Supporting Information for

New oligogermane with five coordinate germanium atom: the preparation of 1-germylgermatrane

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Experimental

Methods and Materials. All manipulations were performed under a dry, oxygen-free argon atmosphere using standard Schlenk techniques. Triethanolamine (Aldrich), triethylamine (Aldrich) were distilled prior to use and stored over activated molecular sieves (4Å). Solvents were dried using usual procedures. Tetrahydrofuran, diethyl ether, triethylamine were stored under solid KOH and than distilled under sodium/benzophenone. Toluene and *n*-hexane were refluxed and distilled under sodium. Dichloromethane and acetonitrile were distilled under CaH_2. C_6D_6 was distilled over sodium under argon. $CDCl_3$ was distilled over CaH_2 under argon.

^{1}H NMR (400.130 MHz), ^{13}C NMR (100.613 MHz), ^{29}Si (79.495 MHz) spectra were recorded with a Bruker 400 spectrometer at 298 K. Chemical shifts are given in ppm relative to internal Me_4Si. Elemental analyses were carried out by the Microanalytical Laboratory of the Chemistry Department of the Moscow State University using Heraeus Vario Elementar instrument. UV/visible spectra were obtained using two ray spectrophotometer Evolution 300 «Thermo Scientific» with cuvette of 0.10 cm long. Mass spectra (EI-MS, 70 eV) were recorded on a quadropoule mass spectrometer FINNIGAN MAT INCOS 50 with direct insertion; all assignments were made with reference to the most abundant isotopes.

X-ray crystallography. Experimental intensities were measured on a Bruker SMART APEX II diffractometer using ω-scan mode. Absorption correction based on measurements of equivalent reflections was applied.[1] The structure was solved be direct methods and refined by full matrix least-squares based on F^2 with anisotropic thermal parameters for all non-hydrogen atoms.[2] All disordered –$SiMe_3$ groups were refined with restrained Si-C distances. All hydrogen atoms were placed in calculated positions and refined using a riding model. The structure of **1** contains three crystallographically independent molecules. One of them occupies general position while two others lie on mirror planes. In all molecules atrane fragments and all –$SiMe_3$ groups are disordered over two positions with occupancy ratios 0.5/0.5. The structure was checked for supercell and low-symmetry space groups. These possibilities were not confirmed.

Table S1 Crystal data for germatrane **1**

Empirical formula	$C_{15}H_{39}Ge_2NO_3Si_3$
M_r	510.92
Crystal system	Monoclinic
Space group	P21/m
a, Å	11.3567(16)
b, Å	27.748(4)
c, Å	16.127(2)
β, degree	102.683(2)
V, Å^3	4957.8(12)
D_{calcd}, g*cm^{-3}	1.369
Z	8
F(000)	2128
μ (Mo Kα), mm^{-1}	2.582
temperature, K	130(2)
Total reflections	30945
Unique reflections (R_{int})	9333 (0.0726)
Parameters	524
Restraints	204
R_1 (I>2σ(I))	0.0592
wR_2 (all reflections)	0.1391
goodness-of-fit on F^2	1.055
Min/max residual electron density, e*Å^{-3}	-0.668 / 1.321

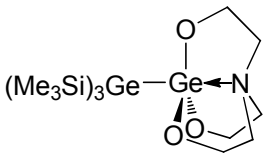
Synthesis. The known compounds $(TMS)_3GeGeCl_3$[3] and $TfOGe(OCH_2CH_2)_3N$[4] were obtained using literature procedure.

Synthesis of 1. *Method 1.* At -78˚C solution of $N(CH_2CH_2OH)_3$ (0.16 ml, 1.17 mmol), Et_3N (0.50 ml, 3.50 mmol) in CH_2Cl_2 (30 ml) was added dropwise over 1 h to solution of $(Me_3Si)_3GeGeCl_3$ (0.55 g, 1.17 mmol) in CH_2Cl_2 (70 ml). The reaction mixture was slowly warmed to room temperature and mixed for 1 h more. All volatiles were removed in vacuum, benzene (50 ml) was added to the residue and the suspension formed was filtered. The solvent was removed, hexane (40 ml) was added, and the mixture was filtered. The volatiles were removed and the solid formed was recrystallized from hexane/CH_2Cl_2 (1:5). After filtration and concentration the solution formed was stored at -25 ^oC for 3 d. The precipitate formed was isolated and dried in high vacuum. The compound **1** was obtained as a white solid (0.11 g, 19%). The crystals suitable for X-ray analysis were obtained by recrystallization from pentane.

Method 2. The solution of $(Me_3Si)_3GeK$[5] generated *in situ* from $(Me_3Si)_4Ge$ (0.91 g, 2.50 mmol) and *t*-BuOK (0.28 g, 2.50 mmol) in THF (50 ml) was added dropwise to slurry of $TfOGe(OCH_2CH_2)_3N$ in xylene (15 ml) during 1 h at room temperature. The reaction mixture was stirred overnight, the volatiles were removed under vacuum, pentane (30 ml) was added and the suspension obtained was filtered. After removal of solvent the residue was recrystallized from acetonitrile at -30 ^oC yielding compound **1** (0.43 g, 34%) as a white powder.

^1H NMR ($CDCl_3$) δ 3.65 (t, J = 5.6 Hz, 6H, $3OCH_2$), 2.68 (t, J = 5.6 Hz, 6H, $3NCH_2$), 0.25 (s, 27H, $3Si(CH_3)_3$). ^{13}C NMR ($CDCl_3$) δ 57.84 (OCH_2), 53.53 (NCH_2), 2.67 ($SiCH_3$). ^1H NMR (C_6D_6) δ 3.43 (t, J = 5.4 Hz, 6H, $3OCH_2$), 2.04 (t, J = 5.4 Hz, 6H, $3NCH_2$), 0.26 (s, 27H, $3Si(CH_3)_3$). ^{13}C NMR (C_6D_6) δ 57.88 (OCH_2), 52.87 (NCH_2), 2.79 ($SiCH_3$). ^{29}Si NMR (C_6D_6) δ -6.37. UV/vis (CH_2Cl_2) λ_{max} nm (ε, M^{-1} $см^{-1}$): 221 (2.3×10^4). MS (EI) *m/z* 513 (M^+, 5), 367 (A = M - 2TMS, 12), 293 ($(Me_3Si)_3Ge$, 4), 220 ($Ge(OCH_2CH_2)_3N$, 6), 219 ($(Me_3Si)_2Ge$ - H, 12), 147 (Me_3SiGe, 15), 132 (Me_3SiGe – Me, 5), 73 (Me_3Si, 100). Calcd., %: C 35.26, H 7.69, N 2.74. Found, %: C 35.18, H 7.79, N 2.70. $C_{15}H_{39}Ge_2NO_3Si_3$.

Fig. S1 ^{1}H NMR Spectrum (400.130 MHz, $CDCl_3$) of Germatrane **1**.



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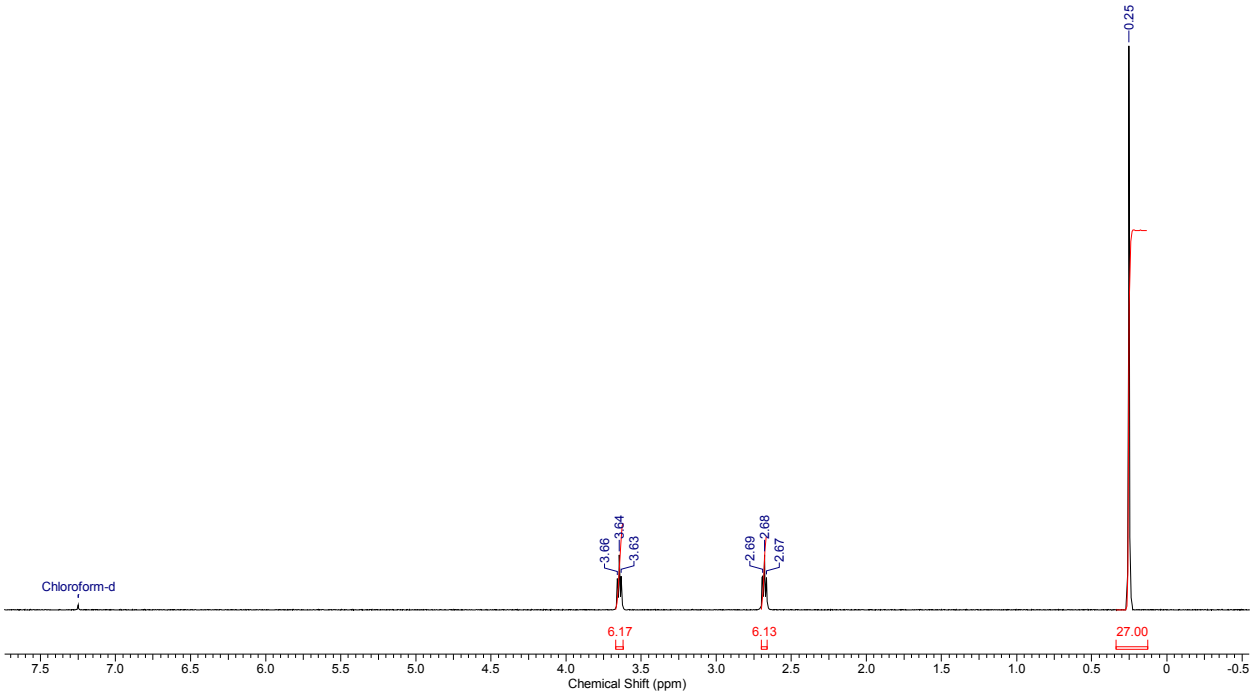
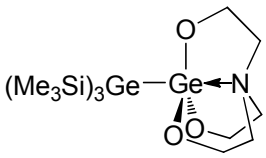


Fig. S2 ^{13}C NMR Spectrum (100.613 MHz, $CDCl_3$) of Germatrane **1**.



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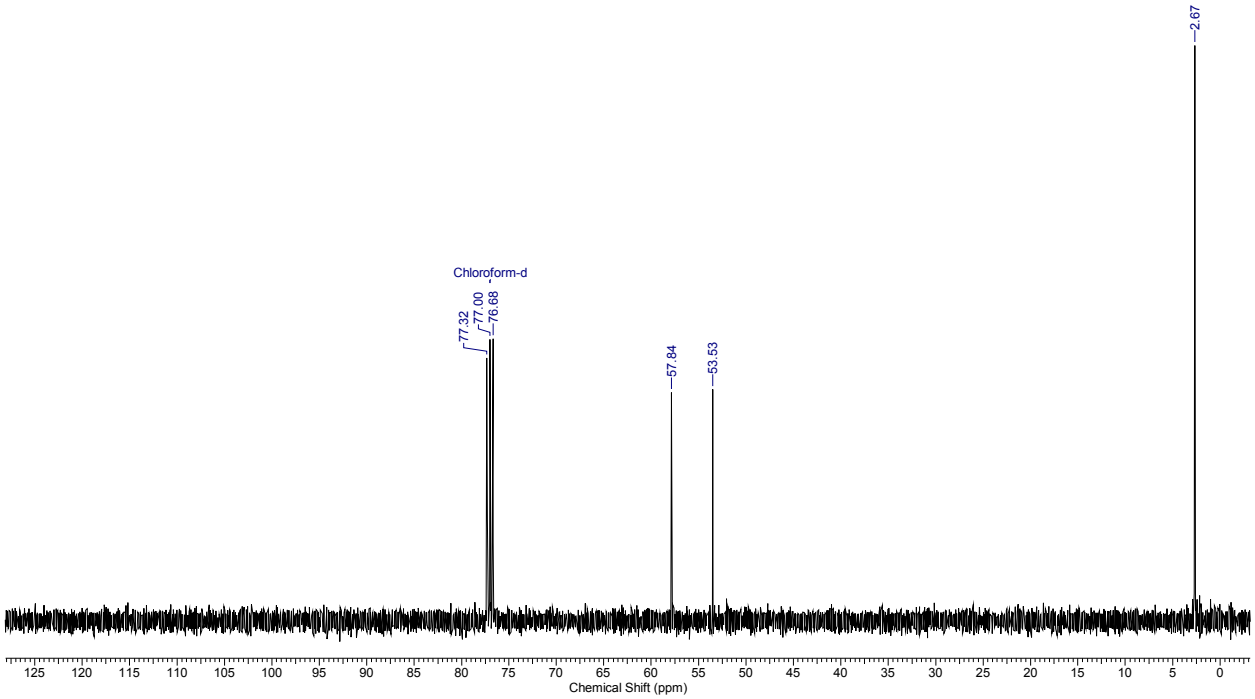
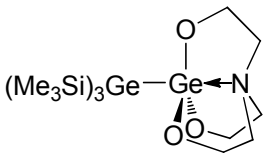


Fig. S3 ^{29}Si NMR Spectrum (79.495 MHz, $CDCl_3$) of Germatrane **1**.



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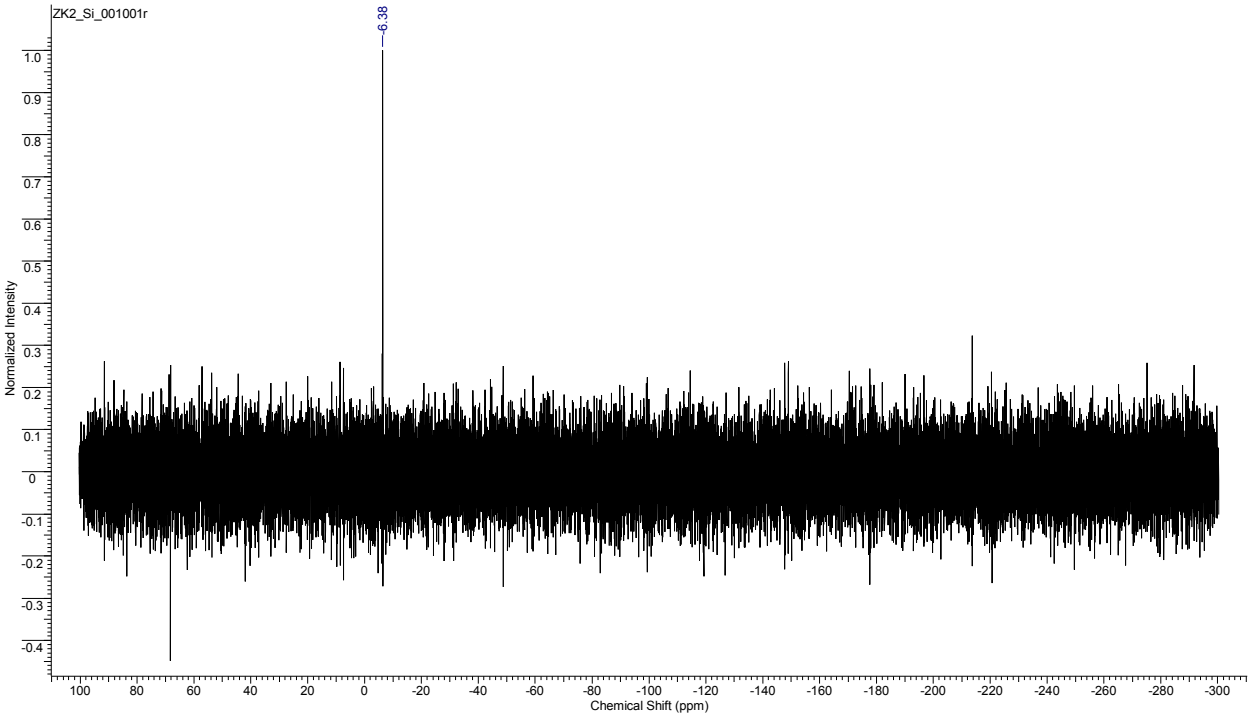


Fig. S4 UV/vis spectrum of germatrane **1** in CH_2Cl_2.

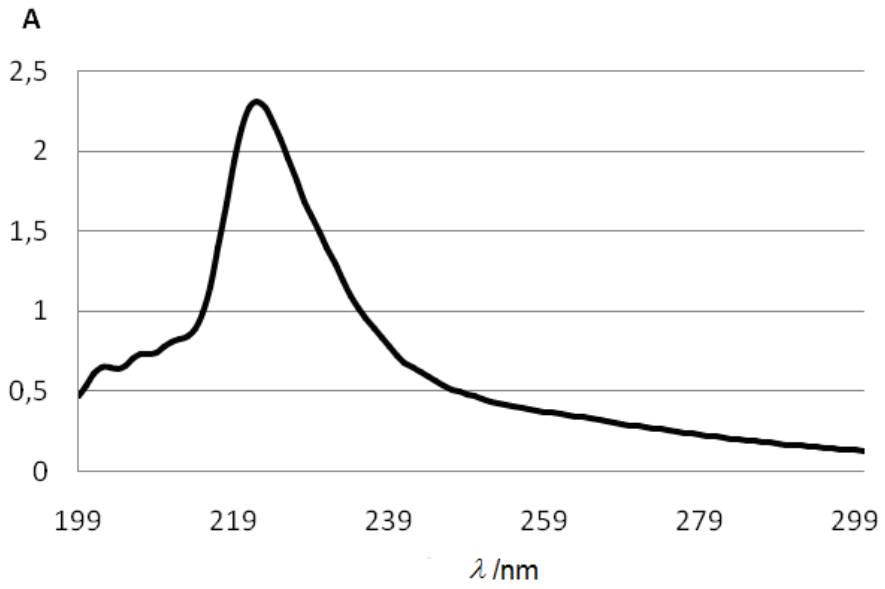
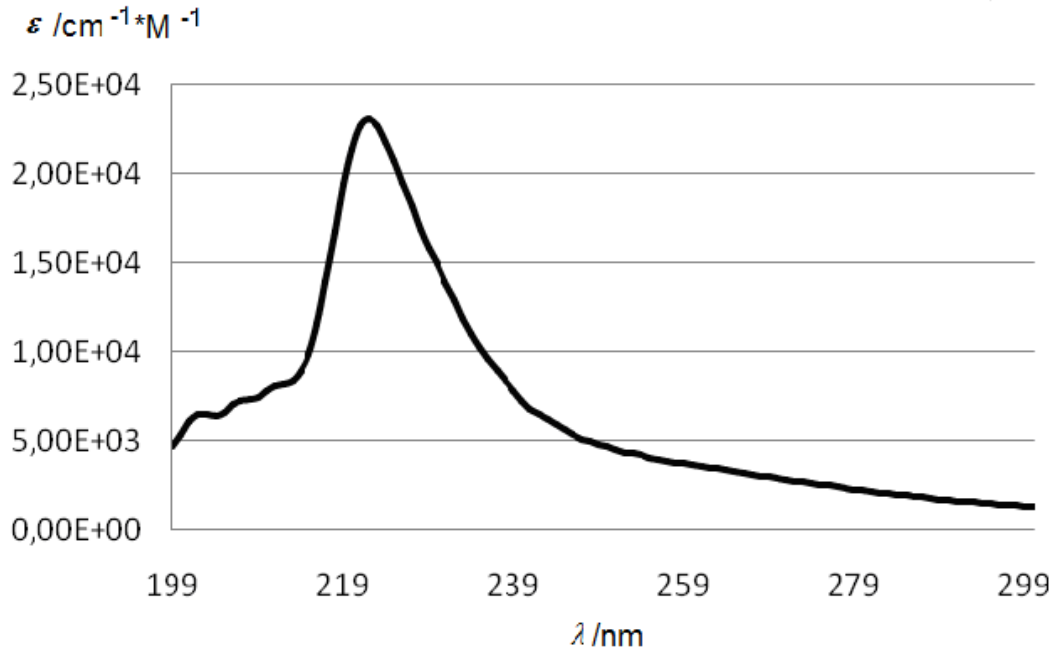


Fig. S5 UV/vis spectrum of compound **1** in CH_2Cl_2.



DFT calculations. The nonlocal hybrid three-parameter B3LYP[6] density functional has been used throughout the study because previous theoretical calculations have shown that B3LYP approach is a cost-effective method for studying metal containing systems.[7] Even at calculations of the thermodynamic parameters, B3LYP results compare well to the highly exact G2 (MP2, SVP) methods, as well as to the experimental values.[8] We have used DGDZVP basis set for all the atoms at the B3LYP level. DGDZVP basis set is all-electron, double-ζ valence polarized basis sets which were optimized specifically for DFT methods.[9]

The calculations were performed with full geometry optimization and used the GAUSSIAN'03 program package.[10] The absence of imaginary vibration frequencies confirmed the stationary character of the structures. The formation enthalpies were corrected for zero-point vibration energy (ZPVE) and reduced to the normal conditions (298.15 K, 1 atm) using a thermal correction to the enthalpy. The electronic structures of the compounds were examined by NBO analysis.[11] The molecular orbitals were constructed using the GaussView program.

Additional single-point calculations have been carried out for Ge dimers using the binding energy partition scheme implemented in the ADF program.[12] This scheme has been widely applied to a large number of systems including metal-containing ones.[13] We have used the BP86 functional of Becke[6] and the correlation functional of Perdew.[14] Scalar relativistic effects have been considered using the ZORA formalism.[15] Uncontracted Slater-type orbitals (STOs) using triple-ζ basis sets augmented by two sets of polarization functions were employed for the SCF calculations.[16]

It is important to recall that in the NBO analysis the electronic wave function is interpreted in terms of a set of occupied Lewis and a set of unoccupied non-Lewis localized orbitals.[11] Delocalization effects can be identified from the presence of off-diagonal elements of the Fock matrix in the NBO basis. The strengths of these delocalization interactions, $E_{ij}^{(2)}$, are estimated by second-order perturbation theory.

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Table S2. The NMR spectroscopy data for germatrane 1

Nucleus	Group	Exp, δ, ppm	Calcd., B3LYP/6-311+G(2d,p) GIAO relative TMS
^{1}H	$SiMe_3$	0.25 ($CDCl_3$), 0.26 (C_6D_6)	0.1-0.8
	NCH_2	2.68 ($CDCl_3$), 2.04 (C_6D_6)	2.6-3.0
	OCH_2	3.65 ($CDCl_3$), 3.43 (C_6D_6)	3.7-4.1
^{13}C	$SiMe_3$	2.67 ($CDCl_3$), 2.79 (C_6D_6)	2.7-3.1
	NCH_2	53.53 ($CDCl_3$), 52.87 (C_6D_6)	60.1; 65.4; 65.8
	OCH_2	57.84 ($CDCl_3$), 57.88 (C_6D_6)	64.6; 68.4; 69.1
^{29}Si		-6.37 (C_6D_6)	2.0; 3.0
^{15}N		-	34.3 (relative to NH_3)
^{17}O		-	95.3; 112.1; 114.1 (relative to H_2O)

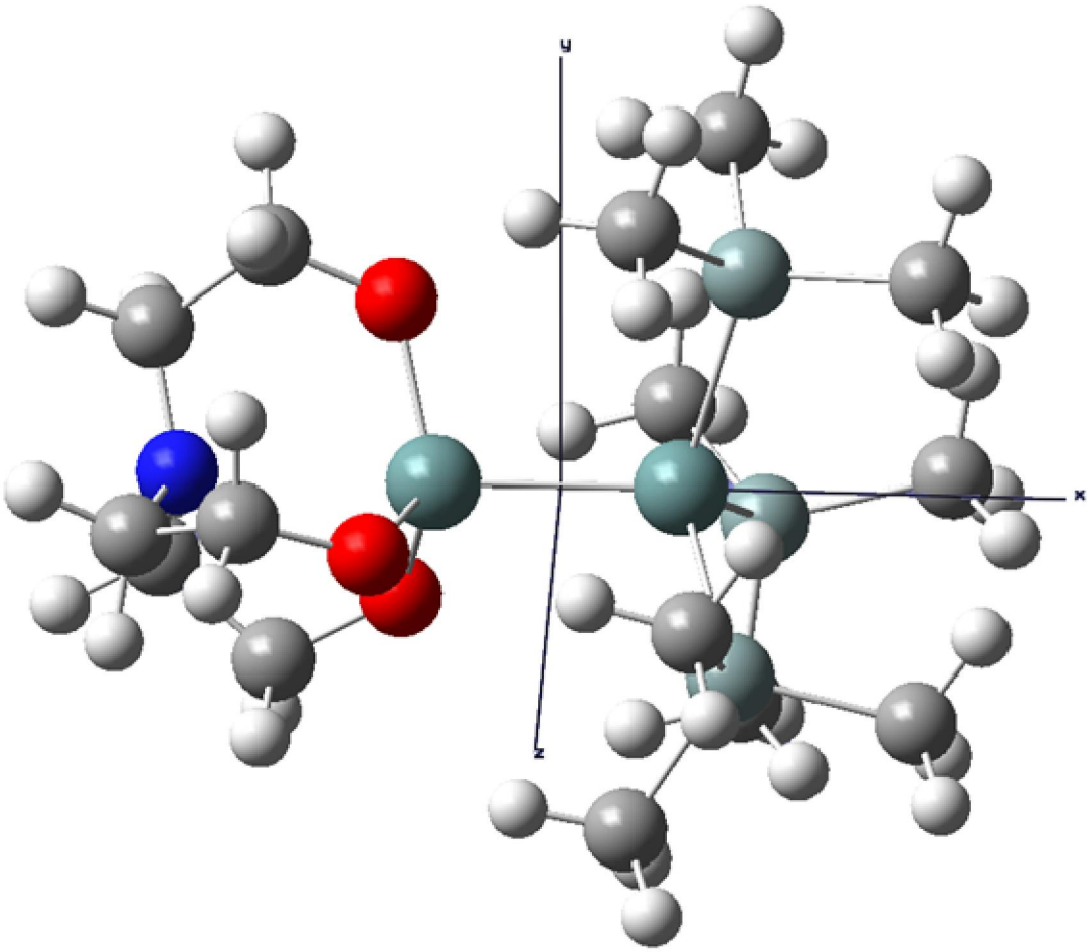
Table S3 NBO analysis of the germatrane 1, calculated at B3LYP/DGDZVP level of the theory

Bond	Hybridization	Population, e	Interaction between N, O lone pairs and anti-bonding Ge-O orbitals	$Eij^{(2)}$, kcal/mol
BD(Ge-Ge)	$sp^{2.4}$	1.860	BD(Ge-Ge)→BD*(Ge-O)	20
BD(Ge-O)	$sp^{3.2}$	1.951	LP(O)→BD*(Ge-O)	38
BD(Ge-Si)	$sp^{2.7}$	1.927	LP(N)→BD*(Ge-O)	17
LP(O)	$sp^{1.2}$	1.949		
LP(O)	p	1.918		
LP(N)	p	1.819		

Table S4 The thermodynamic characteristics of the complexes (kcal/mol)

Reaction	ΔG	ΔE	E_a (B3LYP/DGDZVP)	E_a (BP86/TZ2P+)
$(CH_3)_3SiSiCl_3$*$N(CH_3)_3$ -> $(CH_3)_3SiCl + SiCl_2$*$N(CH_3)_3$	-6	-11	38	42
$(CH_3)_3GeGeCl_3$<---$N(CH_3)_3$	-33	-22	28	22
$(CH_3)_3SnSnCl_3$<---$N(CH_3)_3$	-21	-16	83	72

Fig. S6 Standard orientation of molecule **1**



Standard orientation:

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3	14	0	1.935478	-1.455601	-1.786693
4	14	0	1.793783	-0.824155	2.194323
5	14	0	1.829798	2.314262	-0.348119

6	6	0	3.774482	-1.123424	-2.133711
7	6	0	0.947591	-1.144112	-3.372979
8	6	0	1.723127	-3.269411	-1.282798
9	6	0	3.637988	-1.283869	2.213314
10	6	0	1.477789	0.508265	3.504044
11	6	0	0.774558	-2.358265	2.639094
12	6	0	3.669488	2.534897	0.077366
13	6	0	0.807603	3.466433	0.756510
14	6	0	1.561972	2.811074	-2.157288
15	8	0	-1.689232	1.419896	-1.107428
16	8	0	-1.822983	0.200554	1.712239
17	8	0	-1.624125	-1.745506	-0.635220
18	7	0	-3.821926	-0.103495	-0.216277
19	6	0	-4.211393	0.029703	1.192612
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31	1	0	2.019328	-3.934729	-2.104317
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33	1	0	0.676156	-3.476385	-1.038154
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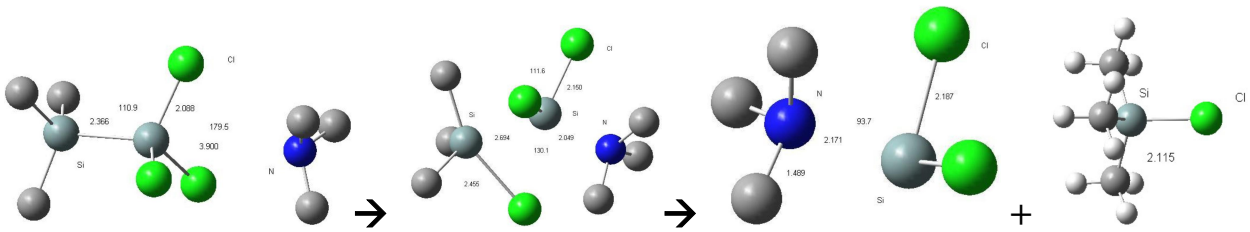
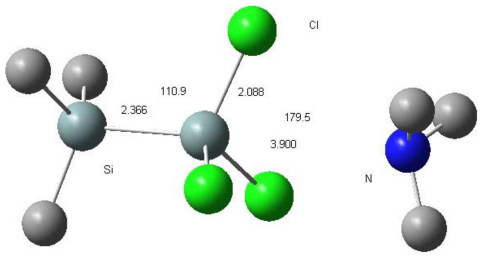


Complex of $Me_3SiSiCl_3$ with NMe_3, $Me_3SiSiCl_3$*NMe_3



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Standard orientation:

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4	1	0	3.074574	1.134442	2.233486
5	6	0	3.439808	0.373804	-1.750037
6	1	0	4.536052	0.384213	-1.791211
7	1	0	3.087807	-0.379119	-2.463073
8	1	0	3.085645	1.352492	-2.090679
9	6	0	3.422288	-1.721285	0.558974
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11	1	0	3.063950	-1.960694	1.565683
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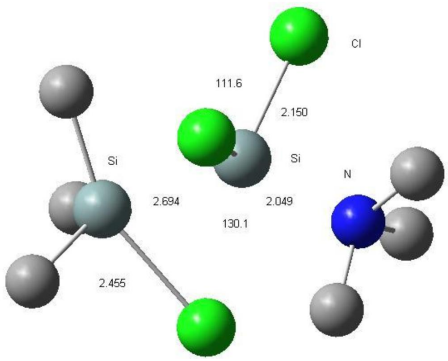
15	17	0	-0.236656	1.867009	-0.600398
16	6	0	-3.850169	1.023720	0.941611
17	1	0	-4.953729	1.096529	1.014326
18	1	0	-3.456319	0.808334	1.940339
19	1	0	-3.464285	2.000312	0.631489
20	1	0	-4.936196	-1.445949	0.447674
21	1	0	-3.429088	-2.084718	-0.261991
22	1	0	-3.447238	-1.547735	1.424904
23	6	0	-3.834425	0.293774	-1.358310
24	1	0	-3.450303	1.273333	-1.661338
25	1	0	-3.426766	-0.454514	-2.045875
26	1	0	-4.936697	0.304710	-1.473609
27	7	0	-3.404560	-0.002558	0.004421
28	6	0	-3.833913	-1.332857	0.423359
29	14	0	2.862801	-0.004087	0.007842
30	14	0	0.496896	0.005479	-0.002696

Transition state (TS) in decomposition of complex $Me_3SiSiCl_3$*NMe_3



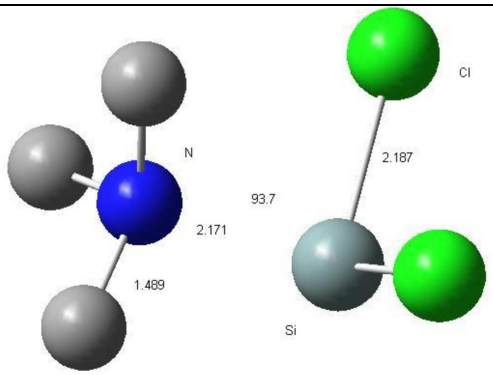
G= -2253.639 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.469284	0.250334	-1.254724
2	1	0	4.182965	-0.576219	-1.358203
3	1	0	3.009951	0.416658	-2.235547
4	1	0	4.001551	1.167128	-0.990089
5	6	0	2.021892	-2.085949	-0.277596

	6	1	0	3.038044	-2.485483	-0.142526
	7	1	0	1.368923	-2.626860	0.416257
	8	1	0	1.714479	-2.334981	-1.299158
	9	6	0	2.634561	-0.036185	1.850193
	10	1	0	3.324726	-0.847757	2.112090
	11	1	0	3.113168	0.925300	2.051507
	12	1	0	1.763989	-0.122146	2.508961
	13	17	0	-1.251440	-1.634174	1.610278
	14	17	0	1.447537	2.164909	-0.093397
	15	17	0	-1.280650	-1.511365	-1.757189
	16	6	0	-1.876975	1.835735	-1.189817
	17	1	0	-2.618749	2.638186	-1.124762
	18	1	0	-0.872688	2.259804	-1.219342
	19	1	0	-2.061184	1.242465	-2.086134
	20	1	0	-2.544587	2.582584	1.282315
	21	1	0	-1.923407	1.146636	2.138911
	22	1	0	-0.796045	2.207189	1.241327
	23	6	0	-3.393581	0.381661	0.048860
	24	1	0	-3.557977	-0.222035	-0.843254
	25	1	0	-3.517674	-0.239741	0.934965
	26	1	0	-4.114223	1.205650	0.073401
	27	7	0	-2.007919	0.953770	0.021434
	28	6	0	-1.799769	1.780482	1.259749
	29	14	0	2.148516	-0.184945	0.032963
	30	14	0	-0.530723	-0.464951	-0.043356

Complex of $SiCl_2$ with NMe_3 – the product of $Me_3SiSiCl_3$*NMe_3 decomposition

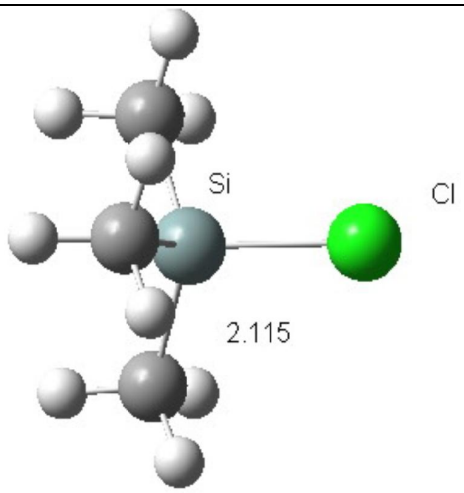


G= -1384.304 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.641571	-0.000120	-0.962328
2	17	0	1.410566	-1.680705	0.207256
3	17	0	1.410195	1.680994	0.207172
4	6	0	-1.989903	-1.216255	-0.444264
5	1	0	-1.475911	-2.106437	-0.078757
6	1	0	-3.027729	-1.220581	-0.089785
7	1	0	-1.983771	-1.226794	-1.537415
8	6	0	-1.238288	-0.000107	1.530598
9	1	0	-0.706594	0.887319	1.875476
10	1	0	-2.257753	-0.000571	1.936586
11	1	0	-0.705834	-0.887120	1.875389
12	6	0	-1.989964	1.216070	-0.444214
13	1	0	-3.027760	1.220315	-0.089655
14	1	0	-1.475976	2.106272	-0.078743
15	1	0	-1.983911	1.226600	-1.537365
16	7	0	-1.282966	-0.000070	0.042695

Me_3SiCl – the product of $Me_3SiSiCl_3$*NMe_3 decomposition

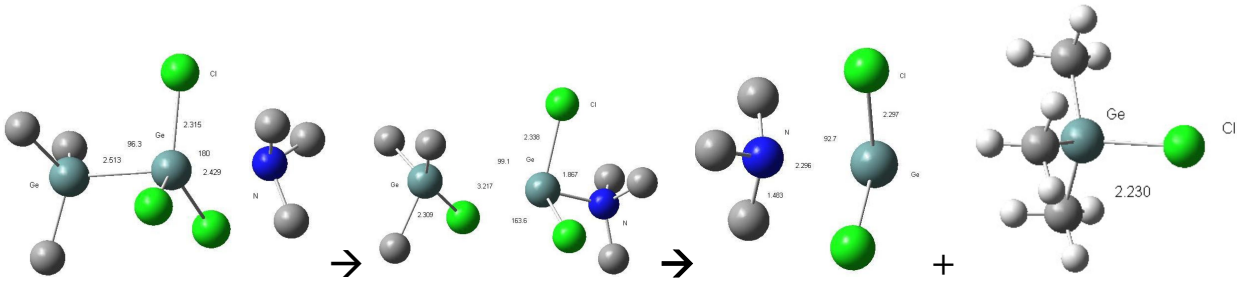


E = -869.484062438 a.e.

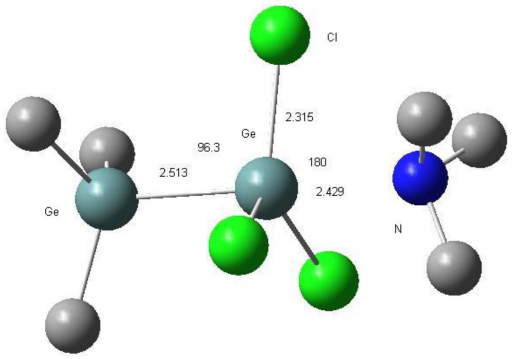
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.343517	0.000073	-0.000343
2	6	0	-0.896657	1.697126	-0.585081
3	1	0	-1.992151	1.755699	-0.612504
4	1	0	-0.534815	2.486228	0.082687
5	1	0	-0.523485	1.913591	-1.591743
6	6	0	-0.897773	-0.341708	1.761543
7	1	0	-1.993232	-0.338593	1.827315
8	1	0	-0.543396	-1.318176	2.108617
9	1	0	-0.517718	0.417384	2.453521
10	6	0	-0.896890	-1.355231	-1.176861
11	1	0	-0.524840	-1.179181	-2.191797
12	1	0	-0.534082	-2.336561	-0.853039
13	1	0	-1.992403	-1.399841	-1.223036
14	17	0	1.771369	-0.000158	0.000422

TS



Complex of $Me_3GeGeCl_3$ with NMe_3, $Me_3GeGeCl_3$*NMe_3



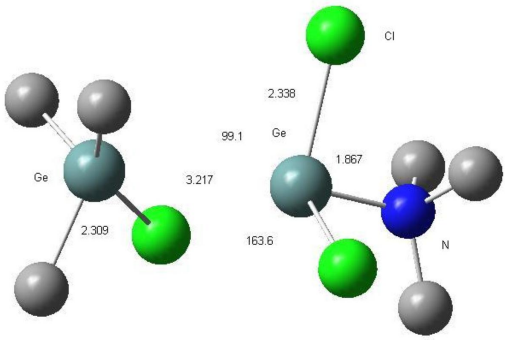
G= -5827.929 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.771528	1.624454	0.959643
2	1	0	-3.866066	1.664406	0.979922
3	1	0	-2.398641	1.610563	1.986356
4	1	0	-2.394109	2.516048	0.453631
5	6	0	-2.772939	-1.644212	0.926356
6	1	0	-3.867555	-1.680043	0.953190
7	1	0	-2.402572	-2.526211	0.398811
8	1	0	-2.393309	-1.654188	1.950686
9	6	0	-2.772403	0.020018	-1.887011
10	1	0	-3.866965	0.017314	-1.931087
11	1	0	-2.400116	0.917270	-2.386765
12	1	0	-2.395189	-0.862803	-2.408336
13	17	0	0.562893	-1.974391	-1.181098
14	17	0	0.560783	2.011343	-1.118336
15	17	0	0.561186	-0.035689	2.300573

16	6	0	3.246055	1.197964	0.720036
17	1	0	4.344494	1.193337	0.714837
18	1	0	2.890412	2.102712	0.227817
19	1	0	2.893795	1.184892	1.751230
20	1	0	4.343820	0.023384	-1.391681
21	1	0	2.890626	-0.855609	-1.933931
22	1	0	2.891734	0.922699	-1.903350
23	6	0	3.245776	-1.222156	0.676990
24	1	0	2.890771	-1.247199	1.706770
25	1	0	2.892667	-2.108718	0.150926
26	1	0	4.344175	-1.215480	0.674706
27	7	0	2.736357	0.000378	-0.000307
28	6	0	3.245401	0.024369	-1.397964
29	32	0	-2.205241	-0.000513	-0.000131
30	32	0	0.307825	-0.000397	0.000155

Transition state (TS) in decomposition of complex $Me_3GeGeCl_3*NMe_3$



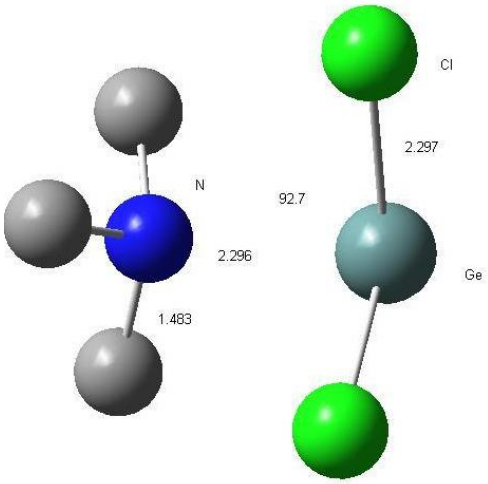
G= -5827.884

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.097339	-1.636311	0.714275
2	1	0	-4.182190	-1.669506	0.562671
3	1	0	-2.651592	-2.524198	0.259249
4	1	0	-2.889140	-1.639898	1.785656
5	6	0	-2.623507	-0.005213	-2.071719
6	1	0	-3.698702	-0.011878	-2.281161

	7	1	0	-2.177217	0.886099	-2.518483
	8	1	0	-2.167274	-0.893668	-2.514177
	9	6	0	-3.097679	1.641219	0.705911
	10	1	0	-4.181703	1.676077	0.548959
	11	1	0	-2.894427	1.647916	1.778245
	12	1	0	-2.648199	2.526847	0.250099
	13	17	0	1.242262	2.017521	-1.151170
	14	17	0	-0.964794	-0.003581	1.709932
	15	17	0	1.233511	-2.006790	-1.164194
	16	6	0	2.984978	-1.222530	1.315402
	17	1	0	4.063587	-1.216993	1.519615
	18	1	0	2.441915	-1.232807	2.260721
	19	1	0	2.732752	-2.114700	0.743326
	20	1	0	4.068659	1.189795	1.532089
	21	1	0	2.738547	2.100523	0.769868
	22	1	0	2.448404	1.200339	2.276738
	23	6	0	3.398640	0.001336	-0.733535
	24	1	0	3.155795	-0.882580	-1.320915
	25	1	0	3.161207	0.895323	-1.308081
	26	1	0	4.472279	-0.003691	-0.502084
	27	7	0	2.616597	-0.005452	0.538735
	28	6	0	2.989670	1.200614	1.330264
	29	32	0	-2.375364	0.000506	-0.118244
	30	32	0	0.840236	0.002897	-0.034403

Complex of $GeCl_2$ with NMe_3 – the product of $Me_3GeGeCl_3$*NMe_3 decomposition

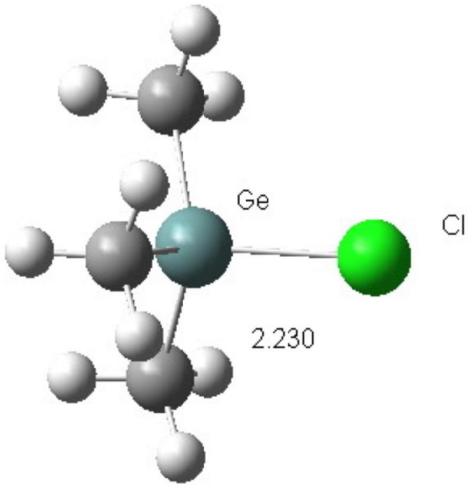


G= -3171.465 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.296052	-1.765393	0.510349
2	17	0	1.295899	1.765510	0.510333
3	6	0	-2.156428	-1.217504	-0.411601
4	1	0	-1.642675	-2.103181	-0.033055
5	1	0	-3.209754	-1.247984	-0.102410
6	1	0	-2.109764	-1.220595	-1.504383
7	6	0	-1.510967	-0.000196	1.596682
8	1	0	-0.993281	0.886524	1.965096
9	1	0	-2.547486	-0.000041	1.961253
10	1	0	-0.993637	-0.887218	1.964880
11	6	0	-2.156437	1.217541	-0.411389
12	1	0	-3.209768	1.247950	-0.102207
13	1	0	-1.642685	2.103144	-0.032689
14	1	0	-2.109765	1.220832	-1.504173
15	7	0	-1.491536	-0.000024	0.112600
16	32	0	0.618106	-0.000009	-0.793571

Me_3GeCl – the product of $Me_3GeGeCl_3$*NMe_3 decomposition

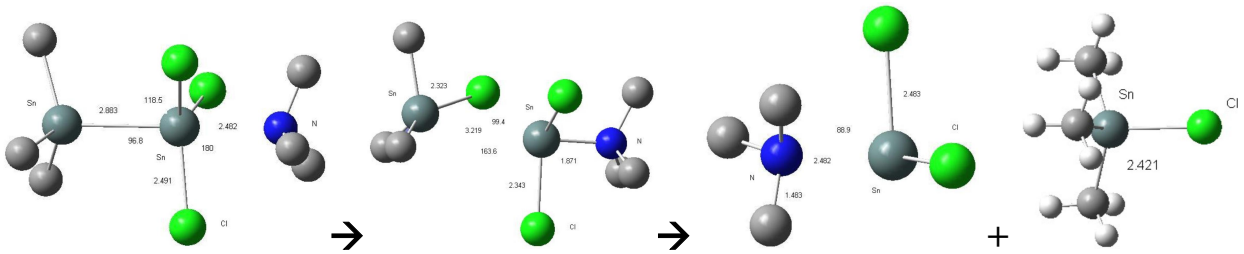


E = -2656.59400261 a.e.

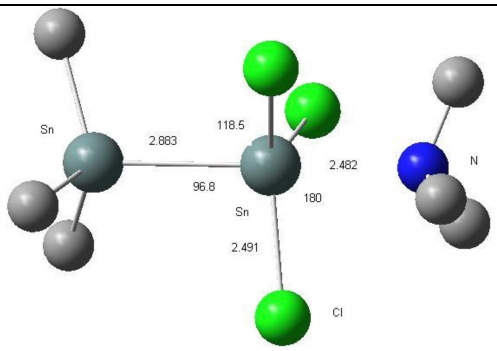
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.835848	-1.540369	-1.088521
2	1	0	1.928841	-1.591980	-1.132940
3	1	0	0.455051	-2.465867	-0.649676
4	1	0	0.444173	-1.442553	-2.103937
5	6	0	0.836774	-0.172448	1.877751
6	1	0	1.929741	-0.192899	1.943316
7	1	0	0.462850	0.673950	2.459061
8	1	0	0.438992	-1.097259	2.302662
9	6	0	0.834857	1.713300	-0.789646
10	1	0	0.444353	1.801426	-1.806408
11	1	0	0.452193	2.542939	-0.190184
12	1	0	1.927835	1.773414	-0.822588
13	17	0	-1.936601	-0.000428	0.000612
14	32	0	0.293541	0.000100	-0.000225

TS



Complex of $Me_3GeGeCl_3$ with NMe_3, $Me_3GeGeCl_3$*NMe_3



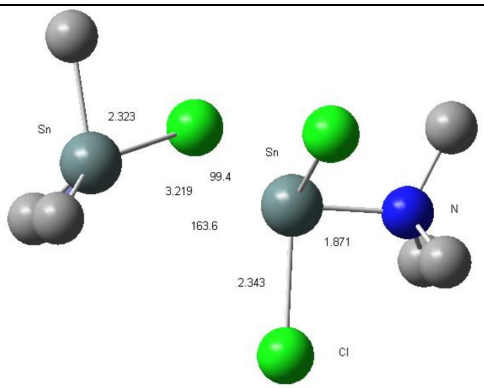
G= -13724.275 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.930569	-2.041286	0.432271
2	1	0	4.024062	-2.091914	0.427524
3	1	0	2.565412	-2.350163	1.414904
4	1	0	2.540048	-2.727039	-0.323743
5	6	0	2.931627	1.394250	1.550646
6	1	0	4.025277	1.427645	1.584842
7	1	0	2.552566	2.396545	1.336249
8	1	0	2.555803	1.072891	2.525190
9	6	0	2.936803	0.645282	-1.982406
10	1	0	4.030667	0.659726	-2.023719
11	1	0	2.562291	-0.042477	-2.744659
12	1	0	2.560380	1.649338	-2.193205
13	17	0	-0.888117	2.411461	-0.550792
14	17	0	-0.894755	-1.685371	-1.808038
15	17	0	-0.889105	-0.727529	2.363213

16	6	0	-3.588022	-1.364574	0.307424
17	1	0	-4.685773	-1.353846	0.307312
18	1	0	-3.234840	-2.067023	-0.447676
19	1	0	-3.231208	-1.676326	1.289162
20	1	0	-4.683862	0.421932	-1.326965
21	1	0	-3.225165	1.420594	-1.571204
22	1	0	-3.236007	-0.279771	-2.098087
23	6	0	-3.585437	0.952047	1.029177
24	1	0	-3.230779	0.649627	2.014623
25	1	0	-3.228581	1.957868	0.807413
26	1	0	-4.683243	0.947442	1.021952
27	50	0	2.288998	-0.000264	-0.000713
28	50	0	-0.594165	-0.000299	-0.000608
29	7	0	-3.075905	0.001499	-0.000501
30	6	0	-3.586167	0.418788	-1.337930

Transition state (TS) in decomposition of complex $Me_3GeGeCl_3*NMe_3$



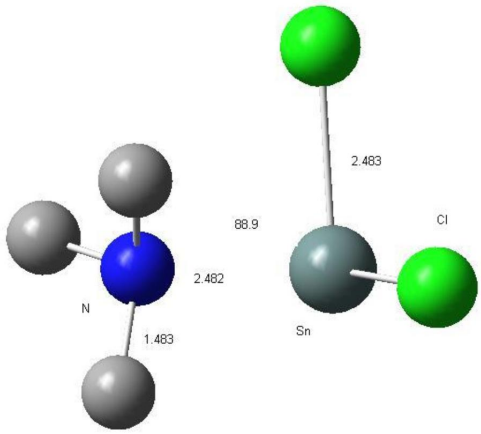
G= -13724.002 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.966476	-1.656994	0.761909
2	1	0	-4.052807	-1.697003	0.622713
3	1	0	-2.523229	-2.546644	0.307720
4	1	0	-2.749737	-1.659190	1.832088
5	6	0	-2.535886	-0.003165	-2.068917

	6	1	0	-3.612279	-0.009409	-2.274602
	7	1	0	-2.095684	0.887886	-2.522555
	8	1	0	-2.085994	-0.890398	-2.520594
	9	6	0	-2.967079	1.659392	0.757117
	10	1	0	-4.052616	1.701420	0.612519
	11	1	0	-2.755424	1.662374	1.828328
	12	1	0	-2.520079	2.547782	0.304086
	13	17	0	1.372613	2.024160	-1.140815
	14	17	0	-0.811168	-0.006136	1.730515
	15	17	0	1.367233	-2.011392	-1.157133
	16	6	0	3.135214	-1.224848	1.304382
	17	1	0	4.217546	-1.220062	1.488214
	18	1	0	2.610124	-1.237283	2.259642
	19	1	0	2.872827	-2.116183	0.735711
	20	1	0	4.222681	1.190514	1.503319
	21	1	0	2.878926	2.101305	0.766974
	22	1	0	2.616741	1.200599	2.278297
	23	6	0	3.512983	0.002250	-0.749009
	24	1	0	3.261067	-0.880825	-1.333606
	25	1	0	3.266833	0.896259	-1.319536
	26	1	0	4.590268	-0.003003	-0.536015
	27	7	0	2.752322	-0.005618	0.537013
	28	6	0	3.140009	1.200962	1.321886
	29	50	0	-2.249711	0.000153	-0.093432
	30	50	0	0.968601	0.002505	-0.028761

Complex of $GeCl_2$ with NMe_3 – the product of $Me_3GeGeCl_3$*NMe_3 decomposition

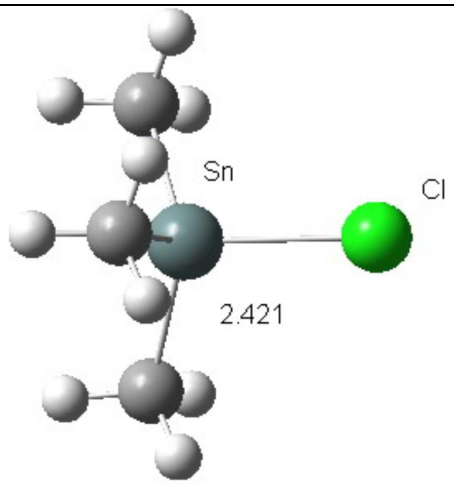


G= -7119.642 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.133513	-1.895937	0.818684
2	17	0	1.133382	1.896049	0.818619
3	6	0	-2.341127	-1.217645	-0.432390
4	1	0	-1.839189	-2.104118	-0.038704
5	1	0	-3.403398	-1.251262	-0.153611
6	1	0	-2.265430	-1.222143	-1.523765
7	6	0	-1.775306	0.000411	1.595297
8	1	0	-1.274369	0.887516	1.985809
9	1	0	-2.826529	-0.000374	1.916399
10	1	0	-1.272839	-0.885545	1.986460
11	6	0	-2.341326	1.217133	-0.433119
12	1	0	-3.403049	1.251893	-0.152398
13	1	0	-1.838107	2.103922	-0.041762
14	1	0	-2.267692	1.219798	-1.524635
15	7	0	-1.693267	-0.000042	0.111983
16	50	0	0.649056	-0.000014	-0.709011

Me_3SnCl – the product of $Me_3SnSnCl_3$*NMe_3 decomposition



E = -6604.74002240 a.e.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.841047	2.011627	-0.585109
2	1	0	-1.932299	2.093930	-0.609345
3	1	0	-0.445934	2.738022	0.129684
4	1	0	-0.445463	2.241938	-1.577661
5	6	0	-0.843488	-0.498860	2.033817
6	1	0	-1.934807	-0.517204	2.116708
7	1	0	-0.450533	-1.481917	2.305639
8	1	0	-0.447246	0.244665	2.730141
9	6	0	-0.842191	-1.512370	-1.449140
10	1	0	-0.442895	-1.260310	-2.434922
11	1	0	-0.451610	-2.488096	-1.148849
12	1	0	-1.933481	-1.570425	-1.511753
13	17	0	2.160024	-0.000676	0.000755
14	50	0	-0.261516	0.000170	-0.000198

Fig. S7 Interaction of O lone electron pairs with the Ge-O antibonding orbitals