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Crystallographic report

1,1-Diphenyl-3-(triphenylgermyl)-3-(4-chlorophenyl) propanol

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The germanium atom in $[(C_6H_5)_3GeCH(4\text{-}ClC_6H_4)CH_2C(C_6H_5)_2OH]$ is in a distorted tetrahedral geometry. Steric hindrance precludes O–H···O intra- or inter-molecular bonding. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organogermanium; germylpropanol

COMMENT

The crystallization of monoalcohols in low symmetry groups with a single molecule defining the asymmetric unit is rare owing to packing considerations associated with O–H···O hydrogen bonding.[1,2] A single molecule of $[(C_6H_5)_3GeCH(4\text{-}ClC_6H_4)CH_2C(C_6H_5)_2OH]$ (Fig. 1) comprises the asymmetric unit in the title compound, as steric reasons preclude OH···O hydrogen bond formation. The germanium atom is four-coordinated within a distorted tetrahedral geometry with a mean $Ge–C_{aromatic}$ distance 1.948(2) Å which is significantly shorter than $Ge–C_{benzyl}$ distance of 1.996(2) Å.

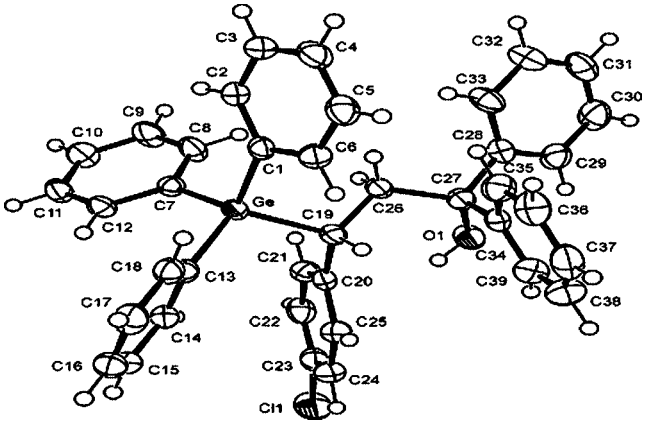

Figure 1. Molecular structure of $[(C_6H_5)_3GeCH(4\text{-}ClC_6H_4)CH_2C(C_6H_5)_2OH]$. Key geometric parameters: Ge–C1 1.949(2), Ge–C7 1.945(2), Ge–C13 1.949(2), O1–C27, 1.437(2) Å; C1–Ge–C7 111.14(9), C1–Ge–C13 112.12(9), C7–Ge–C13 108.68(9), C7–Ge–C19 113.41(8)°.

EXPERIMENTAL

$[C_{39}H_{33}ClGeO]$ was synthesized from the 1:6 reaction between $Cl_3GeCH(4\text{-}ClC_6H_4)CH_2COOH$ and C_6H_5MgBr as per the literature method,[3] and the crystals were grown from a $CHCl_3$/acetone (3:1) solution of the compound; m.p.: 419–421 K. Anal. Found: C, 74.71; H, 5.32. Calc.: C, 74.86; H, 5.27% Data were collected at 173(2) K on a Nonius Kappa CCD diffractometer. $C_{39}H_{33}ClGeO$, $M = 625.69$, monoclinic, space group $P2_1/c$, $a = 11.661(2)$, $b = 19.181(4)$, $c = 14.861(3)$ Å, $V = 3101.8(10)$ Å^3, $Z = 4$, $R = 0.038$ (3101 reflections with $I \geq 2\sigma(I)$, $\theta_{max} = 27.5°$), $wR = 0.094$ (all 7066 data). Programs used: SHELXL–97 and ORTEP II. CCDC deposition number: 246934.

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