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CRYSTAL AND MOLECULAR STRUCTURE OF 13,13-DIMETHYL-8,13-DIHYDRO-5*H*-DIBENZO[*d,g*][1.2.6]DISELENAGERMONINE AND 13,13-DIPHENYL-8,13-DIHYDRO-5*H*-DIBENZO[*d,g*][1.2.6]DISELENASILONINE

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Summary

The crystal and molecular structures of 13,13-dimethyl-8,13-dihydro-5*H*-dibenzo[*d,g*][1.2.6]diselenagermonine and 13,13-diphenyl-8,13-dihydro-5*H*-dibenzo[*d,g*][1.2.6]diselenasilonine have been determined. The intramolecular Ge · · · Se distances in the molecule of the first compound (4.327 and 4.216(1) Å) preclude the possibility of the corresponding transannular interaction. The Si · · · Se distances in the molecule of the second compound are markedly different (3.608 and 4.328(5) Å), the former value corresponding to the transannular attractive Si ← Se interaction. The conformations of the nine-membered heterocycles can be considered as BB → TBB in both cases.

Introduction

The interest in tricyclic compounds with a central heterocycle stems mainly from their structural similarity to well-known compounds that exhibit bioactivity (neuroleptic, psychotropic, etc., for example, to phenathiazine and imipramine derivatives). To study the relation between structure and bioactivity the structural analogues of tricyclic systems mentioned with other heteroatoms were synthesized [1–4]. The character and efficiency of the biological activity are supposed to depend on the value of the dihedral angle between the benzene rings in these tricyclic systems [5].

Our investigations of compounds of analogous structure are also directed towards determining the correlations between molecular structure and biological activity – this requires an investigation of specific electronic effects and features of the spatial structure, including intramolecular transannular interactions.

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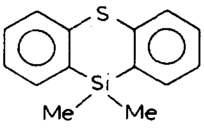
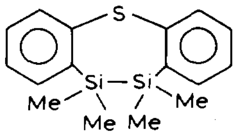
A study of the photoelectronic spectra of tricyclic systems with six- and seven-membered heterocycles, including silicon and sulphur atoms, provides sufficient evidence for the conclusion on the absence of the Si ← S transannular interaction in these molecules in the gas phase [6,7]. The spectra of the charge-transfer complexes of these compounds with tetracyanoethylene confirm this conclusion [8].

X-Ray studies of phenathiazine and thiadisilepine II type compounds also does not reveal any indication of a transannular interaction, viz. characteristic distorsions of the tetrahedral geometry of the silicon atom [9,10].



(I)



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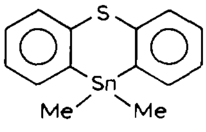
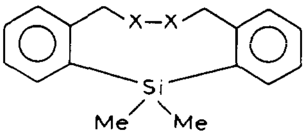


(III)

At the same time, electron-impact fragmentation of phenathiasiline and its analogues suggests the possibility of transannular interaction in these molecules, at least in the excited state [11]. The transannular Sn ← S interaction was also suspected in molecule III on the basis of an X-ray study [12] (the Sn · · · S distance is 3.351(1) Å while the sum of the Van der Waals radii of Sn and S equals 4.04 Å [13]; the tetrahedral geometry of the Sn atom is distorted considerably).

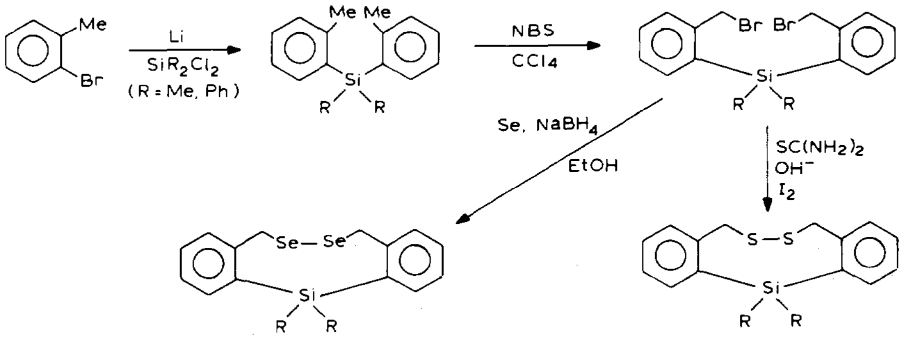
The study of compounds containing heterocycles of increased size allowed the first observation of the transannular Si ← S interaction in the nine-membered cycle of molecule IV [14].



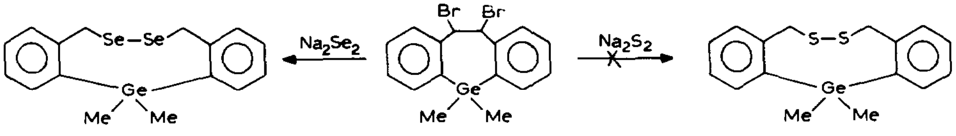
(IV, X = S;
V, X = Se)

However, in the analogous diselenasilonine V the transannular Si ← Se interaction is absent [15].

The synthesis of dichalcogenosilonines was performed in the following way:



An attempt to synthesize dichalcogenogermonines by the same method gave unexpected results. Dibromide VI turned out to be the main product in the bromination stage of bis-(*o*-tolyl)-dimethylgermane. The reaction of VI with sodium diselenide in situ allowed diselenagermonine VII to be obtained, but attempts to synthesize dithiagermonine VIII in a similar way were unsuccessful.



(VII) (VI) (VIII)

To clarify the possibility of a transannular interaction we carried out an X-ray study of compounds VII and IX (Ph analogue of compound V).

Results and discussion

The Ge · · · Se(1) and Ge · · · Se(2) distances of 4.327(1) and 4.216(1) Å in molecule VII (Fig. 1) exceed the sum of the Van der Waals radii of the Ge and Se atoms noticeably (2.02 + 1.97 = 3.99 Å) [13], thus excluding the transannular Ge ← Se interaction in this molecule. The Ge atom has a slightly distorted tetrahedral geometry (Table 1).

The intramolecular Si · · · Se distances in molecule IX (Fig. 2) are considerably different. If the Si · · · Se(2) distance of 4.382(5) Å is significantly larger than the sum of the Van der Waals radii of the Si and Se atoms (1.97 + 1.97 = 3.94 Å) [13], then the Si · · · Se(1) distance of 3.608(5) Å is $\Delta \approx 0.33$ Å smaller than this sum and is indicative of the intramolecular transannular interaction, resulting in a (4 + 1)-coordination of the Si atom and a (2 + 1)-coordination of the Se(1) atom. The Si · · · S distance in molecule IV, which is characterized by the intramolecular Si ← S

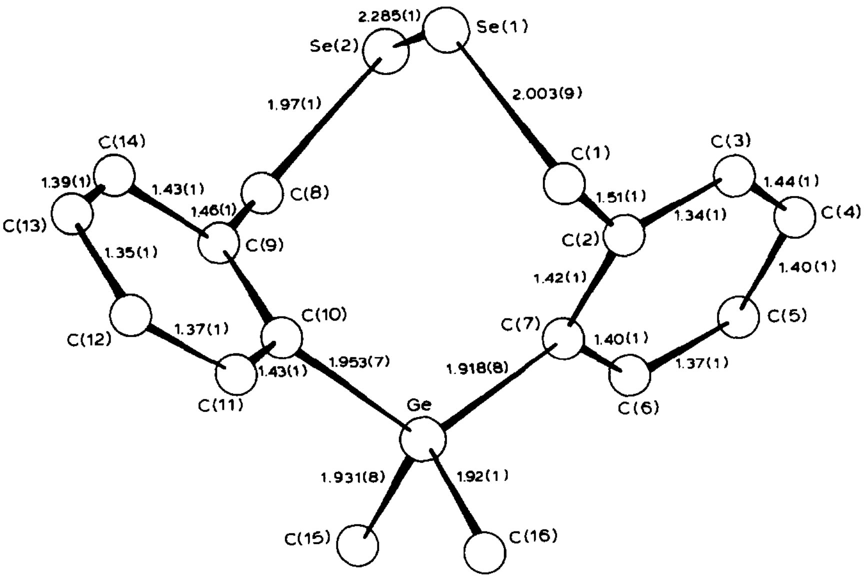


Fig. 1. Structure of molecule VII.

TABLE 1

BONDS ANGLES ω (°) IN MOLECULE VII

C(1)Se(1)Se(2)	104.3(2)	C(8)C(9)C(14)	118.7(7)	C(12)C(13)C(14)	120.9(8)
Se(1)Se(2)C(8)	104.1(3)	C(2)C(3)C(4)	119.5(8)	C(13)C(14)C(9)	120.9(8)
Se(2)C(8)C(9)	116.9(6)	C(3)C(4)C(5)	116.4(9)	C(14)C(9)C(10)	118.9(7)
C(8)C(9)C(10)	122.2(7)	C(4)C(5)C(6)	121.6(9)	GeC(7)C(6)	119.2(6)
C(9)C(10)Ge	124.5(6)	C(5)C(6)C(7)	123.4(8)	GeC(10)C(11)	117.4(5)
C(10)GeC(7)	113.6(3)	C(6)C(7)C(2)	113.5(7)	C(7)GeC(15)	109.9(4)
GeC(7)C(2)	126.4(6)	C(7)C(2)C(3)	125.4(7)	C(7)GeC(16)	109.3(4)
C(7)C(2)C(1)	118.2(7)	C(9)C(10)C(11)	124.5(6)	C(10)GeC(15)	109.1(4)
C(2)C(1)Se(1)	113.9(5)	C(10)C(11)C(12)	122.1(7)	C(10)GeC(16)	109.1(4)
C(1)C(2)C(3)	116.2(7)	C(11)C(12)C(13)	119.6(8)	C(15)GeC(16)	106.4(4)

interaction, is shortened by the value of $\Delta \approx 0.37$ Å in comparison with the sum of the Van der Waals radii, which is close to the contraction observed in IX. As in molecule IV, the tetrahedral coordination of the Si atom in molecule IX is noticeably distorted towards a trigonal-bipyramid coordination, with the Se(1) and C(21) atoms in the axial positions (Table 2). The Si and C(21) atoms are situated on one side of the equatorial plane passing through the C(7), C(10) and C(15) atoms at distances of 0.549(4) and 2.44(1) Å from it. The Se(1) atom is situated on the other side at a distance of 3.047(2) Å. Earlier, only an intermolecular donor–acceptor Si ← Se interaction was observed in the crystal of $H_3SiSeSiH_3$ (X) [16], where the Se atom is coordinated by two Si atoms at distances of 3.61(1) and 3.58(1) Å, which are somewhat longer than in the case of IX. In crystal X the two Si atoms have distorted trigonal-bipyramid (4 + 1)-coordination and the Se atom has (2 + 2)-coordination.

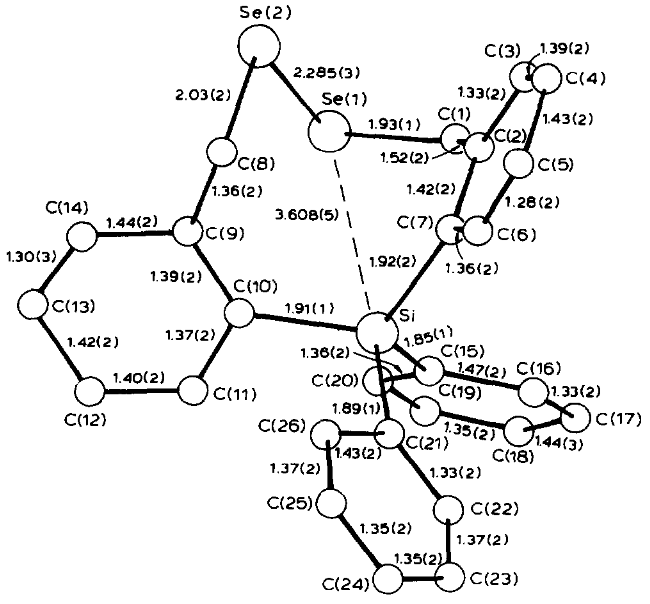


Fig. 2. Structure of molecule IX.

TABLE 2

BOND ANGLES ω (°) IN MOLECULE IX

C(1)Se(1)Se(2)	102.7(4)	C(5)C(6)C(7)	126(1)	C(7)SiC(21)	104.7(6)
Se(1)Se(2)C(8)	100.4(5)	C(7)C(2)C(13)	122(1)	C(10)SiC(15)	110.8(6)
Se(2)C(8)C(9)	114(1)	C(9)C(10)C(11)	121(1)	C(10)SiC(21)	104.7(6)
C(8)C(9)C(10)	128(1)	C(10)C(11)C(12)	122(1)	C(15)SiC(21)	108.8(6)
C(9)C(10)Si	127(1)	C(11)C(12)C(13)	116(1)	C(20)C(15)C(16)	118(1)
C(10)SiC(7)	115.6(6)	C(12)C(13)C(14)	122(2)	C(15)C(16)C(17)	119(1)
SiC(7)C(2)	125(1)	C(13)C(14)C(9)	123(1)	C(16)C(17)C(18)	123(2)
C(7)C(2)C(1)	122(1)	C(14)C(9)C(10)	115(1)	C(17)C(18)C(19)	117(2)
C(2)C(1)Se(1)	115(1)	C(6)C(7)Si	115(1)	C(18)C(19)C(20)	121(1)
Se(2)Se(1)Si	93.3(1)	C(11)C(10)Si	111(1)	C(19)C(20)C(15)	121(1)
C(1)Se(1)Si	66.6(4)	Se(1)SiC(7)	72.9(5)	C(26)C(21)C(22)	116(1)
C(1)C(2)C(3)	119(1)	Se(1)SiC(10)	69.8(4)	C(21)C(22)C(23)	121(1)
C(8)C(9)C(14)	117(1)	Se(1)SiC(15)	77.2(4)	C(22)C(23)C(24)	124(2)
C(2)C(3)C(4)	123(1)	Se(1)SiC(21)	173.3(5)	C(23)C(24)C(25)	117(2)
C(3)C(4)C(5)	116(1)	C(7)SiC(15)	109.5(6)	C(24)C(25)C(26)	120(2)
C(4)C(5)C(6)	120(4)			C(25)C(26)C(21)	121(1)

In both the IX and X structures the C–Si $\cdots$ Se and Se–Si $\cdots$ Se angles, respectively, between the axial substituents are close to 180°.

The Se–Se distances in molecules VII and IX are equal (2.285(3) Å) and in fact coincide with those found in molecule V (2.288(1) Å).

The endocyclic torsion angles around the Se–Se (S–S) bonds depend evidently on the presence of the transannular interaction. Whereas in molecule IX, as well as in IV, these angles are close to the ideal value of 90° (87.9 and 88.6°, respectively), in VII and V they are decreased to 75.6 and 73.7°, respectively [15].

The nine-membered GeC(7)C(2)C(1)Se(1)Se(2)C(8)C(9)C(10) heterocycle of molecule VII is characterized by the following Cremer–Pople parameters [17]: φ_2 273.3°, q_2 2.424 Å, φ_3 93.4°, q_3 0.396 Å, φ_4 280.0°, q_4 0.247 Å, Q 2.469 Å. In fact, these values coincide with those observed in molecule V. The conformation of the heterocycle in VII is defined mainly by the contributions of the canonical TBB and BB forms ($q_2 \geqslant q_3$, q_4), with the former type predominating. Noteworthy is also the approximate C_2 symmetry of molecule VII, also observed in molecule V.

Further, the Cremer–Pople parameters of the heterocycle in the molecule IX (φ_2 112.9°, q_2 2.318 Å, φ_3 262.8°, q_3 0.435 Å, φ_4 128.4°, q_4 0.315 Å, Q 2.379 Å) allow the same conformation (intermediate between TBB and BB) as the heterocycle in IV to be ascribed to it. The difference of the heterocycles in V and VII from the heterocycles in IV and IX lies in the different positioning of the corresponding atoms around the contour of heterocycles of a similar form.

The dihedral angles between the planes of the benzene rings in the pairs of molecules V and VII (80.0 and 83.1°), and accordingly IV and IX (97.1 and 98.1°), are similar.

In crystal VII a number of intermolecular Se $\cdots$ C contacts are observed at distances which are close to the sum of the Van der Waals radii (3.67 Å [13]): Se(1) $\cdots$ C(12)($-$x, $1-y$, $-z$) 3.75(1) Å, Se(1) $\cdots$ C(11)($-x$, $1-y$, $-z$) 3.79(1) Å, Se(2) $\cdots$ C(3)(x, y, $1+z$) 3.86(1) Å, Se(2) $\cdots$ C(4)(x, $1/2-y$, $1/2+z$) 3.92(1) Å. In crystal IX all the intermolecular distances involving Se atoms exceed 4 Å.

Experimental

Synthesis of dibromide VI

15.96 g (0.095 mol) of *N*-bromosuccinimide and 0.1 g of benzoyl peroxide were added in small portions to a solution of 9 g (0.0477 mol) of bis(*o*-tolyl)dimethylgermane in 50 ml of absolute CCl_4. The mixture was refluxed under stirring for 4 h. The succinimide was filtered off and the solvent was evaporated. The crystallizing oil obtained was chromatographed on a silica gel column, with petroleum ether as eluant. 9 g of a crystalline product was obtained, m.p. 134–135°C, *M* 442 (mass

TABLE 3

ATOMIC COORDINATES ($\times 10^5$ for Ge and Se; $\times 10^4$ for C; $\times 10^3$ for H) AND THERMAL PARAMETERS (B_{iso}^{eq} for non-H, B_{iso} for H atoms)

Atom	x	y	z	B (Å^2)
Ge	15674(2)	59386(6)	1906(13)	2.26(2)
Se(1)	4468(3)	40557(7)	11713(14)	3.94(3)
Se(2)	11102(3)	38076(6)	29999(15)	4.01(3)
C(1)	765(3)	4515(5)	−1033(13)	3.5(3)
C(2)	1297(2)	4277(5)	−1280(11)	2.6(3)
C(3)	1382(3)	3531(5)	−2024(13)	3.9(3)
C(4)	1890(3)	3249(6)	−2258(15)	5.5(4)
C(5)	2263(3)	3770(6)	−1611(16)	6.2(4)
C(6)	2157(3)	4531(5)	−879(13)	3.9(3)
C(7)	1668(2)	4821(5)	−617(11)	2.5(3)
C(8)	1305(3)	4920(6)	3846(12)	4.2(3)
C(9)	969(3)	5608(6)	3408(11)	3.0(3)
C(10)	1014(2)	6054(5)	1858(11)	2.1(2)
C(11)	656(2)	6697(5)	1512(12)	2.8(3)
C(12)	263(2)	6851(5)	2645(12)	3.1(3)
C(13)	215(3)	6399(6)	4145(13)	4.0(3)
C(14)	556(3)	5777(6)	4557(13)	3.9(3)
C(15)	2174(3)	6332(7)	1292(14)	5.4(4)
C(16)	1449(3)	6650(6)	−1811(14)	4.7(3)
H(1.1)	68(2)	485(5)	−79(11)	5(2)
H(1.2)	56(2)	422(3)	−207(8)	2(1)
H(3)	116(2)	313(3)	−239(8)	1(1)
H(4)	202(5)	262(5)	−283(11)	5(2)
H(5)	256(3)	349(5)	−150(2)	11(3)
H(6)	239(2)	484(3)	−39(8)	1(1)
H(8.1)	157(2)	501(4)	369(5)	4(2)
H(8.2)	137(2)	486(5)	511(12)	6(2)
H(11)	67(1)	704(3)	57(8)	1(1)
H(12)	1(2)	728(5)	260(10)	5(2)
H(13)	−7(2)	648(4)	510(10)	4(2)
H(14)	51(2)	529(4)	543(10)	3(2)
H(15.1)	237(2)	613(4)	111(8)	2(2)
H(15.2)	215(2)	646(5)	223(12)	9(2)
H(15.2)	218(2)	706(2)	102(13)	15(3)
H(16.1)	159(2)	622(4)	−244(10)	6(2)
H(16.2)	151(2)	728(5)	−150(11)	8(2)
H(16.3)	122(2)	655(4)	−222(10)	5(2)

TABLE 4

ATOMIC COORDINATES (10^4 for Si, Se and C; $\times 10^3$ for H) AND THERMAL PARAMETERS ($B_{\rm iso}^{\rm eq}$ for non-H, $B_{\rm iso}$ for H atoms)

Atom	x	y	z	B (Å^2)
Si	1775(3)	3002(2)	3253(5)	2.7(1)
Se(1)	1920(2)	2236(1)	6975(3)	4.75(5)
Se(2)	791(2)	1374(1)	6260(3)	5.57(6)
C(1)	2952(9)	1851(10)	5962(16)	3.5(4)
C(2)	2571(9)	1484(8)	4441(17)	3.1(4)
C(3)	2731(10)	735(9)	4256(18)	3.5(5)
C(4)	2432(11)	347(9)	2906(19)	4.1(5)
C(5)	2006(12)	820(10)	1658(19)	4.3(6)
C(6)	1883(10)	1546(7)	1853(18)	2.8(4)
C(7)	2120(9)	1930(9)	3182(17)	3.0(4)
C(8)	93(11)	1877(11)	4334(19)	4.6(5)
C(9)	44(10)	2622(9)	4403(15)	3.0(4)
C(10)	649(9)	3203(9)	3972(14)	2.6(4)
C(11)	469(10)	3780(9)	3992(17)	3.0(4)
C(12)	−325(11)	4275(10)	4444(18)	4.3(5)
C(13)	−925(10)	3721(10)	4908(17)	4.2(5)
C(14)	−767(10)	2983(11)	4871(16)	4.0(5)
C(15)	2783(9)	3556(8)	4339(15)	2.8(4)
C(16)	3694(9)	3472(10)	3886(17)	3.6(5)
C(17)	4442(10)	3856(12)	4639(20)	4.9(6)
C(18)	4404(11)	4374(10)	5851(21)	4.8(6)
C(19)	3571(11)	4444(10)	6277(19)	4.3(5)
C(20)	2744(10)	4036(9)	5502(18)	3.8(5)
C(21)	1506(10)	3372(8)	1265(16)	2.9(4)
C(22)	2078(10)	3794(10)	615(17)	3.9(5)
C(23)	1789(12)	4038(11)	−839(20)	5.4(6)
C(24)	918(12)	3909(10)	−1685(16)	4.7(6)
C(25)	323(11)	3470(12)	−1073(18)	5.1(6)
C(26)	579(10)	3229(11)	385(18)	4.7(5)
H(1.1)	348(10)	128(9)	665(10)	1(4)
H(1.2)	304(10)	234(9)	581(10)	9(5)
H(3)	254(8)	38(7)	491(10)	1(3)
H(4)	216(10)	−28(9)	277(10)	12(4)
H(5)	130(10)	50(9)	59(10)	2(4)
H(6)	177(10)	184(10)	122(10)	4(4)
H(8.1)	−39(9)	166(8)	417(10)	6(4)
H(8.2)	36(10)	191(9)	379(10)	13(4)
H(11)	86(7)	436(5)	391(10)	1(2)
H(12)	−16(8)	501(8)	453(10)	6(4)
H(13)	−177(10)	386(9)	483(10)	5(5)
H(14)	−83(7)	235(6)	506(10)	2(2)
H(16)	374(7)	301(6)	337(10)	1(2)
H(17)	496(10)	378(9)	476(10)	15(4)
H(18)	516(10)	466(9)	650(10)	15(4)
H(19)	358(10)	499(10)	694(10)	8(5)
H(20)	216(10)	394(8)	565(10)	5(3)
H(22)	240(10)	389(9)	131(10)	8(4)
H(23)	193(10)	440(9)	−100(10)	6(4)
H(24)	65(7)	429(6)	−251(10)	4(2)
H(25)	−10(10)	330(9)	−136(10)	11(4)
H(26)	4(10)	285(10)	95(10)	9(5)

spectrum). ^{1}H NMR spectrum (ppm): 0.85 s (6H, $GeMe_2$), 6.40s (2H, CBrH), 7.17–8.00 m (8H, aromatic protons).

Synthesis of diselenagermonine VII

50 ml of absolute ethanol was added to a cooled (to 0°C) mixture of 1.07 g (0.0135 mol) of selenium and 0.342 g (0.009 mol) of $NaBH_4$. The mixture was stirred under reflux for 1.5 h and then 2 g (0.0045 mol) of dibromide VI in 30 ml of absolute ethanol was added gradually. The mixture was refluxed under stirring for 5–6 h. After the solvent was evaporated, the residue was chromatographed on a silica gel column, with petroleum ether/chloroform (20/1) mixture as eluant. Recrystallization from petroleum ether yielded 0.6 g of a yellow crystalline powder of VII, m.p. 154–156°C.

X-Ray structural study of VII and IX

Crystals of VII are orthorhombic, a 26.755(2), b 16.090(2), c 7.5661(6) Å, V 3257.1(5) Å^3, d_{calc} 1.48 g cm^{-3}, $Z = 8$; $C_{16}H_{18}GeSe_2$, space group $Pccn$. Crystals of IX are monoclinic, a 14.4877(8), b 17.274(1), c 9.1623(7) Å, β 102.228(5)°, V 2241.0(3) Å^3, d_{calc} 1.54 g cm^{-3}, $Z = 8$; $C_{26}H_{22}Se_2Si$, space group $C2/c$.

The unit cell parameters and intensities of 1527 (VII) and 2287 (IX) independent reflections were measured with a four-circle Hilger & Watts autodiffractometer at 20°C (λ(Mo-K_α)) graphite monochromator, $\theta/2\theta$ scan, $\theta_{max} = 25°$ (VII) and 28° (IX)). The structure of VII was solved by the heavy atom technique, the initial Ge and Se coordinates being taken equal to those of Si and Se in the isostructural analogue V. The structure of IX was solved by direct methods using the MULTAN program. Both structures were refined by full-matrix least-squares with anisotropic thermal parameters for non-hydrogen atoms, whose positions in structure VII were calculated (benzene rings) or located in the difference maps (Me groups); in structure IX they were calculated. For the structure VII (μ(Mo-K_α) 43.8 cm^{-1}) an absorption correction was applied using the DIFABS program [18]. The final values of the discrepancy factors were: VII: $R = 0.039$ ($R_w = 0.034$) for 1435 reflections with $I \geqslant 2\sigma$; IX: $R = 0.075$ ($R_w = 0.071$) for 2080 reflections with $I \geqslant 2\sigma$. All calculations were performed with an Eclipse S/200 computer using INEXTL programs [19]. The atomic coordinates are given in Tables 3 and 4.

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