© 2001 American Chemical Society, Organometallics, Tacke om010816o Supporting Info Page 1

Reinhold Tacke,* Thomas Schmid, Christian Burschka, Martin Penka, and Horst Surburg

Syntheses, Structures, and Sensory Characteristics of the Perfume Ingredient Majantol® and Its Analogs Sila-majantol and Germa-majantol: A Study on C/Si/Ge Bioisosterism

Organometallics

Table 1. Crystal data and structure refinement for **1a**.

Identification code	**1a**
Empirical formula	C12 H18 O
Formula weight	178.26
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 25.127(5) A alpha = 90 deg. b = 9.784(2) A beta = 104.11(3) deg. c = 8.9928(18) A gamma = 90 deg.
Volume	2144.1(7) A^3
Z, Calculated density	8, 1.104 Mg/m^3
Absorption coefficient	0.068 mm^-1
F(000)	784
Crystal size	.5 x .4 x .4 mm
Theta range for data collection	2.24 to 26.37 deg.
Limiting indices	-31<=h<=31, -12<=k<=12, -11<=l<=11
Reflections collected / unique	10881 / 2181 [R(int) = 0.0513]
Completeness to theta = 26.37	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2181 / 0 / 128
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R1 = 0.0440, wR2 = 0.1204
R indices (all data)	R1 = 0.0530, wR2 = 0.1262
Largest diff. peak and hole	0.279 and -0.174 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	894(1)	7541(1)	806(1)	29(1)
C(2)	773(1)	8979(1)	1285(1)	30(1)
C(3)	506(1)	7186(2)	-735(2)	42(1)
C(4)	1482(1)	7539(2)	626(2)	38(1)
C(5)	819(1)	6466(1)	2001(1)	33(1)
C(6)	1197(1)	6607(1)	3575(1)	28(1)
C(7)	1706(1)	5971(1)	3936(1)	30(1)
C(8)	2067(1)	6088(1)	5368(1)	31(1)
C(9)	1912(1)	6887(1)	6466(1)	35(1)
C(10)	1405(1)	7518(1)	6140(2)	39(1)
C(11)	1049(1)	7375(1)	4714(2)	34(1)
C(12)	2608(1)	5356(2)	5719(2)	40(1)
O(1A)	208(1)	9201(1)	1235(2)	43(1)
O(1)	208(1)	9201(1)	1235(2)	43(1)

Table 3. Bond lengths [A] and angles [deg] for **1a**.

C(1)-C(2)	1.5225(17)
C(1)-C(4)	1.5266(17)
C(1)-C(3)	1.5272(17)
C(1)-C(5)	1.5475(17)
C(2)-O(1A)	1.4264(16)
C(5)-C(6)	1.5060(17)
C(6)-C(7)	1.3889(17)
C(6)-C(11)	1.3912(18)
C(7)-C(8)	1.3881(18)
C(8)-C(9)	1.3884(18)
C(8)-C(12)	1.4994(18)
C(9)-C(10)	1.381(2)
C(10)-C(11)	1.380(2)
C(2)-C(1)-C(4)	107.18(10)
C(2)-C(1)-C(3)	109.88(10)
C(4)-C(1)-C(3)	108.91(10)
C(2)-C(1)-C(5)	111.46(10)
C(4)-C(1)-C(5)	110.91(10)
C(3)-C(1)-C(5)	108.47(10)
O(1A)-C(2)-C(1)	113.39(11)
C(6)-C(5)-C(1)	115.80(10)
C(7)-C(6)-C(11)	117.76(11)
C(7)-C(6)-C(5)	120.79(11)
C(11)-C(6)-C(5)	121.45(11)
C(8)-C(7)-C(6)	122.45(11)
C(7)-C(8)-C(9)	118.25(11)
C(7)-C(8)-C(12)	120.61(11)
C(9)-C(8)-C(12)	121.14(11)
C(10)-C(9)-C(8)	120.34(12)
C(11)-C(10)-C(9)	120.48(12)
C(10)-C(11)-C(6)	120.70(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	24(1)	33(1)	28(1)	-1(1)	5(1)	2(1)
C(2)	30(1)	29(1)	32(1)	7(1)	8(1)	3(1)
C(3)	34(1)	55(1)	34(1)	-7(1)	2(1)	2(1)
C(4)	28(1)	50(1)	36(1)	-1(1)	10(1)	5(1)
C(5)	29(1)	26(1)	40(1)	2(1)	4(1)	0(1)
C(6)	30(1)	22(1)	34(1)	6(1)	9(1)	0(1)
C(7)	34(1)	23(1)	34(1)	1(1)	10(1)	3(1)
C(8)	32(1)	23(1)	36(1)	6(1)	8(1)	1(1)
C(9)	44(1)	31(1)	28(1)	5(1)	6(1)	1(1)
C(10)	52(1)	36(1)	32(1)	4(1)	19(1)	10(1)
C(11)	35(1)	33(1)	39(1)	9(1)	16(1)	9(1)
C(12)	34(1)	37(1)	45(1)	5(1)	3(1)	7(1)
O(1A)	35(1)	47(1)	48(1)	10(1)	14(1)	17(1)
O(1)	35(1)	47(1)	48(1)	10(1)	14(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1a**.

	x	y	z	U(eq)
H(2A)	994	9149	2341	36
H(2B)	890	9646	600	36
H(3A)	528	7896	-1486	63
H(3B)	129	7129	-616	63
H(3C)	612	6304	-1092	63
H(4A)	1514	8181	-185	57
H(4B)	1579	6618	354	57
H(4C)	1732	7818	1594	57
H(5A)	436	6515	2100	39
H(5B)	873	5547	1600	39
H(7)	1811	5435	3173	36
H(9)	2156	7001	7448	42
H(10)	1300	8054	6902	46
H(11)	700	7805	4507	41
H(12A)	2684	4988	6763	60
H(12B)	2899	5996	5633	60
H(12C)	2593	4605	4988	60
H(1A)	53(17)	9710(40)	560(40)	64
H(1)	147(17)	9320(40)	2030(50)	64

Table 6. Crystal data and structure refinement for **1b**.

Identification code	**1b**
Empirical formula	C11 H18 O Si
Formula weight	194.34
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 9.7441(19) A alpha = 90 deg. b = 27.492(6) A beta = 92.46(3) deg. c = 8.9331(18) A gamma = 90 deg.
Volume	2390.9(8) A^3
Z, Calculated density	8, 1.080 Mg/m^3
Absorption coefficient	0.161 mm^-1
F(000)	848
Crystal size	.5 x .5 x .4 mm
Theta range for data collection	2.09 to 26.38 deg.
Limiting indices	-12<=h<=11, -27<=k<=34, -11<=l<=11
Reflections collected / unique	13824 / 4848 [R(int) = 0.0504]
Completeness to theta = 26.38	99.3 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4848 / 0 / 247
Goodness-of-fit on F^2	0.973
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.1063
R indices (all data)	R1 = 0.0579, wR2 = 0.1142
Largest diff. peak and hole	0.234 and -0.260 e.A^-3

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(2)	6220(2)	1709(1)	-2104(2)	36(1)
C(3)	8369(2)	2218(1)	-68(3)	60(1)
C(4)	8390(2)	1107(1)	-478(2)	46(1)
C(5)	6150(2)	1602(1)	1316(2)	37(1)
C(6)	5093(2)	1205(1)	1151(2)	34(1)
C(7)	5358(2)	741(1)	1697(2)	37(1)
C(8)	4399(2)	367(1)	1576(2)	40(1)
C(9)	3141(2)	464(1)	858(2)	45(1)
C(10)	2856(2)	920(1)	284(2)	46(1)
C(11)	3815(2)	1291(1)	434(2)	41(1)
C(12)	4708(2)	-127(1)	2248(2)	53(1)
C(22)	3128(2)	2834(1)	-807(2)	47(1)
C(23)	3283(2)	3915(1)	-27(2)	47(1)
C(24)	1517(2)	3239(1)	1798(2)	50(1)
C(25)	678(2)	3441(1)	-1487(2)	38(1)
C(26)	-272(2)	3856(1)	-1157(2)	32(1)
C(27)	-85(2)	4315(1)	-1785(2)	34(1)
C(28)	-940(2)	4705(1)	-1492(2)	35(1)
C(29)	-1991(2)	4635(1)	-520(2)	39(1)
C(30)	-2200(2)	4182(1)	119(2)	40(1)
C(31)	-1347(2)	3795(1)	-206(2)	37(1)
C(32)	-744(2)	5191(1)	-2235(2)	48(1)
O(1)	5362(1)	2131(1)	-2093(1)	43(1)
O(2)	4386(2)	2739(1)	19(1)	49(1)
Si(1)	7299(1)	1659(1)	-312(1)	33(1)
Si(2)	2165(1)	3369(1)	-85(1)	32(1)

Table 8. Bond lengths [A] and angles [deg] for **1b**.

C(2)-O(1)	1.4304(19)
C(2)-Si(1)	1.8823(17)
C(3)-Si(1)	1.865(2)
C(4)-Si(1)	1.8614(19)
C(5)-C(6)	1.504(2)
C(5)-Si(1)	1.8792(19)
C(6)-C(7)	1.387(2)
C(6)-C(11)	1.395(2)
C(7)-C(8)	1.389(2)
C(8)-C(9)	1.384(3)
C(8)-C(12)	1.511(3)
C(9)-C(10)	1.379(3)
C(10)-C(11)	1.387(3)
C(22)-O(2)	1.428(2)
C(22)-Si(2)	1.8738(18)
C(23)-Si(2)	1.854(2)
C(24)-Si(2)	1.8567(19)
C(25)-C(26)	1.506(2)
C(25)-Si(2)	1.8842(18)
C(26)-C(31)	1.387(2)
C(26)-C(27)	1.395(2)
C(27)-C(28)	1.391(2)
C(28)-C(29)	1.384(3)
C(28)-C(32)	1.506(2)
C(29)-C(30)	1.389(2)
C(30)-C(31)	1.388(2)
O(1)-C(2)-Si(1)	111.06(10)
C(6)-C(5)-Si(1)	114.36(11)
C(7)-C(6)-C(11)	117.82(16)
C(7)-C(6)-C(5)	121.15(15)
C(11)-C(6)-C(5)	121.03(15)
C(6)-C(7)-C(8)	122.56(16)
C(9)-C(8)-C(7)	118.30(16)
C(9)-C(8)-C(12)	120.91(17)
C(7)-C(8)-C(12)	120.77(17)
C(10)-C(9)-C(8)	120.42(18)
C(9)-C(10)-C(11)	120.64(17)
C(10)-C(11)-C(6)	120.25(17)
O(2)-C(22)-Si(2)	113.41(11)
C(26)-C(25)-Si(2)	114.28(10)
C(31)-C(26)-C(27)	118.10(15)
C(31)-C(26)-C(25)	121.02(15)
C(27)-C(26)-C(25)	120.88(15)
C(28)-C(27)-C(26)	122.18(16)
C(29)-C(28)-C(27)	118.36(15)
C(29)-C(28)-C(32)	120.80(16)
C(27)-C(28)-C(32)	120.83(16)
C(28)-C(29)-C(30)	120.59(17)
C(31)-C(30)-C(29)	120.12(17)
C(26)-C(31)-C(30)	120.63(16)
C(4)-Si(1)-C(3)	111.25(11)
C(4)-Si(1)-C(5)	110.87(8)
C(3)-Si(1)-C(5)	109.06(10)
C(4)-Si(1)-C(2)	106.99(8)
C(3)-Si(1)-C(2)	109.09(9)
C(5)-Si(1)-C(2)	109.53(8)
C(23)-Si(2)-C(24)	110.60(9)
C(23)-Si(2)-C(22)	110.00(10)
C(24)-Si(2)-C(22)	110.87(10)
C(23)-Si(2)-C(25)	111.55(8)
C(24)-Si(2)-C(25)	109.95(9)
C(22)-Si(2)-C(25)	103.68(7)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **1b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(2)	42(1)	32(1)	33(1)	-2(1)	5(1)	11(1)
C(3)	62(1)	50(1)	67(1)	-1(1)	-1(1)	-19(1)
C(4)	43(1)	47(1)	47(1)	3(1)	-1(1)	11(1)
C(5)	45(1)	32(1)	32(1)	-1(1)	0(1)	2(1)
C(6)	37(1)	37(1)	28(1)	0(1)	7(1)	2(1)
C(7)	40(1)	39(1)	31(1)	3(1)	3(1)	4(1)
C(8)	49(1)	38(1)	34(1)	0(1)	12(1)	-2(1)
C(9)	41(1)	48(1)	45(1)	-6(1)	11(1)	-8(1)
C(10)	35(1)	56(1)	48(1)	-3(1)	3(1)	2(1)
C(11)	41(1)	40(1)	42(1)	2(1)	4(1)	8(1)
C(12)	68(1)	39(1)	53(1)	8(1)	14(1)	-4(1)
C(22)	51(1)	44(1)	46(1)	-17(1)	-10(1)	17(1)
C(23)	48(1)	39(1)	55(1)	0(1)	0(1)	-1(1)
C(24)	58(1)	53(1)	39(1)	6(1)	4(1)	6(1)
C(25)	44(1)	35(1)	34(1)	-4(1)	0(1)	2(1)
C(26)	34(1)	34(1)	28(1)	-1(1)	-4(1)	-1(1)
C(27)	32(1)	41(1)	29(1)	3(1)	-1(1)	-3(1)
C(28)	37(1)	35(1)	35(1)	5(1)	-6(1)	-3(1)
C(29)	36(1)	37(1)	45(1)	1(1)	0(1)	5(1)
C(30)	34(1)	42(1)	46(1)	5(1)	8(1)	2(1)
C(31)	38(1)	33(1)	40(1)	5(1)	3(1)	-3(1)
C(32)	55(1)	41(1)	47(1)	13(1)	-5(1)	-1(1)
O(1)	59(1)	41(1)	30(1)	-3(1)	-3(1)	22(1)
O(2)	57(1)	52(1)	36(1)	-15(1)	-10(1)	26(1)
Si(1)	34(1)	29(1)	35(1)	2(1)	-1(1)	0(1)
Si(2)	38(1)	26(1)	31(1)	-2(1)	2(1)	5(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1b**.

	x	y	z	U(eq)
H(2A)	6827	1728	-2963	43
H(2B)	5641	1415	-2232	43
H(3A)	8892	2202	892	90
H(3B)	7771	2505	-84	90
H(3C)	9005	2240	-886	90
H(4A)	8880	1123	-1412	69
H(4B)	7809	816	-484	69
H(4C)	9056	1092	374	69
H(5A)	6727	1541	2236	44
H(5B)	5671	1916	1448	44
H(7)	6229	675	2171	44
H(9)	2469	214	760	53
H(10)	1994	981	-219	55
H(11)	3602	1605	46	49
H(12A)	4400	-137	3278	79
H(12B)	5700	-187	2253	79
H(12C)	4226	-378	1650	79
H(22A)	2536	2542	-771	57
H(22B)	3330	2893	-1869	57
H(23A)	2764	4195	324	71
H(23B)	3599	3982	-1033	71
H(23C)	4078	3856	659	71
H(24A)	2296	3203	2521	75
H(24B)	980	2938	1761	75
H(24C)	935	3509	2107	75
H(25A)	1045	3492	-2492	45
H(25B)	141	3135	-1521	45
H(27)	650	4362	-2434	41
H(29)	-2574	4899	-288	47
H(30)	-2928	4137	780	48
H(31)	-1502	3485	227	44
H(32A)	-1621	5301	-2694	72
H(32B)	-67	5158	-3009	72
H(32C)	-415	5428	-1484	72
H(1)	5040(20)	2165(9)	-2940(30)	65
H(2)	4840(30)	2541(10)	-480(30)	73

Table 11. Crystal data and structure refinement for **1c**.

Identification code	**1c**
Empirical formula	C11 H18 Ge O
Formula weight	238.84
Temperature	263(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 9.774(2) A alpha = 90 deg. b = 27.597(6) A beta = 91.26(3) deg. c = 9.0082(18) A gamma = 90 deg.
Volume	2429.3(8) A^3
Z, Calculated density	8, 1.306 Mg/m^3
Absorption coefficient	2.486 mm^-1
F(000)	992
Crystal size	.5 x .5 x .4 mm
Theta range for data collection	2.38 to 24.71 deg.
Limiting indices	-11<=h<=7, -32<=k<=32, -10<=l<=10
Reflections collected / unique	11159 / 4115 [R(int) = 0.0782]
Completeness to theta = 24.71	99.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4115 / 0 / 248
Goodness-of-fit on F^2	0.938
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.0925
R indices (all data)	R1 = 0.0572, wR2 = 0.1004
Largest diff. peak and hole	0.506 and -0.544 e.A^-3

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1c**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(2)	6491(4)	3278(1)	7011(3)	50(1)
C(3)	8376(5)	2797(2)	4579(5)	78(1)
C(4)	8379(5)	3944(1)	5127(5)	70(1)
C(5)	5785(4)	3420(1)	3578(3)	54(1)
C(6)	4811(4)	3825(1)	3887(3)	45(1)
C(7)	4977(4)	4279(1)	3247(3)	49(1)
C(8)	4082(4)	4664(1)	3514(3)	52(1)
C(9)	3030(4)	4589(1)	4484(4)	58(1)
C(10)	2857(4)	4142(2)	5140(4)	60(1)
C(11)	3718(4)	3765(1)	4837(4)	54(1)
C(12)	4292(5)	5145(1)	2759(4)	73(1)
C(22)	3318(5)	2757(2)	10357(6)	89(2)
C(23)	3401(5)	3885(1)	9572(4)	68(1)
C(24)	1177(5)	3200(2)	7986(4)	76(1)
C(25)	969(4)	3406(1)	11438(4)	58(1)
C(26)	-34(4)	3812(1)	11231(3)	47(1)
C(27)	260(4)	4278(1)	11736(3)	52(1)
C(28)	-660(4)	4658(1)	11593(4)	55(1)
C(29)	-1893(4)	4568(2)	10865(4)	61(1)
C(30)	-2200(4)	4117(2)	10317(4)	65(1)
C(31)	-1292(4)	3742(1)	10511(4)	58(1)
C(32)	-325(5)	5151(2)	12237(4)	76(1)
O(1)	5646(3)	2858(1)	7054(2)	64(1)
O(2)	4674(3)	2771(1)	9902(3)	65(1)
Ge(1)	7274(1)	3360(1)	5053(1)	45(1)
Ge(2)	2232(1)	3326(1)	9793(1)	47(1)

Table 13. Bond lengths [A] and angles [deg] for **1c**.

C(2)-O(1)	1.424(4)
C(2)-Ge(1)	1.951(3)
C(3)-Ge(1)	1.944(4)
C(4)-Ge(1)	1.940(4)
C(5)-C(6)	1.499(5)
C(5)-Ge(1)	1.956(4)
C(6)-C(7)	1.389(4)
C(6)-C(11)	1.393(5)
C(7)-C(8)	1.401(5)
C(8)-C(9)	1.379(5)
C(8)-C(12)	1.508(5)
C(9)-C(10)	1.379(5)
C(10)-C(11)	1.371(5)
C(22)-O(2)	1.396(6)
C(22)-Ge(2)	1.956(4)
C(23)-Ge(2)	1.933(4)
C(24)-Ge(2)	1.939(4)
C(25)-C(26)	1.499(5)
C(25)-Ge(2)	1.961(4)
C(26)-C(27)	1.391(5)
C(26)-C(31)	1.391(5)
C(27)-C(28)	1.386(5)
C(28)-C(29)	1.383(5)
C(28)-C(32)	1.511(5)
C(29)-C(30)	1.369(5)
C(30)-C(31)	1.371(5)
O(1)-C(2)-Ge(1)	111.0(2)
C(6)-C(5)-Ge(1)	113.7(2)
C(7)-C(6)-C(11)	117.4(3)
C(7)-C(6)-C(5)	121.0(3)
C(11)-C(6)-C(5)	121.5(3)
C(6)-C(7)-C(8)	122.2(3)
C(9)-C(8)-C(7)	118.1(3)
C(9)-C(8)-C(12)	121.9(4)
C(7)-C(8)-C(12)	119.9(4)
C(8)-C(9)-C(10)	120.5(4)
C(11)-C(10)-C(9)	120.8(3)
C(10)-C(11)-C(6)	120.9(3)
O(2)-C(22)-Ge(2)	114.5(3)
C(26)-C(25)-Ge(2)	114.3(2)
C(27)-C(26)-C(31)	117.0(3)
C(27)-C(26)-C(25)	121.4(3)
C(31)-C(26)-C(25)	121.6(3)
C(28)-C(27)-C(26)	122.8(3)
C(29)-C(28)-C(27)	117.6(3)
C(29)-C(28)-C(32)	121.6(4)
C(27)-C(28)-C(32)	120.8(4)
C(30)-C(29)-C(28)	121.1(4)
C(29)-C(30)-C(31)	120.2(4)
C(30)-C(31)-C(26)	121.2(4)
C(4)-Ge(1)-C(3)	111.1(2)
C(4)-Ge(1)-C(2)	107.16(16)
C(3)-Ge(1)-C(2)	109.57(18)
C(4)-Ge(1)-C(5)	111.08(18)
C(3)-Ge(1)-C(5)	108.99(18)
C(2)-Ge(1)-C(5)	108.86(16)
C(23)-Ge(2)-C(24)	111.14(18)
C(23)-Ge(2)-C(22)	110.4(2)
C(24)-Ge(2)-C(22)	110.5(2)
C(23)-Ge(2)-C(25)	111.80(18)
C(24)-Ge(2)-C(25)	108.83(18)
C(22)-Ge(2)-C(25)	103.95(18)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters (A^2 x 10^3) for **1c**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(2)	65(2)	45(2)	38(2)	-3(1)	-2(2)	-10(2)
C(3)	81(3)	58(3)	96(3)	-12(2)	4(2)	22(2)
C(4)	77(3)	55(2)	79(3)	1(2)	9(2)	-19(2)
C(5)	76(3)	47(2)	39(2)	-2(1)	1(2)	1(2)
C(6)	54(2)	42(2)	38(2)	-3(1)	-9(1)	-3(2)
C(7)	54(2)	51(2)	42(2)	4(1)	-3(1)	0(2)
C(8)	57(2)	53(2)	46(2)	3(2)	-15(2)	4(2)
C(9)	58(3)	57(2)	59(2)	2(2)	-8(2)	11(2)
C(10)	48(2)	70(3)	62(2)	7(2)	9(2)	-1(2)
C(11)	57(2)	48(2)	57(2)	9(2)	-1(2)	-10(2)
C(12)	99(4)	54(2)	67(2)	17(2)	-16(2)	5(2)
C(22)	72(3)	69(3)	125(4)	43(3)	21(3)	18(3)
C(23)	66(3)	57(2)	80(3)	6(2)	-7(2)	-6(2)
C(24)	93(4)	81(3)	52(2)	-10(2)	8(2)	-12(3)
C(25)	67(3)	65(2)	42(2)	4(2)	6(2)	8(2)
C(26)	50(2)	54(2)	38(2)	-2(1)	10(1)	4(2)
C(27)	50(2)	64(2)	42(2)	-6(2)	2(2)	-3(2)
C(28)	62(3)	56(2)	47(2)	-6(2)	11(2)	-3(2)
C(29)	56(3)	65(3)	62(2)	-4(2)	13(2)	12(2)
C(30)	47(2)	79(3)	70(2)	-5(2)	-1(2)	-1(2)
C(31)	58(3)	58(2)	57(2)	-9(2)	3(2)	-6(2)
C(32)	94(4)	62(3)	74(3)	-19(2)	17(2)	-4(2)
O(1)	94(2)	60(2)	39(1)	-3(1)	7(1)	-33(2)
O(2)	67(2)	75(2)	53(1)	23(1)	17(1)	33(2)
Ge(1)	54(1)	34(1)	46(1)	-1(1)	7(1)	1(1)
Ge(2)	50(1)	42(1)	48(1)	6(1)	4(1)	7(1)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1c**.

	x	y	z	U(eq)
H(2A)	7223	3248	7750	59
H(2B)	5953	3561	7252	59
H(3A)	8569	2799	3539	117
H(3B)	7884	2508	4820	117
H(3C)	9219	2808	5145	117
H(4A)	8931	3961	4261	105
H(4B)	8960	3938	6000	105
H(4C)	7792	4223	5158	105
H(5A)	6174	3470	2609	65
H(5B)	5278	3117	3542	65
H(7)	5706	4328	2619	59
H(9)	2434	4841	4696	70
H(10)	2147	4097	5797	72
H(11)	3570	3464	5271	65
H(12A)	3486	5227	2184	110
H(12B)	5061	5123	2118	110
H(12C)	4462	5391	3495	110
H(22A)	3315	2724	11429	106
H(22B)	2882	2471	9937	106
H(23A)	3803	3878	8610	101
H(23B)	4111	3879	10325	101
H(23C)	2869	4175	9672	101
H(24A)	1785	3173	7167	113
H(24B)	550	3462	7806	113
H(24C)	676	2904	8090	113
H(25A)	466	3106	11562	70
H(25B)	1500	3462	12344	70
H(27)	1108	4336	12188	62
H(29)	-2525	4818	10745	73
H(30)	-3027	4065	9811	78
H(31)	-1522	3436	10156	69
H(32A)	-732	5398	11620	114
H(32B)	649	5194	12280	114
H(32C)	-681	5174	13219	114
H(1)	5230(50)	2837(17)	7930(50)	96
H(2)	5100(60)	2587(18)	10360(50)	97