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N-Phenyl-2-(triphenylstannylseleno)benzamide and 2-Methylseleno-*N*-phenylbenzamide

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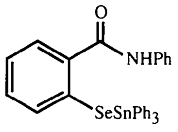
Abstract

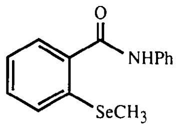
The two independent molecules of *N*-phenyl-2-(triphenylstannylseleno)benzamide, $C_{31}H_{25}NOSeSn$, differ significantly in the conformations of the *N*-phenylbenzamide groups. For 2-methylseleno-*N*-phenylbenzamide, $C_{14}H_{13}NOSe$, the *N*-phenylbenzamide group is oriented such that the O atom is in close contact with the Se atom [Se···O 2.829 (2) Å] and the N atom is pointed away. In both compounds, the amide N atom is involved in hydrogen bonding with the O atom of an adjacent molecule, forming zigzag chains which lie along the *a* axis.

Comment

Recently, we reported that triphenylstannane selenides react with peroxides to afford diaryl diselenides in good yield (Fong & Schiesser, 1995). During the course of this work, we prepared *N*-phenyl-2-(triphenylstannylseleno)benzamide, (1). This selenide was subsequently reacted with benzoyl peroxide to afford 2,2′-diselenobis(*N*-phenylbenzamide), which in turn was converted into the anti-inflammatory compound ebselen and varying quantities of 2-methylseleno-*N*-phenylbenzamide, (2), upon treatment with di-*tert*-butyl peroxide. Given the aromatic nature of compound (1), its structure was difficult to elucidate by NMR spectroscopy. In order to confirm the identities of (1) and (2), X-ray structural analyses were carried out on both compounds.



(1)



(2)

The two independent molecules of (1) differ significantly in the conformations of the *N*-phenylbenzamide groups (Fig. 1). In one molecule, the Se atom is in close contact with the O atom [Se···O 3.155 (4) Å], while the N atom lies more distant [Se···N 4.231 (5) Å]. The two aromatic rings (C1–C6 and C8–C13) are almost perpendicular, the dihedral angle between them being 88.5 (2)°. The amide group is inclined at angles of 52.4 (2) and 36.2 (3)° with respect to these two rings. In the second molecule, the O atom is pointed away from the Se atom [Se′···O′ 3.988 (4) Å], which now has a close contact with the N atom [Se′···N′ 3.384 (5) Å]. This Se atom also has an O atom of an adjacent molecule as a near neighbour [Se′···O′^{i} 3.554 (4) Å; symmetry code: (i) $-\frac{1}{2}+x, y, \frac{1}{2}-z$]. The dihedral angle between the two aromatic rings C1′–C6′ and C8′–C13′ is 55.5 (2)°, while the dihedral angles between these two rings and the amide group are 66.4 (3) and 11.3 (9)°, respectively.

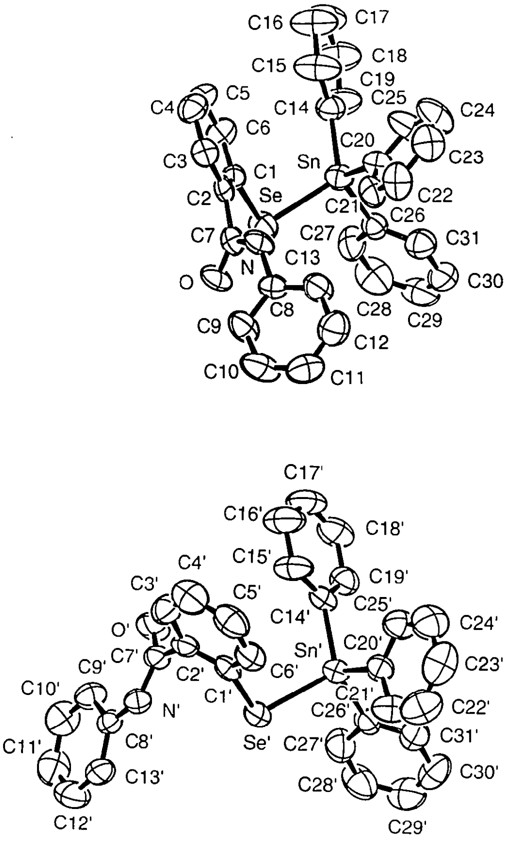


Fig. 1. An *ORTEP*II (Johnson, 1976) drawing of the two independent molecules of compound (1). Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

For both molecules, the amide N atom is involved in hydrogen bonding with the O atom of an adjacent molecule, forming zigzag chains which lie along the *a* axis; N···O^{ii} 2.941 (5), N—H(N) 0.81 (4), H(N)···O^{ii} 2.16 (4) Å and N—H(N)···O^{ii} 164 (4)°; N′···O′^{i} 2.936 (6), N′—H(N′) 0.76 (4), H(N′)···O′^{i}

2.19 (4) Å and N′—H(N′)···O′ⁱ 168 (4)° [symmetry code: (ii) $-\frac{1}{2}+x$, $\frac{1}{2}-y$, $-z$]. The Se···O and Se···N distances of 3.155 (4) and 3.384 (5) Å, respectively, are just within the sum of the van der Waals radii (3.5 Å; Bondi, 1964), indicating that there is little interaction between these atoms. As the bond lengths and angles found for both molecules are similar (Table 2), the differing molecular conformations are presumably due to either the requirements of hydrogen bonding or to crystal packing effects.

In compound (2) (Fig. 2), the *N*-phenylbenzamide group is oriented such that the O atom is in close contact with the Se atom [Se···O 2.829 (2) Å] and the N atom is pointed away [Se···N 4.349 (2) Å]. The two aromatic rings, C1–C6 and C8–C13, are not coplanar, with the dihedral angle between them being 47.42 (10)°. The amide group lies out of the plane of both aromatic rings, the respective dihedral angles between the amide group and the C1–C6 and C8–C13 rings being 35.9 (2) and 13.4 (4)°. Similar to compound (1), the amide N atom is involved in hydrogen bonding with the O atom of an adjacent molecule [N···O^{iii} 2.893 (3), N—H 0.71 (2), H(N)···O^{iii} 2.20 (3) Å and N—H(N)···O^{iii} 167 (2)°; symmetry code: (iii) $\frac{1}{2}+x$, y, $\frac{1}{2}-z$], forming zigzag chains which lie along the *a* axis. Apart from the shorter Se···O interaction, the bond lengths and angles (Table 4) are similar to those of compound (1).

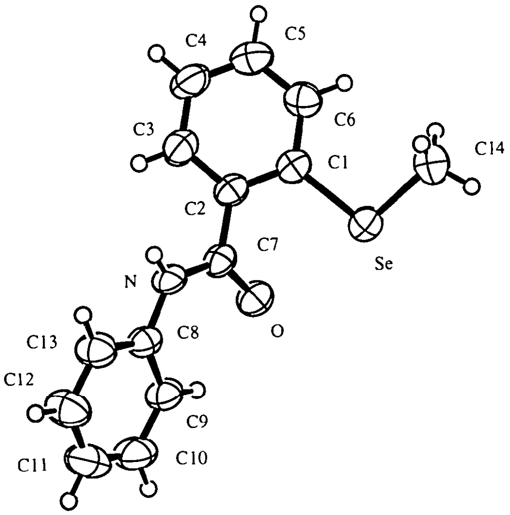


Fig. 2. An *ORTEP*II (Johnson, 1976) drawing of compound (2) with displacement ellipsoids drawn at the 50% probability level.

The bond lengths and angles of compounds (1) and (2) are similar to those found for the the related compound 2-(acetonylseleno)benzanilide (Dupont, Dideberg & Jacquemin, 1990), except for a much shorter Se···O interaction [2.636 (4) Å] being found in the latter compound. The similarity of the structures of the three compounds also extends to the amide group being involved in hydrogen bonding, which links the molecules into chains.

Experimental

Compounds (1) and (2) were prepared according to Fong & Schiesser (1995). Compound (1) was crystallized from an ether–hexane (2:1) solution and compound (2) was recrystallized from ethanol.

Compound (1)

Crystal data

$C_{31}H_{25}NOSeSn$
$M_r = 625.195$
Orthorhombic
Pbca
$a = 9.9321 (10)$ Å
$b = 35.972 (6)$ Å
$c = 30.363 (4)$ Å
$V = 10848 (3)$ Å^3
$Z = 16$
$D_x = 1.531$ Mg m^{-3}
D_m not measured

Mo *Kα* radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9.3$–$14.1°$
$\mu = 2.307$ mm^{-1}
$T = 293 (1)$ K
Plate
0.36 × 0.32 × 0.18 mm
Colourless

Data collection

Enraf–Nonius CAD-4 MachS diffractometer
$\omega/2\theta$ scans
Absorption correction: Gaussian integration from crystal shape (*SHELX76*; Sheldrick, 1976)
$T_{min} = 0.4574$, $T_{max} = 0.6911$
11 506 measured reflections
7182 independent reflections

5124 observed reflections [$I > 2\sigma(I)$]
$R_{int} = 0.0333$
$\theta_{max} = 24.99°$
$h = -1 \rightarrow 11$
$k = -1 \rightarrow 42$
$l = -1 \rightarrow 36$
3 standard reflections
frequency: 150 min
intensity decay: 2%

Refinement

Refinement on F^2
$R(F) = 0.0390$
$wR(F^2) = 0.0786$
$S = 1.022$
7182 reflections
687 parameters
All coordinates refined for H(N) and H(N′); other H atoms riding with all parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 12.18P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.001$
$\Delta\rho_{max} = 0.392$ e Å^{-3}
$\Delta\rho_{min} = -0.294$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (1)*

$U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Sn	0.09321 (4)	0.217941 (11)	0.161675 (12)	0.05020 (11)
Se	0.26083 (6)	0.23904 (2)	0.10403 (2)	0.0580 (2)
O	0.2685 (3)	0.24226 (11)	0.00023 (12)	0.0583 (10)

N	0.0480 (5)	0.23450 (14)	−0.0165 (2)	0.0506 (13)
C1	0.1555 (5)	0.27984 (14)	0.0815 (2)	0.0457 (13)
C2	0.1095 (5)	0.28015 (14)	0.0379 (2)	0.0401 (12)
C3	0.0290 (5)	0.3097 (2)	0.0244 (2)	0.0537 (15)
C4	0.0006 (6)	0.3390 (2)	0.0518 (2)	0.065 (2)
C5	0.0487 (6)	0.3388 (2)	0.0942 (2)	0.072 (2)
C6	0.1260 (6)	0.3095 (2)	0.1084 (2)	0.061 (2)
C7	0.1512 (6)	0.25064 (14)	0.0061 (2)	0.0434 (13)
C8	0.0600 (5)	0.2051 (2)	−0.0467 (2)	0.0456 (14)
C9	0.1647 (6)	0.2026 (2)	−0.0764 (2)	0.064 (2)
C10	0.1685 (7)	0.1733 (2)	−0.1050 (2)	0.085 (2)
C11	0.0710 (8)	0.1464 (2)	−0.1055 (2)	0.081 (2)
C12	−0.0319 (8)	0.1493 (2)	−0.0763 (2)	0.081 (2)
C13	−0.0394 (6)	0.1783 (2)	−0.0477 (2)	0.065 (2)
C14	0.0426 (6)	0.2573 (2)	0.2115 (2)	0.058 (2)
C15	−0.0484 (7)	0.2849 (2)	0.2053 (2)	0.099 (3)
C16	−0.0847 (9)	0.3090 (2)	0.2388 (3)	0.114 (3)
C17	−0.0315 (8)	0.3044 (2)	0.2793 (3)	0.104 (3)
C18	0.0584 (9)	0.2780 (2)	0.2868 (3)	0.107 (3)
C19	0.0959 (8)	0.2543 (2)	0.2528 (2)	0.088 (2)
C20	−0.0925 (6)	0.20231 (15)	0.1316 (2)	0.0524 (14)
C21	−0.1042 (6)	0.1921 (2)	0.0881 (2)	0.060 (2)
C22	−0.2275 (7)	0.1825 (2)	0.0703 (2)	0.069 (2)
C23	−0.3398 (7)	0.1833 (2)	0.0951 (2)	0.079 (2)
C24	−0.3316 (7)	0.1926 (2)	0.1384 (3)	0.094 (2)
C25	−0.2063 (6)	0.2022 (2)	0.1559 (2)	0.089 (2)
C26	0.2018 (6)	0.1735 (2)	0.1904 (2)	0.0494 (14)
C27	0.3308 (6)	0.1784 (2)	0.2061 (2)	0.069 (2)
C28	0.4017 (8)	0.1495 (2)	0.2237 (2)	0.093 (2)
C29	0.3457 (10)	0.1147 (3)	0.2267 (2)	0.097 (3)
C30	0.2200 (9)	0.1094 (2)	0.2106 (2)	0.089 (2)
C31	0.1479 (7)	0.1382 (2)	0.1927 (2)	0.068 (2)
Sn′	0.35931 (4)	0.000542 (11)	0.088104 (12)	0.05312 (11)
Se′	0.22203 (6)	0.00401 (2)	0.15852 (2)	0.0636 (2)
O′	0.4810 (4)	−0.01202 (12)	0.25709 (13)	0.0755 (13)
N′	0.2614 (5)	0.00124 (14)	0.26917 (15)	0.0510 (13)
C1′	0.2537 (5)	−0.04480 (14)	0.1820 (2)	0.0466 (14)
C2′	0.3186 (5)	−0.0498 (2)	0.2217 (2)	0.0492 (14)
C3′	0.3484 (6)	−0.0859 (2)	0.2355 (2)	0.073 (2)
C4′	0.3100 (8)	−0.1163 (2)	0.2107 (3)	0.086 (2)
C5′	0.2407 (8)	−0.1108 (2)	0.1723 (3)	0.083 (2)
C6′	0.2140 (6)	−0.0760 (2)	0.1576 (2)	0.065 (2)
C7′	0.3617 (6)	−0.0181 (2)	0.2508 (2)	0.0509 (14)
C8′	0.2700 (5)	0.03167 (14)	0.2979 (2)	0.0451 (13)
C9′	0.3872 (6)	0.0425 (2)	0.3180 (2)	0.063 (2)
C10′	0.3877 (8)	0.0721 (2)	0.3466 (2)	0.082 (2)
C11′	0.2738 (9)	0.0920 (2)	0.3548 (2)	0.089 (2)
C12′	0.1559 (8)	0.0816 (2)	0.3350 (2)	0.089 (2)
C13′	0.1538 (6)	0.0514 (2)	0.3067 (2)	0.063 (2)
C14′	0.5594 (5)	−0.0171 (2)	0.1017 (2)	0.0507 (14)
C15′	0.5822 (7)	−0.0487 (2)	0.1261 (2)	0.077 (2)
C16′	0.7116 (8)	−0.0607 (2)	0.1351 (3)	0.101 (3)
C17′	0.8191 (7)	−0.0420 (2)	0.1184 (3)	0.091 (2)
C18′	0.7979 (7)	−0.0112 (2)	0.0944 (2)	0.084 (2)
C19′	0.6679 (6)	0.0017 (2)	0.0855 (2)	0.064 (2)
C20′	0.2704 (6)	−0.0375 (2)	0.0431 (2)	0.0544 (15)
C21′	0.1376 (7)	−0.0346 (2)	0.0309 (2)	0.079 (2)
C22′	0.0810 (9)	−0.0586 (2)	0.0002 (3)	0.098 (2)
C23′	0.1587 (10)	−0.0857 (2)	−0.0182 (3)	0.098 (3)
C24′	0.2897 (9)	−0.0892 (2)	−0.0070 (3)	0.093 (2)
C25′	0.3453 (7)	−0.0650 (2)	0.0236 (2)	0.071 (2)
C26′	0.3277 (5)	0.0553 (2)	0.0643 (2)	0.0536 (15)
C27′	0.3261 (7)	0.0861 (2)	0.0918 (2)	0.083 (2)
C28′	0.2938 (8)	0.1211 (2)	0.0769 (3)	0.101 (3)
C29′	0.2643 (8)	0.1263 (2)	0.0336 (3)	0.098 (3)
C30′	0.2642 (7)	0.0972 (3)	0.0053 (3)	0.085 (2)
C31′	0.2975 (6)	0.0621 (2)	0.0210 (2)	0.066 (2)

Table 2. *Selected geometric parameters (Å, °) for (1)*

Sn—C26	2.117 (5)	Sn′—C26′	2.122 (6)
Sn—C14	2.134 (6)	Sn′—C20′	2.126 (6)
Sn—C20	2.134 (5)	Sn′—C14′	2.127 (5)
Sn—Se	2.5320 (7)	Sn′—Se′	2.5389 (7)
Se—C1	1.927 (5)	Se′—C1′	1.921 (5)
O—C7	1.217 (6)	O′—C7′	1.220 (6)
N—C7	1.363 (6)	N′—C7′	1.338 (6)
N—C8	1.403 (6)	N′—C8′	1.401 (6)
C26—Sn—C14	109.3 (2)	C26′—Sn′—C20′	108.5 (2)
C26—Sn—C20	114.7 (2)	C26′—Sn′—C14′	118.8 (2)
C14—Sn—C20	106.0 (2)	C20′—Sn′—C14′	108.8 (2)
C26—Sn—Se	100.13 (15)	C26′—Sn′—Se′	99.31 (15)
C14—Sn—Se	116.5 (2)	C20′—Sn′—Se′	110.49 (15)
C20—Sn—Se	110.56 (15)	C14′—Sn′—Se′	110.64 (15)
C1—Se—Sn	96.68 (14)	C1′—Se′—Sn′	100.33 (14)
C7—N—C8	125.8 (5)	C7′—N′—C8′	128.3 (5)
O—C7—N	122.8 (5)	O′—C7′—N′	124.4 (6)
O—C7—C2	122.4 (5)	O′—C7′—C2′	120.3 (5)
N—C7—C2	114.9 (5)	N′—C7′—C2′	115.3 (5)
C26—Sn—Se—C1	−178.4 (2)	C26′—Sn′—Se′—C1′	−178.1 (2)
C14—Sn—Se—C1	−60.7 (2)	C20′—Sn′—Se′—C1′	68.1 (2)
C20—Sn—Se—C1	60.3 (2)	C14′—Sn′—Se′—C1′	−52.4 (2)
C8—N—C7—O	4.4 (9)	C8′—N′—C7′—O′	1.0 (9)
C8—N—C7—C2	−177.0 (5)	C8′—N′—C7′—C2′	179.3 (5)
C3—C2—C7—O	125.7 (6)	C1′—C2′—C7′—O′	−113.8 (6)
C1—C2—C7—O	−51.3 (7)	C3′—C2′—C7′—O′	65.1 (7)
C3—C2—C7—N	−52.9 (6)	C1′—C2′—C7′—N′	67.8 (7)
C1—C2—C7—N	130.1 (5)	C3′—C2′—C7′—N′	−113.3 (6)
C7—N—C8—C13	142.7 (6)	C7′—N′—C8′—C9′	−12.1 (9)
C7—N—C8—C9	−39.8 (8)	C7′—N′—C8′—C13′	168.8 (5)

Compound (2)

Crystal data

$C_{14}H_{13}NOSe$
$M_r = 290.22$
Orthorhombic
Pbca
$a = 9.777$ (2) Å
$b = 16.692$ (2) Å
$c = 15.8203$ (14) Å
$V = 2581.8$ (7) Å^3
$Z = 8$
$D_x = 1.493$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation (nickel filtered)
$\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 18.8$–$34.6°$
$\mu = 3.794$ mm^{-1}
$T = 293$ (1) K
Plate
0.66 × 0.22 × 0.04 mm
Colourless

Data collection

Enraf–Nonius CAD-4 MachS diffractometer
$\omega/2\theta$ scans
Absorption correction: Gaussian integration from crystal shape (*SHELX*76; Sheldrick, 1976)
$T_{\min} = 0.3036$, $T_{\max} = 0.8599$
3400 measured reflections
2659 independent reflections

2149 observed reflections [$I > 2\sigma(I)$]
$R_{\rm int} = 0.0125$
$\theta_{\max} = 74.92°$
$h = -1 \rightarrow 12$
$k = -1 \rightarrow 20$
$l = -19 \rightarrow 1$
3 standard reflections
frequency: 150 min
intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0290$
$wR(F^2) = 0.0795$
$S = 1.049$
2659 reflections
170 parameters
All coordinates refined for H(N); other H atoms riding with all parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 1.0801P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.216$ e Å^{-3}
$\Delta\rho_{\min} = -0.425$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Se	0.04443 (3)	0.21728 (2)	0.05502 (2)	0.05538 (11)
O	0.0492 (2)	0.16221 (11)	0.22408 (12)	0.0621 (5)
N	0.2559 (2)	0.14000 (12)	0.28273 (13)	0.0463 (4)
C1	0.1760 (2)	0.28094 (13)	0.11507 (15)	0.0442 (5)
C2	0.2232 (2)	0.25693 (13)	0.19475 (14)	0.0429 (5)
C3	0.3160 (3)	0.3049 (2)	0.2381 (2)	0.0553 (6)
C4	0.3620 (3)	0.3760 (2)	0.2032 (2)	0.0666 (7)
C5	0.3163 (3)	0.3993 (2)	0.1248 (2)	0.0644 (7)
C6	0.2254 (3)	0.35232 (14)	0.0807 (2)	0.0542 (6)
C7	0.1687 (2)	0.18249 (14)	0.23479 (14)	0.0438 (5)
C8	0.2294 (2)	0.07190 (13)	0.33304 (14)	0.0450 (5)
C9	0.0989 (3)	0.0437 (2)	0.3504 (2)	0.0558 (6)
C10	0.0834 (3)	−0.0219 (2)	0.4035 (2)	0.0696 (8)
C11	0.1936 (4)	−0.0598 (2)	0.4384 (2)	0.0739 (8)
C12	0.3228 (3)	−0.0320 (2)	0.4211 (2)	0.0733 (8)
C13	0.3404 (3)	0.0333 (2)	0.3687 (2)	0.0600 (6)
C14	0.0722 (5)	0.2586 (3)	−0.0579 (2)	0.0875 (11)

Table 4. *Selected geometric parameters (Å, °) for (2)*

Se—C1	1.920 (2)	N—C7	1.343 (3)
Se—C14	1.935 (3)	N—C8	1.412 (3)
O—C7	1.228 (3)		
C1—Se—C14	99.55 (13)	O—C7—C2	120.7 (2)
C7—N—C8	128.8 (2)	N—C7—C2	116.9 (2)
O—C7—N	122.4 (2)		
C14—Se—C1—C6	19.8 (2)	C1—C2—C7—O	−34.2 (3)
C14—Se—C1—C2	−160.9 (2)	C3—C2—C7—N	−37.0 (3)
C8—N—C7—O	−5.4 (4)	C1—C2—C7—N	146.2 (2)
C8—N—C7—C2	174.2 (2)	C7—N—C8—C13	172.5 (2)
C3—C2—C7—O	142.6 (2)	C7—N—C8—C9	−9.6 (4)

Of the 11 506 reflections measured for compound (1) (9535 of which are unique), 3088 reflections with either large negative F^2 values or showing evidence of overlap with adjacent reflections were omitted from the refinement. Of these 8418 reflections, 7182 were unique and used in the refinement.

For both compounds, program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*93.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry, least-squares-planes data and torsion angles have been deposited with the IUCr (Reference: TA1069). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tetrabenzylgermanium

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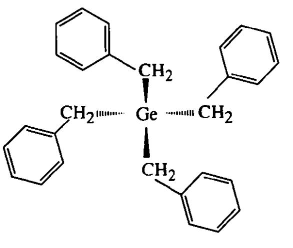
Abstract

Tetrabenzylgermanium, $[Ge(C_7H_7)_4]$, crystallizes with approximate $\bar{4}$ (S_4) molecular symmetry and with almost perfect staggering about the Ge—C bonds. The Ge—C—C angles are significantly larger than the tetrahedral value, with a mean value of 115 (1)°.

Comment

Few tribenzyl or tetrabenzyl derivatives of the elements have been structurally characterized. For germanium, the sole examples appear to be $O[(PhCH_2)_3Ge]_2$ (Glidewell & Liles, 1979) and $S[(PhCH_2)_3Ge]_2$ (Glidewell & Liles, 1982). In the oxo compound, the $(PhCH_2)_3Ge$ fragments have precise threefold rotation symmetry, with the molecule as a whole having $\bar{3}$ (S_6) symmetry, while in the thio compound, although the whole molecule has only twofold rotation symmetry, the $(PhCH_2)_3Ge$ fragments again have approximate threefold local symmetry. In both cases, the benzyl groups are arranged so as to give almost perfect staggering about the Ge—C bonds, but the core conformations of the two compounds are entirely different (see Fig. 2 of Glidewell & Liles, 1982). These observations lead naturally to the question of the conformational behaviour of the corresponding homoleptic tetrabenzyl compound and we report here the structure of tetrabenzylgermanium, $(PhCH_2)_4Ge$, (I).



(I)

The title compound crystallizes in space group $P2_1/n$, with a single molecule in the asymmetric unit. Although no crystallographic symmetry is imposed by the space group, the molecules nonetheless exhibit near $\bar{4}$ (S_4) symmetry (Table 2 and Fig. 1). The lack of crystallographic symmetry in (I) may be contrasted with both

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