ELECTRONIC SUPPLEMENTARY INFORMATION

Arsagermene, a compound with As=Ge double bond

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Contents of the Supporting Information:

1. Experimental Section.

General procedures. All experimental manipulations were performed using high-vacuum line techniques, or in an argon atmosphere of MBRAUN MB 150B-G glove box. All solvents were predried by conventional methods and finally dried and degassed over a potassium mirror in vacuum immediately prior to use. NMR spectra were recorded on Bruker AV-400FT (^{1}H NMR at 400.1 MHz; ^{13}C NMR at 100.6 MHz; ^{29}Si NMR at 79.5 MHz) NMR spectrometer. UV-Vis spectrum was recorded on a Shimadzu UV-3150 UV-Vis spectrophotometer in hexane. High-resolution mass spectra were measured on Bruker Daltonics micrOTOF-TU mass spectrometer with atmospheric pressure chemical ionization (APCI) method. Starting 1,1-dilithiogermane derivative $(^{t}Bu_2MeSi)_2GeLi_2$ was prepared according to a previously published procedure.[1]

(a) Experimental procedure, spectroscopic and crystallographic data for arsagermene 1.

A mixture of bis[di-*tert*-butyl(methyl)silyl]dilithiogermane $(^{t}Bu_2MeSi)_2GeLi_2$ [prepared from 1,1-bis[di-*tert*-butyl(methyl)silyl]2,3-bis(trimethylsilyl)-1-germacycloprop-2-ene (207.7 mg, 0.37 mmol) and Li (27.0 mg, 3.9 mmol) in THF/Et_2O (1.6 mL/0.4 mL)] and (2,4,6-tri-*tert*-butylphenyl)difluoroarsane (152.8 mg, 0.43 mmol) was placed in a reaction tube with a magnetic stirring bar. Dry, oxygen-free THF (2 mL) was introduced by vacuum transfer, and the dark-red reaction mixture was stirred for 1 hour at room temperature. Then the inorganic salts were filtered off and the solvent was evaporated. The pure arsagermene was isolated by recrystallization from hexane as orange crystals (50.0 mg, 19%). Mp > 190°C (dec.). ^{1}H NMR (400 MHz, C_6D_6, δ, ppm) −0.28 (s, 3 H, Me), 0.57 (s, 3 H, Me), 0.97 (s, 18 H, 2 ^{t}Bu), 1.36 (s, 18 H, 2 ^{t}Bu), 1.42 (s, 9 H, ^{t}Bu), 1.69 (s, 18 H, 2 ^{t}Bu), 7.53 (s, 2 H, H_{meta}); ^{13}C NMR (C_6D_6, δ, ppm) −5.8, −2.8, 22.5, 22.8, 30.3, 30.4, 31.9, 34.2, 34.9, 39.2, 122.0, 144.1, 148.6, 153.7; ^{29}Si NMR (C_6D_6, δ, ppm) 26.5, 34.4; HRMS (APCI): *m/z* calcd for $C_{36}H_{71}Si_2GeAs$ 708.3525, found 708.3534; UV/Vis (hexane) λ_{max}/nm (ε) = 392 (3000).

The X-ray crystallographic data for **1** have been deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition no. CCDC 1852834. These data can be obtained free of charge from the CCDC (www.ccdc.cam.ac.uk/data_request/cif).

(b) X-ray crystallography of 1.

Table S1. Crystallographic data for arsagermene **1**.

Identification code	AsGe	
Empirical formula	$C_{36}H_{71}AsGeSi_2$	
Formula weight	707.61	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 11.871(2) Å	α = 90°
	b = 17.675(4) Å	β = 90°
	c = 19.376(4) Å	γ = 90°
Volume	4065.5(14) $Å^3$	
Z	4	
Density (calculated)	1.156 $Mg•m^{-3}$	
Absorption coefficient	1.641 mm^{-1}	
F(000)	1520	
Crystal size	0.55 x 0.40 x 0.25 mm	
Theta range for data collection	2.067 to 27.933°	
Index ranges	0<=h<=15, 0<=k<=23, 0<=l<=25	
Reflections collected	5341	
Independent reflections	5340 [R(int) = 0.074]	
Completeness to theta = 25.242	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5340 / 0 / 385	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1248	
R indices (all data)	R1 = 0.0608, wR2 = 0.1328	
Absolute structure parameter	0.450(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.408 and -1.251 $e•Å^{-3}$	

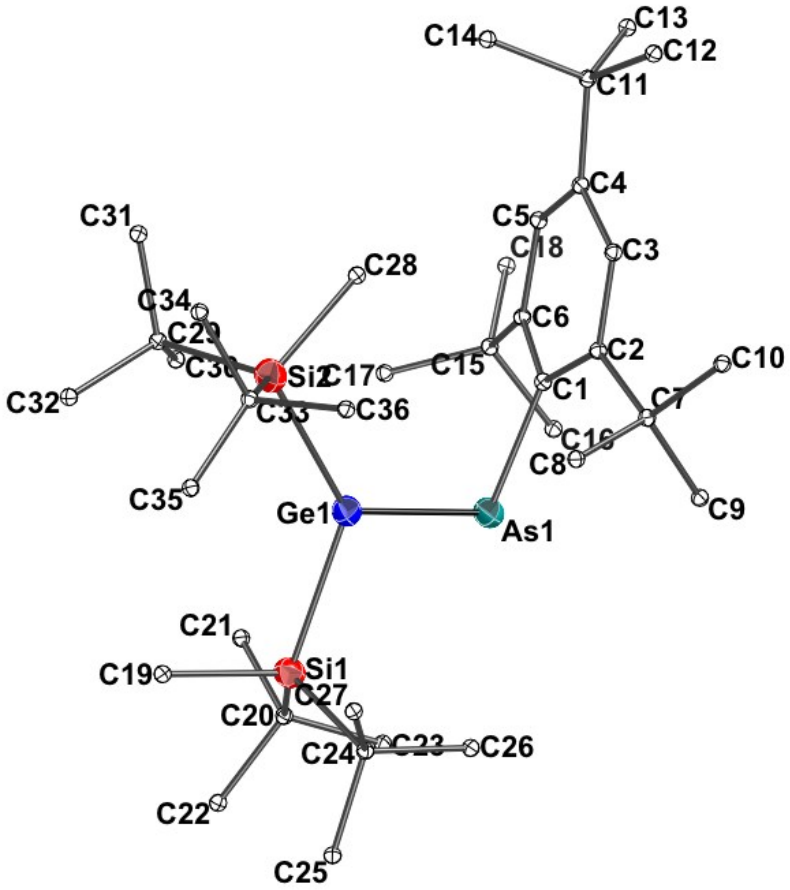

Figure S1. Crystal structure of the arsagermene **1** (ORTEP view with the thermal ellipsoids drawn at the 30% probability level), hydrogen atoms are not shown.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic atomic displacement parameters (Å^2 x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
As(1)	7136(1)	372(1)	199(1)	32(1)
Ge(1)	5868(1)	-115(1)	957(1)	30(1)
Si(1)	4808(1)	-1031(1)	296(1)	32(1)
Si(2)	5646(1)	212(1)	2169(1)	39(1)
C(1)	8068(5)	1140(3)	693(3)	31(1)
C(2)	9043(5)	922(3)	1069(3)	32(1)
C(3)	9487(5)	1448(3)	1542(3)	32(1)
C(4)	9050(5)	2170(3)	1640(3)	35(1)
C(5)	8195(5)	2395(3)	1189(3)	36(1)
C(6)	7716(5)	1915(3)	693(3)	30(1)
C(7)	9686(5)	165(3)	968(3)	36(1)
C(8)	9080(6)	-511(4)	1313(3)	44(1)
C(9)	9881(6)	7(4)	203(3)	45(1)
C(10)	10868(5)	194(4)	1308(3)	44(1)
C(11)	9451(5)	2699(4)	2208(3)	40(1)
C(12)	10553(6)	2423(4)	2553(4)	52(2)
C(13)	9677(7)	3504(4)	1916(4)	54(2)
C(14)	8527(7)	2756(5)	2767(4)	60(2)
C(15)	6908(5)	2277(3)	154(3)	35(1)
C(16)	7271(6)	2034(4)	-582(3)	49(2)
C(17)	5664(5)	2105(4)	277(4)	51(2)
C(18)	7021(7)	3147(4)	148(4)	53(2)
C(19)	3575(6)	-1347(4)	841(4)	51(2)
C(20)	4159(5)	-576(3)	-517(3)	40(1)
C(21)	3644(6)	190(4)	-331(4)	53(2)
C(22)	3190(6)	-1072(4)	-791(4)	56(2)
C(23)	5017(7)	-454(4)	-1114(3)	53(2)

C(24)	5759(6)	-1897(3)	123(3)	44(1)
C(25)	5136(7)	-2507(4)	-297(5)	67(2)
C(26)	6843(6)	-1702(4)	-252(4)	57(2)
C(27)	6103(10)	-2218(5)	820(4)	86(3)
C(28)	6799(7)	903(6)	2360(4)	70(3)
C(29)	4236(6)	731(4)	2302(3)	50(2)
C(30)	3995(10)	1211(6)	1658(5)	90(4)
C(31)	4329(8)	1274(5)	2921(4)	67(2)
C(32)	3234(5)	193(5)	2420(4)	55(2)
C(33)	5860(6)	-664(5)	2755(3)	54(2)
C(34)	5685(7)	-423(6)	3511(3)	67(2)
C(35)	5067(9)	-1317(5)	2586(4)	66(2)
C(36)	7076(7)	-935(7)	2682(4)	78(3)

Table S3. Bond lengths [Å] and bond angles [°] for **1**.

As(1)-C(1)	1.996(5)
As(1)-Ge(1)	2.2727(8)
Ge(1)-Si(1)	2.4174(16)
Ge(1)-Si(2)	2.4336(17)
Si(1)-C(19)	1.889(7)
Si(1)-C(20)	1.928(6)
Si(1)-C(24)	1.931(6)
Si(2)-C(28)	1.872(7)
Si(2)-C(29)	1.926(8)
Si(2)-C(33)	1.937(8)
C(1)-C(2)	1.421(7)
C(1)-C(6)	1.432(8)
C(2)-C(3)	1.408(8)
C(2)-C(7)	1.554(8)
C(3)-C(4)	1.391(8)
C(4)-C(5)	1.396(8)
C(4)-C(11)	1.520(8)
C(5)-C(6)	1.403(8)
C(6)-C(15)	1.555(8)
C(7)-C(9)	1.527(8)
C(7)-C(8)	1.546(8)
C(7)-C(10)	1.550(8)
C(11)-C(14)	1.544(10)
C(11)-C(12)	1.547(9)
C(11)-C(13)	1.555(9)
C(15)-C(17)	1.527(8)
C(15)-C(18)	1.544(8)
C(15)-C(16)	1.549(9)
C(20)-C(21)	1.528(9)
C(20)-C(22)	1.541(8)
C(20)-C(23)	1.558(10)

C(24)-C(26)	1.517(10)
C(24)-C(27)	1.521(10)
C(24)-C(25)	1.539(9)
C(29)-C(30)	1.536(11)
C(29)-C(31)	1.539(10)
C(29)-C(32)	1.540(10)
C(33)-C(35)	1.525(12)
C(33)-C(36)	1.528(11)
C(33)-C(34)	1.540(9)

C(1)-As(1)-Ge(1)	108.33(16)
As(1)-Ge(1)-Si(1)	104.85(5)
As(1)-Ge(1)-Si(2)	127.25(5)
Si(1)-Ge(1)-Si(2)	127.90(6)
C(19)-Si(1)-C(20)	105.7(3)
C(19)-Si(1)-C(24)	108.4(3)
C(20)-Si(1)-C(24)	115.0(3)
C(19)-Si(1)-Ge(1)	107.8(2)
C(20)-Si(1)-Ge(1)	111.18(18)
C(24)-Si(1)-Ge(1)	108.6(2)
C(28)-Si(2)-C(29)	107.3(4)
C(28)-Si(2)-C(33)	108.1(4)
C(29)-Si(2)-C(33)	114.6(3)
C(28)-Si(2)-Ge(1)	105.5(2)
C(29)-Si(2)-Ge(1)	109.7(2)
C(33)-Si(2)-Ge(1)	111.2(2)
C(2)-C(1)-C(6)	119.8(5)
C(2)-C(1)-As(1)	120.9(4)
C(6)-C(1)-As(1)	119.2(4)
C(3)-C(2)-C(1)	117.4(5)
C(3)-C(2)-C(7)	117.8(5)
C(1)-C(2)-C(7)	124.8(5)
C(4)-C(3)-C(2)	123.7(5)

C(3)-C(4)-C(5)	116.5(5)
C(3)-C(4)-C(11)	123.1(5)
C(5)-C(4)-C(11)	120.4(6)
C(4)-C(5)-C(6)	123.5(6)
C(5)-C(6)-C(1)	117.3(5)
C(5)-C(6)-C(15)	117.6(5)
C(1)-C(6)-C(15)	125.0(5)
C(9)-C(7)-C(8)	110.5(5)
C(9)-C(7)-C(10)	106.3(5)
C(8)-C(7)-C(10)	105.3(5)
C(9)-C(7)-C(2)	110.7(5)
C(8)-C(7)-C(2)	112.5(5)
C(10)-C(7)-C(2)	111.2(5)
C(4)-C(11)-C(14)	109.0(5)
C(4)-C(11)-C(12)	112.6(6)
C(14)-C(11)-C(12)	108.6(6)
C(4)-C(11)-C(13)	110.6(5)
C(14)-C(11)-C(13)	108.5(6)
C(12)-C(11)-C(13)	107.4(6)
C(17)-C(15)-C(18)	106.4(6)
C(17)-C(15)-C(16)	111.0(6)
C(18)-C(15)-C(16)	104.2(5)
C(17)-C(15)-C(6)	114.2(5)
C(18)-C(15)-C(6)	111.2(5)
C(16)-C(15)-C(6)	109.5(5)
C(21)-C(20)-C(22)	106.7(5)
C(21)-C(20)-C(23)	108.3(6)
C(22)-C(20)-C(23)	108.1(5)
C(21)-C(20)-Si(1)	109.7(4)
C(22)-C(20)-Si(1)	110.0(5)
C(23)-C(20)-Si(1)	113.8(4)
C(26)-C(24)-C(27)	106.4(7)
C(26)-C(24)-C(25)	108.3(6)

C(27)-C(24)-C(25)	109.7(7)
C(26)-C(24)-Si(1)	113.5(5)
C(27)-C(24)-Si(1)	107.4(5)
C(25)-C(24)-Si(1)	111.4(5)
C(30)-C(29)-C(31)	107.6(7)
C(30)-C(29)-C(32)	108.5(7)
C(31)-C(29)-C(32)	108.9(6)
C(30)-C(29)-Si(2)	108.4(5)
C(31)-C(29)-Si(2)	109.8(6)
C(32)-C(29)-Si(2)	113.4(5)
C(35)-C(33)-C(36)	109.0(8)
C(35)-C(33)-C(34)	109.3(7)
C(36)-C(33)-C(34)	107.6(6)
C(35)-C(33)-Si(2)	113.5(5)
C(36)-C(33)-Si(2)	108.7(6)
C(34)-C(33)-Si(2)	108.6(6)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic atomic displacement parameters ($Å^2$ x 10^3) for **1**. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
As(1)	31(1)	34(1)	30(1)	-2(1)	0(1)	-5(1)
Ge(1)	27(1)	34(1)	30(1)	-2(1)	0(1)	-2(1)
Si(1)	30(1)	28(1)	37(1)	-2(1)	-1(1)	-1(1)
Si(2)	34(1)	52(1)	32(1)	-5(1)	4(1)	-6(1)
C(1)	26(3)	34(3)	33(2)	2(2)	-5(2)	-3(2)
C(2)	28(3)	37(3)	30(3)	3(2)	2(2)	-3(2)
C(3)	28(3)	39(3)	28(2)	1(2)	-4(2)	-1(2)
C(4)	33(3)	39(3)	32(3)	1(2)	-2(2)	-7(3)
C(5)	37(3)	33(3)	39(3)	-1(2)	-5(2)	-3(2)
C(6)	31(3)	29(3)	32(2)	0(2)	0(2)	0(2)
C(7)	31(3)	39(3)	39(3)	1(3)	-2(2)	2(2)
C(8)	38(3)	44(3)	50(3)	11(3)	0(3)	8(3)
C(9)	46(3)	47(4)	42(3)	0(3)	1(3)	10(3)
C(10)	30(3)	48(3)	54(3)	0(3)	-8(3)	6(3)
C(11)	43(3)	43(3)	33(3)	-2(2)	-4(2)	-8(3)
C(12)	57(4)	52(4)	48(4)	-2(3)	-17(3)	-10(3)
C(13)	72(5)	42(4)	48(4)	0(3)	-17(4)	-10(4)
C(14)	56(5)	78(6)	46(4)	-15(4)	-2(3)	-15(4)
C(15)	35(3)	33(3)	38(3)	7(2)	-8(2)	-1(2)
C(16)	53(4)	58(4)	36(3)	4(3)	-8(3)	4(3)
C(17)	32(3)	48(4)	72(5)	2(3)	-4(3)	4(3)
C(18)	63(4)	37(3)	59(4)	11(3)	-19(4)	1(3)
C(19)	47(4)	50(4)	57(4)	-4(3)	6(3)	-13(3)
C(20)	36(3)	35(3)	50(3)	-11(2)	-13(3)	1(3)
C(21)	52(4)	47(4)	60(4)	-8(3)	-22(3)	15(3)
C(22)	52(4)	54(4)	60(4)	-6(3)	-19(3)	-5(3)
C(23)	63(4)	56(4)	40(3)	5(3)	-12(3)	-5(4)

C(24)	51(4)	31(3)	49(3)	-9(3)	-5(3)	9(3)
C(25)	70(5)	35(3)	94(6)	-21(4)	12(5)	1(4)
C(26)	47(4)	52(4)	73(5)	-14(4)	7(4)	13(3)
C(27)	134(9)	63(5)	61(5)	8(4)	-4(6)	58(6)
C(28)	63(5)	102(7)	45(4)	-30(4)	19(3)	-39(5)
C(29)	56(4)	52(4)	42(3)	-1(3)	13(3)	3(3)
C(30)	113(8)	83(7)	73(6)	20(5)	36(6)	53(7)
C(31)	68(5)	61(5)	72(5)	-16(4)	30(4)	-11(4)
C(32)	34(3)	70(5)	61(4)	-19(4)	1(3)	7(3)
C(33)	53(4)	75(5)	35(3)	8(3)	4(3)	11(4)
C(34)	60(5)	114(7)	28(3)	8(4)	1(3)	8(5)
C(35)	86(6)	59(5)	54(4)	15(4)	10(4)	-3(5)
C(36)	52(5)	137(9)	44(4)	20(5)	2(4)	30(6)

Table S6. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$ x 10^3) for **1**.

	x	y	z	U(eq)
H(3)	10119	1300	1811	38
H(5)	7924	2899	1221	43
H(8A)	8364	-605	1077	66
H(8B)	8936	-394	1799	66
H(8C)	9557	-962	1281	66
H(9A)	10308	-464	151	68
H(9B)	10307	426	-2	68
H(9C)	9154	-41	-32	68
H(10A)	10786	243	1809	66
H(10B)	11285	630	1128	66
H(10C)	11280	-271	1200	66
H(12A)	10423	1930	2771	79
H(12B)	10789	2790	2904	79
H(12C)	11143	2375	2202	79
H(13A)	10060	3810	2267	81
H(13B)	8960	3743	1793	81
H(13C)	10155	3466	1505	81
H(14A)	8389	2255	2965	90
H(14B)	7831	2948	2558	90
H(14C)	8774	3103	3131	90
H(16A)	7107	1496	-648	74
H(16B)	8081	2121	-639	74
H(16C)	6855	2332	-924	74
H(17A)	5208	2371	-68	76
H(17B)	5450	2276	740	76
H(17C)	5536	1559	239	76

H(18A)	7816	3286	96	80
H(18B)	6730	3353	582	80
H(18C)	6588	3354	-239	80
H(19A)	3177	-1759	605	77
H(19B)	3060	-921	910	77
H(19C)	3850	-1526	1289	77
H(21A)	3239	392	-731	80
H(21B)	4244	541	-197	80
H(21C)	3119	126	56	80
H(22A)	2671	-1191	-413	83
H(22B)	3499	-1543	-980	83
H(22C)	2785	-799	-1154	83
H(23A)	4647	-185	-1494	80
H(23B)	5289	-945	-1278	80
H(23C)	5655	-153	-946	80
H(25A)	5572	-2977	-290	100
H(25B)	5046	-2334	-774	100
H(25C)	4392	-2596	-93	100
H(26A)	7231	-1293	-6	86
H(26B)	6668	-1538	-723	86
H(26C)	7330	-2149	-269	86
H(27A)	5429	-2381	1072	129
H(27B)	6496	-1828	1087	129
H(27C)	6604	-2652	751	129
H(28A)	6674	1369	2096	105
H(28B)	7526	683	2230	105
H(28C)	6802	1020	2855	105
H(30A)	3851	878	1264	135
H(30B)	4648	1533	1558	135
H(30C)	3333	1530	1741	135
H(31A)	3611	1537	2986	100
H(31B)	4925	1645	2833	100
H(31C)	4512	984	3338	100

H(32A)	3393	-135	2816	82
H(32B)	3119	-118	2007	82
H(32C)	2553	490	2512	82
H(34A)	4884	-322	3592	101
H(34B)	6122	36	3604	101
H(34C)	5938	-830	3818	101
H(35A)	5196	-1484	2110	99
H(35B)	4284	-1148	2636	99
H(35C)	5209	-1738	2903	99
H(36A)	7215	-1350	3006	117
H(36B)	7591	-516	2782	117
H(36C)	7203	-1113	2209	117

2. Computations.

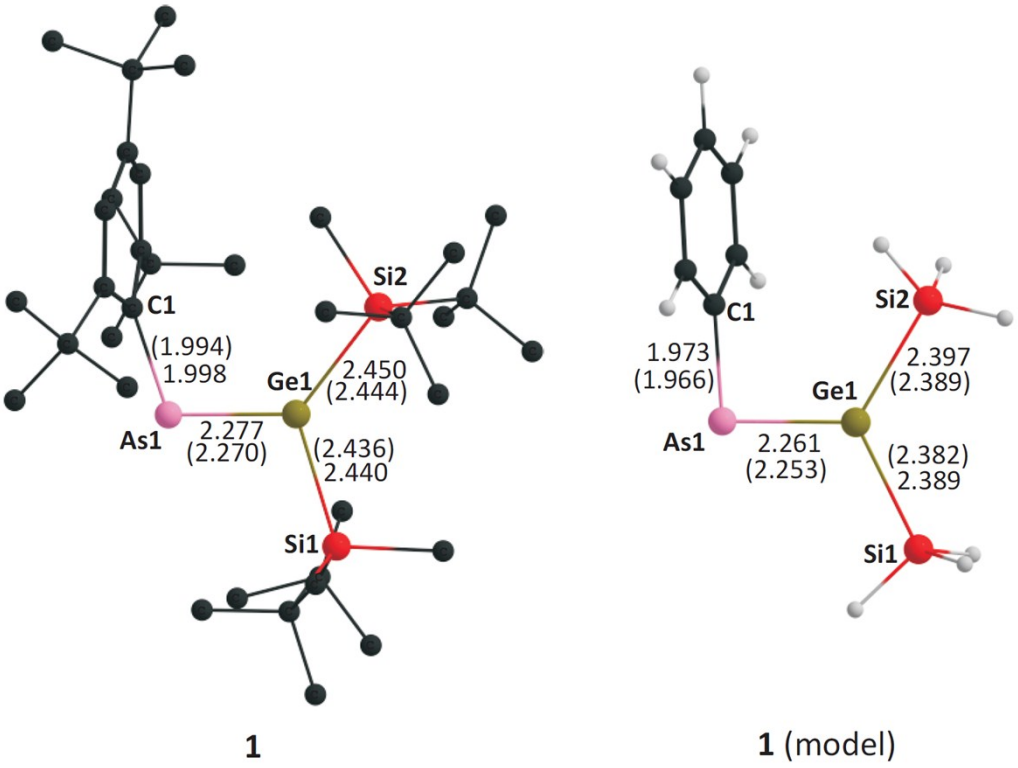

Figure S2. Optimized geometries for **1** and **1′** (model) at the DFT1 (DFT2) levels. In the left structure **1**, hydrogen atoms are omitted.

Cartesian coordinates [NI – number of imaginary frequencies, ω_1 – lowest harmonic frequency (cm^{-1}), E – total electronic energy (a.u)]:

Compound 1: M06/6-311+G**, NI = 0, ω_1 = 19.8, E = –6305.584119

As,0,0.0803993608,-1.9106646282,-0.0579578467
Ge,0,1.1849585928,0.0800039247,-0.0808700606
Si,0,3.5489275334,-0.5196401337,-0.0212102518
Si,0,0.2723465016,2.3532537618,-0.128848941
C,0,4.5521130645,1.0841145019,-0.0670750196
H,0,4.4995615169,1.5490742025,-1.0578382533
H,0,5.6097427545,0.894060062,0.1486083523

H,0,4.1903747675,1.8152843111,0.6628100262
C,0,3.9576476334,-1.3936358412,1.6598634031
C,0,3.653779867,-0.4071564961,2.7898935812
H,0,4.229903959,0.5220269,2.7045608503
H,0,3.9126061733,-0.8631051198,3.7567927755
H,0,2.5873093632,-0.1485643459,2.8316351749
C,0,5.4457649607,-1.7475937349,1.7228232071
H,0,5.7168933842,-2.5340469622,1.0095638889
H,0,5.6903566625,-2.1265290356,2.726179044
H,0,6.094839079,-0.8832577016,1.5387770499
C,0,3.1488938643,-2.6625615992,1.9193694651
H,0,3.3287313622,-3.4401267343,1.1704927595
H,0,2.0703653695,-2.4687552869,1.9411320463
H,0,3.4285215452,-3.0789360077,2.8986799419
C,0,4.0335651036,-1.5141511185,-1.6102092703
C,0,5.5473893851,-1.4237904308,-1.8285365544
H,0,6.1202136166,-1.8409793805,-0.9935432224
H,0,5.8827512687,-0.3918955934,-1.9813474165
H,0,5.8233700192,-1.9920832262,-2.7290017332
C,0,3.6343632963,-2.9859126368,-1.5407948588
H,0,4.1955361942,-3.5311197908,-0.7740484696
H,0,3.8490507356,-3.4714199483,-2.5044191548
H,0,2.563665801,-3.1207437429,-1.3392263949
C,0,3.3477135641,-0.8916411789,-2.8274015769
H,0,3.5801847346,0.1752129796,-2.9389400525
H,0,2.2569040371,-1.0001354028,-2.7859346812
H,0,3.6957393131,-1.393196974,-3.742583182
C,0,-1.5635763071,2.1864384227,-0.5022795752
H,0,-2.0353421845,1.4142726486,0.1128174476
H,0,-1.7304599183,1.9096087279,-1.5484291535
H,0,-2.0786998565,3.137886289,-0.318947608
C,0,1.0508340042,3.4136490319,-1.5480990557
C,0,0.0792240619,4.5367032033,-1.9238850581

H,0,-0.8763193572,4.1496589749,-2.2939875254
H,0,0.5183591733,5.1455933908,-2.7280533983
H,0,-0.1339793742,5.2097449897,-1.0856794784
C,0,2.3926290242,4.0357009152,-1.1740956025
H,0,3.1283603913,3.285541713,-0.8641430076
H,0,2.2996468716,4.7721307598,-0.3684616444
H,0,2.8111588335,4.5626015979,-2.0446279059
C,0,1.2552345856,2.5333170124,-2.7802676394
H,0,2.0063084006,1.7527566898,-2.6063390268
H,0,1.6087500712,3.1473176669,-3.621878687
H,0,0.3297523322,2.0415867789,-3.1032614858
C,0,0.4490775138,3.1041855153,1.6377475377
C,0,-0.0813930925,4.537887598,1.6674691934
H,0,0.5220974021,5.2192953864,1.0571960139
H,0,-0.0565096425,4.9189456626,2.6991137345
H,0,-1.1210160917,4.6040824783,1.3246541175
C,0,1.8888609072,3.0987626748,2.1467424858
H,0,2.5541926878,3.7156892693,1.5344114056
H,0,2.3054892373,2.0851557929,2.1836597016
H,0,1.9226193958,3.4974301595,3.1714175707
C,0,-0.3928921249,2.253932504,2.5897401108
H,0,-1.4528249302,2.2213766721,2.3054771291
H,0,-0.336108715,2.6671963776,3.6077040404
H,0,-0.0286450269,1.2207668071,2.6361811939
C,0,-1.8679306724,-1.4659914282,-0.0542149878
C,0,-2.5510743068,-1.3549404724,1.1912262779
C,0,-3.7220088114,-0.6068870825,1.2227198658
C,0,-4.2944367508,-0.0389925317,0.0878900678
C,0,-3.7355721931,-0.3856556872,-1.1280086772
H,0,-4.2187764172,-0.0440649909,-2.0344994571
C,0,-2.5504840717,-1.1220451005,-1.2413219921
C,0,-2.1352820954,-2.0846662826,2.4931643654
C,0,-1.0342917695,-1.3508848425,3.2622662706

H,0,-1.3711955063,-0.3442601865,3.5374360922
H,0,-0.1107613295,-1.2567181115,2.6843509974
H,0,-0.8018304988,-1.8928258073,4.1878390738
C,0,-1.7053734796,-3.5271629374,2.1938738666
H,0,-0.7722250003,-3.5972921089,1.6289554624
C,0,-2.1178169537,-1.507179608,-2.6779111927
C,0,-3.3575121883,-1.7457983794,-3.5575646829
H,0,-4.0338168199,-2.4791466592,-3.1040307814
H,0,-3.0370628262,-2.1366615992,-4.5292743294
H,0,-3.9277358681,-0.8354350052,-3.7611834951
C,0,-1.2983872574,-0.3905971837,-3.3278067023
H,0,-1.0352404119,-0.6633352759,-4.3578529462
H,0,-0.3697544711,-0.2046082144,-2.7787060162
H,0,-1.8715327662,0.5445915498,-3.36440325
C,0,-1.3290548665,-2.8197347251,-2.7441704855
H,0,-1.8267106824,-3.6122922127,-2.1728907022
H,0,-0.3032138655,-2.7295320402,-2.3772621068
H,0,-1.2590700729,-3.1482358741,-3.7875560188
C,0,-3.3214281166,-2.2126417508,3.4602766404
C,0,-5.5232103893,0.8547691438,0.2200096246
C,0,-6.7060416705,0.0241297821,0.7274792372
C,0,-5.2321937495,1.9848815234,1.2128178961
C,0,-5.9198911767,1.4931049573,-1.10772569
H,0,-2.4835972444,-4.0527781854,1.628276309
H,0,-1.5482556467,-4.0661490648,3.1354721153
H,0,-3.6282002199,-1.251971735,3.8861945381
H,0,-3.0226252924,-2.8479398113,4.3008475659
H,0,-4.1921770174,-2.6763754476,2.9831244248
H,0,-6.9349602494,-0.7909391079,0.0312961216
H,0,-7.6011205958,0.6509336106,0.8256818549
H,0,-6.4994554853,-0.4210747241,1.7065098118
H,0,-6.2253963617,0.7464290276,-1.8491107469
H,0,-6.7711133895,2.1655861979,-0.9524415371

H,0,-5.0998778179,2.0849936909,-1.5320618729
H,0,-4.9979232505,1.6084457648,2.2135391753
H,0,-6.1054934692,2.6420883389,1.3031896128
H,0,-4.383405163,2.5912445902,0.874947691
H,0,-4.2203363981,-0.4585673065,2.1733862554

Compound 1: M06/Def2TZVP, NI = 0, ω_1 = 19.9, E = –6305.818504
As,0,-0.0696006269,-1.900099485,0.0798575884
Ge,0,-1.1875048033,0.0755165671,0.0795859342
Si,0,-3.5429116514,-0.5424824926,0.0257186174
Si,0,-0.2886665884,2.348558389,0.1011847831
C,0,-4.5475437742,1.0523695758,0.0567194102
H,0,-4.4964239751,1.5239157458,1.0412269632
H,0,-5.6015341839,0.8589085813,-0.158634426
H,0,-4.1858861752,1.7762368325,-0.676164154
C,0,-3.9448594984,-1.4304778869,-1.640176898
C,0,-3.6466614669,-0.4544298154,-2.7769271537
H,0,-4.2252784318,0.4704298974,-2.6991400558
H,0,-3.9032450541,-0.9193496844,-3.7368419691
H,0,-2.5840261639,-0.1918762597,-2.8206605445
C,0,-5.4286623913,-1.7907467265,-1.7001847878
H,0,-5.6957943934,-2.5692646504,-0.9810501287
H,0,-5.6700011517,-2.178609139,-2.6976997931
H,0,-6.0789364766,-0.9292906834,-1.5238070136
C,0,-3.1326276948,-2.6955282909,-1.8896293906
H,0,-3.3077131517,-3.4652734994,-1.1357819651
H,0,-2.0575791272,-2.497306066,-1.9138125703
H,0,-3.41111111,-3.1195306198,-2.8626968353
C,0,-4.0213924617,-1.5215037948,1.6161184143
C,0,-5.5327487994,-1.4367242532,1.8345594558
H,0,-6.1025757377,-1.8586133686,1.003642702
H,0,-5.8707253353,-0.4080264459,1.9826538347
H,0,-5.8037553829,-2.0009455337,2.7355475846

C,0,-3.616387324,-2.9891818536,1.5600763561
H,0,-4.1751450148,-3.5422365954,0.801229851
H,0,-3.8265363001,-3.4645593786,2.5264169848
H,0,-2.548252396,-3.1203689823,1.3569111708
C,0,-3.3402324248,-0.8865232269,2.8257927349
H,0,-3.5725017552,0.1787082387,2.9240343598
H,0,-2.2518752694,-0.9943275415,2.7874307486
H,0,-3.6891139895,-1.3774090165,3.7429371062
C,0,1.541793485,2.1865385483,0.4692451632
H,0,2.0087595909,1.413289851,-0.1438160295
H,0,1.7109023346,1.912875479,1.5129840475
H,0,2.0556123569,3.1342848503,0.2809131634
C,0,-1.0612040802,3.4147414407,1.508119992
C,0,-0.0932454055,4.540600118,1.8729043243
H,0,0.8590218864,4.1586382024,2.2481960326
H,0,-0.534079725,5.1556423767,2.6674565448
H,0,0.1206620017,5.2022110753,1.0294117187
C,0,-2.4028132318,4.0298216261,1.134684581
H,0,-3.1353148878,3.2770533852,0.8328652487
H,0,-2.3135889863,4.7580971464,0.3250976227
H,0,-2.818280599,4.5602918808,2.0008126675
C,0,-1.2603328486,2.5446519432,2.7446098023
H,0,-2.0108699947,1.7654106256,2.5785587691
H,0,-1.6090571445,3.1631197273,3.581160183
H,0,-0.3360355538,2.0555076176,3.0653190854
C,0,-0.4707645363,3.0812666904,-1.6641094101
C,0,0.0590233191,4.5117569338,-1.707544958
H,0,-0.5425678627,5.1965125241,-1.1042530516
H,0,0.0334733571,4.8816925394,-2.7401215352
H,0,1.0959195366,4.5798566388,-1.3658035433
C,0,-1.9085541273,3.0714822882,-2.1694653192
H,0,-2.5707390177,3.6939207196,-1.5644678591
H,0,-2.3244223927,2.0600073471,-2.1937969255

H,0,-1.942992663,3.4576564018,-3.1957847185
C,0,0.3662495013,2.2244016553,-2.6099455614
H,0,1.4243365472,2.1924858292,-2.3295992637
H,0,0.3062664116,2.6287443172,-3.6281169223
H,0,0.001143848,1.1939352603,-2.6464924658
C,0,1.8755820087,-1.4619321914,0.0686057489
C,0,2.5553944893,-1.3641147747,-1.1759163777
C,0,3.7227367816,-0.6169032688,-1.2170293849
C,0,4.2950373087,-0.0369033538,-0.0924222484
C,0,3.7391835641,-0.370231719,1.1247978926
H,0,4.2224188343,-0.0198873469,2.025333563
C,0,2.5581232319,-1.1048619618,1.2477877744
C,0,2.1383025926,-2.1042333591,-2.4683623252
C,0,1.0445124242,-1.372153538,-3.2428247775
H,0,1.3845102459,-0.3699441995,-3.5191109527
H,0,0.1212924015,-1.2733568696,-2.6694798324
H,0,0.8139133024,-1.9154531727,-4.1646285667
C,0,1.7007095182,-3.5387240687,-2.1580773182
H,0,0.7696909231,-3.5983793135,-1.5932291865
C,0,2.1286968401,-1.4738464836,2.6866169483
C,0,3.3666448108,-1.6982489393,3.5673228877
H,0,4.043380677,-2.4327844955,3.1231489765
H,0,3.0467442465,-2.0782540153,4.5402809805
H,0,3.9319658816,-0.7858721236,3.7597577146
C,0,1.3090021356,-0.3534872334,3.3222030216
H,0,1.0475923698,-0.6135449888,4.3528483241
H,0,0.3818794041,-0.1765417211,2.7723850318
H,0,1.8787122304,0.5809082723,3.3463447607
C,0,1.3451877578,-2.7851012565,2.7699001817
H,0,1.8448818093,-3.5819871571,2.2119736415
H,0,0.3215067712,-2.7049451093,2.401385394
H,0,1.2757479259,-3.0971787037,3.8153309758
C,0,3.3222387223,-2.2470794373,-3.431459365

C,0,5.5200371192,0.8560141864,-0.2349658655
C,0,6.7033182722,0.0236869186,-0.7294417924
C,0,5.2287111046,1.9705518804,-1.2406240727
C,0,5.9140390776,1.5121415285,1.0814677547
H,0,2.4739723436,-4.0630360325,-1.5899159352
H,0,1.541026001,-4.0817583298,-3.0935395734
H,0,3.6317989435,-1.2947082453,-3.8664407951
H,0,3.0213862531,-2.8895133077,-4.2620958465
H,0,4.1885426776,-2.7068459333,-2.9487661317
H,0,6.933628084,-0.7785790041,-0.02325296
H,0,7.5936281757,0.6510032862,-0.8352618917
H,0,6.4983534564,-0.4340708117,-1.6998468592
H,0,6.2198229025,0.7782150803,1.8312088628
H,0,6.7614076713,2.1825307563,0.9164094836
H,0,5.0939567365,2.1060537192,1.4957243926
H,0,4.9966421715,1.5810948196,-2.2337796497
H,0,6.0987861943,2.6262154651,-1.3375669608
H,0,4.3804004733,2.5777353866,-0.9117106091
H,0,4.218583095,-0.4790044094,-2.1681543304

Model Compound 1′: M06/6-311+G**, NI = 0, ω_1 = 24.5, E = –5126.791364
As,0,0.0051144574,-1.646433759,0.4743798198
Ge,0,-1.3638014634,0.0898690811,0.002022106
Si,0,-3.7089892302,-0.3658106178,0.0130946099
Si,0,-0.4598333754,2.2527417718,-0.4987807359
H,0,-4.4045714647,0.4492000568,1.0375283784
H,0,-4.3004308407,-0.0671834722,-1.3130425014
H,0,-3.8763341982,-1.8049079588,0.3226831716
H,0,0.8090111211,2.09253527,-1.2431089736
H,0,-0.2182645234,3.0007514182,0.7577270609
H,0,-1.4412879863,3.0028365609,-1.3198098201
C,0,1.6541558737,-0.5784963816,0.2932784336
C,0,2.4685297348,-0.7601101965,-0.8248115256

C,0,3.6160725032,0.0020980409,-0.9954328498
C,0,3.9722734855,0.9495160866,-0.0442366287
C,0,3.1824463176,1.121337911,1.0839518553
H,0,3.4598727703,1.8538660277,1.8366557495
C,0,2.0326141905,0.3601166808,1.2541954238
H,0,2.1933503976,-1.4931647533,-1.5799569833
H,0,1.4201663887,0.5034536016,2.1418112866
H,0,4.8680187312,1.5480483982,-0.1792006194
H,0,4.2331231106,-0.1414937664,-1.8777382576

Model Structure 1′: M06/Def2TZVP, NI = 0, ω_1 = 25.0, E = –5126.912287
As,0,0.0082040593,-1.6154366438,0.361446143
Ge,0,-1.3827016026,0.1186632937,-0.0039823266
Si,0,-3.7126067119,-0.3752131707,0.0426773322
Si,0,-0.5365244993,2.3027251229,-0.472861546
H,0,-4.3940871441,0.3841233742,1.1133874556
H,0,-4.340778425,-0.0329583767,-1.2517334607
H,0,-3.8535883496,-1.8243550028,0.2970387476
H,0,0.6911657611,2.1764810519,-1.2837922737
H,0,-0.2394735641,3.0264126661,0.7815975746
H,0,-1.5620646078,3.0589380177,-1.2249819019
C,0,1.6625452614,-0.5617807085,0.2312489808
C,0,2.540434735,-0.8060158619,-0.8206667036
C,0,3.7094622603,-0.0753711797,-0.9488732462
C,0,4.0245701298,0.9022589635,-0.0190843246
C,0,3.1683635585,1.1405122999,1.0423249822
H,0,3.4123566796,1.8981408508,1.7786332883
C,0,1.9969256245,0.4111314314,1.1693300389
H,0,2.2998018333,-1.5670732787,-1.5567923764
H,0,1.3318760376,0.6034455013,2.0057672241
H,0,4.9398456464,1.473828573,-0.1191543874
H,0,4.3775093178,-0.2696869237,-1.7803202202

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