7 109.09(6), O1–Ge–C13 108.83(7), C1–Ge–C7 111.16(7), C1–Ge–C13 111.91(7), C7–Ge–C13 114.53(7)°.

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