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Crystallographic report

2-Furfurylgermatrane

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The germanium atom is penta-coordinated and adopts a trigonal bipyramidal geometry. The 2-furfuryl group and the nitrogen atom each occupy an apical position with a transannular N→Ge bond distance of 2.173(3) Å. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: germatrane; crystal structure; transannular N→Ge bond

COMMENT

As a part of a systematic study of five-coordinated organogermanium and organosilicon compounds,[1,2] the title compound, 2-furfurylgermatrane (**I**), a new representative of five-coordinated organogermanium compounds with a heterocyclic substituent at the central atom, has been investigated. The structure of **I** reveals germanium to be penta-coordinated and trigonal bipyramidal; the deviation of the germanium atom from the trigonal plane is 0.2219(4) Å (Fig. 1). The 2-furfuryl group and the nitrogen atom each occupy an apical position. The transannular N→Ge bond of 2.173(3) Å in **I** is comparable to that in 2-furylgermatrane (2.158(5) Å)[3] and the deviation of the germanium atom from O(2)–O(8)–O(9) plane in germatrane **I** is more expressed than in 2-furylgermatrane (0.185(1) Å).[3] The structural parameters of the furan ring in **I** are C(13)–C(14) 1.331(4) Å and C(14)–C(15) 1.466(6) Å, whereas those for 2-furylgermatrane[3] are 1.350(9) Å and 1.437(10) Å respectively.

EXPERIMENTAL

I was prepared according to a literature procedure.[4] Single crystals were grown from the slow evaporation of a chloroform solution of **I**; m.p. 196–197 °C. Intensity data were collected at 298 K on a Nonius Kappa CCD diffractometer using Mo Kα radiation for a yellow crystal $0.15 \times 0.15 \times 0.20$ mm^3, $C_{11}H_{17}GeNO_4$, $M = 299.85$, monoclinic space group, $P2_1/c$, $a = 10.3637(3)$, $b = 11.2812(4)$, $c = 13.5920(5)$ Å, $\beta = 128.488(2)°$, $V = 1243.85(7)$ Å^3, $Z = 4$, $\mu = 2.46$ mm^{-1}, 3013 unique data ($2\theta_{\max} = 55.0°$), $R = 0.044$ (2222 reflections with $I > 3\sigma(I)$). Programs used: SIR97, maXus, ORTEP. CCDC deposition number 221046.

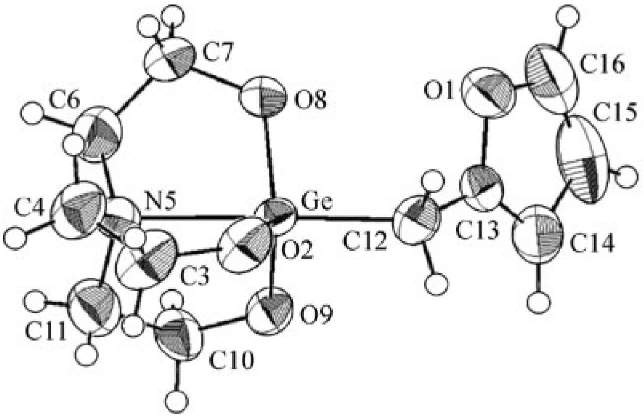

Figure 1. Molecular structure of **I**. Key geometric parameters: Ge–O2 1.803(2), Ge–O8 1.795(2), Ge–O9 1.795(2), Ge–N5 2.173(3), Ge–C12 1.955(3), O2–C3 1.405(4), O8–C7 1.403(4), O9–C10 1.418(4), N5–C4 1.483(4), N5–C6 1.457(4), N5–C11 1.467(5) Å; O2–Ge–O8 117.8(1), O2–Ge–O9 117.20(9), O2–Ge–N5 82.86(9), O8–Ge–O9 120.45(9), O8–Ge–N5 82.89(9), O8–Ge–C12 99.4(1), O9–Ge–N5 82.9(1), N5–Ge–C12 177.0(1), Ge–C12–C13 117.7(2)°.

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