Supporting Information

for

Unsaturated Amido-Substituted Six-Vertex Mixed Silicon Germanium Clusters

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1. Supplementary data for $[Si_{3.72}Ge_{2.28}\{N(SiMe_3)Dipp\}_4]$ (1)

EI-MS

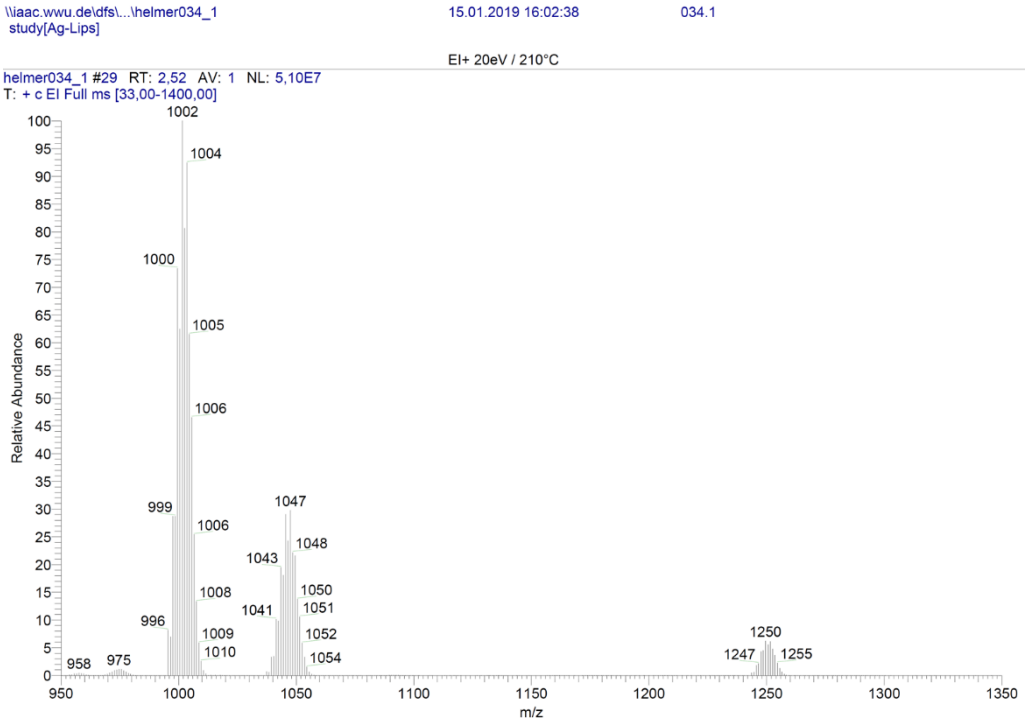


Figure S1. EI-MS spectrum of $[Si_{3.72}Ge_{2.28}\{N(SiMe_3)Dipp\}_4]$ (**1**).

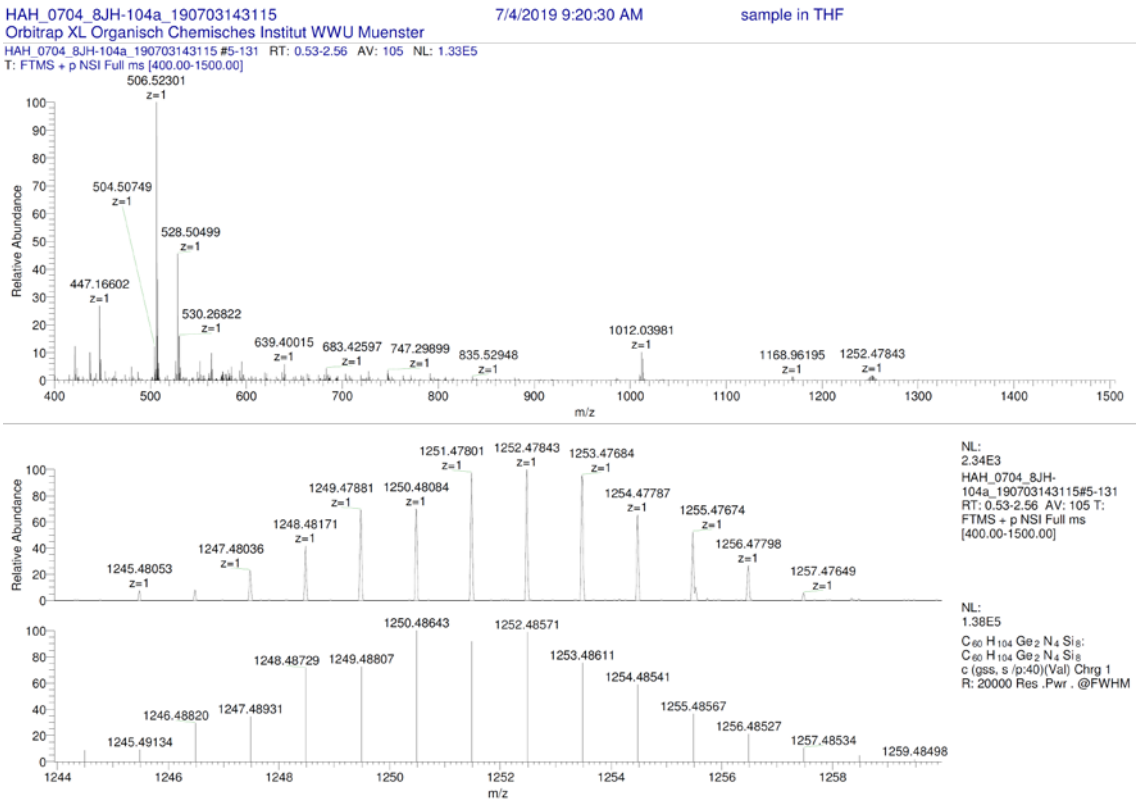


Figure S2. ESI-MS spectrum of **1** with zoom into the $Si_4Ge_2R_4$ cluster.

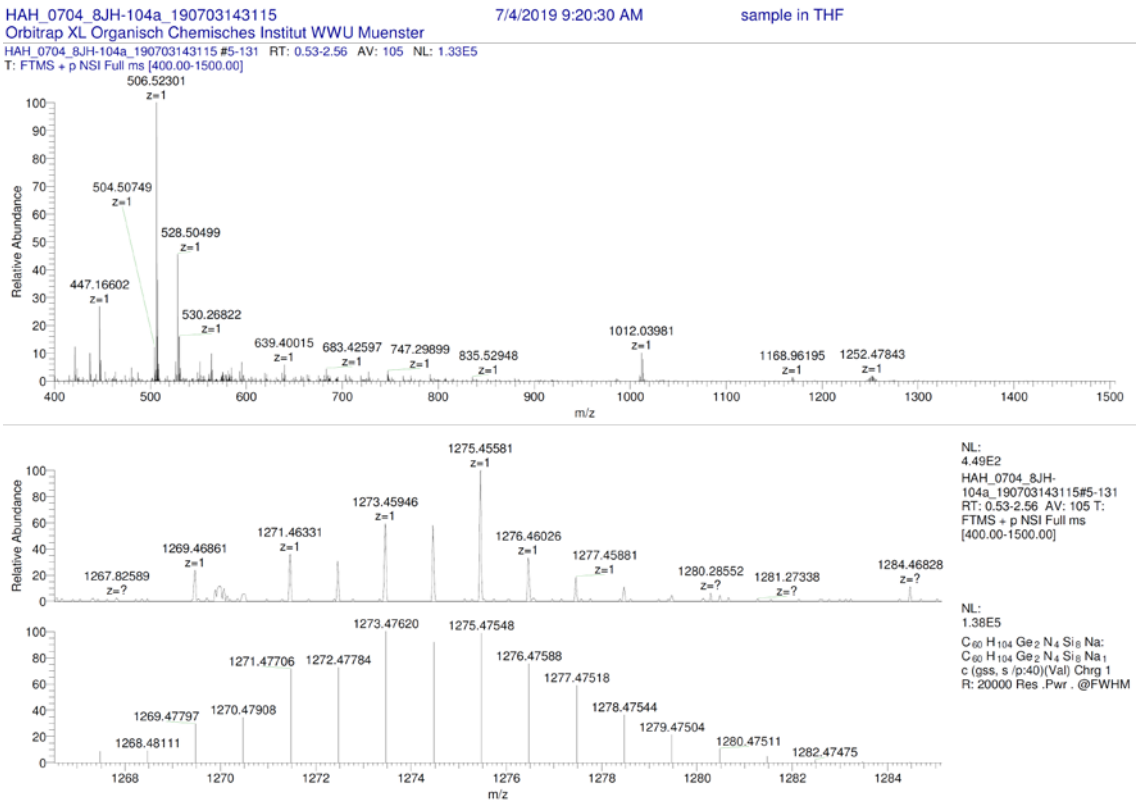


Figure S3. ESI-MS spectrum of **1** with zoom into the $Si_4Ge_2R_4$ cluster anion.

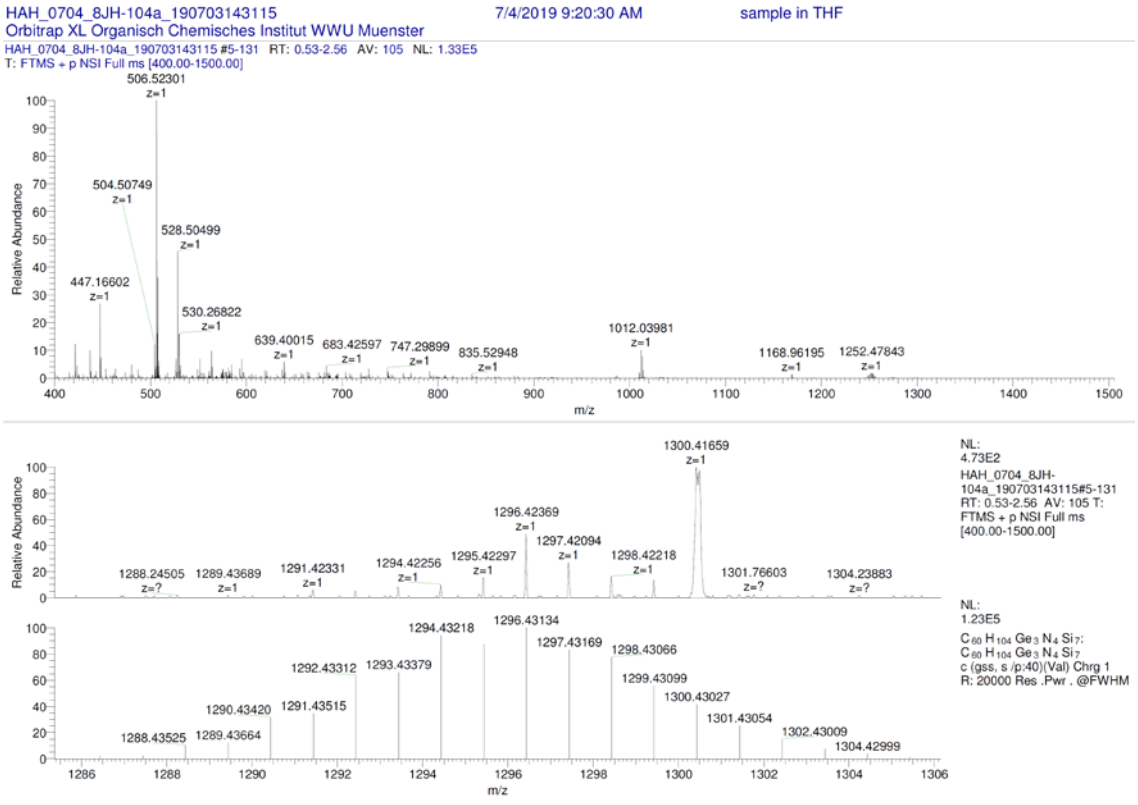


Figure S4. ESI-MS spectrum of **1** with zoom into the $Si_3Ge_3R_4$ cluster.

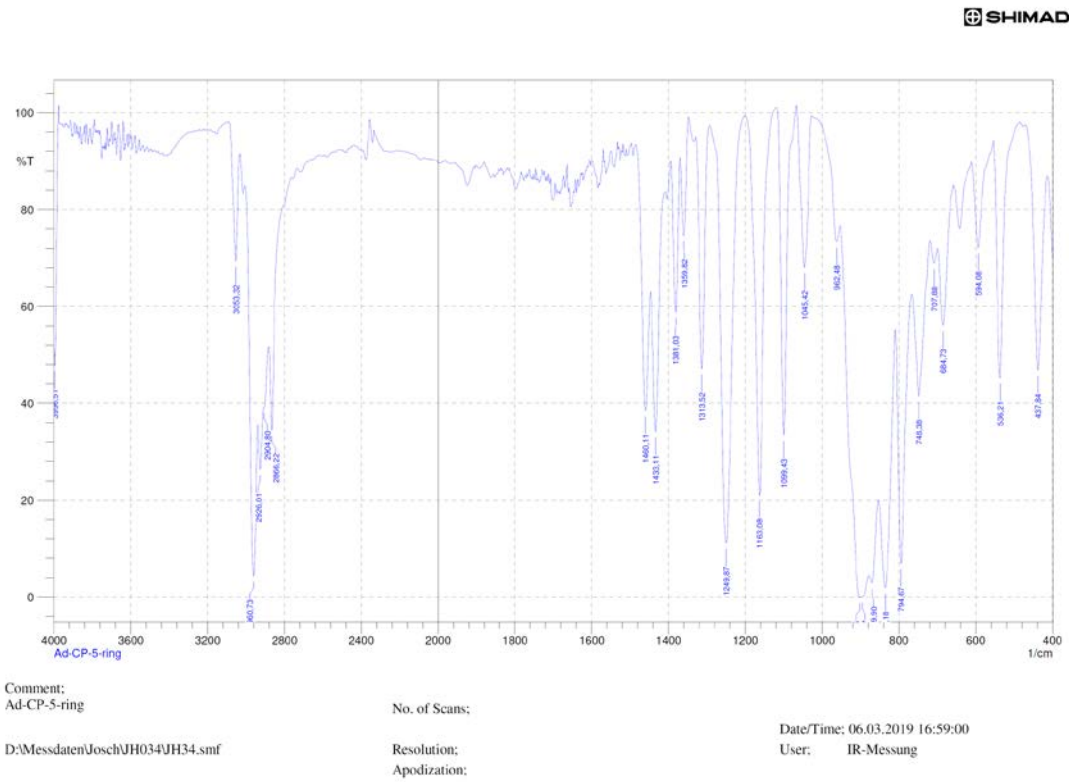


Figure S5. IR spectrum of $[Si_{3.72}Ge_{2.28}\{N(SiMe_3)Dipp\}_4]$ (**1**).

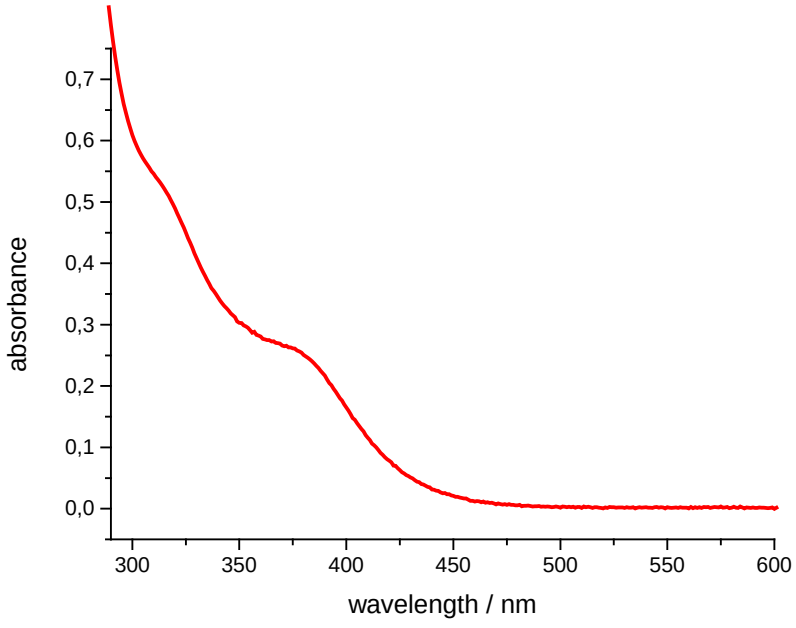


Figure S6. UV/Vis spectrum of $[Si_{3.72}Ge_{2.28}\{N(SiMe_3)Dipp\}_4]$ (**1**)

2. Supplementary data for $[Si_{3.10}Ge_{2.90}\{N(SiMe_3)Dipp\}_4]$ (2)

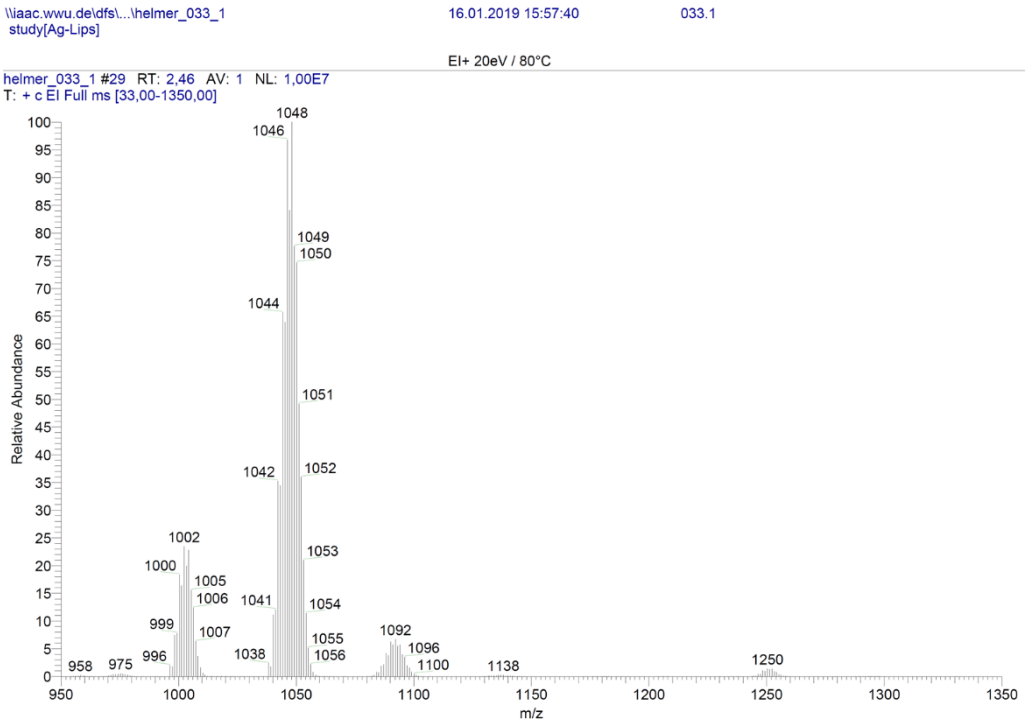


Figure S7. EI-MS spectrum of $[Si_{3.10}Ge_{2.90}\{N(SiMe_3)Dipp\}_4]$ (**2**).

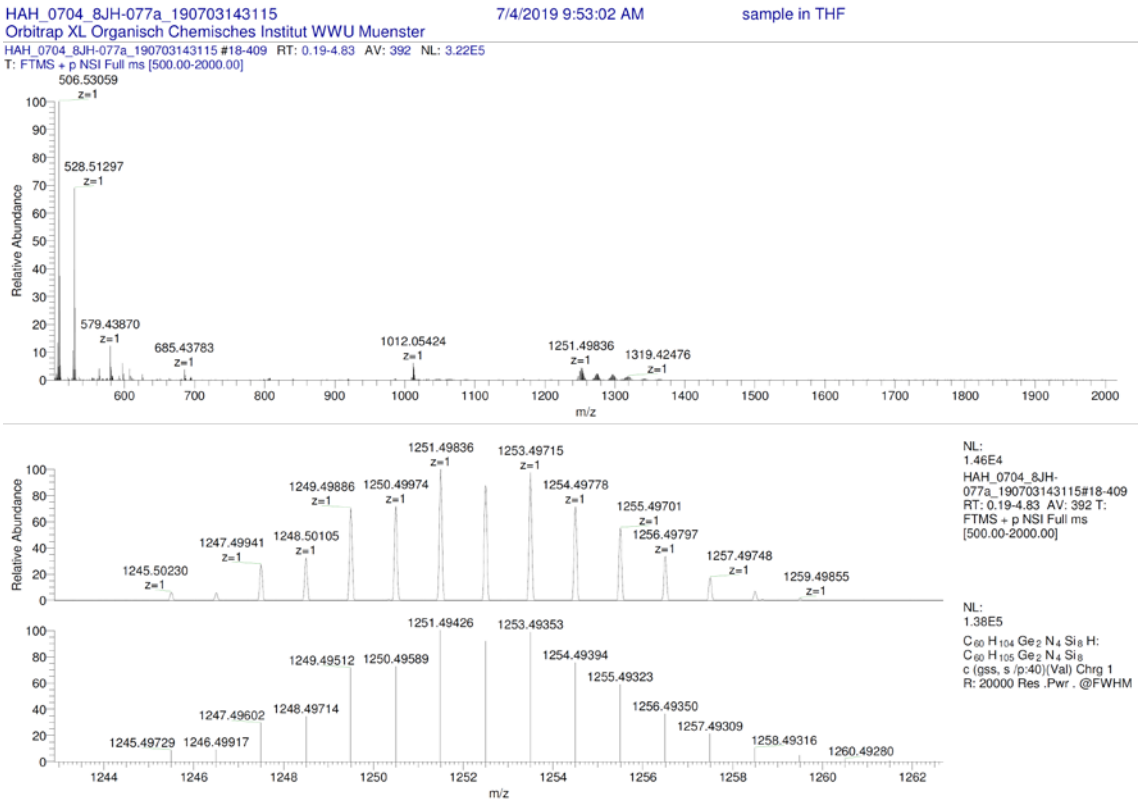


Figure S8. ESI-MS spectrum of **2** with zoom into the protonated $Si_4Ge_2R_4$ cluster.

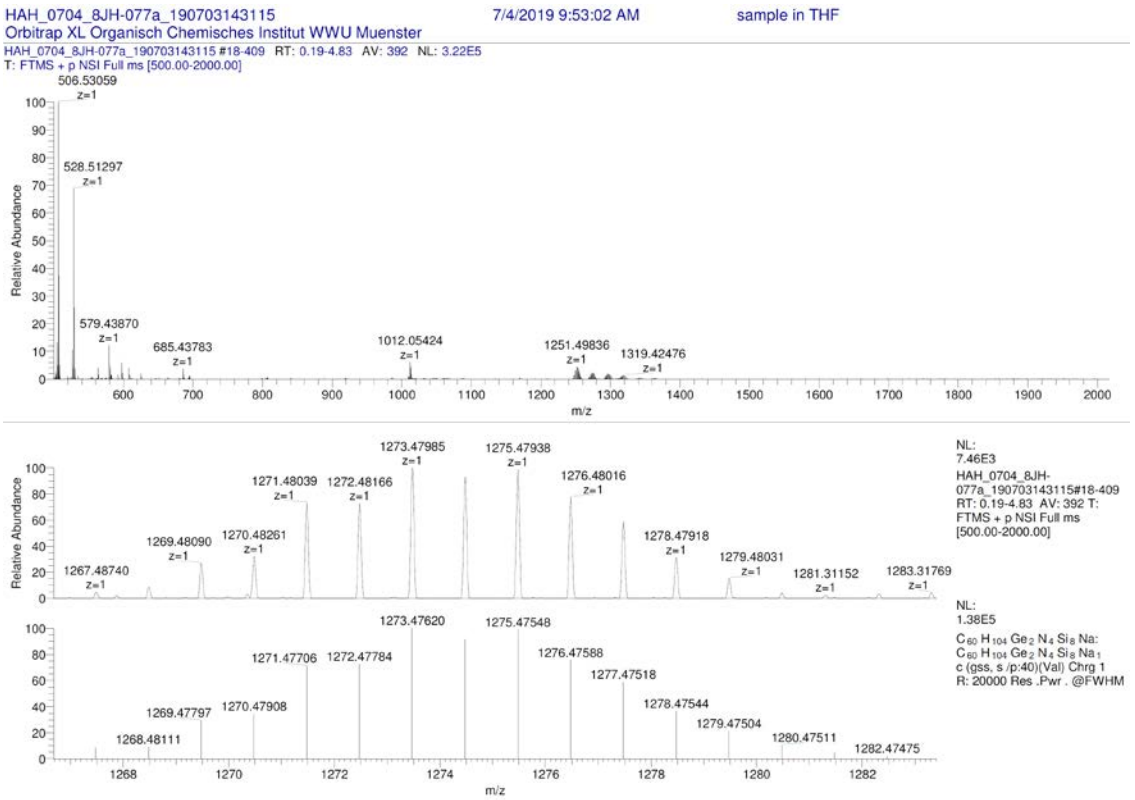


Figure S9. ESI-MS spectrum of **2** with zoom into the $Si_4Ge_2R_4$ cluster anion.

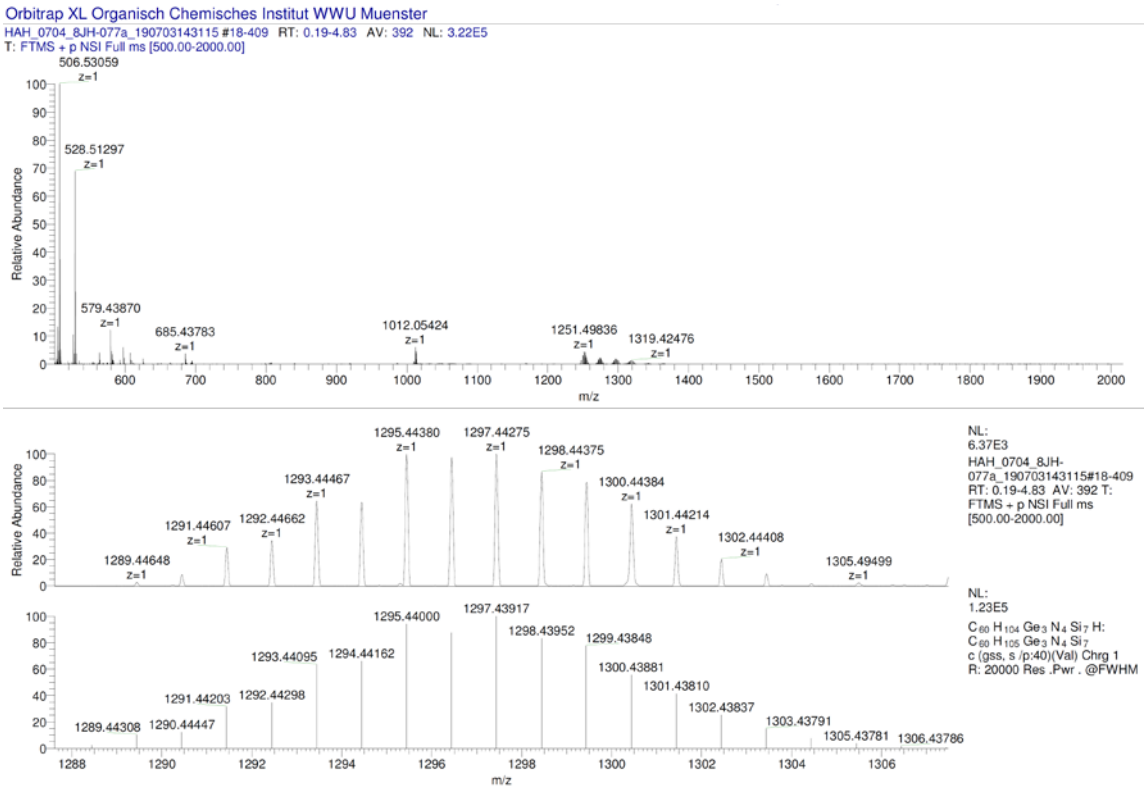


Figure S10. ESI-MS spectrum of **2** with zoom into the protonated $Si_3Ge_3R_4$ cluster.

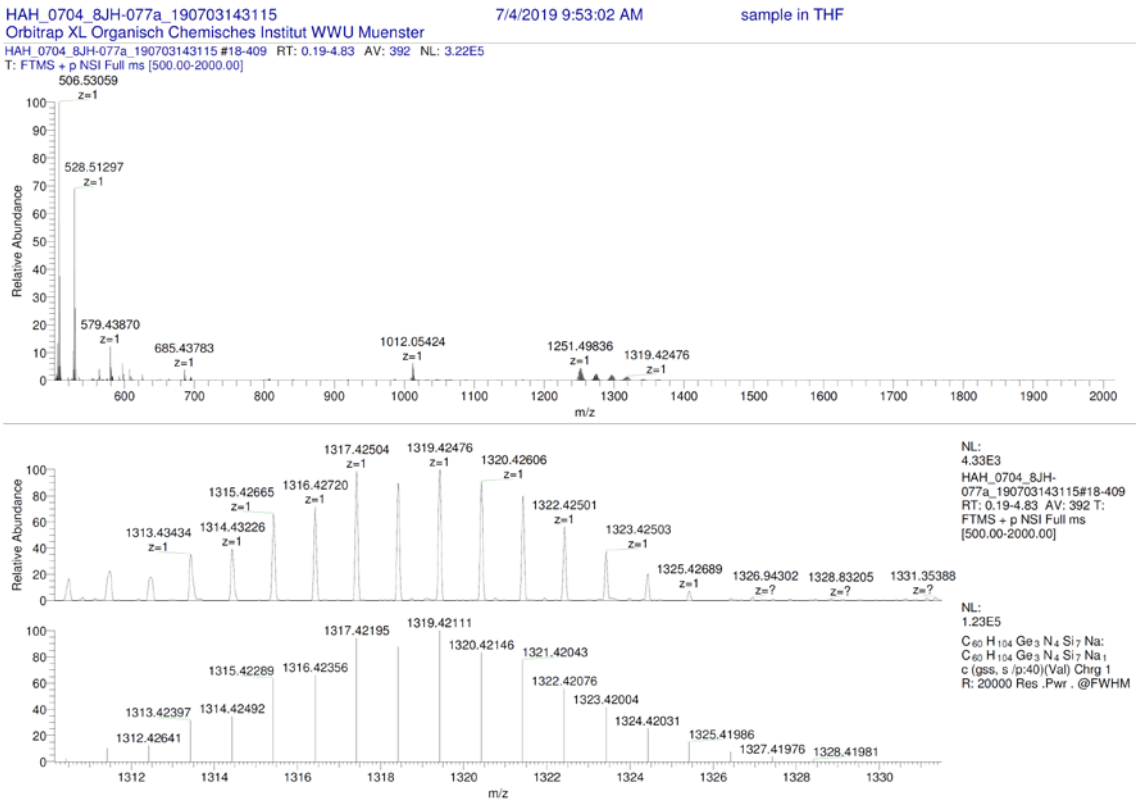


Figure S11. ESI-MS spectrum of **2** with zoom into the $Si_3Ge_3R_4$ cluster anion.

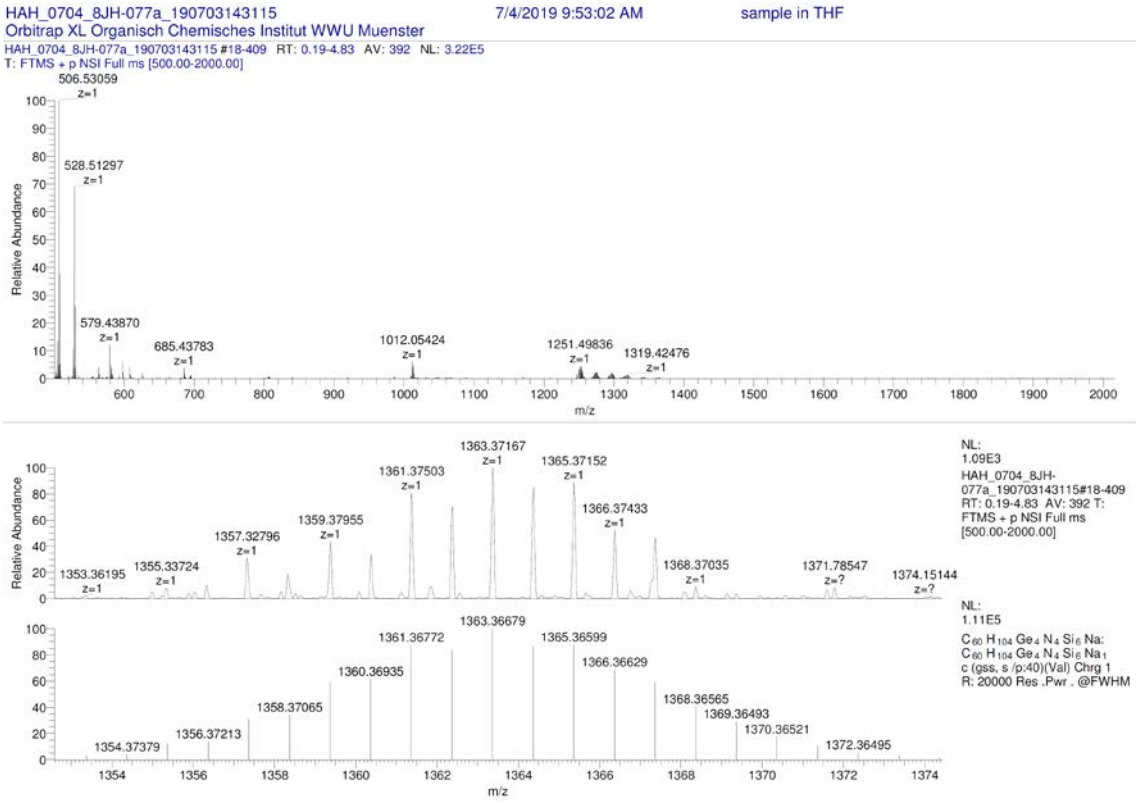


Figure S12. ESI-MS spectrum of **2** with zoom into the $Si_2Ge_4R_4$ cluster anion.

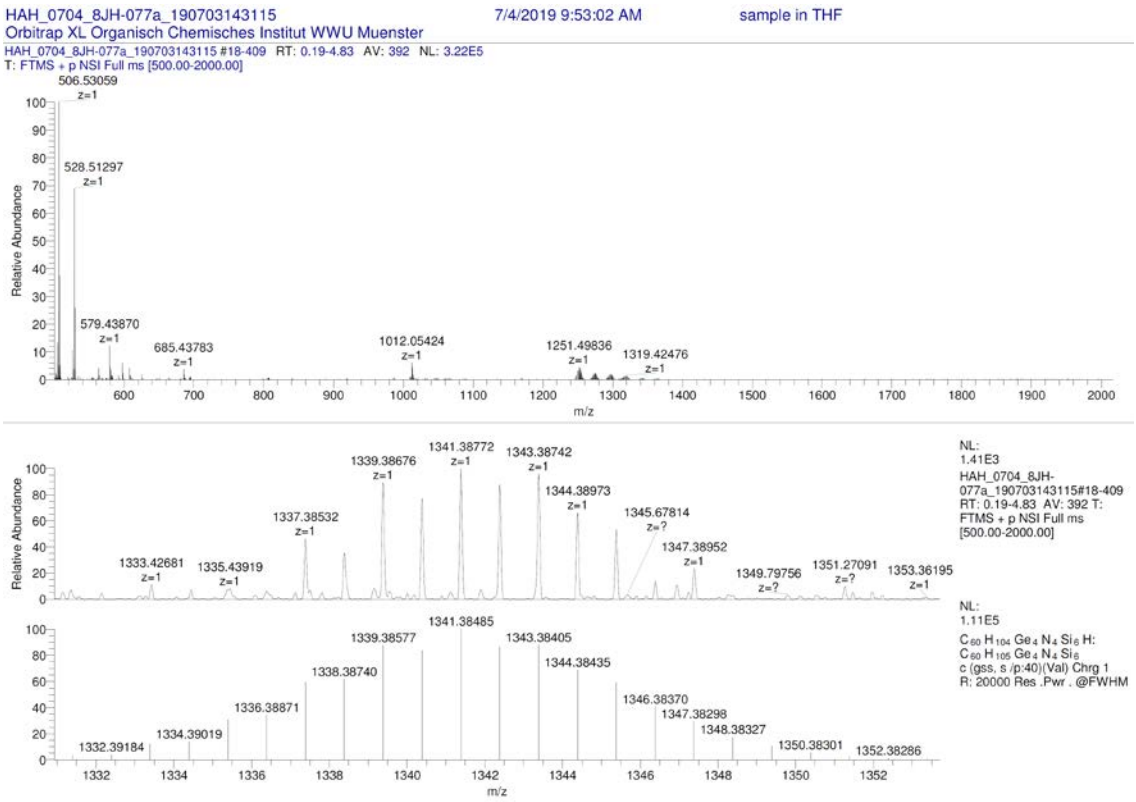


Figure S13. ESI-MS spectrum of **2** with zoom into the protonated $Si_2Ge_4R_4$ cluster.

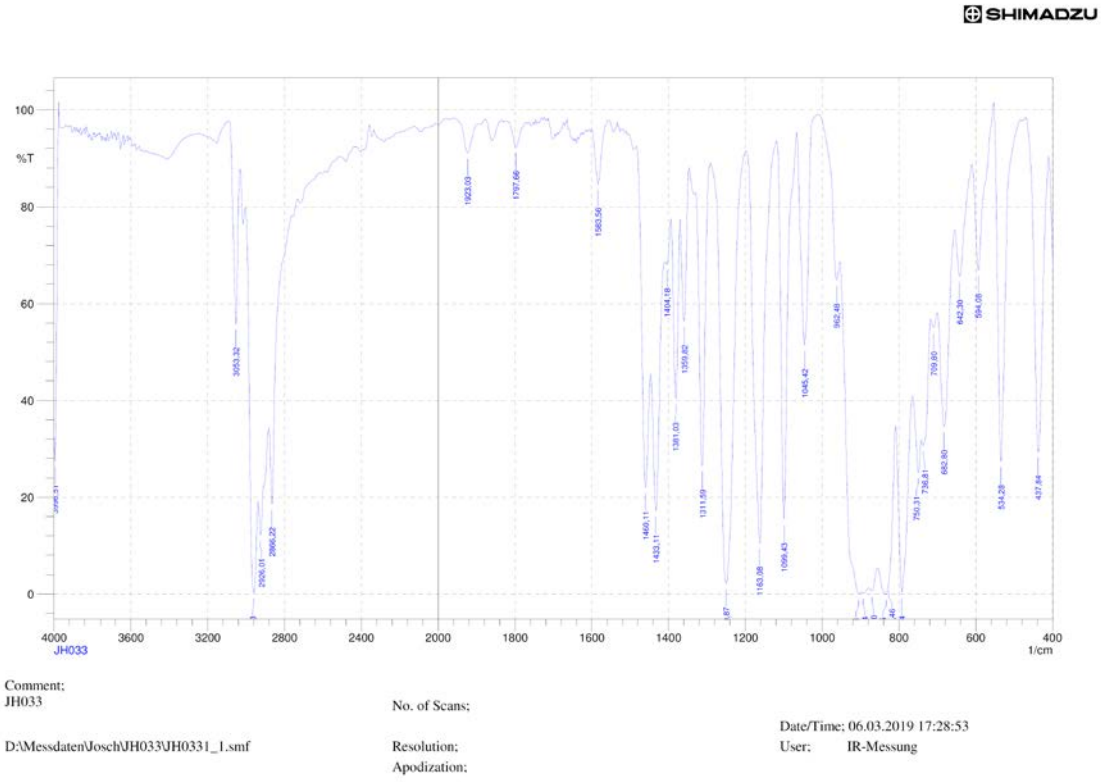


Figure S14. IR spectrum of $[Si_{3.10}Ge_{2.90}\{N(SiMe_3)Dipp\}_4]$ (**2**).

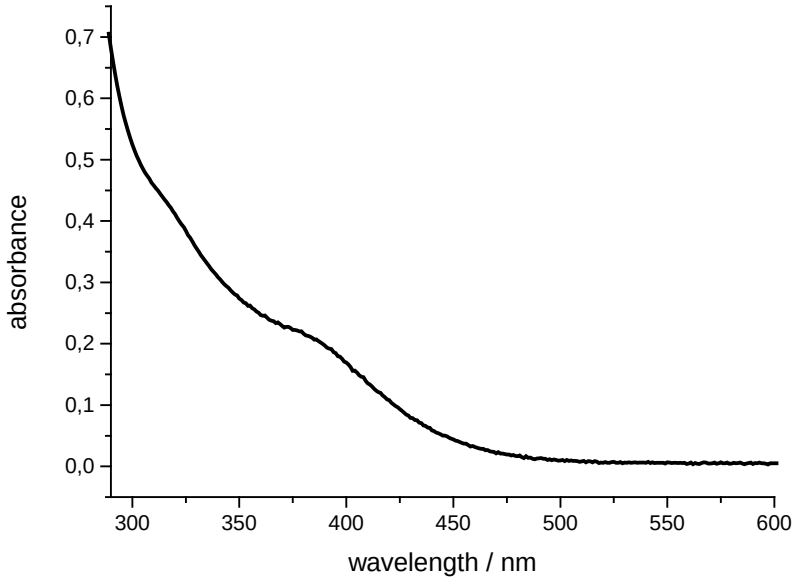


Figure S15. UV/Vis spectrum of $[Si_{3.10}Ge_{2.90}\{N(SiMe_3)Dipp\}_4]$ (**2**).

3. Supplementary data for $[Si_{2.11}Ge_{3.89}\{N(SiMe_3)Dipp\}_4]$ (3)

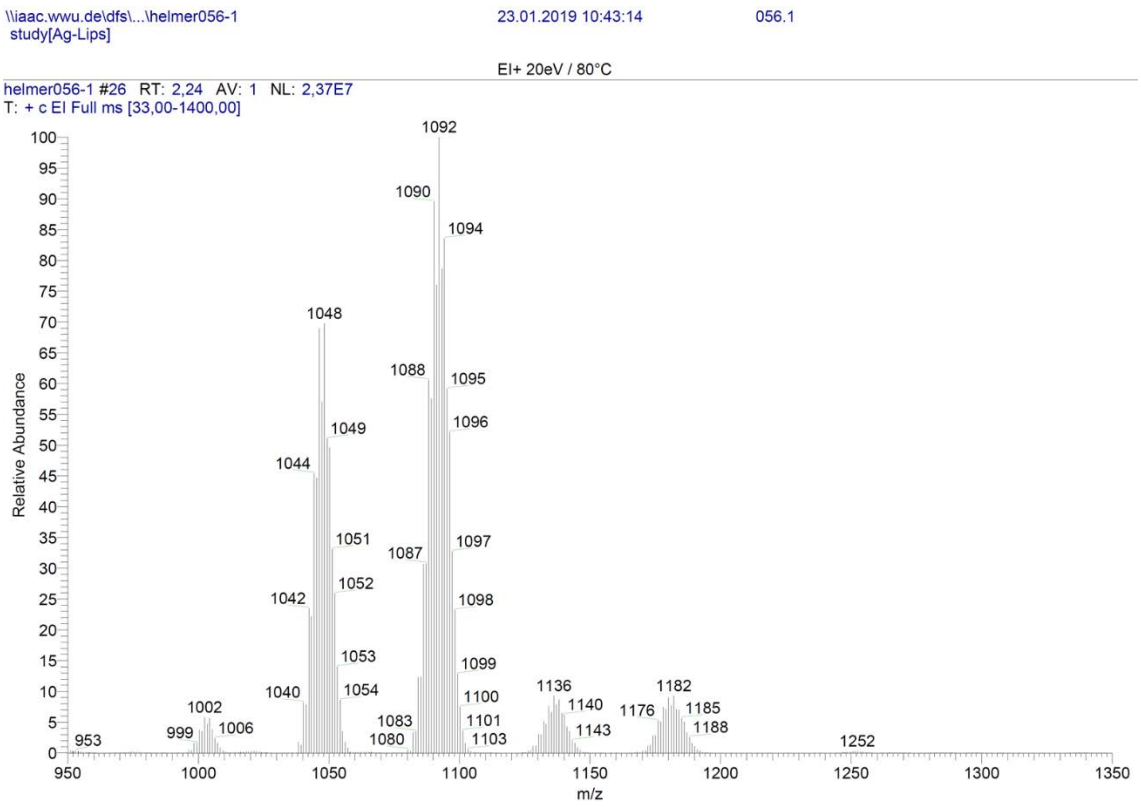


Figure S16. EI-MS spectrum of $[Si_{2.11}Ge_{3.89}\{N(SiMe_3)Dipp\}_4]$ (**3**).

4. Details of the single crystal x-ray diffraction analysis

4.1. Refinement details

For **1**(·solvent), **2**(·solvent), **3**(·solvent) all positions of the six-vertex cluster core were refined with split positions and free refinement of the occupancy by silicon or germanium atoms using PART instructions. All three crystal structures were refined as two-component inversion twins and the Flack parameters are given in Table S1. Additionally, these crystal structures each contain 0.5 hexane solvent molecule per asymmetric unit which were treated with the Platon squeeze routine.[S1]

Table S1. Crystal data and structure refinement for **1**(·solvent), **2**(·solvent) and **3**(·solvent).

Compound	**1**(·solvent)	**2**(·solvent)	**3**(·solvent)
CCDC number	2093200	2093201	2093202
Empirical formula	$C_{60}H_{104}Ge_{2.28}N_4Si_{7.72}$	$C_{60}H_{104}Ge_{2.90}N_4Si_{7.10}$	$C_{60}H_{104}Ge_{3.89}N_4Si_{6.11}$
Formula weight /g·mol^{-1}	1263.60	1291.53	1335.47
Crystal color, shape	yellow, rod	yellow, rod	yellow, rod
Crystal size /mm^3	0.176×0.289×0.584	0.170×0.194×0.566	0.140×0.201×0.388
Crystal system	tetragonal	tetragonal	tetragonal
Space group	*P*-42$_1$*c*	*P*-42$_1$*c*	*P*-42$_1$*c*
a /Å *b* /Å *c* /Å	16.3651(5) 16.3651(5) 27.0314(9)	16.3758(5) 16.3758(5) 27.0498(9)	16.3876(8) 16.3876(8) 27.0831(13)
α /° *β* /° *γ* /°	90 90 90	90 90 90	90 90 90
V /Å^3	7239.5(5)	7253.9(5)	7273.3(8)
Z	4	4	4
T /K	100(2)	100(2)	100(2)
Completeness to *θ* 25.24° /%	99.9	99.9	99.8
ρ_{calc} /g·cm^{-3}	1.159	1.183	1.220
μ(Mo) /mm^{-1}	1.106	1.348	1.729
2*Θ* range /°	4.64-54.34	4.63-54.39	3.90-54.27
Reflections measured	91036	92304	85997
Independent reflections	8000	8055	8042
R(int)	0.0372	0.0401	0.0536
Ind. reflections ($I > 2\sigma(I)$)	7813	7822	7658
Parameters	339	339	343
Restraints	-	-	-
R_1 ($I > 2\sigma(I)$)	0.0175	0.0179	0.0267
wR_2 (all data)	0.0493	0.0479	0.0641
GooF (all data)	1.080	1.030	1.078
Max. peak/hole /e$^-$·Å^{-3}	0.179 /-0.396	0.199 /-0.367	0.398 /-0.437
Absorption correction type	multi-scan	multi-scan	multi-scan
Min. /Max. transmission	0.5839 /0.7455	0.5883 /0.7455	0.5539 /0.7358
Flack parameter	0.021(7)	0.017(6)	0.055(9)

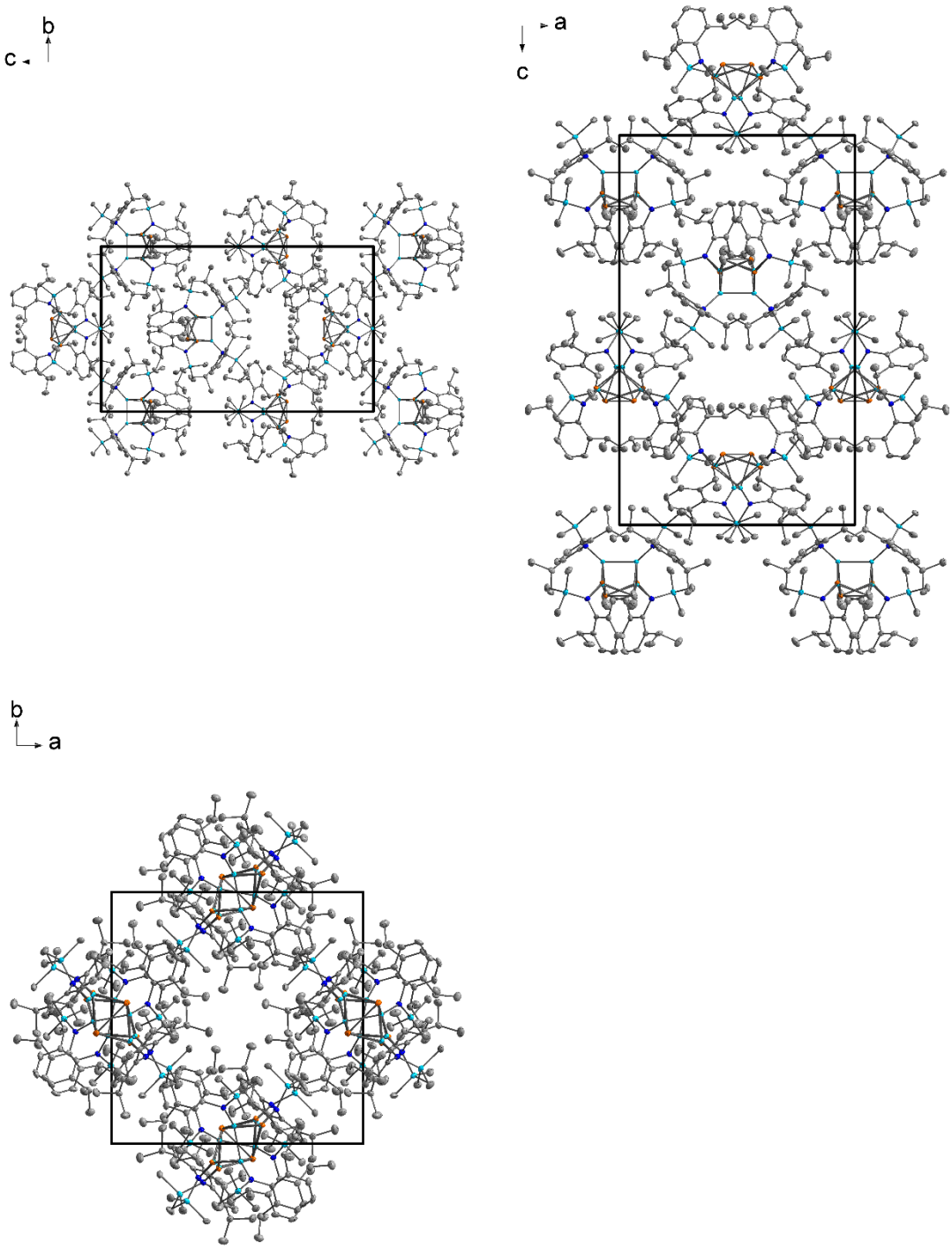


Figure S17. Packing of the crystal structures of **1**. Views along a, b and c axis. Hydrogen atoms and disordered hexane molecules are omitted for clarity. Color code: silicon (turquoise), germanium (orange), nitrogen (blue), carbon (gray).

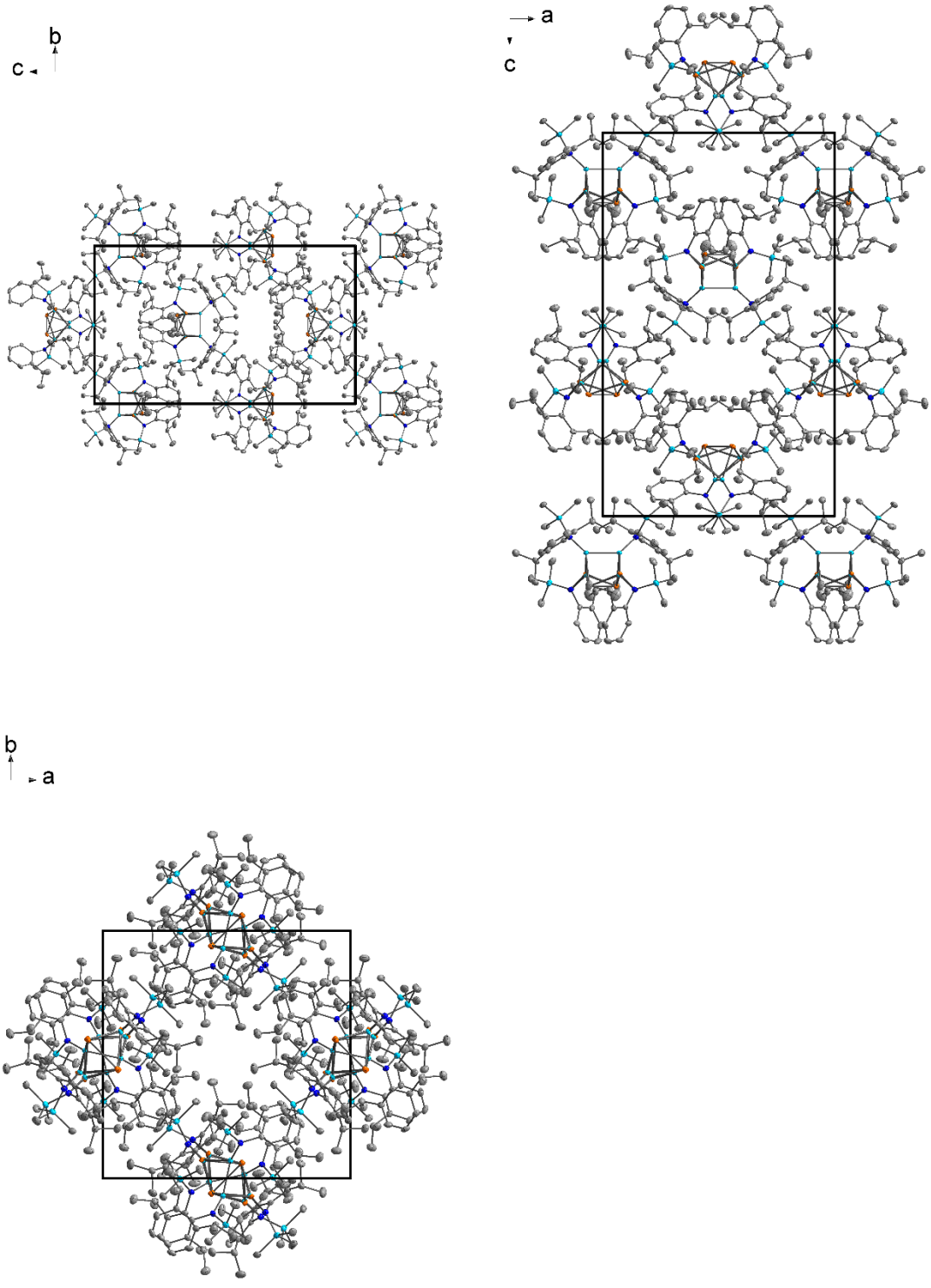


Figure S18. Packing of the crystal structures of **2**. Views along a, b and c axis. Hydrogen atoms and disordered hexane molecules are omitted for clarity. Color code: silicon (turquoise), germanium (orange), nitrogen (blue), carbon (gray).

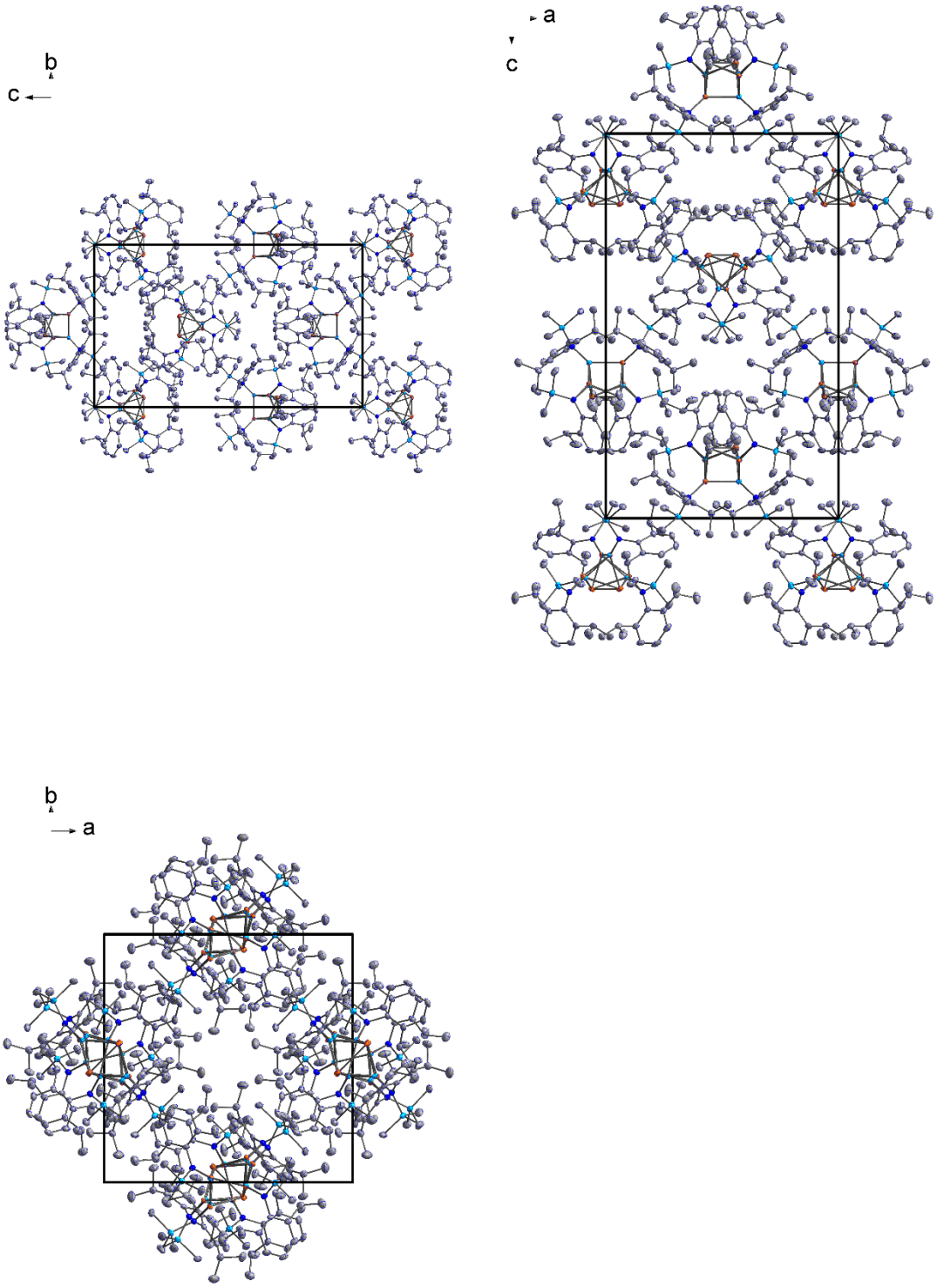
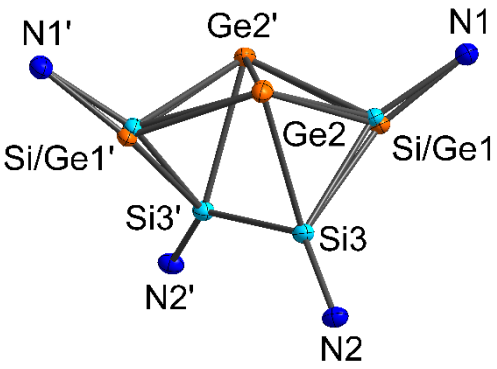
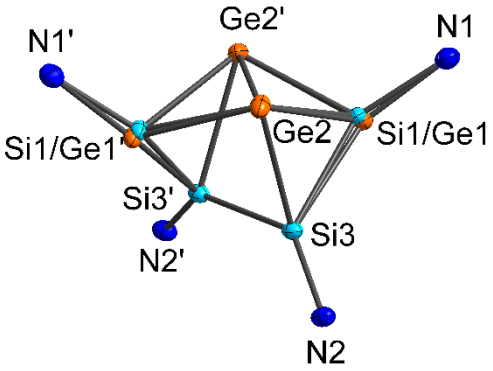


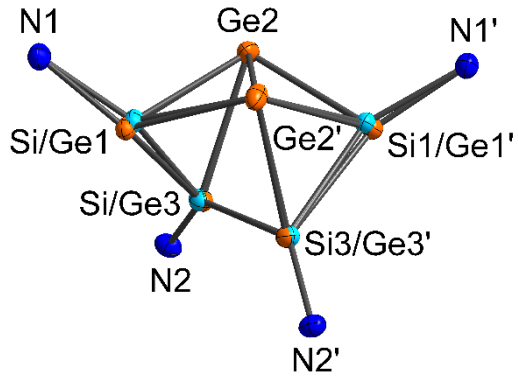
Figure S19. Packing of the crystal structures of **3**. Views along a, b and c axis. Hydrogen atoms and disordered hexane molecules are omitted for clarity. Color code: silicon (turquoise), germanium (orange), nitrogen (blue), carbon (gray).



1 (3:1)

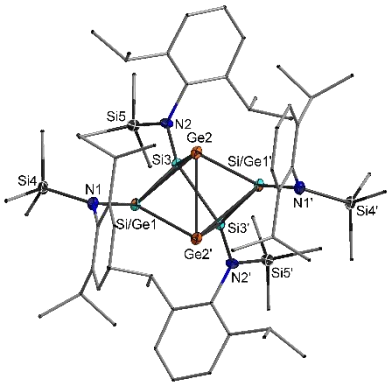


2 (1:1)



3 (1:3)

Figure S20. Cluster cores of **1**-**3** showing the mixed silicon germanium sites.



1

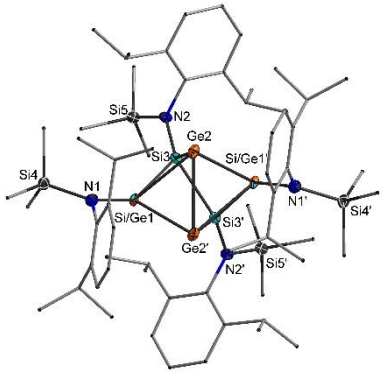
Figure S21. Molecular structure of **1**.

Selected distances /Å

Ge2–Si1B 2.626(3), Ge2–Ge1A 2.786(9), Ge2–Si1B' 2.352(4), Ge2–Ge1A' 2.453(10), Ge2–Si3 2.4823(5), Ge2–Ge2' 2.7868(4), Ge1A–Si3 2.350(10), Si1B–Si3 2.341(4), Ge1A'–Ge2 2.453(10), Si1B'–Ge2 2.352(4), Si3–Si3‘ 2.3843(9), Ge1A–N1 1.747(10), Si1B–N1 1.753(4), Si3–N2 1.7402(14), Si5–N2 1.7649(14), Si4–N1 1.7631(16), Si4–C13 1.862(2), Si4–C14 1.862(2), Si4–C15 1.861(2), Si5–C28 1.8654(19), Si5–C29 1.858(2), Si5–C30 1.857(2).

Selected angles /°

Si3-Ge2-Si1B 54.45(8), Si3-Ge2-Ge1A 52.6(2), Si3-Si1B-Ge2 59.64(9), Si3-Ge1A-Ge2 57.0(2), Si1B-Si3-Ge2 65.91(7), Ge1A-Si3-Ge2 70.4(2), Si1B-Ge2‘-Si3‘ 80.38(9), Ge1A-Ge2‘-Si3‘ 78.8(2), Si1B-Ge2-Si1B‘ 100.78(14), Ge1A-Ge2-Ge1A' 101.8(3), Si1B‘-Ge2-Ge2‘ 60.77(9), Ge1A‘-Ge2-Ge2‘ 63.9(2), Si3‘-Ge2-Ge2 80.306(11), Si3‘-Si3-Ge2 88.799(13), Si3‘-Si1B‘-Ge2 93.07(14), Si3'-Ge1A'-Ge2 90.3(3), Ge2-Si1B-Ge2‘ 67.83(8), Ge2-Ge1A-Ge2‘ 63.9(2), Si1B-Ge2-Ge2' 51.40(9), Ge1A-Ge2-Ge2' 52.2(2), Si1B-Si3-Si3‘ 82.68(11), Ge1A-Si3-Si3‘ 82.9(3), N1-Si1B-Si3 144.3(2), N1-Ge1A-Si3 144.0(6), N1-Si1B-Ge2 116.06(17), N1-Ge1A-Ge2 109.2(4), N1-Ge1A-Ge2' 114.4(5), N1-Si1B-Ge2' 119.1(2), N2-Si3-Si1B 134.53(11), N2-Si3-Ge1A 132.5(3), N2-Si3-Si3‘ 137.55(5), N2-Si3-Ge2 121.67(5).



2

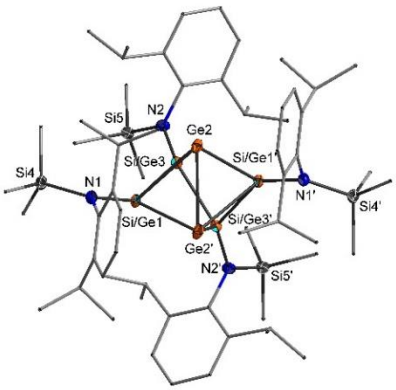
Figure S22. Molecular structure of **2**.

Selected distances /Å

Ge1A–Si3 2.383(4), Si1B–Si3 2.360(8), Ge1A–Ge2' 2.449(3), Si1B–Ge2' 2.338(8), Ge1A–Ge2 2.773(3), Si1B–Ge2 2.622(8), Ge2'–Ge1A 2.449(3), Ge2–Si1B 2.338(8), Ge2'–Si3 2.4832(5), Ge2'–Ge2 2.7798(4), Ge1A–N1 1.781(4), Si1B–N1 1.813(8), Si3–N2 1.7396(16), Si3–Si3' 2.3950(10), Si4–N1 1.7585(18), Si4–C13 1.865(2), Si4–C14 1.864(3), Si4–C15 1.860(2), Si5–N2 1.7653(16), Si5–C28 1.864(2), Si5–C29 1.857(2), Si5–C30 1.858(2).

Selected angles /°

Si3-Ge1A-Ge2' 90.21(11), Si3-Ge1A-Ge2 56.97(8), Ge2-Ge1A-Ge2' 63.97(7), Ge2'-Si1B-Si3 93.5(3), Ge2-Si1B-Ge2' 67.90(19), Si3-Si1B-Ge2 59.51(19), Ge1A'-Ge2-Si3 78.63(8), Si1B'-Ge2-Si3 79.7(2), Ge1A-Ge2-Ge1A' 101.88(12), Si1B-Ge2-Si1B' 100.2(3), Si3-Ge2-Ge1A 53.57(7), Si3-Ge2-Si1B 55.00(17), Ge1A-Ge2-Ge2' 63.70(9), Si1B-Ge2-Ge2' 60.9(2), Si3-Ge2-Ge2' 80.937(13), Ge1A-Ge2-Ge2' 52.33(8), Si1B-Ge2-Ge2' 51.18(18), Ge1A-Si3-Si3' 81.69(9), Si1B-Si3-Si3' 81.0(2), Ge1A-Si3-Ge2 69.45(8), Si1B-Si3-Ge2 65.50(18), Si3-Si3'-Ge2 89.121(15), N1-Ge1A-Si3 144.0(2), N1-Si1B-Si3 143.3(4), N1-Ge1A-Ge2' 115.30(17), N1-Si1B-Ge2' 119.3(4), N1-Ge1A-Ge2 110.19(16), N1-Si1B-Ge2 115.6(4), N2-Si3-Ge1A 132.43(10), N2-Si3-Si1B 134.8(2), N2-Si3-Si3' 137.77(5), N2-Si3-Ge2 122.77(6).



3

Figure S23. Molecular structure of **3**.

Selected distances /Å

Ge1A–Ge2 2.7641(18), Si1B–Ge2 2.592(19), Si1B–Ge2' 2.34(2), Ge1A–Ge2' 2.441(2), Ge1A–Ge3A 2.428(18), Si1B–Si3B 2.36(2), Ge2–Si3B 2.500(11), Ge2–Ge3A 2.497(18), Ge2'–Si1B' 2.592(19), Ge2'–Ge1A' 2.7641(18), Ge2–Ge2' 2.7715(7), Si3B–Si3B' 2.44(2), Ge3A–Ge3A' 2.42(3), Si3B'–Si1B' 2.36(2), Ge3A'–Ge1A' 2.428(18), Si1B–N1 1.87(2), Ge1A–N1 1.829(4), Si3B–N2 1.762(11), Ge3A–N2 1.759(18), Si4–N1 1.753(3), Si5–N2 1.762(3), Si4–C13 1.862(4), Si4–C14 1.861(4), Si4–C15 1.868(4), Si5–C28 1.857(3), Si5–C29 1.856(3), Si5–C30 1.858(4).

Selected angles /°

Si3B-Si1B-Ge2 60.4(6), Ge3A-Ge1A-Ge2 57.1(4), Ge3A'-Ge1A'-Ge2 90.5(4), Ge2-Si1B'-Si3B' 94.6(8), Ge3A'-Ge3A-Ge1A 79.8(7), Si1B-Si3B-Si3B' 80.5(7), Ge2-Ge1A-Ge2' 63.99(4), Ge2-Si1B-Ge2‘ 68.2(5), Si1B-Ge2'-Si3B 79.6(6), Ge1A-Ge2'-Ge3A 78.0(4), Si1B-Ge2-Si1B' 99.6(8), Ge1A-Ge2-Ge1A' 101.61(9), Si3B-Ge2-Si1B 55.2(6), Ge3A-Ge2-Ge1A 54.7(4), Si1B'-Ge2-Ge2' 60.2(5), Ge1A'-Ge2-Ge2' 63.68(5), Si1B-Ge2-Ge2' 51.6(5), Ge1A-Ge2-Ge2' 52.34(6), Si3B-Ge2-Ge2‘ 81.7(3), Ge3A-Ge2-Ge2' 81.9(4), Si1B-Si3B-Ge2 64.4(5), Ge1A-Ge3A-Ge2 68.3(5), Si3B'-Si3B-Ge2 88.7(3), Ge3A'-Ge3A-Ge2 89.4(5), N1-Si1B-Si3B 143.7(13), N1-Ge1A-Ge3A 143.9(4), N1-Si1B-Ge2' 118.8(11), N1-Ge1A-Ge2' 115.72(14), N1-Si1B-Ge2 117.0(10), N1-Ge1A-Ge2 110.94(12), N2-Si3B-Si3B' 137.6(4), N2-Ge3A-Ge3A' 138.7(7), N2-Si3B-Si1B 135.4(8), N2-Ge3A-Ge1A 131.5(9), N2-Si3B-Ge2 123.9(5), N2-Ge3A-Ge2 124.2(9).

5. Quantum chemical investigations of isomers of clusters present in 1 and 2

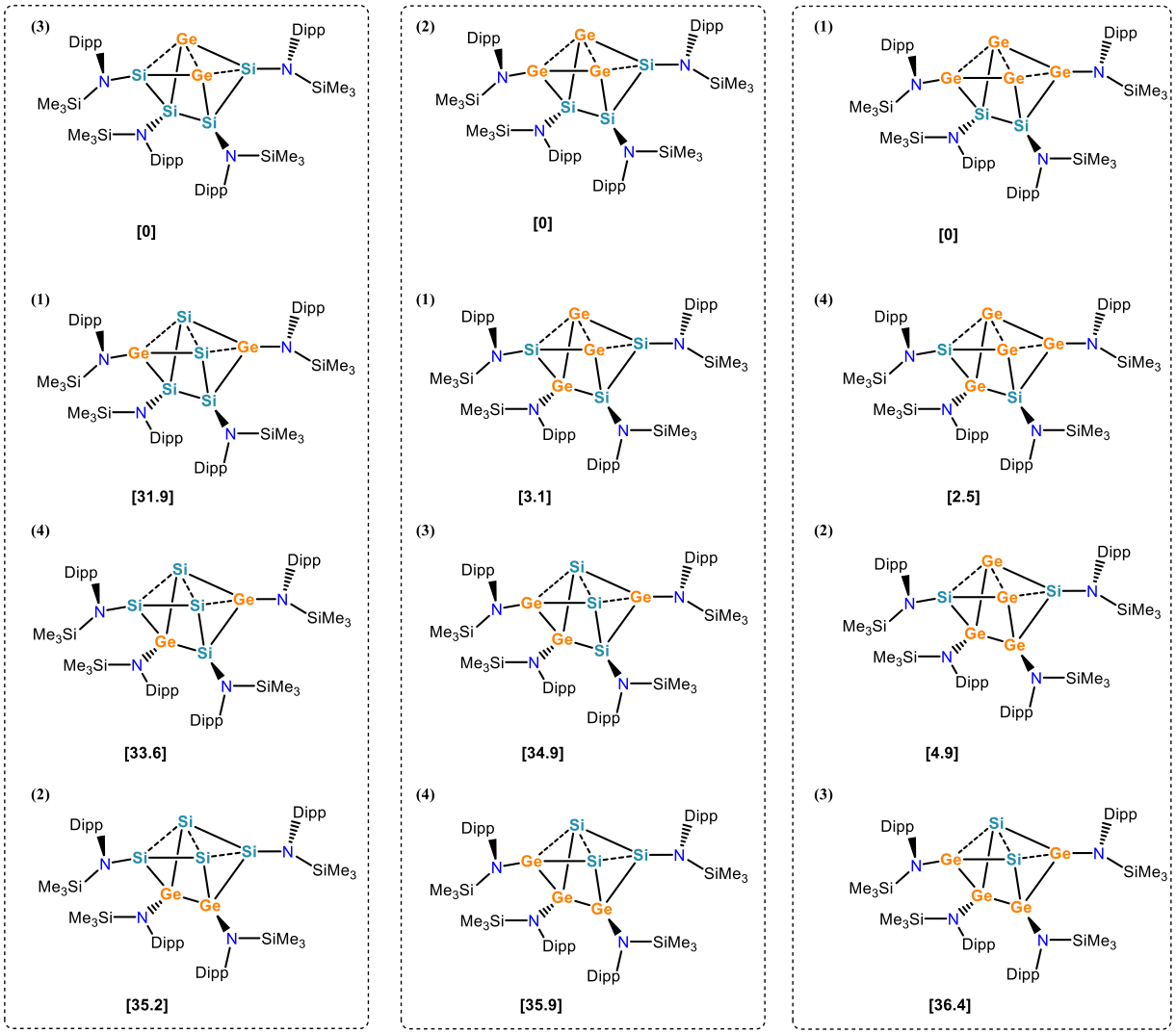


Table S2. Energies of isomers of clusters with core compositions Si_4Ge_2, Si_3Ge_3 and Si_2Ge_4.

	E /Hartree	**ΔE /Hartree**	**ΔE /kcal·mol^{-1}**
Si4Ge2			
Si4Ge2_1	-9040.341433711	0.050845749	31.90
Si4Ge2_2	-9040.336121606	0.056157854	35.20
Si4Ge2_3	**-9040.392279460**	0.000000000	0
Si4Ge2_4	-9040.338758010	0.053521450	33.60
Si3Ge3			
Si3Ge3_1	-10827.845643420	0.004920220	3.10
Si3Ge3_2	**-10827.850563640**	0.000000000	0
Si3Ge3_3	-10827.794962940	0.055600700	34.90
Si3Ge3_4	-10827.793303230	0.057260410	35.90
Si2Ge4			
Si2Ge4_1	**-12615.307725020**	0.000000000	0
Si2Ge4_2	-12615.299889170	0.007835850	4.90
Si2Ge4_3	-12615.249655250	0.058069770	36.40
Si2Ge4_4	-12615.303771300	0.003953720	2.50

6. Results from $^{29}Si\{^{1}H\}$ CP/MAS NMR spectroscopy of 1 and 2

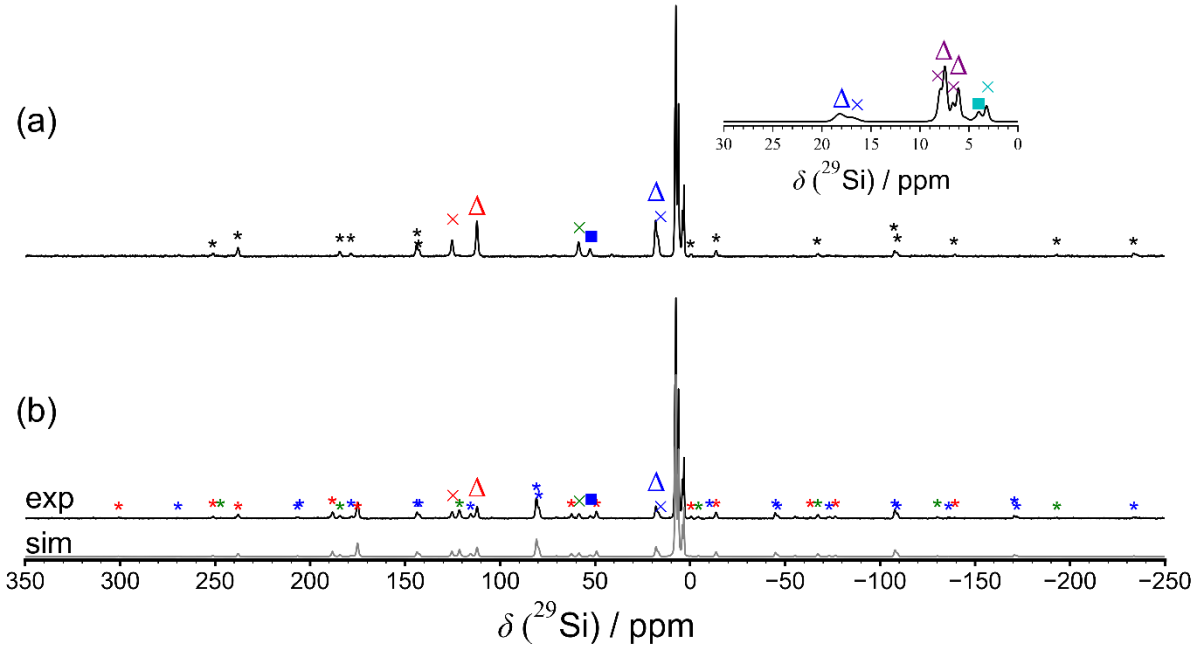


Figure S24. $^{29}Si\{^{1}H\}$ CP/MAS NMR spectra of **2** recorded at 9.4 T employing spinning frequencies of (a) 10.0 and (b) 5.0 kHz, respectively. In (b) the corresponding fit is shown in grey. The spinning side-bands are marked by an asterisk. The inset shows an enlargement of the TMS groups. The different colors mark the Si positions. The cross, triangle, and square represent the signals corresponding to Si_3Ge_3, Si_4Ge_2 and Si_2Ge_4, respectively.

The $^{29}Si\{^{1}H\}$ CP/MAS NMR spectra of **1** and **2** are shown in Figure S24 and S25. In **1** only Si_3Ge_3 and Si_4Ge_2 are present whereas **2** also contains some amount of Si_2Ge_4. By comparison of the relative intensities the signals at 125, 58, and 3.2 ppm can be assigned to Si_3Ge_3 and the signals at 112 and 18 ppm correspond to Si_4Ge_2. The signals at 52 and 4.0 ppm can be assigned to Si_2Ge_4 since they are only present in **2**. The signals at 7.4, 6.1, 7.9, and 6.6 ppm can be assigned to the $SiMe_3$ groups of Si_4Ge_2 and Si_3Ge_3, respectively. However, the $SiMe_3$ signals of Si_2Ge_4 cannot be distinguished since they overlap with the other $SiMe_3$ signals.

Table S3. Relative intensities of the ^{29}Si signals. The intensities were normalized to the signal at δ^{29}Si = 125 and 112 ppm, respectively to reveal the signals belonging to the same compound.

	2 (with Si_4Ge_2, Si_3Ge_3 and Si_2Ge_4)		**1** (with Si_4Ge_2 and Si_3Ge_3)	
δ(^{29}Si) / ppm	**normalized to 125 ppm**	**normalized to 112 ppm**	**normalized to 125 ppm**	**normalized to 112 ppm**
125	1.00	0.53	1.00	0.16
112	1.87	1.00	6.23	1.00
59	0.84	0.45	0.83	0.13
52	0.40	0.21		
18	1.46	0.78	4.46	0.72
17	0.86	0.46	1.85	0.30
4.0	1.36	0.73		
3.2	1.04	0.56	1.12	0.18

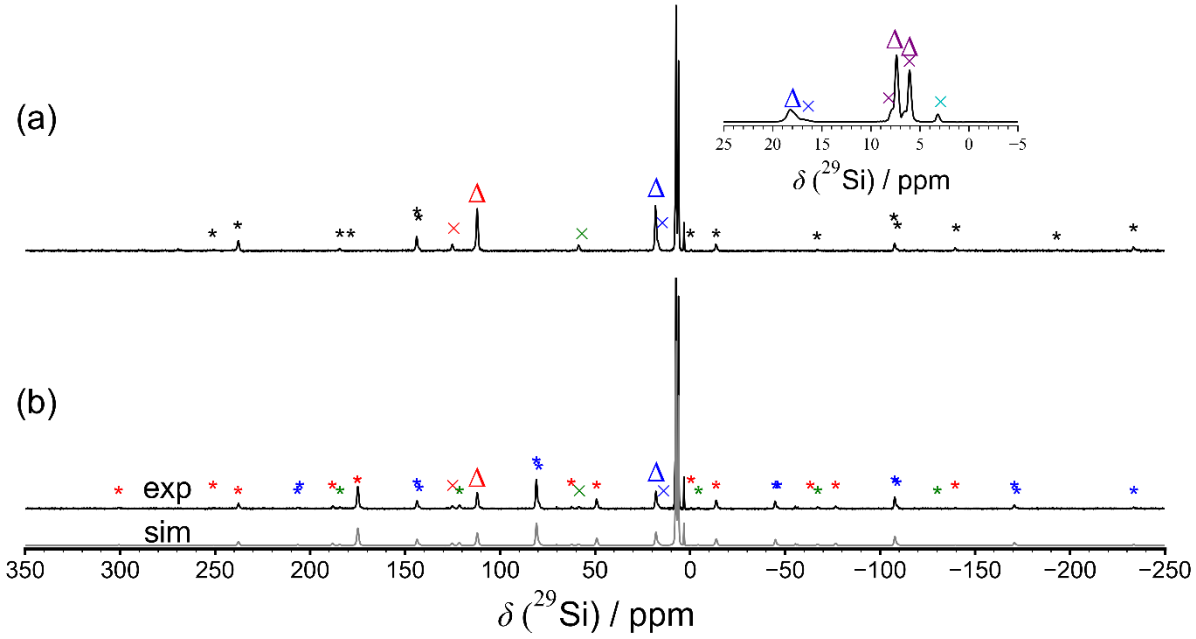


Figure S25. ^{29}Si{^{1}H} CP/MAS NMR spectra of **1** recorded at 9.4 T employing spinning frequencies of (a) 10.0 and (b) 5.0 kHz, respectively. In (b) the corresponding fit is shown in grey. The spinning side-bands are marked by an asterisk. The inset shows an enlargement of the $SiMe_3$ groups. The different colors mark the Si positions. The cross and triangle represent the signals corresponding to Si_3Ge_3, Si_4Ge_2, respectively. Si_2Ge_4 is not present in this sample.

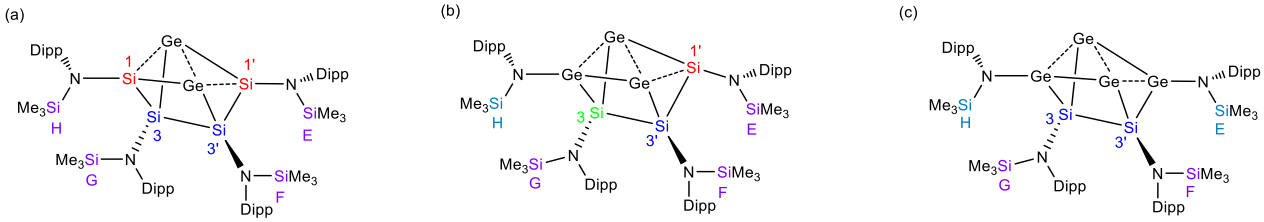


Figure S26. Chemical structure of (a) Si_4Ge_2, (b) Si_3Ge_3, and (c) Si_2Ge_4 with the corresponding labels of the Si atoms. The color code is identical to the assignment used in Figure S22 and S23.

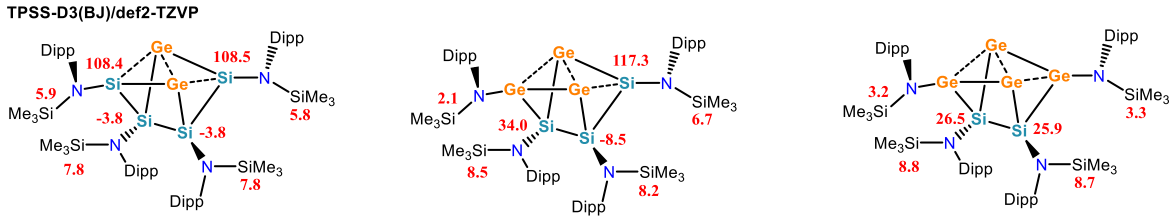


Table S4. Calculated (TPSS-D3(BJ)/def2-TZVP) isotropic chemical shift and anisotropic chemical shift parameters (R = $N(SiMe_3)Dipp$).

	$Si_4Ge_2R_4$			$Si_3Ge_3R_4$			$Si_2Ge_4R_4$		
Site	**$\delta(^{29}Si)$ / ppm**	**δ_σ / ppm**	**η_σ**	**$\delta(^{29}Si)$ / ppm**	**δ_σ / ppm**	**η_σ**	**$\delta(^{29}Si)$ / ppm**	**δ_σ / ppm**	**η_σ**
Si1'	108.5	-176.4	0.4	117.3	-162.2	0.7	-	-	-
Si3'	-3.7	-201.1	0.1	-8.5	-211.5	0.2	25.9	-206.0	0.2
Si3	-3.8	-201.1	0.1	34.0	-196.0	0.2	26.5	-206.3	0.2
Si1	108.4	-176.4	0.4	-	-	-	-	-	-
SiE	7.8	-19.1	0.4	8.5	-18.0	0.4	8.7	-18.1	0.3
SiF	7.8	-19.1	0.4	8.2	-19.4	0.3	8.8	-18.2	0.3
SiG	5.9	-14.0	0.5	6.7	-13.5	0.5	3.2	-17.9	0.5
SiH	5.9	-14.1	0.5	2.1	-18.4	0.5	3.3	-17.9	0.5

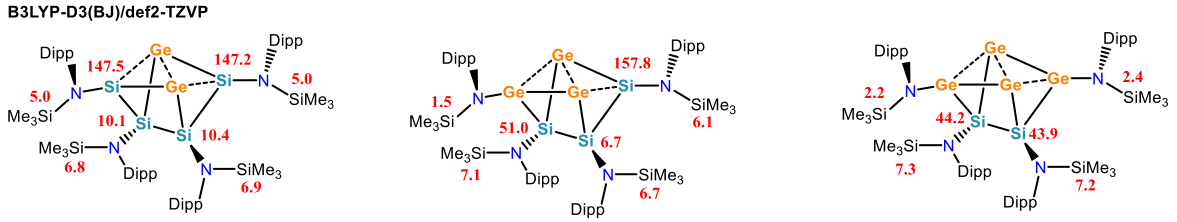


Table S5. Calculated (B3LYP-D3(BJ)/def2-TZVP) isotropic chemical shift and anisotropic chemical shift parameters (R = $N(SiMe_3)Dipp$).

	$Si_4Ge_2R_4$			$Si_3Ge_3R_4$			$Si_2Ge_4R_4$		
Site	**$\delta(^{29}Si)$ / ppm**			**$\delta(^{29}Si)$ / ppm**			**$\delta(^{29}Si)$ / ppm**		
Si1'	147.2			157.8			-		
Si3'	10.4			6.7			43.9		
Si3	10.1			51.0			44.2		
Si1	147.5			-			-		
SiE	5.0			6.1			2.4		
SiF	6.9			6.7			7.2		
SiG	6.8			7.1			7.3		
SiH	5.0			1.5			2.2		

Table S6. Experimental determined ^{29}Si isotropic chemical shifts (δ), chemical shift anisotropy parameters (δ_σ, η_σ) for the mixed Si_4Ge_2, Si_3Ge_3 and Si_4Ge_2 clusters.

	2 (with Si_4Ge_2, Si_3:Ge_3 and Si_2Ge_4)				**1** (with Si_4Ge_2 and Si_3:Ge_3)		
Site	**δ(^{29}Si) / ppm**	**δ_σ / ppm**	**η_σ**	***Cluster***	**δ(^{29}Si) / ppm**	**δ_σ / ppm**	**η_σ**
Si1'	125.4 ± 0.2	-176 ± 20	0.6 ± 0.05	Si_3Ge_3	125.1 ± 0.2	-176 ± 20	0.5 ± 0.05
Si1'/Si1	112.1 ± 0.2	-201 ± 20	0.4 ± 0.05	Si_4Ge_2	112.0 ± 0.2	-195 ± 20	0.4 ± 0.05
Si3'/Si3	58.5 ± 0.2	-226 ± 20	0 ± 0.05	Si_3Ge_3	58.5 ± 0.2	-233 ± 20	0 ± 0.05
Si3	52.6 ± 0.2	-233 ± 20	0 ± 0.05	Si_2Ge_4			
Si3'	18.0 ± 0.2	-220 ± 20	0 ± 0.05	Si_4Ge_2	18.0 ± 0.2	-214 ± 20	0 ± 0.05
Si3'	16.7 ± 0.2	-226 ± 20	0 ± 0.05	Si_3Ge_3	16.9 ± 0.2	-208 ± 20	0 ± 0.05
$SiMe_3$ (Si)	8.0 ± 0.2	19 ± 20	0 ± 0.05		7.9 ± 0.2	31 ± 20	0 ± 0.05
	7.5 ± 0.2	19 ± 20	0 ± 0.05		7.4 ± 0.2	19 ± 20	0 ± 0.05
	6.6 ± 0.2	19 ± 20	0.8 ± 0.05		6.6 ± 0.2	31 ± 20	0 ± 0.05
	6.1 ± 0.2	13 ± 20	0.7 ± 0.05		6.1 ± 0.2	13 ± 20	0.6 ± 0.05
$SiMe_3$ (Ge)	4.0 ± 0.2	13 ± 20	0.6 ± 0.05	Si_2Ge_4			
	3.2 ± 0.2	19 ± 20	1 ± 0.05	Si_3Ge_3	3.2 ± 0.2	19 ± 20	0 ± 0.05

Footnote: The CSA parameters are defined as $\delta_{iso} = 1/3(\delta_{xx} + \delta_{yy} + \delta_{zz})$, $\delta_\sigma = \delta_{iso} - \delta_{zz}$, $\eta_\sigma = (\delta_{xx} + \delta_{yy})/\delta_\sigma$, with $|\delta_{zz} - \delta_{iso}| \geq |\delta_{xx} - \delta_{iso}| \geq |\delta_{yy} - \delta_{iso}|$. The asymmetry parameter η_σ describes the symmetry of the CSA tensor. The CSA tensor is axial symmetric if $\eta_\sigma = 0$ and deviates from axial symmetry for $0 < \eta_\sigma < 1$.

For the $SiMe_3$ groups, the calculated and experimental anisotropic chemical shift parameters deviate from each other since only a "frozen" structure is calculated and the dynamic of the $SiMe_3$ groups is not included in these calculations. However, depending whether the amido ligand is bonded to Si or Ge in the **1** or **1'** positions in the clusters, different isotropic chemical shifts were obtained. Those signals at 3.2 and 4.0 ppm with a low chemical shift anisotropy can be assigned to the $SiMe_3$ groups in Si_3Ge_3 and Si_2Ge_4 that are connected to Ge via nitrogen.

7. Results from NMR spectroscopy of 1 and 2 in solution

7.1 General experimental procedures

All NMR data were obtained on Bruker Avance I and III spectrometer and were referenced to the deuterated solvent (C_6D_6, THF-d_8, PhMe-d_8) according to an IUPAC recommendation. Additionally, the ^{1}H and ^{13}C NMR spectra were referenced internally to residual solvent resonances at 300 K. ^{1}H, ^{13}C and ^{29}Si NMR spectra were referenced to tetramethylsilane (TMS; δ = 0 ppm). Further explanation of the ^{29}Si NMR experiments: ^{29}Si DEPT 19.5 = ^{29}Si NMR measurement with Distortionless Enhancement Polarization Transfer method, pulse angle 19.5°, coupling to 9 protons as polarization source with coupling $^{2}J_{Si-H}$ = 7 Hz; $^{29}Si\{^{1}H\}IG$ = Inverse gated decoupled ^{29}Si proton decoupled NMR measurement; $^{29}Si\{/\}$ = ^{29}Si proton coupled NMR measurement. ^{13}C DEPT 135 = Distortionless Enhancement of Polarization Transfer using a 135 degree decoupler pulse. All ^{13}C NMR spectra were recorded proton decoupled.

7.2 Assignment of signals to clusters with core composition Si4:Ge2, Si3:Ge3 and Si2:Ge4

The following signals were assigned based on NMR spectroscopy of both **1** and **2** in toluene-d_8. Variable temperature, two-dimensional correlated NMR spectroscopy and comparison of the ^{29}Si NMR spectra was performed to identify each mixed silicon germanium cluster and the occurrence of minor conformers for clusters with the core composition Si2:Ge4 and Si4:Ge2.

[Si_4Ge_2{N(SiMe$_3$)Dipp}$_4$]

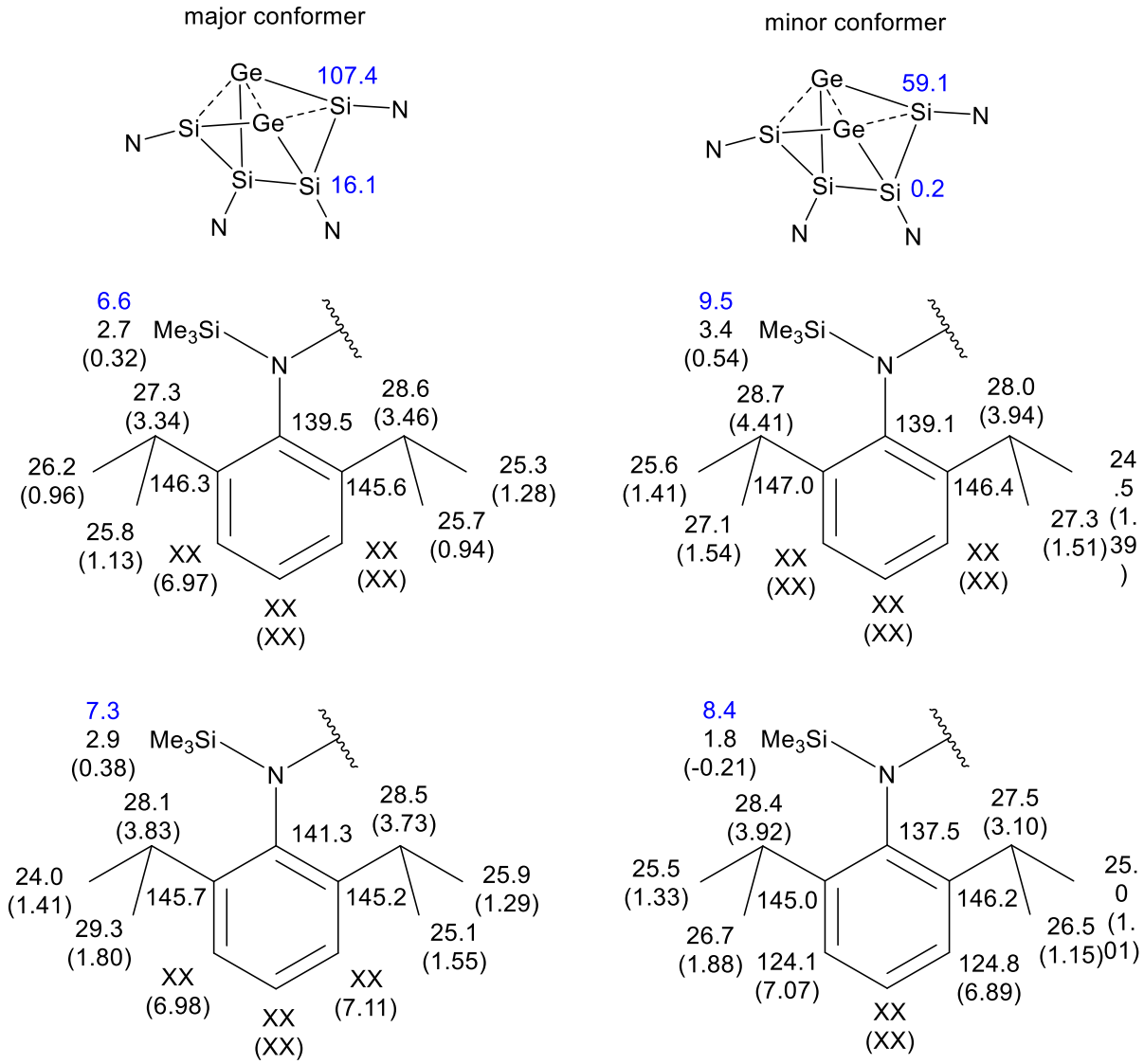


Figure S27. Result from multinuclear NMR spectroscopy of **1** and **2** in toluene-d_8 at 220 K. Assignment of signals to the cluster Si_4Ge_2{N(SiMe$_3$)Dipp}$_4$. ^{1}H (in brackets), ^{13}C (black), ^{29}Si (blue).

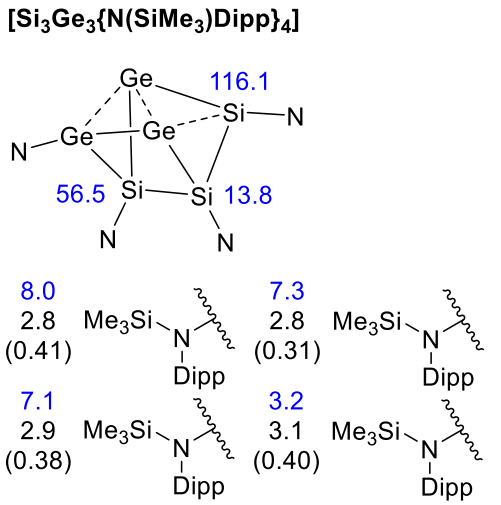


Figure S28. Result from multinuclear NMR spectroscopy of **1** and **2** in toluene-d_8 at 220 K. Assignment of signals to the cluster $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$. ^1H (in brackets), ^{13}C (black), ^{29}Si (blue).

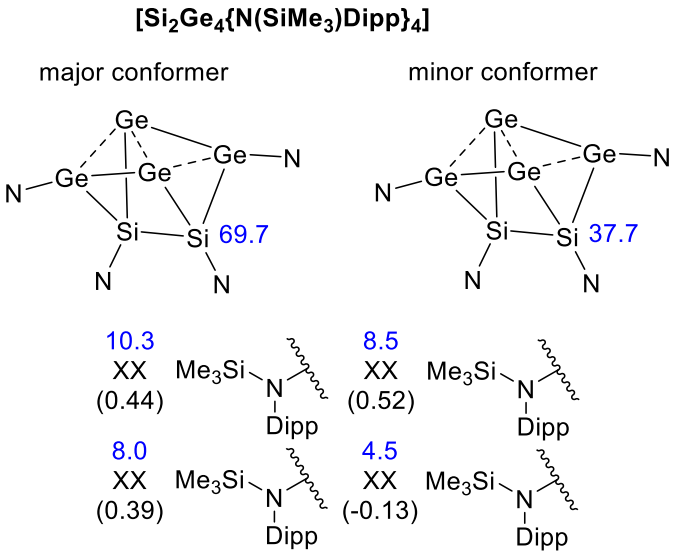


Figure S29. Result from multinuclear NMR spectroscopy of **1** and **2** in toluene-d_8 at 220 K. Assignment of signals to the cluster $Si_2Ge_4\{N(SiMe_3)Dipp\}_4$. ^1H (in brackets), ^{13}C (black), ^{29}Si (blue).

Signals assigned to $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

^{1}H-NMR: (400 MHz, toluene-d_8, 220 K): δ (ppm) = 7.15-6.87 (12H, m, ü.l.); 4.41 (1H, br); 3.94 (1H, br), 3.92 (1H, br); 3.83 (1H, br), 3.73 (1H, br); 3.46 (1H, br); 3.34 (1H, br); 3.10 (1H, br); 1.88 (3H, br); 1.80 (3H, br); 1.54 (6H, br); 1.51 (3H, br); 1.43-1.38 (9H, m); 1.33-1.27 (9H, m); 1.16-1.12 (6H, m); 1.01 (3H, br); 0.98-0.93 (6H, m); 0.54 (9H, s); 0.38 (9H, s); 0.32 (9H, s); −0.21 (9H, s).

^{13}C-NMR: (101 MHz, toluene-d_8, 220 K): δ (ppm) = 147.0; 146.4; 146.3; 146.2; 145.7; 145.5; 145.2; 145.0; 141.3; 139.5; 139.1; 137.5; 125.7; 124.1; 29.3; 28.7; 28.6; 28.5; 28.4; 28.1; 28.0; 27.5; 27.3; 27.3; 27.1; 26.7; 26.5; 26.2; 25.9; 25.8; 25.7; 25.6; 25.5; 25.3; 25.1; 25.0; 24.5; 24.0; 3.4; 2.9; 2.7; 1.8.

^{29}Si{^{1}H}DEPT19.5-NMR: (79 MHz, toluene-d_8, 220 K): δ (ppm) = 9.5; 8.4; 7.3; 6.6.

^{29}Si{^{1}H}IG-NMR: (79 MHz, toluene-d_8, 220 K, nur Signale von [$Si_4Ge_2\{N(SiMe_3)Dipp\}_4$]): δ (ppm) = 107.4; 59.1; 16.1; 9.5; 8.4; 7.3; 6.6; 0.2.

Signals assigned to $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$

^{1}H-NMR: (400 MHz, toluene-d_8,): δ (ppm) = 7.16-7.93 (12H, ü.l.); 3.91 (1H, ü.l.); 3.78 (2H, ü.l.); 3.68 (2H, ü.l.); 3.52 (1H, ü.l.); 3.35 (1H, ü.l.); 3.25 (1H, ü.l.); 1.81 (3H, ü.l.); 1.75 3H, ü.l.); 1.70 (3H, ü.l.); 1.57 (3H, ü.l.); 1.52 (6H, ü.l.); 1.42-1.15 (15H, m, ü.l.); 1.02 (6H, ü.l.); 0.97 (3H, ü.l.); 0.94 (3H, ü.l.); 0.78 (3H, d, $^3J_{H\text{-}H}$ = 6.5 Hz); 0.41 (9H, s); 0.40 (9H, s); 0.38 (9H, s); 0.31 (9H, s).

^{13}C-NMR: (101 MHz, toluene-d_8, 220 K,): δ (ppm) = 3.1; 2.9; 2.9; 2.9.

^{29}Si{^{1}H}DEPT19.5-NMR: (79 MHz, toluene-d_8, 220 K,): δ (pm) = 8.0; 7.3; 7.1; 3.2.

^{29}Si{^{1}H}IG-NMR: (79 MHz, toluene-d_8, 220 K, nur Signale von [$Si_3Ge_3\{N(SiMe_3)Dipp\}_4$]):

δ (ppm) = 116.1; 56.5; 13.8; 8.0; 7.3; 7.1; 3.2.

Signals assigned to $Si_2Ge_4\{N(SiMe_3)Dipp\}_4$

^{1}H-NMR: (400 MHz, toluene-d_8): δ (ppm) = 7.16-7.93 (12H, ü.l.); 4.27 (1H, br); 4.14 (1H, br); 3.96-3.22 (5H, ü.l.); 2.97 (1H, br); 1.89-0.76 (48H, ü.l.); 0.52 (9H, s); 0.44 (9H, s); 0.39 (9H, s); −0.31 (9H, s).

^{29}Si{^{1}H}DEPT19.5-NMR: (79 MHz, toluene-d_8, 220 K): δ (ppm) = 10.3; 8.5; 8.0; 4.5.

^{29}Si{^{1}H}IG-NMR: (79 MHz, toluene-d_8, 220 K): δ (ppm) = 69.7; 37.7; 10.3; 8.5; 8.0; 4.5.

7.3 Solution NMR spectra of 1

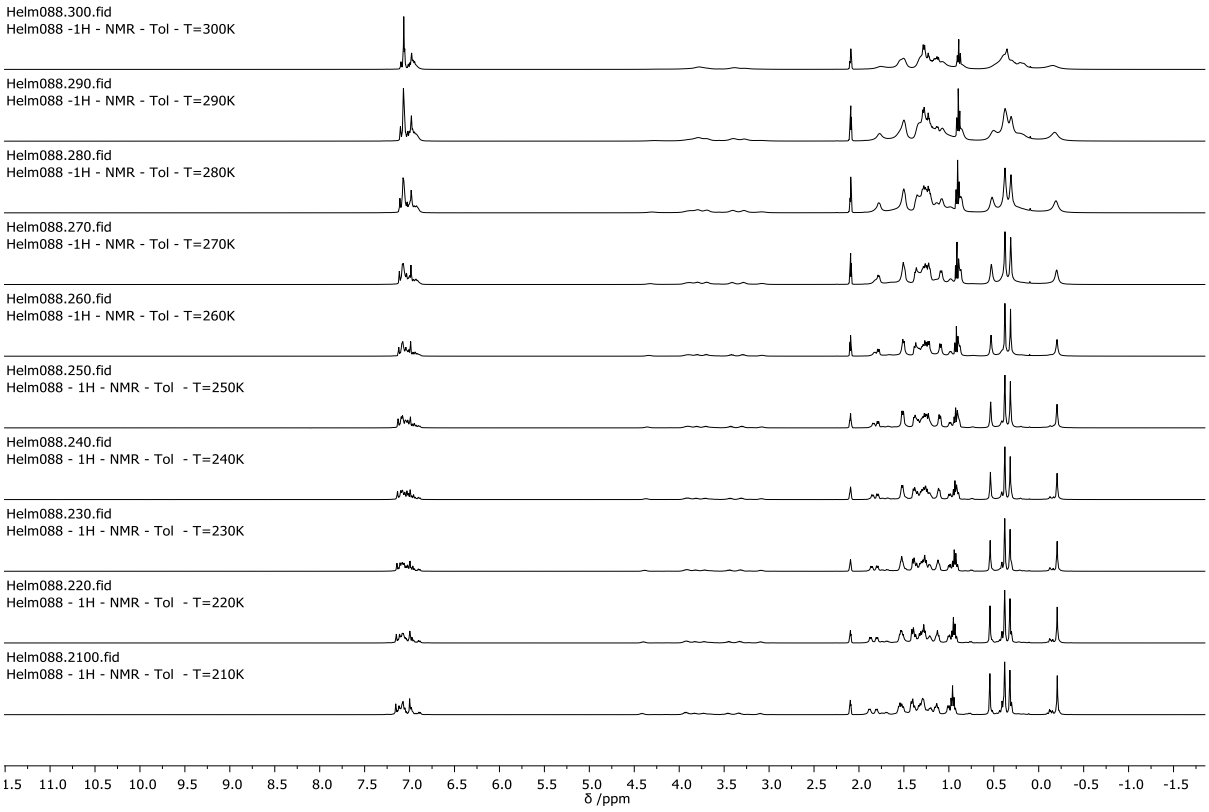


Figure S30. Variable temperature ^{1}H-NMR spectra (d_8-toluene, 300-210 K, 400 MHz) of **1**.

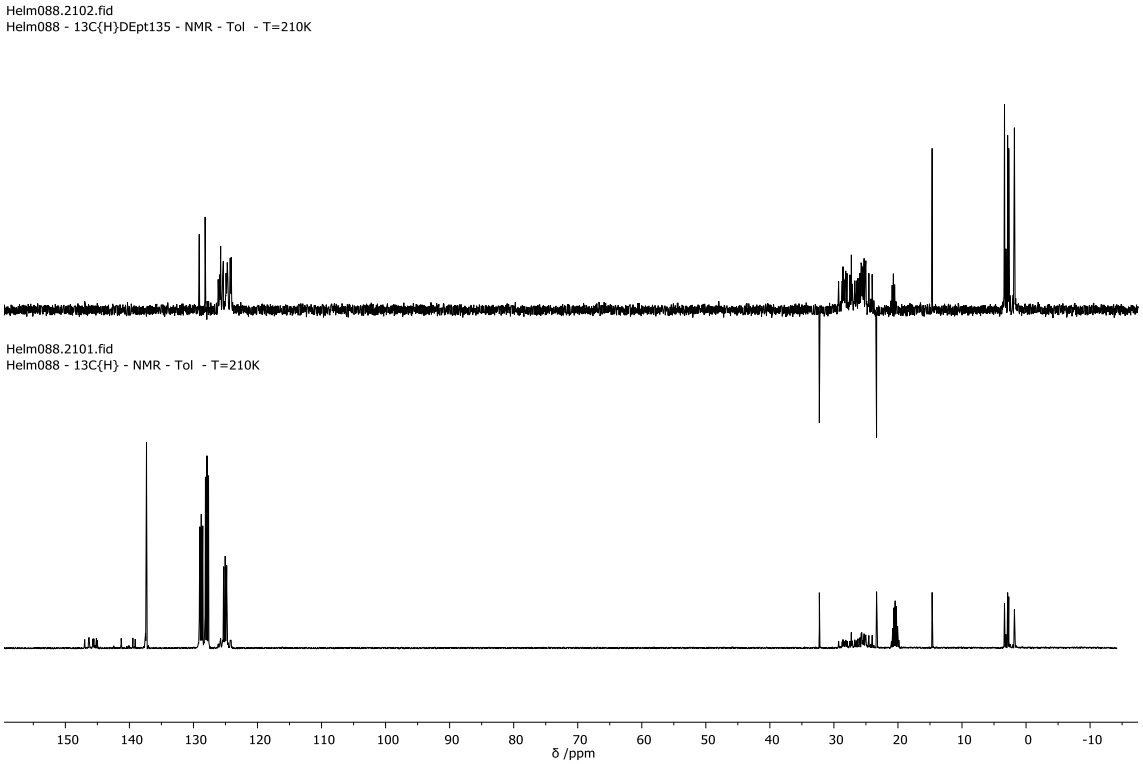


Figure S31. $^{13}C\{^{1}H\}$-NMR and $^{13}C\{^{1}H\}$DEPT135-NMR spectra (d_8-toluene, 210 K, 100 MHz) of **1**.

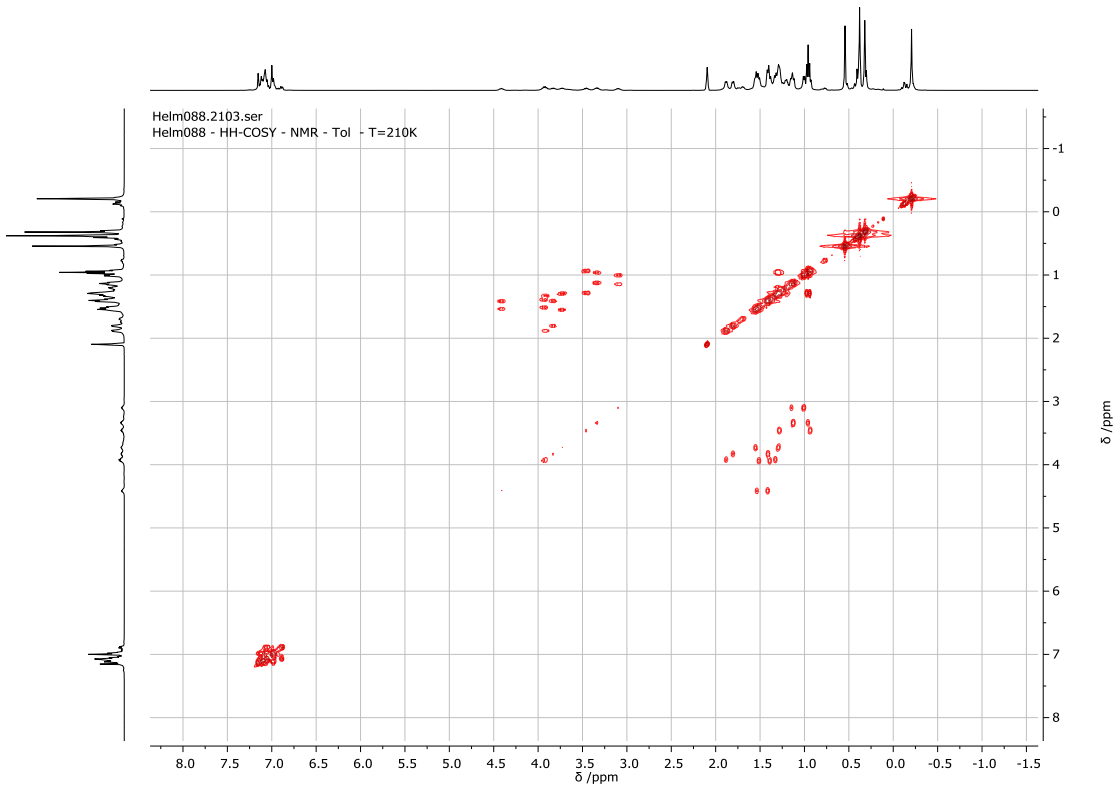


Figure S32. H,H-COSY-NMR spectrum (d_8-toluene, 210 K) of **1**.

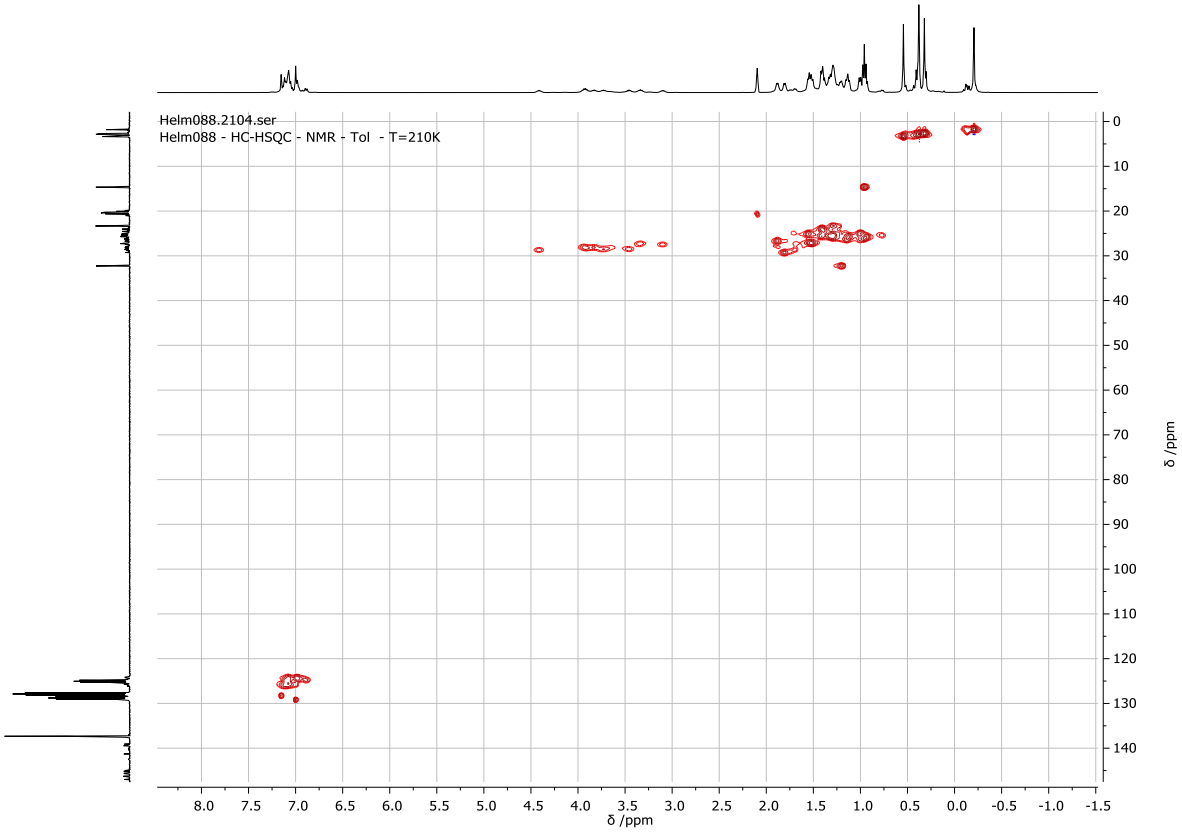


Figure S33. H,C-HSQC-NMR spectrum (d_8-toluene, 210 K) of **1**.

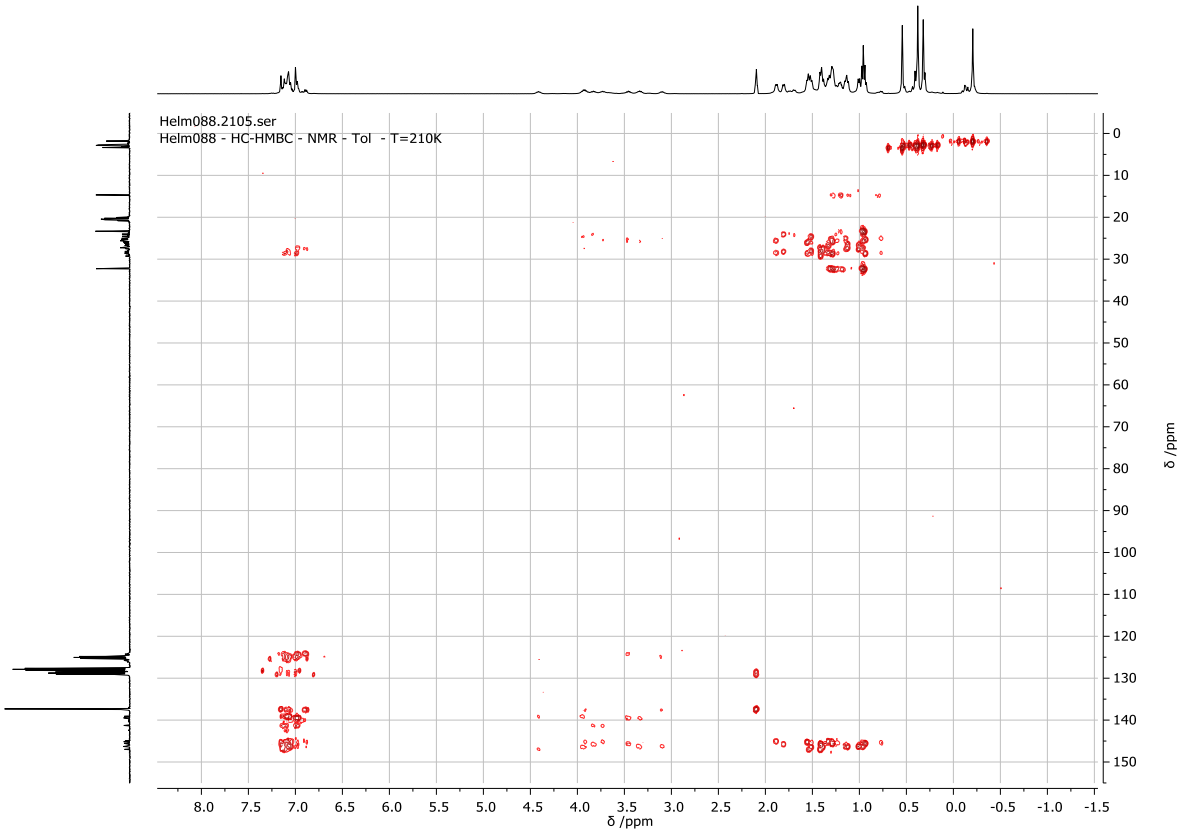


Figure S34. H,C-HMBC-NMR spectrum (d_8-toluene, 210 K) of **1**.

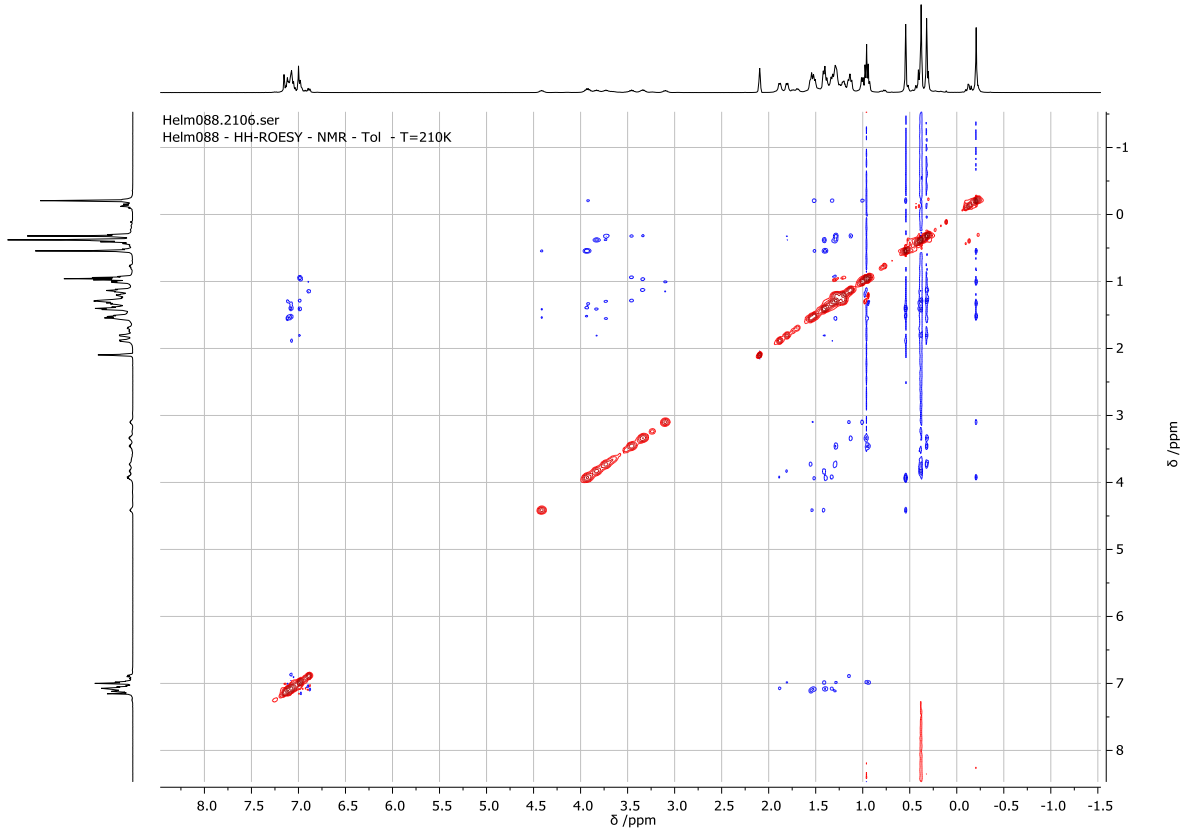


Figure S35. H,H-ROESY-NMR spectrum (d_8-toluene, 210 K) of **1**.

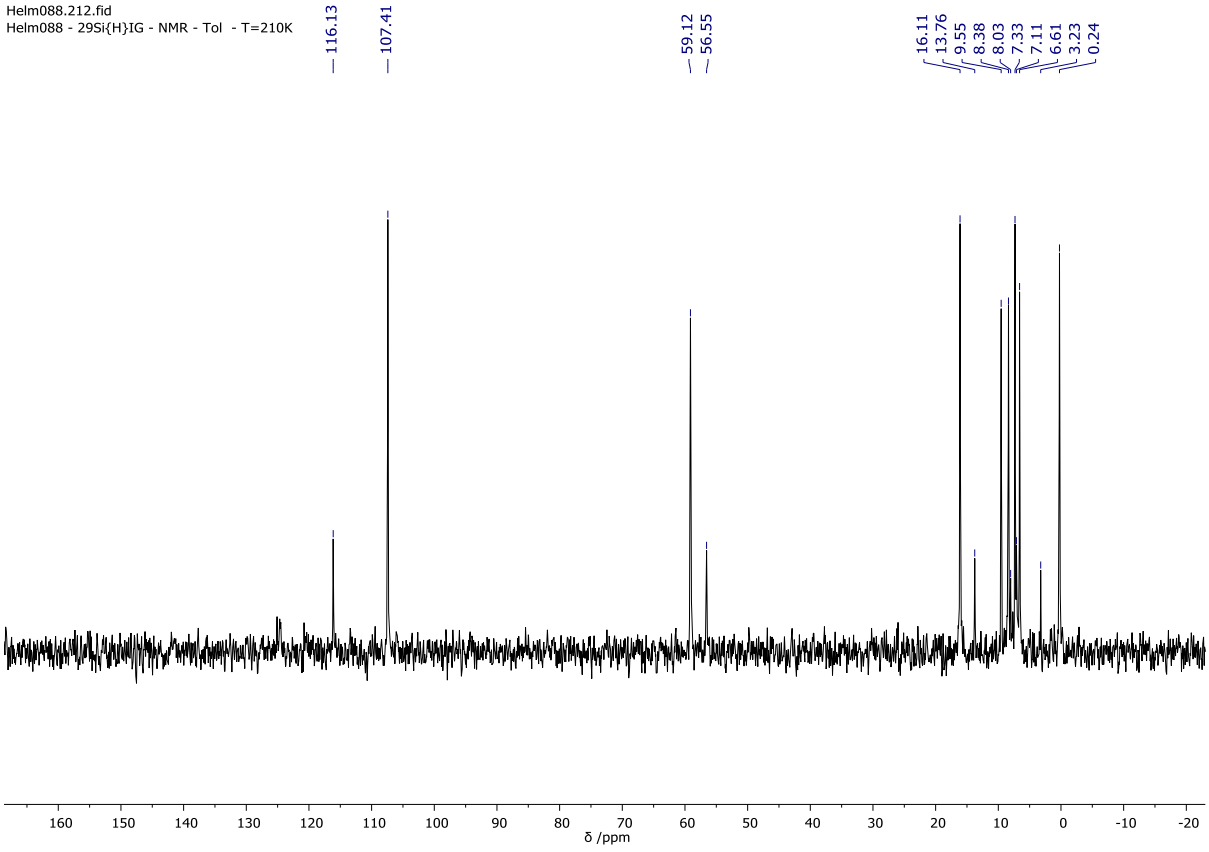


Figure S36. $^{29}Si\{^1H\}$IG-NMR spectrum (d_8-toluene, 210 K, 80MHz) of **1**.

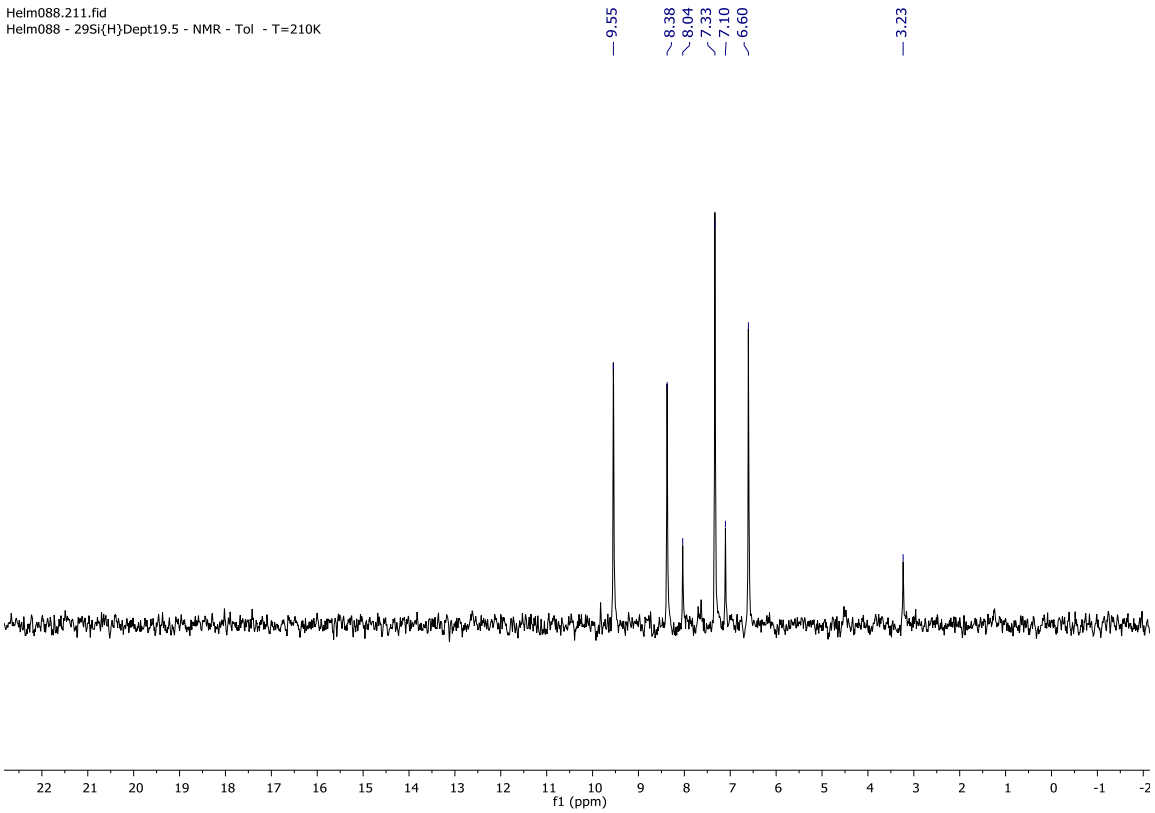


Figure S37. $^{29}Si\{^{1}H\}$DEPT19.5 NMR spectrum (d_8-toluene, 210 K, 80MHz) of **1**.

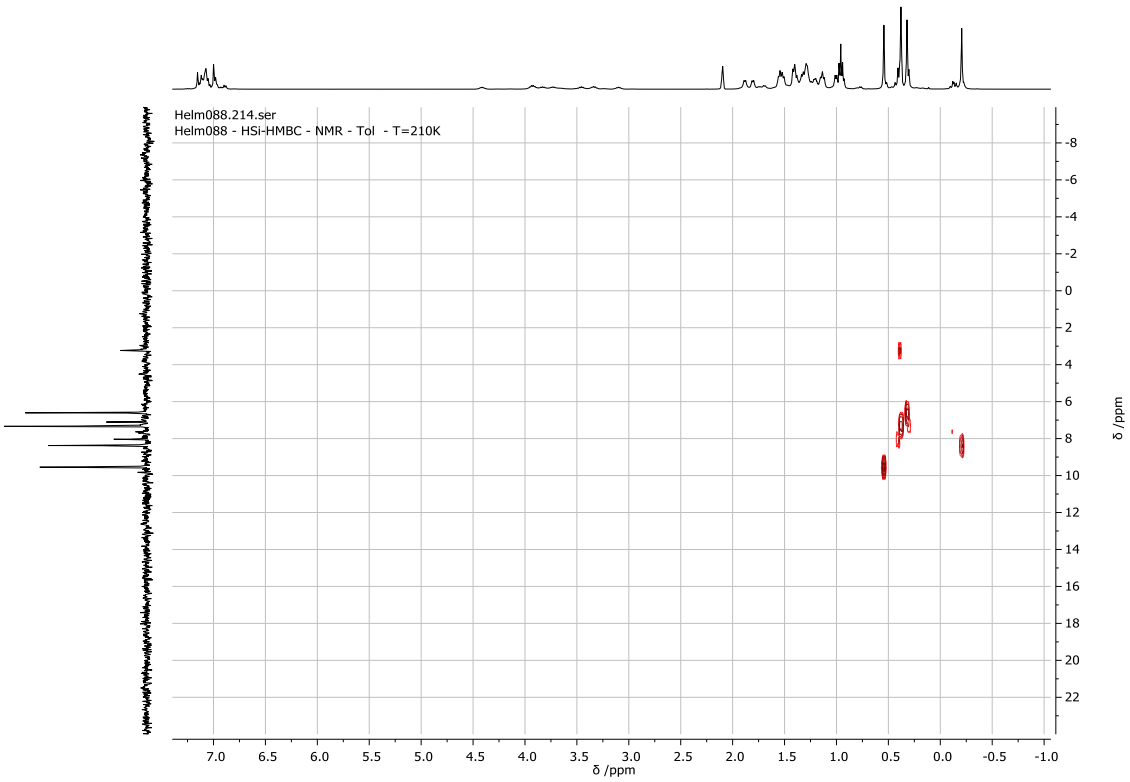


Figure S38. H,Si-HMBC-NMR spectrum (d_8-toluene, 210 K) of **1**.

7.4 Solution NMR spectra of 2

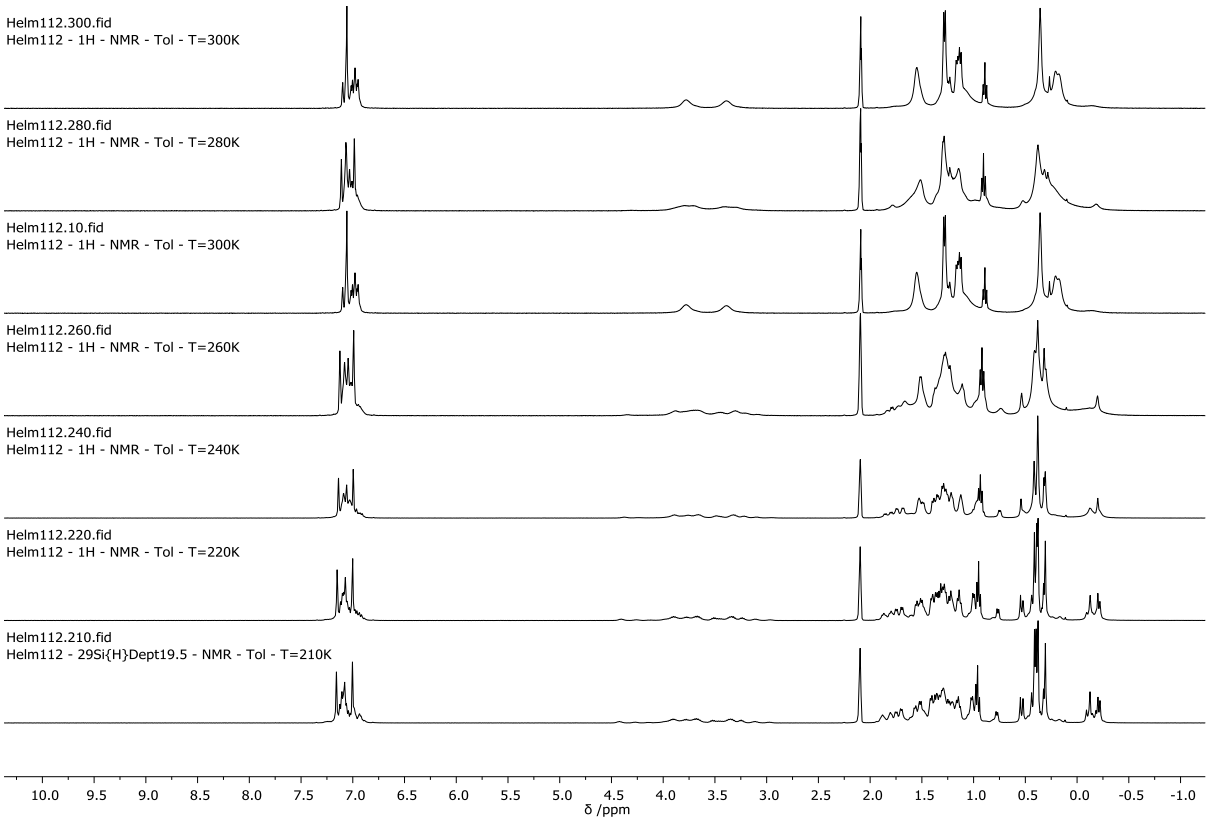


Figure S39. Variable temperature ^{1}H-NMR spectra (d_8-toluene, 300-210 K, 400 MHz) of **2**.

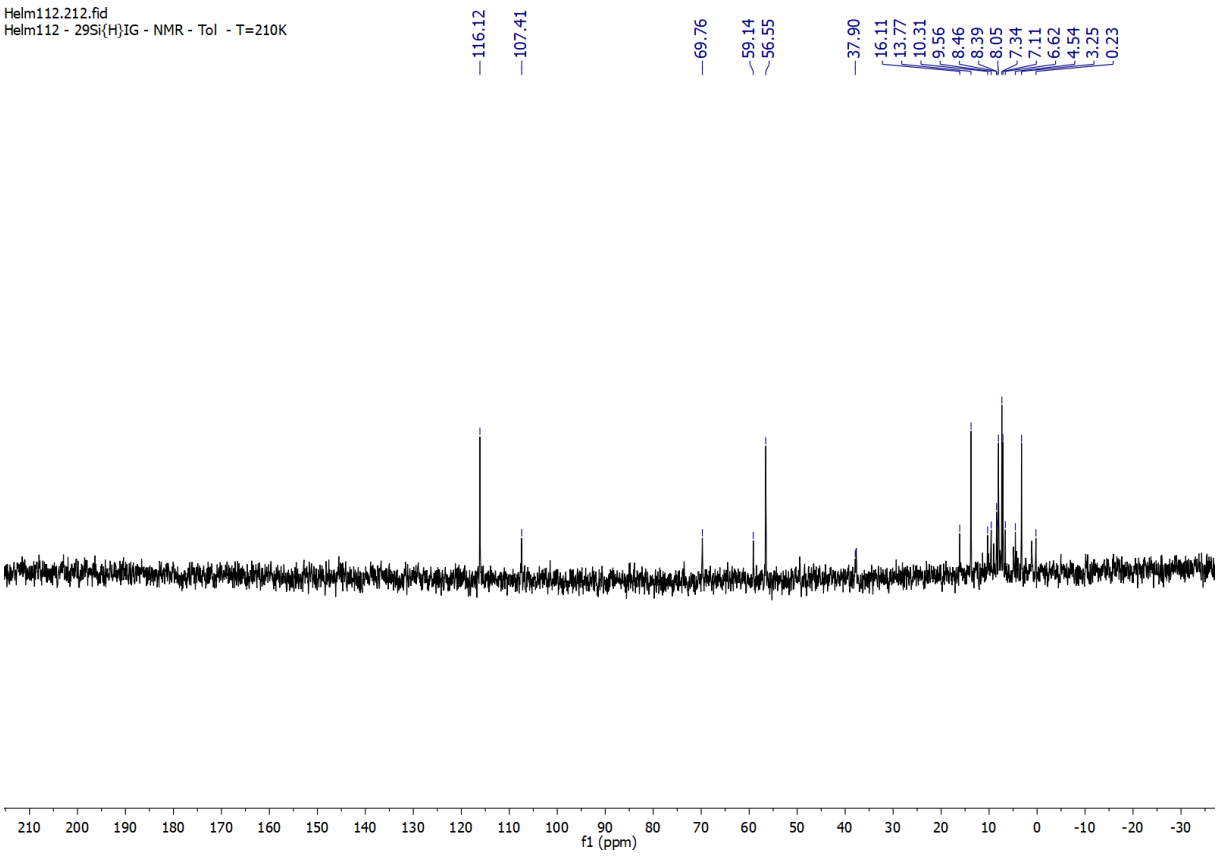


Figure S40. $^{29}Si\{^{1}H\}$IG NMR spectrum (d_8-toluene, 210 K, 80 MHz) of **2**.

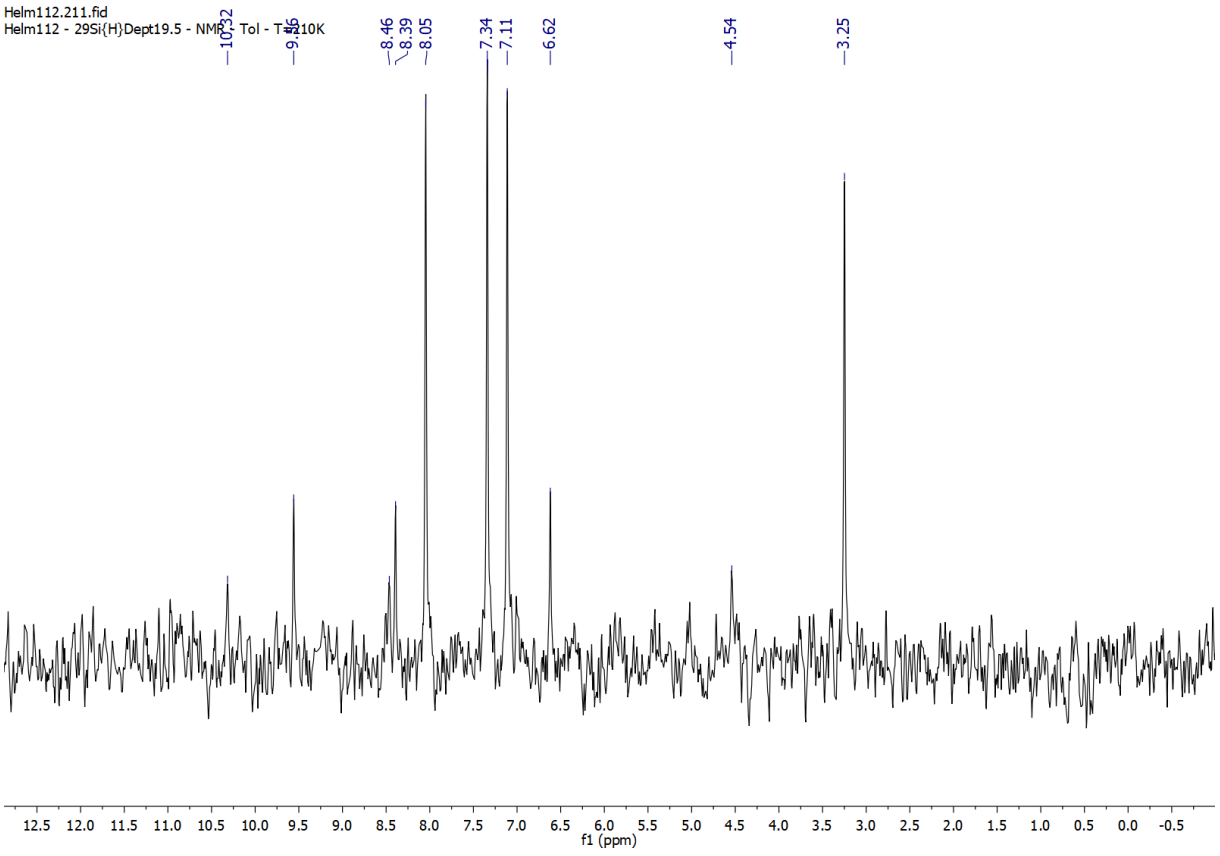


Figure S41. $^{29}Si\{^{1}H\}$DEPT19.5 NMR spectrum (d_8-toluene, 210 K, 80 MHz) of **2**.

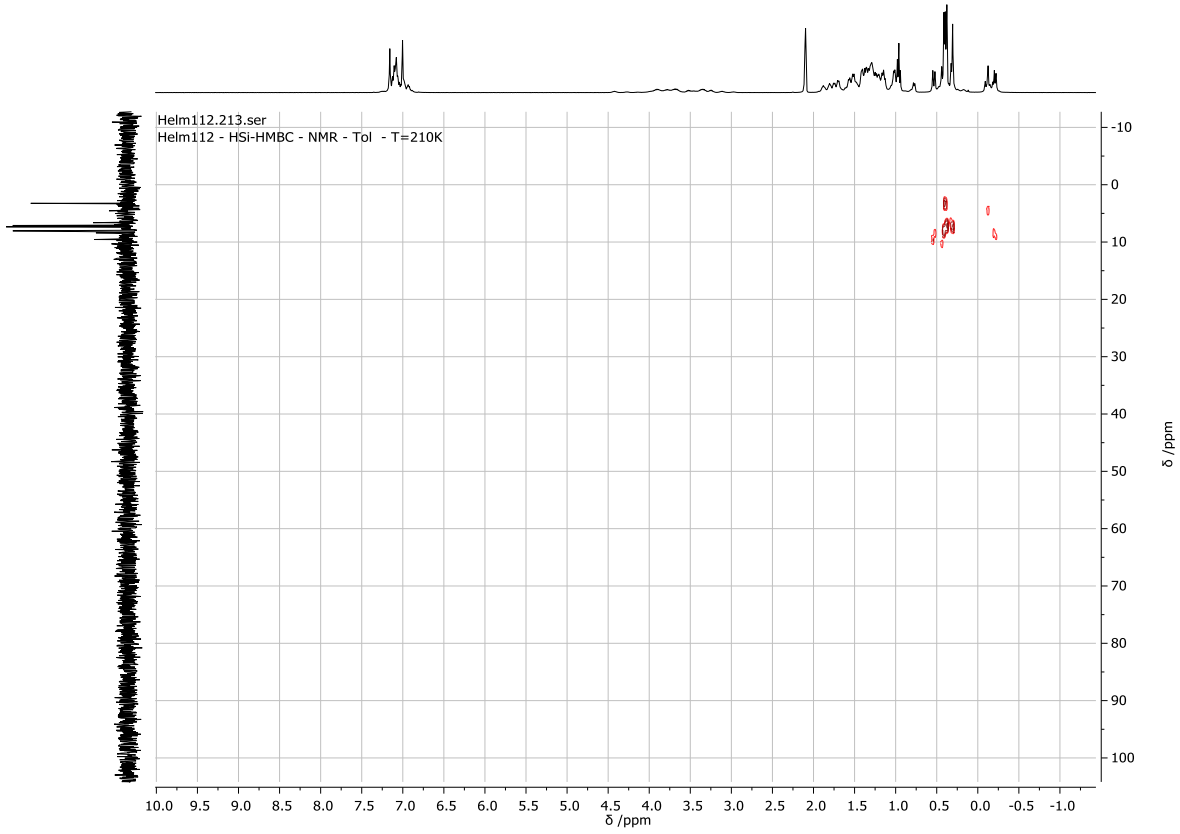


Figure S42. H,Si-HMBC-NMR spectrum (d_8-toluene, 210 K) of **2**.

8. Results from TDDFT calculations of models with $N(SiH_3)CH_3$ substituents

8.1 TDDFT calculation for $Si_4Ge_2\{N(SiH_3)CH_3\}_4$, $Si_3Ge_3\{N(SiH_3)CH_3\}_4$ and $Si_4Ge_2\{N(SiH_3)CH_3\}_4$

General procedure

We have performed a TDDFT calculation with ORCA on the optimized structures of $Si_4Ge_2\{N(SiH_3)CH_3\}_4$, $Si_3Ge_3\{N(SiH_3)CH_3\}_4$ and $Si_4Ge_2\{N(SiH_3)CH_3\}_4$ using the CAM-B3LYP functional, a double zeta basis set (def2-SVP) and the CPCM implicit solvent model for hexane solving for 140 excited states.

$Si_4Ge_2\{N(SiH_3)CH_3\}_4$

The HOMO → LUMO transition at 368.4 nm (State 1) is very weak. The second intense absorption at 331.8 nm (State 2) is related to the HOMO−1 → LUMO transition (Figure S43). The weak absorptions at 302.8 and 301.1 nm (State 3 and State 4) represent mixed excitations that are mainly related to HOMO−2 → LUMO (State 3) and HOMO−3 → LUMO and HOMO−4 → LUMO (State 4).

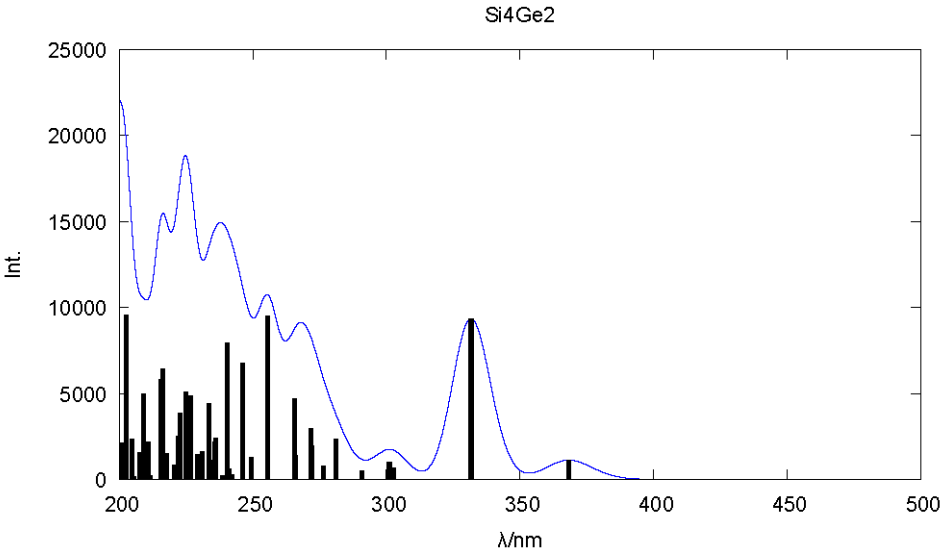


Figure S43. Calculated UV-Vis spectrum of $Si_4Ge_2\{N(SiH_3)CH_3\}_4$.

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	27147.2	368.4	0.007715121	0.09356	0.09579	-0.28331	-0.06420
2	30143.0	331.8	0.064704280	0.70668	-0.55827	0.62839	-0.01215
3	33021.7	302.8	0.004706263	0.04692	0.07106	-0.11983	-0.16586
4	33207.8	301.1	0.006938690	0.06879	-0.13511	0.22346	-0.02443
5	34384.2	290.8	0.003269125	0.03130	-0.15772	0.07972	0.00829
6	35573.1	281.1	0.016310369	0.15094	-0.30596	0.21477	-0.10585
7	36181.5	276.4	0.005500002	0.05004	-0.19874	0.06728	0.07758
8	36779.5	271.9	0.020534998	0.18381	-0.05427	0.35349	0.23644
9	36768.1	272.0	0.013376252	0.11977	-0.28958	0.12545	0.14204
10	37607.0	265.9	0.009577822	0.08384	0.04016	-0.17956	-0.22359

11	37656.4	265.6	0.032431869	0.28354	0.07418	0.52201	-0.07440
12	39103.1	255.7	0.065787236	0.55387	0.34907	0.65728	0.00044
13	40097.0	249.4	0.008790874	0.07218	-0.26247	0.04671	0.03325
14	40625.2	246.2	0.046666707	0.37817	-0.19198	0.51975	-0.26678
15	41289.5	242.2	0.001772186	0.01413	-0.07583	0.07134	0.05736
16	41595.3	240.4	0.054964382	0.43502	0.30527	-0.53291	-0.24051
17	41474.2	241.1	0.004304950	0.03417	0.16442	-0.08417	0.00727
18	41895.5	238.7	0.001501798	0.01180	-0.05029	-0.03521	0.08963
19	42365.8	236.0	0.016779231	0.13039	0.08471	0.24779	-0.24861
20	42425.5	235.7	0.015078015	0.11700	0.10639	0.21305	0.24554
21	42511.8	235.2	0.007811100	0.06049	0.16003	0.17274	0.07100
22	42791.1	233.7	0.030424703	0.23407	0.29111	-0.11141	0.37002
23	43250.9	231.2	0.011182476	0.08512	-0.18674	0.13609	0.17812
24	43630.9	229.2	0.009942876	0.07502	0.24768	-0.11596	-0.01514
25	44105.0	226.7	0.033452442	0.24970	-0.34494	0.26110	0.25009
26	44298.1	225.7	0.019007828	0.14126	0.28516	-0.22619	-0.09373
27	44442.3	225.0	0.035127831	0.26021	0.29844	-0.40494	-0.08468
28	44870.2	222.9	0.026632741	0.19540	0.29391	-0.24881	0.21707
29	45000.3	222.2	0.017482113	0.12790	0.19896	0.28886	0.06977
30	45110.9	221.7	0.004469863	0.03262	0.04180	-0.17450	-0.02053
31	45309.4	220.7	0.005724657	0.04159	-0.08333	0.18518	-0.01898
32	45948.0	217.6	0.010500268	0.07523	0.13869	0.02325	0.23549
33	46247.4	216.2	0.044492943	0.31672	-0.28879	0.44177	-0.19535
34	46388.3	215.6	0.040261890	0.28573	0.09416	0.50893	-0.13362
35	47260.8	211.6	0.001588891	0.01107	-0.02269	0.00226	0.10270
36	47443.0	210.8	0.015136364	0.10503	0.07109	-0.30724	-0.07471
37	47832.5	209.1	0.034440836	0.23704	0.15146	-0.45887	-0.05952
38	48132.8	207.8	0.010606644	0.07255	-0.19119	0.17399	-0.07563
39	48653.5	205.5	0.001120516	0.00758	0.05161	-0.03674	0.05974
40	48797.9	204.9	0.016159343	0.10902	0.12409	-0.30200	-0.04915
41	49349.7	202.6	0.065981967	0.44017	0.46668	-0.45572	-0.12125
42	49593.6	201.6	0.005731788	0.03805	0.01802	-0.19422	-0.00195
43	49661.8	201.4	0.014713753	0.09754	-0.23467	0.18513	-0.09051
44	49752.2	201.0	0.006772587	0.04481	0.14302	0.01058	-0.15572
45	50087.3	199.7	0.037313785	0.24525	0.03315	0.45228	0.19898
46	50177.9	199.3	0.017422428	0.11431	0.02907	0.33453	0.03940
47	50487.1	198.1	0.003747726	0.02444	-0.05601	0.14440	-0.02119
48	50785.2	196.9	0.031386597	0.20346	0.02035	-0.43429	-0.12018
49	51140.8	195.5	0.030967335	0.19935	-0.20625	0.34448	0.19530
50	51355.1	194.7	0.042075123	0.26972	-0.50588	-0.03781	0.11125
51	51381.5	194.6	0.049808317	0.31913	-0.46568	-0.09078	0.30665
52	51820.4	193.0	0.022273760	0.14150	0.05479	-0.37146	0.02283
53	52388.1	190.9	0.011739322	0.07377	0.17829	-0.05271	-0.19801
54	52370.7	190.9	0.057763423	0.36311	-0.22294	0.10800	-0.54931
55	52798.6	189.4	0.087112556	0.54317	0.44289	-0.45596	-0.37299
56	53310.4	187.6	0.013755952	0.08495	0.24334	-0.04790	-0.15310
57	53597.2	186.6	0.216998850	1.33288	0.79838	-0.82126	0.14493
58	54643.5	183.0	0.062408203	0.37599	0.28373	-0.32602	0.43497
59	54730.6	182.7	0.013531544	0.08139	-0.22901	-0.15627	-0.06728
60	55475.5	180.3	0.200722089	1.19116	-0.86189	0.65997	-0.11291
61	55360.3	180.6	0.034900243	0.20754	-0.29215	0.26208	-0.23131
62	55691.4	179.6	0.007753886	0.04584	0.00539	0.10655	0.18562
63	56044.1	178.4	0.134838508	0.79206	0.02566	0.83862	0.29686
64	56230.0	177.8	0.035406258	0.20729	0.38831	-0.18546	-0.14870
65	56712.0	176.3	0.020513765	0.11908	0.19567	0.23745	0.15625
66	56783.4	176.1	0.048965073	0.28388	0.19722	0.46607	-0.16663
67	57275.4	174.6	0.010630105	0.06110	0.18648	-0.15813	-0.03636
68	57269.4	174.6	0.053426764	0.30712	-0.05616	0.54616	-0.07532
69	57729.3	173.2	0.045461158	0.25925	0.43018	0.07515	-0.26182
70	58041.9	172.3	0.003395273	0.01926	0.06388	0.09837	-0.07416
71	57696.3	173.3	0.051876123	0.29600	-0.36612	-0.29111	-0.27787
72	58556.7	170.8	0.045173566	0.25397	0.38091	0.30610	0.12321
73	58110.2	172.1	0.159676016	0.90461	-0.04269	0.85503	-0.41438
74	58461.4	171.1	0.058220803	0.32786	-0.44555	0.23943	-0.26837
75	59179.5	169.0	0.035527217	0.19764	-0.02063	-0.30295	-0.32470
76	59405.8	168.3	0.048462478	0.26857	-0.44212	0.25941	-0.07619
77	58992.5	169.5	0.104342003	0.58229	0.35769	-0.52286	-0.42539
78	59531.2	168.0	0.085690492	0.47387	-0.58164	0.28330	0.23519
79	59846.0	167.1	0.117778617	0.64790	0.13593	-0.15369	-0.77833
80	60038.3	166.6	0.166953559	0.91547	-0.62326	-0.36352	0.62839
81	60461.4	165.4	0.125086741	0.68110	-0.14887	0.03690	-0.81091
82	60467.7	165.4	0.029453722	0.16036	-0.38718	-0.09763	-0.03025
83	60767.4	164.6	0.074393767	0.40303	0.01505	-0.20222	0.60159
84	60629.1	164.9	0.035389402	0.19216	0.21153	0.16120	0.34847
85	60909.4	164.2	0.094286910	0.50962	-0.68951	0.12689	0.13450
86	60529.8	165.2	0.046518344	0.25301	-0.02524	0.35214	0.35829
87	60999.9	163.9	0.003073859	0.01659	-0.06562	0.02165	-0.10869
88	61699.2	162.1	0.106353968	0.56748	-0.63437	-0.32352	-0.24574
89	61795.1	161.8	0.044518233	0.23717	0.17432	0.39911	-0.21792
90	61916.6	161.5	0.026614926	0.14151	0.18910	-0.32371	-0.03108
91	61689.7	162.1	0.074685807	0.39857	0.27048	0.03798	-0.56918
92	61924.8	161.5	0.123160231	0.65476	0.15460	0.47920	0.63342
93	62314.4	160.5	0.090855616	0.48000	0.37311	-0.41291	-0.41266
94	62579.7	159.8	0.000324349	0.00171	0.03015	-0.02684	0.00877
95	62611.0	159.7	0.077245141	0.40616	0.20099	-0.40248	0.45141
96	62519.5	160.0	0.031485791	0.16580	0.26899	0.29642	0.07467

97	62785.4	159.3	0.102554315	0.53774	0.10498	0.23998	-0.68493
98	62668.1	159.6	0.007313083	0.03842	-0.16237	0.05279	-0.09626
99	63315.2	157.9	0.066788257	0.34727	-0.44286	0.21820	0.32177
100	63333.7	157.9	0.071232885	0.37027	-0.19451	0.18162	0.54722
101	63250.9	158.1	0.086333665	0.44935	0.26594	-0.13056	0.60132
102	63445.1	157.6	0.037293826	0.19351	0.11832	-0.40783	0.11486
103	63538.3	157.4	0.075401652	0.39068	-0.49026	0.05463	-0.38385
104	63553.7	157.3	0.061791803	0.32009	0.27179	-0.48566	0.10172
105	64222.5	155.7	0.040101877	0.20557	0.03982	0.32228	0.31641
106	64343.3	155.4	0.053154228	0.27196	-0.43585	0.27256	-0.08781
107	64407.9	155.3	0.079938610	0.40859	-0.25352	0.15903	-0.56483
108	64482.4	155.1	0.010017295	0.05114	0.09628	0.09339	-0.18208
109	64084.4	156.0	0.012363138	0.06351	0.17106	0.12724	-0.13439
110	64501.2	155.0	0.031045808	0.15846	0.07449	-0.11301	0.37435
111	64965.6	153.9	0.005694444	0.02886	-0.15109	-0.06743	-0.03850
112	65081.6	153.7	0.078072760	0.39493	-0.07249	0.62127	-0.06075
113	64809.8	154.3	0.005643858	0.02867	0.11908	-0.03049	0.11644
114	64772.4	154.4	0.114785633	0.58341	-0.28512	0.67006	0.23052
115	65279.1	153.2	0.037073141	0.18697	-0.35637	0.23689	0.06205
116	65589.5	152.5	0.065686720	0.32970	-0.39214	0.37491	0.18807
117	65035.0	153.8	0.010139174	0.05133	-0.00499	-0.19809	-0.10982
118	65284.3	153.2	0.025108096	0.12661	-0.34015	-0.09106	0.05119
119	65369.5	153.0	0.005237568	0.02638	-0.13585	-0.02540	0.08530
120	65707.1	152.2	0.062899683	0.31515	0.55766	-0.06140	0.01976
121	65934.1	151.7	0.055234139	0.27579	-0.12822	-0.44194	-0.25305
122	65548.3	152.6	0.050548680	0.25388	0.31945	-0.37588	-0.10268
123	65917.8	151.7	0.071586636	0.35752	-0.49499	-0.26924	-0.20004
124	66151.9	151.2	0.003774266	0.01878	0.09404	-0.09638	-0.02548
125	66343.7	150.7	0.021812534	0.10824	0.05205	-0.24881	-0.20887
126	66445.8	150.5	0.107983680	0.53501	0.24459	-0.58071	-0.37144
127	66821.6	149.7	0.016984508	0.08368	0.14470	-0.20042	-0.15023
128	66163.2	151.1	0.174980774	0.87066	0.79341	-0.48031	-0.10231
129	66584.7	150.2	0.002662243	0.01316	0.02763	-0.02618	0.10823
130	67106.3	149.0	0.066710383	0.32727	-0.05137	0.16607	0.54502
131	66624.9	150.1	0.052990106	0.26184	0.40723	-0.30888	0.02447
132	67328.5	148.5	0.040514427	0.19810	0.32265	0.25283	0.17342
133	67125.0	149.0	0.000642336	0.00315	-0.04696	0.00050	-0.03074
134	67425.8	148.3	0.034039020	0.16620	-0.19322	0.05063	0.35539
135	66948.8	149.4	0.060498570	0.29749	0.37779	-0.06931	-0.38725
136	67323.4	148.5	0.014824367	0.07249	-0.18882	-0.19178	0.00769
137	67517.1	148.1	0.018373488	0.08959	-0.18980	0.17091	-0.15606
138	67597.2	147.9	0.042713374	0.20802	0.01909	-0.04401	-0.45357
139	67148.8	148.9	0.005840741	0.02864	0.12096	0.09081	-0.07588
140	67865.5	147.4	0.017018761	0.08256	0.00848	0.06665	0.27936

STATE 1: E= 0.123692 au 3.366 eV 27147.2 cm**-1 (368.4 nm)
124a -> 126a : 0.090635 (c= -0.30105628)
125a -> 126a : 0.860169 (c= -0.92745284) **HOMO → LUMO**

STATE 2: E= 0.137342 au 3.737 eV 30143.0 cm**-1 (331.8 nm)
122a -> 126a : 0.022023 (c= 0.14840013)
124a -> 126a : 0.788191 (c= -0.88780148) **HOMO-1 → LUMO**
124a -> 127a : 0.012310 (c= -0.11095177)
125a -> 126a : 0.068623 (c= 0.26195923)

STATE 3: E= 0.150458 au 4.094 eV 33021.7 cm**-1 (302.8 nm)
121a -> 126a : 0.048726 (c= 0.22074047)
122a -> 126a : 0.179718 (c= 0.42393205)
123a -> 126a : 0.691488 (c= 0.83155752) **HOMO-2 → LUMO**
125a -> 127a : 0.019591 (c= 0.13996878)

STATE 4: E= 0.151306 au 4.117 eV 33207.8 cm**-1 (301.1 nm)
121a -> 126a : 0.234973 (c= -0.48473977) **HOMO-4 → LUMO**
122a -> 126a : 0.415689 (c= -0.64473917) **HOMO-3 → LUMO**
123a -> 126a : 0.188102 (c= 0.43370752)
125a -> 127a : 0.066100 (c= 0.25710000)
125a -> 129a : 0.027815 (c= -0.16677897)

STATE 5: E= 0.156666 au 4.263 eV 34384.2 cm**-1 (290.8 nm)
116a -> 126a : 0.010291 (c= -0.10144268)
121a -> 126a : 0.259556 (c= 0.50946663) **HOMO-4 → LUMO**
122a -> 126a : 0.215365 (c= -0.46407488) **HOMO-3 → LUMO**
123a -> 126a : 0.041023 (c= 0.20254237)
124a -> 127a : 0.080724 (c= -0.28411996)
125a -> 127a : 0.336543 (c= -0.58012305) **HOMO → LUMO+1**

STATE 6: E= 0.162083 au 4.411 eV 35573.1 cm**-1 (281.1 nm)
121a -> 126a : 0.161965 (c= 0.40244909)

```
   122a -> 126a  :     0.033928 (c= -0.18419669)
   124a -> 127a  :     0.511136 (c=  0.71493761)              HOMO-1→ LUMO+1
   124a -> 128a  :     0.033325 (c=  0.18255232)
   125a -> 127a  :     0.025967 (c=  0.16114303)
   125a -> 128a  :     0.134447 (c=  0.36666977)
   125a -> 130a  :     0.014466 (c= -0.12027356)

STATE  7:  E=   0.164855 au      4.486 eV    36181.5 cm**-1 (276.4 nm)
   120a -> 126a  :     0.690896 (c= -0.83120133)              HOMO-5 → LUMO
   121a -> 126a  :     0.018657 (c= -0.13659206)
   124a -> 128a  :     0.071976 (c=  0.26828385)
   124a -> 129a  :     0.067964 (c=  0.26069978)
   125a -> 128a  :     0.051814 (c= -0.22762765)

STATE  8:  E=   0.167580 au      4.560 eV    36779.5 cm**-1 (271.9 nm)
   120a -> 126a  :     0.046556 (c=  0.21576782)
   121a -> 126a  :     0.050273 (c=  0.22421622)
   122a -> 126a  :     0.023977 (c= -0.15484662)
   124a -> 127a  :     0.033885 (c= -0.18408008)
   124a -> 128a  :     0.093915 (c=  0.30645494)
   124a -> 129a  :     0.173257 (c=  0.41624158)              HOMO-1 → LUMO+3
   125a -> 127a  :     0.147282 (c=  0.38377302)              HOMO → LUMO+1
   125a -> 128a  :     0.167883 (c= -0.40973526)              HOMO → LUMO+2
   125a -> 129a  :     0.183816 (c=  0.42873784)              HOMO → LUMO+3
   125a -> 131a  :     0.010287 (c=  0.10142470)

STATE  9:  E=   0.167528 au      4.559 eV    36768.1 cm**-1 (272.0 nm)
   120a -> 126a  :     0.012929 (c=  0.11370769)
   121a -> 126a  :     0.050087 (c=  0.22380158)
   123a -> 126a  :     0.016193 (c= -0.12725006)
   123a -> 129a  :     0.014372 (c= -0.11988335)
   124a -> 127a  :     0.022216 (c=  0.14905119)
   124a -> 129a  :     0.170707 (c= -0.41316746)              HOMO-1 → LUMO+3
   124a -> 130a  :     0.021086 (c= -0.14521182)
   125a -> 128a  :     0.338014 (c= -0.58138948)              HOMO → LUMO+2
   125a -> 129a  :     0.239228 (c= -0.48910954)              HOMO → LUMO+3
   125a -> 131a  :     0.025073 (c=  0.15834486)

STATE 10:  E=   0.171350 au      4.663 eV    37607.0 cm**-1 (265.9 nm)
   120a -> 126a  :     0.016684 (c=  0.12916740)
   121a -> 126a  :     0.010428 (c= -0.10211564)
   124a -> 127a  :     0.040822 (c= -0.20204495)
   124a -> 128a  :     0.651003 (c=  0.80684744)              HOMO-1 → LUMO+2
   124a -> 129a  :     0.048849 (c= -0.22101896)
   124a -> 131a  :     0.030404 (c= -0.17436859)
   125a -> 128a  :     0.066011 (c=  0.25692638)
   125a -> 129a  :     0.026922 (c= -0.16408027)
```

$Si_3Ge_3\{N(SiH_3)CH_3\}_4$

The HOMO → LUMO transition at 376.8 nm (State 1) is weak. The second absorption at 348.4 nm (State 2) is also weak and related to the HOMO−1 → LUMO transition (Figure S44). The more stronger absorption at 271.3 nm (State 10) is related to a mixed excitation involving the transitions HOMO−5 → LUMO and HOMO → LUMO+2.

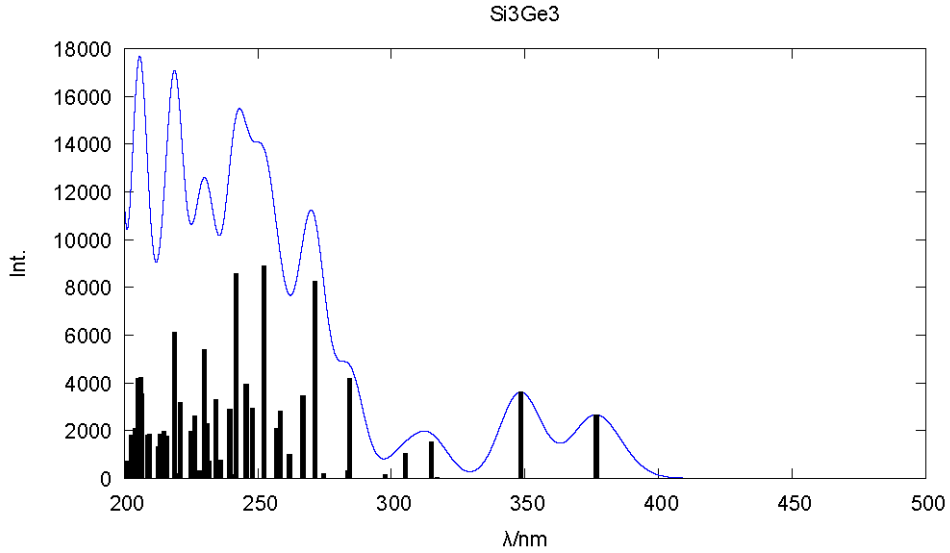


Figure S44. Calculated UV-Vis spectrum of $Si_3Ge_3\{N(SiH_3)CH_3\}_4$.

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	26542.7	376.8	0.018395494	0.22816	-0.11717	-0.45955	-0.05695
2	28702.9	348.4	0.024998196	0.28672	0.29609	0.43474	-0.10029
3	31524.9	317.2	0.000348885	0.00364	0.00410	-0.05146	0.03127
4	31743.4	315.0	0.010620481	0.11015	0.14714	0.29731	0.00996
5	32748.8	305.4	0.007081595	0.07119	0.13038	0.22678	-0.05255
6	33590.3	297.7	0.001104384	0.01082	-0.01911	-0.09729	0.03152
7	35266.1	283.6	0.002057893	0.01921	0.04708	0.11354	-0.06405
8	35170.2	284.3	0.028918354	0.27069	0.11930	0.50542	0.03176
9	36421.3	274.6	0.001352013	0.01222	0.00186	0.10982	-0.01252
10	36855.6	271.3	0.056979538	0.50897	0.58626	0.39569	0.09327
11	37454.2	267.0	0.024011953	0.21106	-0.27782	0.36567	-0.01277
12	38178.9	261.9	0.007045200	0.06075	-0.22467	0.04268	0.09193
13	38674.8	258.6	0.019411809	0.16524	0.18495	-0.33470	-0.13786
14	38898.6	257.1	0.014544388	0.12309	-0.01119	-0.25846	0.23699
15	39622.3	252.4	0.061485776	0.51087	-0.50767	-0.50234	0.02832
16	40321.7	248.0	0.020441540	0.16690	-0.06209	-0.33386	-0.22711
17	40705.4	245.7	0.027241836	0.22032	0.05752	-0.46270	-0.05408
18	41321.5	242.0	0.059352034	0.47286	-0.12495	-0.63821	-0.22347
19	41468.8	241.1	0.001087578	0.00863	-0.08200	-0.01702	0.04024
20	41739.4	239.6	0.020045052	0.15810	-0.17885	0.33036	-0.13030
21	42369.8	236.0	0.005182134	0.04027	-0.05989	0.10084	-0.16282
22	42692.4	234.2	0.022723130	0.17522	-0.11426	-0.25676	0.31023
23	43156.9	231.7	0.005016449	0.03827	0.09596	0.11344	-0.12724
24	43280.9	231.0	0.015727648	0.11963	-0.20273	-0.18451	-0.21092
25	43499.6	229.9	0.037214011	0.28164	-0.39131	-0.31930	0.16300
26	43836.8	228.1	0.002185880	0.01642	-0.01828	0.12440	0.02463
27	44147.5	226.5	0.017987786	0.13414	0.33914	-0.07368	0.11700
28	44287.1	225.8	0.002392278	0.01778	-0.04371	0.02204	-0.12404
29	44466.3	224.9	0.013644671	0.10102	-0.00299	-0.17717	-0.26386
30	45213.6	221.2	0.022112701	0.16101	0.03824	-0.10231	-0.38611
31	45403.8	220.2	0.001224550	0.00888	-0.06107	-0.07137	-0.00747
32	45675.5	218.9	0.042165871	0.30392	0.26945	0.47453	-0.07831
33	45681.7	218.9	0.037147828	0.26771	0.12018	0.45069	-0.22393
34	46271.7	216.1	0.012103116	0.08611	0.10415	0.26623	-0.06623
35	46505.2	215.0	0.013582640	0.09615	-0.11826	0.28175	0.05277
36	46854.8	213.4	0.012670045	0.08902	0.02697	-0.11461	0.27415
37	47002.8	212.8	0.009259364	0.06485	0.03638	0.13291	0.21416

38	47718.4	209.6	0.012856326	0.08870	0.00243	0.29586	-0.03406
39	47928.3	208.6	0.012526215	0.08604	0.02987	0.22008	-0.19160
40	48371.4	206.7	0.024429009	0.16626	-0.16109	-0.28914	-0.23814
41	48733.6	205.2	0.028998322	0.19589	0.39852	-0.01178	0.19219
42	49019.0	204.0	0.014345864	0.09635	0.09853	0.29241	-0.03371
43	48467.4	206.3	0.029252795	0.19870	0.20396	-0.25369	-0.30454
44	49293.7	202.9	0.012483434	0.08337	0.26793	-0.09355	-0.05323
45	48890.2	204.5	0.010388189	0.06995	-0.24736	0.09358	-0.00288
46	49753.2	201.0	0.005070111	0.03355	0.06832	0.16983	-0.00612
47	50106.3	199.6	0.005140174	0.03377	-0.02519	0.10128	-0.15126
48	50391.3	198.4	0.013287802	0.08681	0.17616	-0.14603	0.18562
49	51011.5	196.0	0.101036880	0.65206	-0.52707	-0.59941	0.12235
50	51376.5	194.6	0.083745740	0.53663	-0.16803	-0.71145	-0.04722
51	51485.3	194.2	0.007754870	0.04959	-0.04611	-0.11531	0.18484
52	51640.5	193.6	0.075904903	0.48390	-0.38317	-0.55438	-0.17246
53	51788.1	193.1	0.034395998	0.21865	-0.24646	0.35932	-0.16970
54	52033.6	192.2	0.083462667	0.52806	-0.51320	-0.21569	-0.46708
55	52551.4	190.3	0.045554719	0.28538	0.51536	-0.13220	-0.04808
56	52962.9	188.8	0.027584495	0.17146	0.05442	0.33578	0.23612
57	53150.1	188.1	0.052457969	0.32492	-0.12517	-0.17944	0.52636
58	53436.5	187.1	0.061270057	0.37747	-0.48432	-0.37760	-0.01805
59	53839.4	185.7	0.106557892	0.65157	0.39199	0.67578	-0.20308
60	54377.7	183.9	0.099207775	0.60062	-0.38145	-0.45796	0.49536
61	54620.5	183.1	0.283178772	1.70679	-0.10940	-1.30182	-0.00995
62	54952.2	182.0	0.070501873	0.42237	0.31222	0.37632	-0.42809
63	55173.6	181.2	0.085026767	0.50734	0.12851	0.69616	0.07865
64	55347.8	180.7	0.013440029	0.07994	0.06187	-0.24457	-0.12766
65	55170.8	181.3	0.020535754	0.12254	0.11693	0.25843	0.20514
66	55783.9	179.3	0.028548264	0.16848	-0.35538	-0.20046	0.04470
67	56183.3	178.0	0.021778001	0.12761	0.15159	0.17228	0.27377
68	56380.2	177.4	0.042819973	0.25003	-0.07313	0.48107	-0.11513
69	56332.5	177.5	0.071829937	0.41978	0.14730	-0.59629	0.20620
70	56432.2	177.2	0.016879889	0.09847	0.31201	-0.03324	-0.00436
71	56269.4	177.7	0.048965473	0.28648	-0.05624	0.34102	0.40868
72	56891.9	175.8	0.044879195	0.25970	-0.44773	0.24003	0.04033
73	57861.0	172.8	0.016200386	0.09218	-0.22349	-0.14375	-0.14684
74	57796.1	173.0	0.074087714	0.42201	0.00761	-0.64310	-0.09150
75	58231.5	171.7	0.050933567	0.28795	-0.43505	0.05037	-0.31007
76	57501.5	173.9	0.017319879	0.09916	-0.05030	-0.04423	-0.30769
77	58647.5	170.5	0.022399950	0.12574	-0.07920	-0.04279	0.34298
78	58176.0	171.9	0.055253027	0.31267	0.38824	-0.22915	0.33080
79	59525.0	168.0	0.026626660	0.14726	0.16400	0.33727	0.08135
80	59587.3	167.8	0.062511288	0.34537	-0.52894	-0.14311	0.21239
81	59556.5	167.9	0.073673735	0.40725	0.32166	-0.02667	-0.55052
82	59657.8	167.6	0.178162526	0.98316	-0.90224	0.11386	-0.39516
83	59603.0	167.8	0.034664451	0.19147	0.09513	0.42696	0.01113
84	59843.9	167.1	0.066065193	0.36344	-0.08862	-0.38810	0.45272
85	60279.0	165.9	0.021552204	0.11771	-0.33345	0.01976	0.07826
86	60389.2	165.6	0.048664961	0.26530	0.36677	0.16669	0.32093
87	60747.3	164.6	0.012107693	0.06562	0.20594	-0.13275	-0.07471
88	61027.3	163.9	0.018023838	0.09723	-0.26066	-0.00373	0.17110
89	60552.8	165.1	0.085637824	0.46559	0.52565	-0.19884	0.38697
90	60561.1	165.1	0.005110542	0.02778	0.02232	0.09879	-0.13238
91	61067.1	163.8	0.061926258	0.33384	-0.18837	-0.03145	0.54532
92	61143.9	163.5	0.001822224	0.00981	0.06995	-0.06673	-0.02158
93	60911.7	164.2	0.061371728	0.33170	-0.51364	-0.01813	0.25989
94	61423.8	162.8	0.109568412	0.58725	-0.64668	-0.40055	-0.09283
95	61351.2	163.0	0.015732857	0.08442	0.24751	0.09322	0.12030
96	62312.6	160.5	0.029894953	0.15794	-0.12775	0.02874	-0.37523
97	62268.5	160.6	0.000625733	0.00331	-0.02919	-0.04050	0.02857
98	62459.5	160.1	0.128909551	0.67946	0.55295	0.33391	-0.51207
99	62715.8	159.4	0.059827031	0.31405	-0.18697	-0.27320	-0.45216
100	63132.0	158.4	0.055596501	0.28992	0.42386	-0.01236	-0.33182
101	63160.4	158.3	0.041493442	0.21628	0.18416	-0.21030	-0.37167
102	62986.3	158.8	0.117652650	0.61494	0.44113	0.16691	0.62648
103	63213.4	158.2	0.040171321	0.20921	-0.27592	0.11523	0.34612
104	63391.2	157.8	0.076668145	0.39816	-0.61118	0.04291	0.15093
105	63566.0	157.3	0.214771698	1.11232	0.10454	0.35705	0.98686
106	63870.1	156.6	0.057606061	0.29692	-0.39911	-0.28239	0.24061
107	64184.8	155.8	0.051513914	0.26422	-0.09709	-0.49353	0.10593
108	64167.0	155.8	0.042159410	0.21630	0.28257	0.24867	0.27316
109	64293.0	155.5	0.020964428	0.10735	0.16725	-0.09942	-0.26361
110	61977.0	161.4	0.002732734	0.01452	-0.00998	0.09643	0.07153
111	64024.8	156.2	0.012993921	0.06681	-0.12992	-0.13823	0.17558
112	64335.8	155.4	0.106265256	0.54377	0.36181	0.52026	0.37709
113	63972.1	156.3	0.045338698	0.23332	0.21593	-0.26030	-0.34487
114	64617.0	154.8	0.074139903	0.37773	-0.21610	-0.42339	-0.38958
115	64555.4	154.9	0.022899477	0.11678	-0.16075	-0.20545	-0.22074
116	64877.8	154.1	0.068253186	0.34634	0.37383	0.30190	0.33977
117	64922.9	154.0	0.101742962	0.51592	-0.30173	-0.64721	0.07745
118	64472.2	155.1	0.037629271	0.19214	-0.38787	-0.01854	-0.20337
119	64709.3	154.5	0.011998156	0.06104	-0.24107	-0.05331	0.00920
120	65458.3	152.8	0.001375806	0.00692	0.04622	-0.06253	-0.02954
121	65463.1	152.8	0.015297981	0.07693	0.00688	-0.24951	0.12095
122	65377.0	153.0	0.268209821	1.35059	-0.44853	-1.06725	-0.10191
123	65525.8	152.6	0.114099886	0.57326	0.17962	-0.64969	-0.34481

124	65468.3	152.7	0.127735384	0.64233	-0.51629	-0.53968	-0.29071
125	65515.4	152.6	0.005067836	0.02547	0.09303	-0.07900	-0.10282
126	66055.3	151.4	0.024868434	0.12394	0.16546	-0.02245	0.30994
127	66319.8	150.8	0.049080781	0.24364	0.23165	0.17343	0.39987
128	66178.3	151.1	0.065370859	0.32520	0.49256	0.16239	0.23709
129	66418.7	150.6	0.017335683	0.08593	0.14866	0.25157	0.02319
130	66769.7	149.8	0.128179464	0.63200	0.53070	0.58656	0.07938
131	66922.4	149.4	0.064051695	0.31509	0.33466	0.25593	0.37094
132	67021.7	149.2	0.029917873	0.14696	-0.03018	-0.32131	-0.20689
133	67050.4	149.1	0.141308991	0.69382	-0.24569	-0.57188	-0.55354
134	66941.0	149.4	0.049815282	0.24499	0.42674	-0.16963	-0.18469
135	67304.5	148.6	0.041586190	0.20341	-0.38540	-0.23425	0.00213
136	67167.4	148.9	0.005253090	0.02575	-0.06969	-0.14418	0.01021
137	67617.1	147.9	0.034755609	0.16922	0.11844	0.37248	-0.12826
138	67404.2	148.4	0.054099014	0.26423	0.26469	-0.40404	0.17583
139	67344.0	148.5	0.135682561	0.66329	-0.33295	-0.71197	-0.21337
140	67307.2	148.6	0.011734214	0.05739	0.10651	-0.02038	-0.21362

STATE 1: E= 0.120937 au 3.291 eV 26542.7 cm**-1 (376.8 nm)
130a -> 135a : 0.010393 (c= 0.10194374)
133a -> 135a : 0.086944 (c= 0.29486347)
134a -> 135a : 0.850713 (c= 0.92234110) **HOMO → LUMO**

STATE 2: E= 0.130780 au 3.559 eV 28702.9 cm**-1 (348.4 nm)
133a -> 135a : 0.768328 (c= 0.87654322) **HOMO-1 → LUMO**
133a -> 136a : 0.025966 (c= 0.16113930)
134a -> 135a : 0.059525 (c= -0.24397677)
134a -> 136a : 0.062740 (c= 0.25047863)

STATE 3: E= 0.143638 au 3.909 eV 31524.9 cm**-1 (317.2 nm)
130a -> 135a : 0.010311 (c= 0.10154437)
132a -> 135a : 0.501653 (c= -0.70827450) **HOMO-2 → LUMO**
134a -> 136a : 0.425337 (c= 0.65217829) **HOMO → LUMO+1**

STATE 4: E= 0.144634 au 3.936 eV 31743.4 cm**-1 (315.0 nm)
130a -> 135a : 0.180061 (c= -0.42433642)
131a -> 135a : 0.044725 (c= -0.21148200)
132a -> 135a : 0.309030 (c= -0.55590424) **HOMO-2 → LUMO**
132a -> 136a : 0.049066 (c= 0.22150867)
133a -> 135a : 0.013261 (c= 0.11515741)
134a -> 136a : 0.343273 (c= -0.58589480) **HOMO → LUMO+1**

STATE 5: E= 0.149215 au 4.060 eV 32748.8 cm**-1 (305.4 nm)
125a -> 135a : 0.012680 (c= -0.11260712)
130a -> 135a : 0.023448 (c= 0.15312873)
131a -> 135a : 0.809839 (c= 0.89991074) **HOMO-3 → LUMO**
132a -> 135a : 0.052021 (c= -0.22808108)
133a -> 135a : 0.012492 (c= 0.11176780)
134a -> 136a : 0.018893 (c= -0.13745313)

STATE 6: E= 0.153049 au 4.165 eV 33590.3 cm**-1 (297.7 nm)
130a -> 135a : 0.111045 (c= 0.33323432)
132a -> 135a : 0.010254 (c= -0.10126363)
133a -> 136a : 0.691412 (c= 0.83151216) **HOMO-1 → LUMO+1**
134a -> 136a : 0.015371 (c= -0.12397926)
134a -> 137a : 0.081260 (c= -0.28506145)
134a -> 139a : 0.013110 (c= -0.11449807)

STATE 7: E= 0.160684 au 4.372 eV 35266.1 cm**-1 (283.6 nm)
128a -> 135a : 0.013727 (c= -0.11716238)
128a -> 136a : 0.012593 (c= 0.11221956)
129a -> 135a : 0.125876 (c= -0.35479000)
132a -> 135a : 0.033208 (c= -0.18223146)
132a -> 136a : 0.704431 (c= -0.83930361) **HOMO-2 → LUMO+1**
133a -> 137a : 0.012783 (c= 0.11306367)
134a -> 137a : 0.014880 (c= 0.12198534)

STATE 8: E= 0.160247 au 4.361 eV 35170.2 cm**-1 (284.3 nm)
129a -> 135a : 0.086636 (c= -0.29434035)
130a -> 135a : 0.486336 (c= 0.69737830) **HOMO-4 → LUMO**
130a -> 136a : 0.017407 (c= 0.13193414)
131a -> 135a : 0.049636 (c= -0.22279190)
131a -> 136a : 0.123203 (c= 0.35100299)
132a -> 136a : 0.012096 (c= 0.10997994)
133a -> 136a : 0.036557 (c= -0.19119899)
133a -> 137a : 0.011026 (c= 0.10500712)
134a -> 135a : 0.011936 (c= -0.10925373)

```
   134a -> 136a  :     0.047196 (c= -0.21724747)
   134a -> 137a  :     0.041473 (c=  0.20364959)

STATE  9:  E=   0.165948 au      4.516 eV    36421.3 cm**-1 (274.6 nm)
   129a -> 135a  :     0.244513 (c=  0.49448226)              HOMO-5 → LUMO
   130a -> 136a  :     0.028746 (c=  0.16954772)
   131a -> 137a  :     0.014701 (c= -0.12124577)
   133a -> 137a  :     0.369500 (c=  0.60786551)              HOMO-1 → LUMO+2
   133a -> 138a  :     0.065949 (c=  0.25680610)
   134a -> 137a  :     0.199645 (c=  0.44681654)
   134a -> 138a  :     0.011087 (c=  0.10529325)

STATE 10:  E=   0.167926 au      4.570 eV    36855.6 cm**-1 (271.3 nm)
   129a -> 135a  :     0.249846 (c=  0.49984647)              HOMO-5 → LUMO
   131a -> 135a  :     0.010008 (c= -0.10004216)
   131a -> 136a  :     0.123232 (c=  0.35104461)
   132a -> 136a  :     0.081343 (c= -0.28520747)
   132a -> 137a  :     0.067098 (c=  0.25903240)
   133a -> 135a  :     0.010105 (c=  0.10052172)
   133a -> 136a  :     0.058831 (c= -0.24255128)
   134a -> 137a  :     0.292155 (c= -0.54051345)              HOMO → LUMO+2
```

$Si_2Ge_4\{N(SiH_3)CH_3\}_4$

The HOMO → LUMO transition at 425.3 nm (State 1) is very weak. The second intense absorption at 372.3 nm (State 2) is related to the HOMO−1 → LUMO transition (Figure S45). The other more stronger absorptions at 289.4 nm (State 7) is mainly related to the HOMO−5 → LUMO transition.

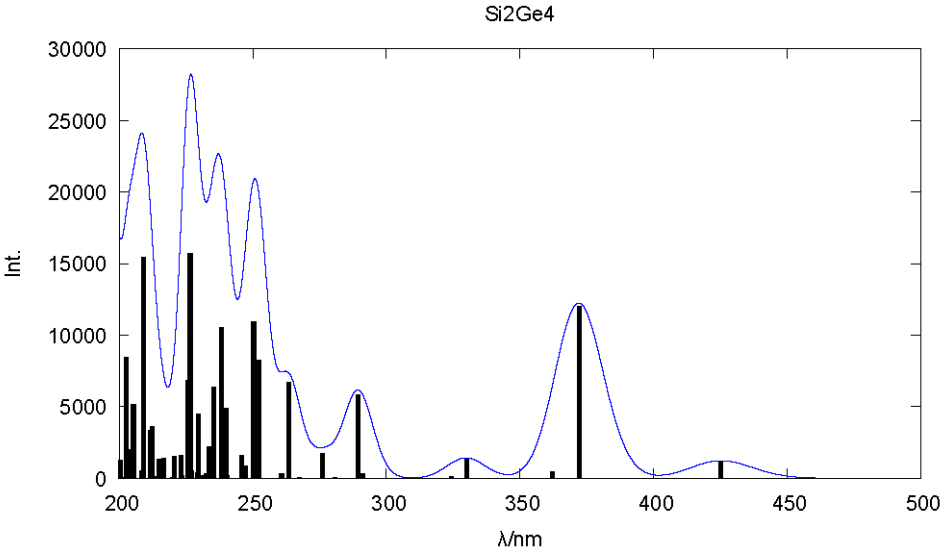


Figure S45. Calculated UV-Vis spectrum of $Si_2Ge_4\{N(SiH_3)CH_3\}_4$.

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	23511.1	425.3	0.008531948	0.11947	0.00180	-0.34503	-0.02040
2	26863.5	372.3	0.083086144	1.01822	0.01174	-0.88935	0.47658
3	27616.5	362.1	0.003053117	0.03640	-0.19022	-0.01123	0.00936
4	30282.6	330.2	0.009197181	0.09999	-0.00179	0.26965	-0.16514
5	30835.7	324.3	0.000957539	0.01022	-0.10109	0.00217	-0.00036
6	34350.3	291.1	0.002187902	0.02097	0.02976	0.12817	-0.06046
7	34551.8	289.4	0.040094606	0.38202	-0.01488	0.56218	-0.25642
8	35609.8	280.8	0.000424208	0.00392	-0.06254	-0.00061	0.00326
9	36202.0	276.2	0.012045589	0.10954	0.00275	0.20357	0.26094
10	37365.3	267.6	0.000225020	0.00198	0.04425	0.00249	0.00431
11	37939.8	263.6	0.046323878	0.40196	-0.00839	-0.13948	-0.61842
12	38342.5	260.8	0.002348537	0.02016	0.14081	0.01385	0.01205
13	39650.5	252.2	0.057236436	0.47523	-0.01026	0.67672	0.13101
14	39648.5	252.2	0.005397553	0.04482	-0.21161	-0.00255	-0.00563
15	39943.0	250.4	0.075530114	0.62252	0.00720	0.73601	-0.28419
16	40665.7	245.9	0.011031715	0.08931	-0.29779	0.02510	0.00123
17	40437.8	247.3	0.006122322	0.04984	0.00979	-0.10736	0.19550
18	41284.1	242.2	0.000044823	0.00036	0.01609	0.00744	-0.00657
19	41666.0	240.0	0.034038610	0.26895	0.00541	-0.48049	0.19504
20	41962.8	238.3	0.072663185	0.57007	-0.01069	0.72030	0.22611
21	41601.1	240.4	0.001293521	0.01024	-0.09566	-0.03161	-0.00934
22	42453.1	235.6	0.044103525	0.34201	-0.58462	-0.01246	0.00883
23	42688.2	234.3	0.008584714	0.06621	-0.02321	0.14268	0.21286
24	42818.1	233.5	0.015207346	0.11692	-0.34166	-0.01007	-0.00959
25	43017.0	232.5	0.002419855	0.01852	0.01030	-0.00722	0.13550
26	43205.5	231.5	0.001493478	0.01138	0.10648	0.00549	-0.00357
27	43545.1	229.6	0.031117345	0.23526	-0.00195	-0.48469	0.01801
28	43628.5	229.2	0.002680101	0.02022	-0.13998	0.02307	0.00991
29	43998.6	227.3	0.003386231	0.02534	0.15665	0.02500	-0.01307
30	44125.1	226.6	0.108765352	0.81149	-0.02087	0.74111	-0.51166
31	44279.0	225.8	0.047369043	0.35219	0.01267	-0.35685	0.47401
32	44732.0	223.6	0.001159701	0.00853	0.00179	-0.03894	0.08376
33	44799.8	223.2	0.010872647	0.07990	-0.28217	-0.01162	0.01196
34	45324.5	220.6	0.010773799	0.07825	-0.27960	0.00876	0.00182
35	45472.5	219.9	0.000603283	0.00437	0.02876	0.05023	-0.03189
36	46137.1	216.7	0.009836034	0.07019	-0.08252	0.23918	-0.07855
37	46182.9	216.5	0.007373545	0.05256	-0.11208	-0.19179	0.05672

38	46549.6	214.8	0.009228285	0.06526	-0.00059	0.20499	0.15246
39	46677.9	214.2	0.000825463	0.00582	-0.07568	-0.00757	0.00604
40	47056.1	212.5	0.024973213	0.17472	0.00264	-0.29489	0.29623
41	47136.6	212.1	0.000070390	0.00049	0.02208	0.00196	-0.00038
42	47270.1	211.6	0.022986933	0.16009	0.39997	0.00184	-0.01059
43	47849.5	209.0	0.106858272	0.73520	0.01552	-0.65510	0.55300
44	47935.3	208.6	0.003565512	0.02449	-0.15204	0.02659	-0.02577
45	48664.6	205.5	0.013123514	0.08878	-0.14536	0.23947	-0.10150
46	48691.7	205.4	0.035696597	0.24135	0.48029	0.09080	-0.04924
47	48921.6	204.4	0.005958773	0.04010	0.01206	0.19945	0.01308
48	49190.0	203.3	0.013941919	0.09331	0.00498	-0.18801	0.24070
49	49656.0	201.4	0.000423710	0.00281	-0.05291	-0.00294	0.00113
50	49365.5	202.6	0.058329723	0.38899	0.00140	0.57877	-0.23240
51	49883.1	200.5	0.008770548	0.05788	0.24008	-0.01469	0.00527
52	50779.1	196.9	0.082182737	0.53281	0.00996	0.12612	0.71889
53	50680.6	197.3	0.001111360	0.00722	0.01203	-0.02142	-0.08134
54	50884.6	196.5	0.046665910	0.30192	0.00173	0.48350	0.26104
55	52043.8	192.1	0.370175183	2.34161	0.04407	1.45059	-0.48525
56	52112.0	191.9	0.052843196	0.33383	-0.56026	0.13454	-0.04290
57	52648.0	189.9	0.187349595	1.17151	-0.00706	-1.05042	0.26092
58	53127.0	188.2	0.017660548	0.10944	0.32954	-0.02870	0.00375
59	53101.6	188.3	0.036547555	0.22658	0.13560	-0.40295	0.21406
60	53182.3	188.0	0.028925231	0.17905	-0.11367	-0.34720	0.21352
61	54435.8	183.7	0.161910173	0.97919	0.00542	0.85963	-0.49009
62	54760.8	182.6	0.008734326	0.05251	0.01172	-0.17755	-0.14439
63	54946.5	182.0	0.026562816	0.15915	-0.39872	0.01070	-0.00763
64	55468.1	180.3	0.010270391	0.06096	0.24566	-0.02028	-0.01395
65	55598.7	179.9	0.065255889	0.38639	0.01042	0.52241	0.33672
66	56315.0	177.6	0.014327787	0.08376	0.00599	0.20128	0.20787
67	56696.0	176.4	0.001263729	0.00734	-0.08537	0.00206	-0.00673
68	56565.6	176.8	0.026538832	0.15446	-0.39274	-0.00425	0.01401
69	57054.1	175.3	0.003427885	0.01978	0.14006	-0.01068	0.00703
70	57152.5	175.0	0.029352016	0.16907	0.00855	-0.33664	0.23596
71	57124.1	175.1	0.011658418	0.06719	0.02131	-0.25296	-0.05238
72	57821.6	172.9	0.010232654	0.05826	0.24038	0.02162	-0.00291
73	57929.0	172.6	0.043272208	0.24592	0.49548	0.00062	0.02042
74	57901.8	172.7	0.151076077	0.85897	-0.00119	-0.08521	0.92288
75	57995.7	172.4	0.218853875	1.24232	0.00715	1.01342	0.46395
76	58104.3	172.1	0.000453515	0.00257	0.03294	-0.00575	-0.03809
77	58404.9	171.2	0.025995050	0.14653	0.38256	-0.00505	-0.01234
78	58413.8	171.2	0.011700083	0.06594	-0.00366	-0.22728	-0.11946
79	59205.5	168.9	0.318076466	1.76866	0.01408	-1.09890	0.74893
80	59009.7	169.5	0.116018825	0.64726	-0.80439	-0.01275	0.00720
81	59293.0	168.7	0.052172984	0.28968	0.10610	-0.34174	0.40204
82	59284.2	168.7	0.055024427	0.30556	-0.54942	-0.02809	0.05388
83	59789.5	167.3	0.078954024	0.43474	0.65921	0.00498	-0.01240
84	59297.9	168.6	0.092355913	0.51274	0.02477	0.68094	-0.22011
85	60127.4	166.3	0.008167762	0.04472	0.21092	0.00081	0.01528
86	60299.4	165.8	0.023399925	0.12775	0.21346	0.08530	0.27370
87	60373.5	165.6	0.025031913	0.13650	0.29050	-0.08339	-0.21249
88	61017.0	163.9	0.272439095	1.46992	0.02860	0.79951	0.91098
89	60964.5	164.0	0.146584014	0.79156	0.00027	-0.49331	0.74041
90	61177.1	163.5	0.001631343	0.00878	0.02033	0.04955	0.07688
91	61314.8	163.1	0.024138959	0.12961	0.34376	0.01884	-0.10526
92	60462.3	165.4	0.020671644	0.11256	0.07106	-0.01344	0.32761
93	61292.6	163.2	0.092785321	0.49836	-0.00356	0.69620	0.11686
94	61402.5	162.9	0.007139781	0.03828	0.06073	0.15374	0.10467
95	60564.6	165.1	0.077391314	0.42068	-0.01090	-0.48937	0.42553
96	61546.0	162.5	0.171502002	0.91737	-0.95634	0.05185	0.01006
97	61924.4	161.5	0.073652192	0.39156	-0.04342	0.48731	-0.39013
98	61461.7	162.7	0.032726182	0.17529	0.41852	0.01045	-0.00508
99	61748.4	161.9	0.028347308	0.15113	0.14892	-0.17700	-0.31246
100	62383.8	160.3	0.095712902	0.50510	-0.70712	-0.06912	-0.01754
101	62760.6	159.3	0.021095981	0.11066	0.00426	-0.09666	0.31827
102	62248.5	160.6	0.009038432	0.04780	0.00865	0.04281	0.21423
103	62963.4	158.8	0.114131298	0.59675	-0.77188	0.01762	0.02536
104	63179.0	158.3	0.063517591	0.33098	0.57390	-0.03918	-0.00899
105	62075.6	161.1	0.026133847	0.13860	0.10423	0.14490	0.32671
106	63094.3	158.5	0.033649003	0.17557	0.02732	0.36885	-0.19691
107	63492.9	157.5	0.031398580	0.16280	-0.02007	0.19296	-0.35379
108	60012.0	166.6	0.004893826	0.02685	0.10252	0.01869	-0.12644
109	59813.5	167.2	0.003174203	0.01747	-0.07513	-0.00436	-0.10866
110	63730.5	156.9	0.116569191	0.60216	0.77583	-0.00895	-0.01290
111	63606.5	157.2	0.029107048	0.15065	-0.09587	-0.27976	-0.25139
112	63831.4	156.7	0.039502821	0.20374	0.44890	-0.03885	-0.02670
113	63600.6	157.2	0.015660106	0.08106	0.02656	-0.05288	-0.27849
114	63652.5	157.1	0.075310246	0.38951	-0.62403	0.00319	0.00915
115	64447.6	155.2	0.009347633	0.04775	0.21828	-0.00980	0.00284
116	64204.1	155.8	0.045885215	0.23528	0.01771	0.28525	-0.39192
117	64671.3	154.6	0.020889525	0.10634	0.04057	0.06630	-0.31670
118	64420.9	155.2	0.051459485	0.26297	-0.51139	0.03114	-0.02197
119	64870.2	154.2	0.042479617	0.21558	0.46380	-0.01801	0.01214
120	65081.8	153.7	0.158721022	0.80288	-0.01781	0.84283	-0.30366
121	64770.5	154.4	0.017805441	0.09050	-0.26670	-0.13272	0.04192
122	64708.6	154.5	0.057708555	0.29360	-0.54181	0.00601	0.00152
123	65307.5	153.1	0.029978869	0.15112	0.03999	-0.38468	0.03934

124	65125.6	153.5	0.003843985	0.01943	0.09723	0.04328	-0.09003
125	65311.5	153.1	0.005069636	0.02555	-0.02110	0.03308	-0.15497
126	64308.0	155.5	0.010545418	0.05399	0.23196	-0.00339	0.01289
127	65391.8	152.9	0.007951920	0.04003	0.20008	-0.00150	-0.00066
128	65531.4	152.6	0.014316404	0.07192	-0.26780	-0.01039	0.00997
129	65546.1	152.6	0.022817218	0.11460	-0.33840	-0.00547	0.00749
130	66070.2	151.4	0.086514922	0.43108	-0.00904	0.40576	-0.51610
131	66233.4	151.0	0.172366584	0.85674	0.01935	-0.82525	0.41874
132	65792.7	152.0	0.022375649	0.11196	0.33431	0.01124	-0.00861
133	66160.4	151.1	0.058774990	0.29246	0.54067	-0.00521	-0.01059
134	66425.1	150.5	0.000971654	0.00482	-0.06891	-0.00373	0.00731
135	66279.0	150.9	0.085333223	0.42386	-0.01439	0.37722	-0.53043
136	65845.2	151.9	0.003666831	0.01833	-0.13127	0.00403	-0.03294
137	65523.5	152.6	0.011913484	0.05986	-0.01724	0.00816	0.24391
138	66792.7	149.7	0.000250451	0.00123	0.01717	0.01237	-0.02805
139	66989.8	149.3	0.058030841	0.28518	0.53360	-0.01515	0.01497
140	67317.6	148.5	0.176796651	0.86461	-0.00887	0.31683	-0.87416

STATE 1: E= 0.107124 au 2.915 eV 23511.1 cm**-1 (425.3 nm)
142a -> 144a : 0.135745 (c= 0.36843524)
143a -> 144a : 0.828242 (c= 0.91007819) **HOMO → LUMO**

STATE 2: E= 0.122399 au 3.331 eV 26863.5 cm**-1 (372.3 nm)
138a -> 144a : 0.031265 (c= -0.17681858)
140a -> 144a : 0.014743 (c= -0.12142052)
141a -> 145a : 0.014862 (c= -0.12191103)
141a -> 147a : 0.010651 (c= -0.10320446)
142a -> 144a : 0.752713 (c= -0.86759061) **HOMO-1 → LUMO**
143a -> 144a : 0.110063 (c= 0.33175707)
143a -> 149a : 0.013224 (c= -0.11499372)

STATE 3: E= 0.125830 au 3.424 eV 27616.5 cm**-1 (362.1 nm)
135a -> 144a : 0.015254 (c= -0.12350845)
139a -> 144a : 0.020531 (c= 0.14328718)
141a -> 144a : 0.924946 (c= 0.96174091) **HOMO-2 → LUMO**

STATE 4: E= 0.137978 au 3.755 eV 30282.6 cm**-1 (330.2 nm)
134a -> 144a : 0.015912 (c= -0.12614142)
140a -> 144a : 0.930437 (c= -0.96459167) **HOMO-3 → LUMO**
143a -> 146a : 0.013650 (c= -0.11683277)

STATE 5: E= 0.140498 au 3.823 eV 30835.7 cm**-1 (324.3 nm)
139a -> 144a : 0.855613 (c= -0.92499326) **HOMO-4 → LUMO**
141a -> 144a : 0.027067 (c= 0.16452165)
143a -> 145a : 0.087887 (c= -0.29645783)

STATE 6: E= 0.156512 au 4.259 eV 34350.3 cm**-1 (291.1 nm)
138a -> 144a : 0.045788 (c= -0.21398211)
139a -> 144a : 0.092209 (c= 0.30365940)
142a -> 145a : 0.105477 (c= -0.32477210)
143a -> 145a : 0.690373 (c= -0.83088717) **HOMO → LUMO+1**

STATE 7: E= 0.157430 au 4.284 eV 34551.8 cm**-1 (289.4 nm)
136a -> 144a : 0.014443 (c= 0.12017844)
138a -> 144a : 0.702349 (c= -0.83806254) **HOMO-5 → LUMO**
141a -> 145a : 0.134467 (c= 0.36669759)
143a -> 145a : 0.043211 (c= 0.20787231)
143a -> 146a : 0.030438 (c= -0.17446473)

STATE 8: E= 0.162250 au 4.415 eV 35609.8 cm**-1 (280.8 nm)
140a -> 145a : 0.014727 (c= -0.12135359)
142a -> 145a : 0.704701 (c= -0.83946449) **HOMO-1 → LUMO+1**
143a -> 145a : 0.089745 (c= 0.29957534)
143a -> 147a : 0.111598 (c= 0.33406233)

STATE 9: E= 0.164948 au 4.488 eV 36202.0 cm**-1 (276.2 nm)
140a -> 146a : 0.020646 (c= 0.14368767)
141a -> 145a : 0.041925 (c= 0.20475717)
142a -> 146a : 0.376144 (c= 0.61330569) **HOMO-1 → LUMO+2**
142a -> 149a : 0.011602 (c= 0.10771110)
143a -> 146a : 0.500311 (c= 0.70732672) **HOMO → LUMO+2**

STATE 10: E= 0.170249 au 4.633 eV 37365.3 cm**-1 (267.6 nm)
142a -> 145a : 0.045981 (c= -0.21443147)
142a -> 147a : 0.060131 (c= 0.24521557)
142a -> 148a : 0.055929 (c= -0.23649304)
143a -> 145a : 0.047162 (c= 0.21716784)
143a -> 147a : 0.463631 (c= -0.68090436) **HOMO → LUMO+3**
143a -> 148a : 0.258898 (c= 0.50882058) **HOMO → LUMO+4**

8.2 TDDFT calculation for $Si_6\{N(SiH_3)CH_3\}_4$ and $Ge_6\{N(SiH_3)CH_3\}_4$

General procedure

We have performed a TDDFT calculation with ORCA on the optimized structures of $Si_6\{N(SiH_3)CH_3\}_4$ and $Ge_6\{N(SiH_3)CH_3\}_4$ using the CAM-B3LYP functional, a double zeta basis set (def2-SVP) and the CPCM implicit solvent model for hexane solving for 140 excited states.

$Si_6\{N(SiH_3)CH_3\}_4$

The HOMO → LUMO transition at 371.6 nm (State 1) is very weak (Figure S46).

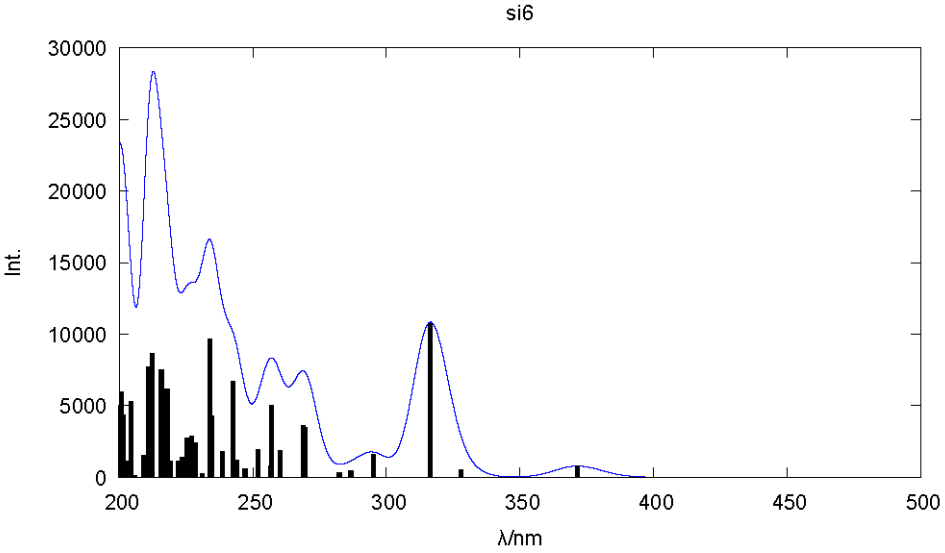


Figure S46. Calculated UV-Vis spectrum of $Si_6\{N(SiH_3)CH_3\}_4$.

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	26907.7	371.6	0.005447872	0.06665	0.14006	-0.20815	-0.06094
2	30494.7	327.9	0.003810617	0.04114	-0.08378	0.01863	-0.18377
3	31598.8	316.5	0.074052135	0.77151	0.63537	-0.60644	0.00681
4	33862.7	295.3	0.011067183	0.10759	-0.15829	0.25019	0.14121
5	34869.5	286.8	0.003117998	0.02944	0.11347	0.12650	0.02367
6	35406.2	282.4	0.002249189	0.02091	0.11435	-0.07444	0.04791
7	37067.6	269.8	0.024280798	0.21565	0.18783	-0.25905	-0.33654
8	37182.6	268.9	0.024798102	0.21956	0.20025	-0.42077	0.04913
9	38431.3	260.2	0.012785502	0.10952	-0.06848	-0.32355	0.01213
10	38928.5	256.9	0.005417557	0.04582	0.02898	0.07683	0.19767
11	38925.5	256.9	0.034790241	0.29424	-0.09458	-0.52727	-0.08535
12	39669.3	252.1	0.013214157	0.10966	0.01777	0.32364	-0.06784
13	40470.2	247.1	0.004143902	0.03371	-0.08963	0.05873	-0.14908
14	40976.2	244.0	0.008154400	0.06551	-0.21491	0.12895	-0.05199
15	41201.5	242.7	0.046255307	0.36959	0.02090	-0.55608	0.24482
16	41895.9	238.7	0.012607541	0.09907	-0.08987	0.28971	0.08403
17	42608.2	234.7	0.029888466	0.23093	0.29116	0.30422	0.23154
18	42764.0	233.8	0.066806220	0.51430	0.50682	-0.47893	-0.16751
19	43275.6	231.1	0.001794351	0.01365	-0.02549	-0.05028	-0.10233
20	43747.5	228.6	0.016692392	0.12561	0.03682	0.31169	-0.16464
21	44002.0	227.3	0.020130203	0.15061	-0.22974	0.29990	-0.08884
22	44196.2	226.3	0.016305329	0.12146	-0.07173	-0.09333	-0.32803
23	44355.3	225.5	0.019006438	0.14107	0.31929	0.10953	-0.16470
24	44698.1	223.7	0.009559994	0.07041	0.14192	-0.22126	-0.03628
25	44938.7	222.5	0.006747575	0.04943	0.11650	-0.00640	-0.18926
26	45029.2	222.1	0.007699532	0.05629	0.06652	-0.16483	0.15716
27	45025.2	222.1	0.007433550	0.05435	0.07580	-0.11135	0.19028

28	45597.5	219.3	0.007843098	0.05663	-0.20126	-0.10255	-0.07488
29	45881.4	218.0	0.042744198	0.30670	-0.52238	0.18375	-0.00768
30	46012.2	217.3	0.018267584	0.13070	0.24932	0.08339	0.24817
31	46340.2	215.8	0.051734807	0.36754	-0.26270	0.54168	0.07147
32	47118.3	212.2	0.059874089	0.41834	-0.07949	0.63525	0.09202
33	47180.1	212.0	0.029710823	0.20732	-0.04294	-0.29439	0.34468
34	47150.8	212.1	0.014225062	0.09932	-0.29755	0.08239	-0.06323
35	47401.7	211.0	0.053408644	0.37093	0.33583	-0.49355	-0.12064
36	47821.5	209.1	0.010566786	0.07274	0.15482	-0.18345	0.12298
37	48559.4	205.9	0.000845227	0.00573	0.01099	0.05458	-0.05129
38	48880.0	204.6	0.036635172	0.24674	-0.16065	0.42155	0.20791
39	49086.6	203.7	0.000388313	0.00260	-0.04786	-0.01751	0.00272
40	49276.1	202.9	0.008014843	0.05355	0.19469	-0.12421	0.01467
41	49016.4	204.0	0.003384247	0.02273	-0.08120	0.12596	0.01645
42	49647.0	201.4	0.029934783	0.19850	0.07288	-0.43511	0.06217
43	49763.2	201.0	0.041405231	0.27392	0.25879	-0.41795	-0.17964
44	49893.8	200.4	0.034629883	0.22850	0.31829	-0.35629	0.01560
45	50428.8	198.3	0.012428404	0.08114	-0.26355	0.10013	-0.04062
46	50334.0	198.7	0.024151949	0.15797	0.15993	0.36259	-0.03036
47	50730.9	197.1	0.007129529	0.04627	-0.10703	0.17504	0.06459
48	51033.4	195.9	0.030918010	0.19945	0.33824	-0.13531	-0.25833
49	51462.0	194.3	0.067191233	0.42984	-0.54570	0.27030	0.24285
50	51642.3	193.6	0.041769474	0.26627	-0.00301	0.20069	-0.47538
51	52071.3	192.0	0.023995836	0.15171	0.29546	0.20803	-0.14537
52	52634.9	190.0	0.032678660	0.20439	-0.18719	0.40791	0.05441
53	52774.8	189.5	0.041348464	0.25793	0.27003	0.25567	0.34591
54	53345.4	187.5	0.022572262	0.13930	-0.32404	0.18341	0.02563
55	53898.5	185.5	0.075598578	0.46176	-0.55943	0.35100	-0.15998
56	53941.2	185.4	0.097475871	0.59491	0.45883	-0.61077	0.10651
57	53749.1	186.0	0.033803940	0.20705	-0.43665	0.07398	0.10445
58	54218.4	184.4	0.008822523	0.05357	0.03511	0.13111	-0.18748
59	55184.9	181.2	0.153888864	0.91804	-0.63651	0.62615	-0.34761
60	55760.4	179.3	0.251972235	1.48766	0.74369	-0.93864	-0.23136
61	55916.9	178.8	0.020063053	0.11812	-0.05034	-0.32060	0.11314
62	56390.6	177.3	0.032025343	0.18697	0.16459	0.09894	0.38741
63	56791.8	176.1	0.027147456	0.15737	-0.28154	-0.16441	-0.22599
64	56684.9	176.4	0.017330179	0.10065	-0.23215	0.18454	0.11270
65	57184.8	174.9	0.009668077	0.05566	-0.13254	0.17026	-0.09542
66	57512.1	173.9	0.039709736	0.22731	0.14129	0.44974	0.07129
67	57256.4	174.7	0.022693064	0.13048	-0.09004	-0.34907	0.02284
68	58104.8	172.1	0.000638109	0.00362	-0.00581	-0.04373	0.04085
69	58462.8	171.0	0.070791096	0.39863	-0.13662	-0.61640	0.00479
70	58855.6	169.9	0.014217947	0.07953	0.14083	0.21678	0.11271
71	58973.4	169.6	0.022603599	0.12618	-0.14611	-0.18820	-0.26347
72	59022.0	169.4	0.023586759	0.13156	-0.21500	0.25518	-0.14219
73	58809.9	170.0	0.115948186	0.64907	0.21064	0.69393	-0.35093
74	59227.1	168.8	0.129461908	0.71961	0.80398	-0.26284	0.06440
75	59948.5	166.8	0.071749434	0.39402	-0.26401	0.15223	-0.54877
76	59840.0	167.1	0.103426109	0.56900	0.68173	-0.28785	-0.14627
77	60160.9	166.2	0.196948097	1.07774	-0.46406	0.39339	0.84121
78	60250.2	166.0	0.002383946	0.01303	0.03129	0.09599	0.05323
79	60724.8	164.7	0.234987834	1.27396	0.05845	0.07209	1.12487
80	60932.6	164.1	0.117212497	0.63329	-0.55935	-0.35754	0.43884
81	61076.3	163.7	0.013839167	0.07460	-0.06214	0.13253	-0.23059
82	61198.5	163.4	0.005660125	0.03045	-0.03164	-0.07739	0.15316
83	60681.0	164.8	0.008608545	0.04670	-0.08367	-0.15340	0.12717
84	60680.7	164.8	0.101376338	0.55000	0.46893	0.33190	0.46898
85	61481.7	162.6	0.050007529	0.26777	-0.49473	-0.06623	0.13648
86	62025.4	161.2	0.048116548	0.25539	0.02816	-0.03420	-0.50341
87	62077.8	161.1	0.047245941	0.25056	0.03671	-0.41699	0.27445
88	61888.4	161.6	0.003858112	0.02052	0.13664	-0.00823	-0.04224
89	62473.6	160.1	0.055838750	0.29425	0.30289	0.19004	-0.40791
90	62387.8	160.3	0.003317971	0.01751	-0.07316	0.02767	-0.10672
91	62375.7	160.3	0.121705229	0.64235	0.74765	-0.28027	-0.06943
92	63029.9	158.7	0.064250972	0.33559	0.04936	0.45988	0.34880
93	62888.8	159.0	0.054456818	0.28507	-0.10299	0.01297	-0.52373
94	63160.3	158.3	0.032000633	0.16680	0.06673	0.13348	0.38017
95	63254.6	158.1	0.052007195	0.27067	0.02475	0.40220	-0.32909
96	63569.3	157.3	0.076535452	0.39636	0.29786	-0.24512	-0.49755
97	63131.5	158.4	0.085151207	0.44404	0.17901	0.22707	0.60036
98	63455.9	157.6	0.019015360	0.09865	0.05855	-0.30440	-0.05068
99	63446.6	157.6	0.017041306	0.08842	0.14184	-0.25382	-0.06230
100	64042.5	156.1	0.053930078	0.27723	0.15590	-0.41505	-0.28400
101	64183.9	155.8	0.041511148	0.21292	-0.29738	-0.14095	0.32344
102	63023.1	158.7	0.018548266	0.09689	0.17173	-0.15923	0.20505
103	63468.7	157.6	0.018849336	0.09777	-0.21018	0.10021	-0.20870
104	63785.6	156.8	0.075100367	0.38761	-0.18267	0.59346	-0.04531
105	64269.9	155.6	0.019646755	0.10064	-0.25266	0.17796	-0.07160
106	64860.3	154.2	0.065637861	0.33316	-0.24663	0.44957	0.26498
107	64535.2	155.0	0.125753451	0.64150	0.48887	-0.32030	0.54764
108	65108.4	153.6	0.079118670	0.40005	0.25414	0.08724	-0.57259
109	64421.8	155.2	0.012690191	0.06485	-0.08863	0.09693	0.21817
110	64660.6	154.7	0.042935490	0.21860	0.43482	0.08191	0.15108
111	65352.1	153.0	0.055026428	0.27720	0.03572	0.52203	-0.05833
112	65196.5	153.4	0.038234690	0.19307	-0.36048	0.19469	0.15879
113	65841.4	151.9	0.009482051	0.04741	0.10444	0.15571	0.11072

114	65403.1	152.9	0.081654315	0.41101	-0.43825	-0.24049	-0.40139
115	65723.3	152.2	0.107798830	0.53997	-0.24589	0.65867	-0.21369
116	64962.9	153.9	0.022473731	0.11389	0.02544	0.24339	0.23239
117	66142.5	151.2	0.017325041	0.08623	-0.27320	0.00412	-0.10761
118	66079.1	151.3	0.010676681	0.05319	-0.22319	-0.02645	0.05177
119	65954.3	151.6	0.037254604	0.18596	0.37368	-0.15061	-0.15374
120	66068.7	151.4	0.016777965	0.08360	-0.19966	0.05376	0.20210
121	66218.7	151.0	0.003818081	0.01898	-0.09865	0.09275	0.02545
122	66618.6	150.1	0.090269152	0.44609	-0.17590	0.61402	0.19527
123	66450.3	150.5	0.013508036	0.06692	-0.20479	-0.05470	-0.14829
124	66588.6	150.2	0.025225299	0.12471	-0.02411	0.33619	0.10539
125	66673.7	150.0	0.012768090	0.06304	0.12150	-0.21753	0.03106
126	66897.1	149.5	0.018349494	0.09030	-0.02635	0.24614	0.17036
127	67196.1	148.8	0.054860724	0.26878	-0.39257	0.24080	0.23808
128	67323.9	148.5	0.191993811	0.93884	-0.48552	0.83171	0.10661
129	66789.5	149.7	0.088731141	0.43736	-0.60330	0.26961	0.02642
130	67174.8	148.9	0.002406527	0.01179	-0.06801	0.07260	0.04357
131	67188.8	148.8	0.030182566	0.14789	0.24265	0.24580	0.16910
132	67330.5	148.5	0.086766510	0.42424	-0.54279	0.15655	0.32422
133	67074.1	149.1	0.009419930	0.04623	-0.11808	-0.07170	-0.16478
134	67603.9	147.9	0.019840187	0.09662	0.15687	-0.26817	0.00948
135	67589.4	148.0	0.042988846	0.20939	-0.34813	0.23713	0.17878
136	63968.9	156.3	0.014790179	0.07612	-0.14156	0.01921	-0.23603
137	66977.8	149.3	0.034288051	0.16853	-0.00931	-0.15931	0.37824
138	68227.3	146.6	0.007980439	0.03851	0.18283	0.06464	0.03004
139	67883.5	147.3	0.030532187	0.14807	0.05633	-0.13986	0.35403
140	68441.2	146.1	0.008941444	0.04301	0.01783	-0.13156	0.15932

STATE 1: E= 0.122600 au 3.336 eV 26907.7 cm**-1 (371.6 nm)
106a -> 108a : 0.045875 (c= 0.21418410)
107a -> 108a : 0.915884 (c= 0.95701848) **HOMO → LUMO**

STATE 2: E= 0.138944 au 3.781 eV 30494.7 cm**-1 (327.9 nm)
105a -> 108a : 0.919024 (c= -0.95865743) **HOMO−2 → LUMO**
106a -> 108a : 0.034858 (c= 0.18670239)
107a -> 109a : 0.010404 (c= 0.10199965)

STATE 3: E= 0.143975 au 3.918 eV 31598.8 cm**-1 (316.5 nm)
104a -> 108a : 0.022106 (c= -0.14867958)
105a -> 108a : 0.026788 (c= -0.16367101)
106a -> 108a : 0.779541 (c= -0.88291594) **HOMO−1 → LUMO**
107a -> 108a : 0.033939 (c= 0.18422416)
107a -> 109a : 0.024762 (c= 0.15736054)
107a -> 112a : 0.011753 (c= -0.10840914)

STATE 4: E= 0.154290 au 4.198 eV 33862.7 cm**-1 (295.3 nm)
99a -> 108a : 0.022423 (c= -0.14974468)
102a -> 108a : 0.110996 (c= -0.33316055)
104a -> 108a : 0.789544 (c= -0.88856309) **HOMO−3 → LUMO**

STATE 5: E= 0.158877 au 4.323 eV 34869.5 cm**-1 (286.8 nm)
98a -> 108a : 0.010743 (c= -0.10364800)
103a -> 108a : 0.884303 (c= -0.94037383) **HOMO−4 → LUMO**
106a -> 111a : 0.017589 (c= 0.13262310)

STATE 6: E= 0.161322 au 4.390 eV 35406.2 cm**-1 (282.4 nm)
98a -> 108a : 0.011397 (c= -0.10675482)
102a -> 108a : 0.585360 (c= -0.76508854) **HOMO−5 → LUMO**
104a -> 108a : 0.057038 (c= 0.23882564)
107a -> 109a : 0.212694 (c= 0.46118769) **HOMO → LUMO+1**
107a -> 110a : 0.063519 (c= 0.25203021)

$Ge_6\{N(SiH_3)CH_3\}_4$

The HOMO → LUMO transition at 459.5 nm (State 1) is very weak (Figure S47).

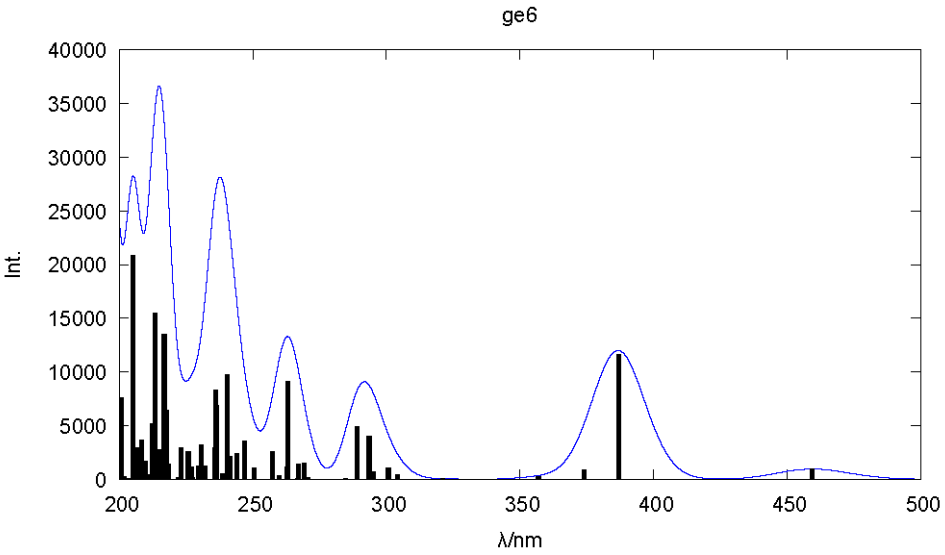


Figure S47. Calculated UV-Vis spectrum of $Ge_6\{N(SiH_3)CH_3\}_4$.

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	21762.9	459.5	0.006617624	0.10011	-0.00079	0.30306	0.09089
2	25829.5	387.2	0.080515447	1.02622	-0.00780	0.85971	-0.53578
3	26721.5	374.2	0.006244041	0.07693	-0.27730	0.00519	0.00196
4	28016.4	356.9	0.001441505	0.01694	-0.00254	-0.08999	0.09399
5	31143.1	321.1	0.000312751	0.00331	0.05671	0.00944	0.00082
6	33245.4	300.8	0.007561514	0.07488	-0.05080	0.22092	0.15327
7	32872.2	304.2	0.002802945	0.02807	0.14303	0.06751	0.05528
8	33877.8	295.2	0.004746599	0.04613	0.05522	-0.16094	-0.13106
9	34060.9	293.6	0.027956558	0.27021	-0.02662	-0.40099	-0.32971
10	34581.6	289.2	0.033735699	0.32116	0.00710	-0.49126	0.28245
11	35103.7	284.9	0.000328392	0.00308	-0.05259	-0.01517	-0.00916
12	36933.0	270.8	0.001057113	0.00942	0.09108	-0.03074	0.01348
13	37124.1	269.4	0.010538814	0.09346	-0.01422	0.04329	-0.30229
14	37430.1	267.2	0.009848195	0.08662	0.01618	0.04410	-0.29054
15	37484.8	266.8	0.000596676	0.00524	0.01867	-0.01213	0.06888
16	38013.3	263.1	0.063187452	0.54723	0.03464	0.69491	-0.25126
17	38043.0	262.9	0.007906284	0.06842	-0.15319	0.19736	-0.07746
18	38469.2	259.9	0.002582456	0.02210	-0.14821	-0.00866	-0.00775
19	38840.8	257.5	0.017733959	0.15031	0.00079	0.34987	-0.16705
20	39897.4	250.6	0.007536904	0.06219	-0.24903	0.01240	0.00464
21	40498.6	246.9	0.024979846	0.20306	0.00124	-0.44939	0.03333
22	40950.8	244.2	0.016826790	0.13527	0.36718	-0.01644	-0.01354
23	41388.1	241.6	0.014782592	0.11758	0.04788	0.28568	-0.18352
24	41437.7	241.3	0.006733051	0.05349	-0.11526	0.08185	-0.18305
25	41450.9	241.2	0.006082193	0.04831	0.04961	0.13669	-0.16481
26	41596.3	240.4	0.067167046	0.53159	0.02094	-0.72754	-0.04284
27	41876.1	238.8	0.003448824	0.02711	0.16376	0.01218	-0.01219
28	42367.7	236.0	0.057606951	0.44763	0.32473	-0.55609	0.18150
29	42320.3	236.3	0.047642430	0.37061	0.37368	0.45904	-0.14234
30	42427.6	235.7	0.020282489	0.15738	0.39654	0.00549	-0.01040
31	43046.2	232.3	0.008353521	0.06389	0.25156	0.01835	-0.01632
32	43347.5	230.7	0.022030683	0.16732	0.00592	-0.40058	0.08258
33	43561.0	229.6	0.008864801	0.06700	0.00348	0.18776	-0.17813
34	43956.5	227.5	0.001404619	0.01052	-0.01103	0.00847	0.10162
35	44029.7	227.1	0.007853244	0.05872	0.02007	0.01535	0.24100
36	44275.1	225.9	0.017732675	0.13185	0.03480	0.32880	0.15011
37	44002.1	227.3	0.003625431	0.02712	-0.12219	0.10450	0.03570
38	44777.2	223.3	0.020085362	0.14767	-0.38373	-0.00603	0.01966
39	45023.5	222.1	0.001335349	0.00976	0.00229	-0.09431	-0.02941
40	45749.0	218.6	0.010022028	0.07212	-0.25989	-0.06171	0.02776
41	45903.4	217.8	0.044360422	0.31815	0.04304	-0.47548	0.30035

42	46117.0	216.8	0.093196882	0.66530	-0.01471	-0.49771	0.64604
43	46541.1	214.9	0.019321781	0.13667	0.36628	-0.04990	-0.00464
44	46850.0	213.4	0.107246896	0.75362	0.00123	-0.86679	0.04791
45	47071.4	212.4	0.035935750	0.25133	0.49670	0.06749	0.00801
46	47480.8	210.6	0.003252943	0.02255	-0.12811	0.07237	0.03009
47	47622.4	210.0	0.011804581	0.08160	-0.00269	-0.25994	-0.11844
48	48010.4	208.3	0.025136748	0.17237	0.00084	0.37452	0.17915
49	48332.2	206.9	0.020187832	0.13751	0.36964	-0.02944	-0.00311
50	48769.0	205.0	0.144402884	0.97478	0.01828	-0.72275	0.67237
51	49205.1	203.2	0.000252948	0.00169	0.00091	0.02201	-0.03475
52	49550.5	201.8	0.001763406	0.01172	0.10283	-0.02186	0.02577
53	49787.5	200.9	0.052722580	0.34862	0.00082	-0.58518	-0.07864
54	50063.2	199.7	0.005095403	0.03351	0.00032	-0.00072	-0.18305
55	50905.8	196.4	0.098866326	0.63938	0.03373	0.64171	-0.47587
56	51076.6	195.8	0.129243558	0.83303	0.00444	-0.38958	0.82537
57	50762.0	197.0	0.039822741	0.25827	-0.17449	0.25178	-0.40549
58	51361.2	194.7	0.029483509	0.18898	-0.42350	-0.02348	0.09530
59	51473.8	194.3	0.003552852	0.02272	-0.14922	0.01932	0.00910
60	52209.6	191.5	0.052491538	0.33099	-0.02686	0.53826	0.20135
61	52355.2	191.0	0.012740372	0.08011	-0.08414	0.27008	0.00930
62	52417.7	190.8	0.262780599	1.65041	0.05185	1.28304	-0.03909
63	52659.6	189.9	0.026256475	0.16415	0.40430	0.00176	-0.02620
64	53103.1	188.3	0.152861557	0.94766	0.02344	-0.86113	0.45340
65	53473.8	187.0	0.081907125	0.50426	0.70991	-0.01124	-0.01259
66	54006.2	185.2	0.151445739	0.92319	0.01827	-0.16925	0.94563
67	54272.4	184.3	0.010346626	0.06276	-0.25051	0.00015	0.00262
68	55126.7	181.4	0.090168218	0.53848	-0.01485	-0.61394	0.40167
69	55316.5	180.8	0.023491414	0.13981	0.37215	-0.01623	0.03235
70	55573.6	179.9	0.029728684	0.17611	-0.01617	0.37234	0.19291
71	55815.3	179.2	0.034534404	0.20369	-0.45126	-0.00618	0.00425
72	55503.2	180.2	0.059362679	0.35210	0.58909	-0.05776	-0.04172
73	56049.4	178.4	0.026443462	0.15532	-0.11341	-0.36457	-0.09769
74	56563.6	176.8	0.054793074	0.31891	0.56398	-0.02809	0.00648
75	56474.9	177.1	0.034277182	0.19981	-0.43000	0.10025	-0.06974
76	56403.5	177.3	0.145856621	0.85133	-0.04406	-0.73540	0.55549
77	57015.7	175.4	0.047178342	0.27241	0.52032	0.03077	-0.02709
78	57448.0	174.1	0.008947431	0.05127	0.22639	-0.00135	-0.00435
79	57313.7	174.5	0.033796961	0.19413	-0.02299	0.40439	-0.17342
80	57699.4	173.3	0.001842809	0.01051	0.10170	-0.00701	0.01110
81	57772.6	173.1	0.041589733	0.23700	0.03192	-0.36811	-0.31697
82	57937.7	172.6	0.045425565	0.25812	-0.10055	-0.22904	-0.44221
83	58390.9	171.3	0.117575975	0.66290	0.81330	-0.02414	-0.02938
84	58851.3	169.9	0.010769501	0.06024	-0.23860	-0.05756	-0.00006
85	58612.5	170.6	0.160855425	0.90349	0.01934	0.84917	-0.42663
86	59009.8	169.5	0.030919083	0.17250	0.38731	0.01337	0.14937
87	59145.6	169.1	0.019839701	0.11043	-0.25535	-0.09986	0.18776
88	58868.4	169.9	0.151050306	0.84472	-0.04391	0.91606	-0.06031
89	59404.2	168.3	0.059217768	0.32818	-0.57189	0.00804	-0.03255
90	59786.9	167.3	0.037025976	0.20388	-0.02129	0.11513	0.43609
91	59823.4	167.2	0.308190762	1.69599	0.00115	0.20803	1.28558
92	59915.1	166.9	0.004114287	0.02261	-0.11824	-0.01260	-0.09202
93	60131.4	166.3	0.139813305	0.76546	-0.01210	-0.85930	-0.16408
94	60291.7	165.9	0.036650260	0.20012	0.03134	0.13804	0.42436
95	60412.5	165.5	0.014068994	0.07667	0.27686	0.00384	0.00042
96	60835.2	164.4	0.101113567	0.54718	-0.73891	0.03274	0.01101
97	60857.7	164.3	0.218195798	1.18034	-0.13864	-0.98002	0.44797
98	60505.0	165.3	0.090188635	0.49072	-0.67138	0.18637	-0.07239
99	61101.5	163.7	0.127632611	0.68768	0.01580	-0.06495	-0.82657
100	61376.6	162.9	0.000183457	0.00098	-0.00047	-0.02983	0.00969
101	61470.1	162.7	0.065940578	0.35315	-0.05963	-0.33791	-0.48520
102	60854.9	164.3	0.009371149	0.05070	0.00168	-0.05085	-0.21933
103	60332.8	165.7	0.150269186	0.81996	0.90306	-0.03223	-0.05840
104	61564.2	162.4	0.004229257	0.02262	-0.14121	0.05113	0.00775
105	61802.4	161.8	0.200364795	1.06731	-0.05054	0.24400	-1.00261
106	61827.4	161.7	0.015716827	0.08369	0.05394	0.07576	-0.27393
107	62244.4	160.7	0.018893674	0.09993	0.29751	-0.06314	0.08619
108	57606.9	173.6	0.004935454	0.02821	-0.05814	0.15718	-0.01093
109	57614.0	173.6	0.005527350	0.03158	-0.05833	-0.16752	0.01089
110	62485.0	160.0	0.067085992	0.35345	0.08824	-0.50338	0.30377
111	62535.0	159.9	0.032401447	0.17058	-0.39506	-0.09987	0.06728
112	62901.6	159.0	0.114016007	0.59673	-0.77218	0.00927	0.01955
113	58882.4	169.8	0.003567291	0.01994	0.14115	0.00394	-0.00237
114	62704.5	159.5	0.028403447	0.14912	-0.08490	-0.31460	-0.20722
115	63224.2	158.2	0.048793400	0.25407	0.50371	-0.00019	-0.01869
116	63582.6	157.3	0.075439435	0.39060	-0.62198	0.03730	0.04854
117	63427.7	157.7	0.024405798	0.12667	0.08750	0.33213	0.09332
118	63689.0	157.0	0.143390899	0.74120	-0.02086	0.63830	-0.57735
119	63657.2	157.1	0.014785891	0.07647	0.00228	-0.22354	0.16276
120	63249.0	158.1	0.004392924	0.02287	0.07648	0.11519	-0.06122
121	64194.1	155.8	0.068412461	0.35085	-0.59169	0.02724	0.00076
122	63780.2	156.8	0.014179157	0.07319	-0.20223	-0.08897	-0.15613
123	63838.3	156.6	0.041821081	0.21567	0.38522	-0.16266	-0.20204
124	63913.9	156.5	0.047636224	0.24537	-0.47352	-0.07059	-0.12712
125	64611.6	154.8	0.121129986	0.61719	-0.01827	0.61384	-0.48996
126	64726.2	154.5	0.230535968	1.17256	-1.08183	-0.01690	0.04374
127	64864.4	154.2	0.137075005	0.69571	-0.83404	0.00442	0.00764

128	64944.3	154.0	0.002390300	0.01212	-0.10548	-0.02786	0.01463
129	65090.7	153.6	0.010997513	0.05562	0.02867	-0.16668	0.16437
130	64756.1	154.4	0.062345477	0.31696	0.21879	-0.40184	0.32804
131	64951.8	154.0	0.116357067	0.58976	0.68257	0.21360	-0.27971
132	65124.3	153.6	0.128972023	0.65197	-0.19563	0.43576	-0.65101
133	65467.6	152.7	0.010090345	0.05074	0.21331	-0.00792	-0.07196
134	65063.9	153.7	0.031569403	0.15974	-0.07910	-0.28157	-0.27239
135	65482.3	152.7	0.053977461	0.27137	0.52078	-0.00694	-0.01064
136	65785.2	152.0	0.036952097	0.18492	0.42861	-0.02113	-0.02767
137	62387.1	160.3	0.009281442	0.04898	0.01657	0.20794	-0.07391
138	65879.5	151.8	0.048177419	0.24075	0.04469	0.48465	-0.06221
139	66043.2	151.4	0.019710163	0.09825	0.31031	0.00154	-0.04424
140	66339.1	150.7	0.286295864	1.42076	0.02737	-1.00117	0.64628

STATE 1: E= 0.099159 au 2.698 eV 21762.9 cm**-1 (459.5 nm)
160a -> 162a : 0.036528 (c= -0.19112200)
161a -> 162a : 0.924559 (c= 0.96153995) **HOMO → LUMO**

STATE 2: E= 0.117688 au 3.202 eV 25829.5 cm**-1 (387.2 nm)
156a -> 162a : 0.027011 (c= 0.16434937)
160a -> 162a : 0.843677 (c= 0.91851911) **HOMO−1 → LUMO**
161a -> 162a : 0.029603 (c= 0.17205590)

STATE 3: E= 0.121752 au 3.313 eV 26721.5 cm**-1 (374.2 nm)
153a -> 162a : 0.020918 (c= 0.14463192)
157a -> 162a : 0.016725 (c= -0.12932542)
159a -> 162a : 0.916136 (c= -0.95714997) **HOMO−2 → LUMO**

STATE 4: E= 0.127652 au 3.474 eV 28016.4 cm**-1 (356.9 nm)
152a -> 162a : 0.014845 (c= 0.12183910)
158a -> 162a : 0.945043 (c= 0.97213313) **HOMO−3 → LUMO**

STATE 5: E= 0.141898 au 3.861 eV 31143.1 cm**-1 (321.1 nm)
157a -> 162a : 0.298341 (c= -0.54620632) **HOMO−4 → LUMO**
159a -> 162a : 0.023801 (c= 0.15427587)
160a -> 163a : 0.016972 (c= 0.13027624)
160a -> 164a : 0.011827 (c= -0.10875084)
161a -> 163a : 0.373904 (c= -0.61147698) **HOMO → LUMO+1**
161a -> 164a : 0.248784 (c= 0.49878252) **HOMO → LUMO+2**

STATE 6: E= 0.151477 au 4.122 eV 33245.4 cm**-1 (300.8 nm)
156a -> 162a : 0.098452 (c= 0.31377104)
157a -> 162a : 0.072855 (c= 0.26991597)
160a -> 163a : 0.025326 (c= 0.15914059)
160a -> 166a : 0.017634 (c= -0.13279215)
161a -> 163a : 0.426535 (c= -0.65309684) **HOMO → LUMO+1**
161a -> 164a : 0.286875 (c= -0.53560753) **HOMO → LUMO+2**

9. Cartesian Coordinates of all calculated structures

9.1 Cartesian Coordinates of mixed silicon germanium clusters with $\{N(SiMe_3)Dipp\}_4$ substituent

(1) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

```
178
Energy = -9040.341433711 Hartree
Si     1.1072150    0.8011386   -1.0163449
Ge     0.9098950   -1.7532666   -0.1607459
Si     1.1847097    0.1264255    1.3007505
Si     3.1087979   -4.0011801   -0.8914795
Si     3.0652353   -0.3349820    3.7347656
N      1.7640674   -2.9559961   -1.3324429
N      2.4584954    0.6311426    2.3778087
C      1.0419426   -3.1322459   -2.5643187
C     -0.0524191   -4.0292754   -2.6226271
C     -0.7099893   -4.2067765   -3.8440183
H     -1.5479048   -4.8974523   -3.8979069
C     -0.3175284   -3.5132586   -4.9830290
H     -0.8381454   -3.6671101   -5.9242641
C      0.7298834   -2.6010496   -4.9036708
H      1.0147445   -2.0366526   -5.7872450
C      1.4144666   -2.3792307   -3.7048420
C     -0.5490611   -4.7926593   -1.4040531
H      0.0395043   -4.4634437   -0.5416768
C     -0.3465961   -6.3109757   -1.5576536
H      0.7054881   -6.5640050   -1.7176277
H     -0.6928082   -6.8331549   -0.6582513
H     -0.9168573   -6.6935803   -2.4116091
C     -2.0250092   -4.4842276   -1.1042665
H     -2.1806800   -3.4102131   -0.9619984
H     -2.6738430   -4.8144218   -1.9232728
H     -2.3431589   -4.9948636   -0.1905420
C      2.5249490   -1.3405814   -3.6591007
H      2.7194957   -1.1225761   -2.6033169
C      3.8290876   -1.8682853   -4.2848664
H      4.6092968   -1.0995705   -4.2392220
H      4.1963947   -2.7577080   -3.7666056
H      3.6721101   -2.1324096   -5.3370664
C      2.1150291   -0.0263396   -4.3428489
H      2.8797867    0.7385411   -4.1699413
H      2.0088096   -0.1519352   -5.4266177
H      1.1693265    0.3525662   -3.9477476
C      2.6997370   -4.9731767    0.6682808
H      3.5703632   -5.5491577    1.0062492
H      2.4045370   -4.3141276    1.4913700
H      1.8776949   -5.6763356    0.4958784
C      3.4359775   -5.2080737   -2.2924283
H      4.2796256   -5.8579387   -2.0274751
H      2.5678630   -5.8462565   -2.4836744
H      3.6807545   -4.7039115   -3.2315387
C      4.6210038   -2.9368063   -0.5625395
H      5.4623728   -3.5358780   -0.1936791
H      4.9435862   -2.4158978   -1.4698796
H      4.3967429   -2.1782178    0.1941966
C      3.0814146    1.9117279    2.0980534
C      2.5808699    3.0723292    2.7281455
C      3.2532501    4.2836896    2.5394027
H      2.8803521    5.1791907    3.0305323
C      4.3833539    4.3611349    1.7325696
H      4.8982786    5.3086333    1.6003356
C      4.8333770    3.2221851    1.0738262
H      5.6994571    3.2888131    0.4207393
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C	4.1945754	1.9873223	1.2316018
C	1.3187942	3.0455225	3.5731549
H	0.9774067	2.0067096	3.6094184
C	0.2103743	3.8793842	2.9096887
H	-0.7200539	3.8105906	3.4840177
H	0.4941089	4.9355607	2.8441662
H	0.0146454	3.5197017	1.8939474
C	1.5595288	3.5177660	5.0162541
H	0.6324685	3.4496271	5.5965546
H	2.3197961	2.9089391	5.5144905
H	1.8955193	4.5602409	5.0394051
C	4.7262022	0.7776626	0.4798493
H	4.0072000	-0.0364458	0.6210562
C	6.0883917	0.3236734	1.0358352
H	6.4440958	-0.5611524	0.4970489
H	6.8340057	1.1180425	0.9174529
H	6.0292527	0.0768710	2.0995027
C	4.8401086	1.0476399	-1.0300596
H	5.1575571	0.1372445	-1.5491475
H	3.8783378	1.3619628	-1.4467204
H	5.5794239	1.8285749	-1.2396494
C	4.4020271	0.6442273	4.6137807
H	4.8228344	0.0389362	5.4264946
H	5.2200511	0.9278752	3.9450580
H	4.0051678	1.5653492	5.0516589
C	3.7384034	-1.9677728	3.0987119
H	3.9904723	-2.6380449	3.9296703
H	2.9867313	-2.4718059	2.4814651
H	4.6364806	-1.8363240	2.4877541
C	1.6645734	-0.7123619	4.9247688
H	1.9939340	-1.4221806	5.6936989
H	1.3058078	0.1900132	5.4295178
H	0.8143548	-1.1616834	4.4012141
Si	-1.1171442	-0.8026940	-1.0055541
Ge	-0.9118769	1.7523723	-0.1535198
Si	-1.1736496	-0.1263022	1.3116648
N	-1.7758989	2.9549119	-1.3181985
N	-2.4383424	-0.6298490	2.4000383
Si	-3.1169527	4.0001070	-0.8663117
C	-1.0642663	3.1309532	-2.5561717
Si	-3.0344358	0.3381884	3.7602853
C	-3.0633075	-1.9108020	2.1264982
C	-2.6946889	4.9723065	0.6897861
C	-3.4557419	5.2065880	-2.2648213
C	-4.6264446	2.9358502	-0.5247149
C	0.0291429	4.0284562	-2.6241555
C	-1.4467806	2.3780524	-3.6934308
C	-4.3637910	-0.6400397	4.6516169
C	-3.7132112	1.9697641	3.1270571
C	-1.6242353	0.7180017	4.9381681
C	-2.5572034	-3.0708485	2.7531937
C	-4.1831809	-1.9874600	1.2687989
H	-3.5629980	5.5464718	1.0366656
H	-2.3900492	4.3134091	1.5095473
H	-1.8757071	5.6771101	0.5095805
H	-4.2980057	5.8556805	-1.9936613
H	-2.5896919	5.8455857	-2.4626493
H	-3.7070469	4.7020083	-3.2019866
H	-5.4645351	3.5349478	-0.1484969
H	-4.9568616	2.4152671	-1.4294245
H	-4.3958614	2.1769966	0.2298529
C	0.6749259	4.2072225	-3.8516359
C	0.5378115	4.7901573	-1.4094958
C	-0.7735861	2.6008686	-4.8985062
C	-2.5563346	1.3388976	-3.6378120
H	-4.7773360	-0.0340586	5.4675378
H	-5.1877485	-0.9238505	3.9902491
H	-3.9634492	-1.5610043	5.0866227
H	-3.9597724	2.6409597	3.9589265

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H    -2.9662056    2.4734501    2.5038773
H    -4.6154836    1.8370548    2.5226047
H    -1.9471817    1.4298753    5.7079075
H    -1.2616541   -0.1831960    5.4422752
H    -0.7781215    1.1657546    4.4066381
C    -3.2303271   -4.2826841    2.5702138
C    -1.2881545   -3.0432578    3.5876919
C    -4.8225897   -3.2227252    1.1167292
C    -4.7211807   -0.7785222    0.5204442
H     1.5115343    4.8988383   -3.9131342
C     0.2722142    3.5140569   -4.9872891
H    -0.0425507    4.4601075   -0.5418947
C     0.3344154    6.3087290   -1.5592905
C     2.0164740    4.4808746   -1.1243393
H    -1.0661094    2.0364542   -5.7795676
H    -2.7412007    1.1206677   -2.5803364
C    -3.8663520    1.8660522   -4.2516719
C    -2.1518874    0.0249399   -4.3253548
H    -2.8528912   -5.1778174    3.0585350
C    -4.3666829   -4.3611423    1.7723316
H    -0.9468911   -2.0043044    3.6208819
C    -0.1849570   -3.8769141    2.9153082
C    -1.5167099   -3.5153016    5.0328479
H    -5.6940177   -3.2900585    0.4708795
H    -4.0014063    0.0359532    0.6554869
C    -6.0790888   -0.3248063    1.0870674
C    -4.8470751   -1.0493940   -0.9883452
H     0.7837930    3.6688288   -5.9333161
H    -0.7190560    6.5622923   -1.7089931
H     0.6892934    6.8296604   -0.6625457
H     0.8967030    6.6922245   -2.4181167
H     2.1731548    3.4066406   -0.9848534
H     2.6575020    4.8117961   -1.9491754
H     2.3436294    4.9903282   -0.2131393
H    -4.6457955    1.0970191   -4.1989107
H    -4.2292921    2.7553468   -3.7300852
H    -3.7190838    2.1302501   -5.3052497
H    -2.9145512   -0.7404423   -4.1455165
H    -2.0556268    0.1506642   -5.4100407
H    -1.2023822   -0.3533950   -3.9389206
H    -4.8821002   -5.3089900    1.6445900
H     0.7501986   -3.8075808    3.4818248
H    -0.4688496   -4.9332115    2.8525085
H     0.0021811   -3.5175053    1.8978468
H    -0.5848622   -3.4468031    5.6053899
H    -2.2729675   -2.9066192    5.5373300
H    -1.8521826   -4.5578709    5.0589897
H    -6.4394774    0.5595776    0.5506837
H    -6.8252593   -1.1195780    0.9750634
H    -6.0115592   -0.0774652    2.1501128
H    -5.1692645   -0.1394695   -1.5053228
H    -3.8884822   -1.3633151   -1.4125724
H    -5.5875567   -1.8308925   -1.1916029
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(2) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

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178
Energy = -9040.336121606 Hartree
Si    1.1135076    0.8024089   -1.0454615
Si    0.8794049   -1.6965375   -0.3203277
Ge    1.2587923    0.0146867    1.3106785
Si    3.0417126   -3.8989236   -0.8555187
Si    3.2091319   -0.3656646    3.8002416
N     1.6905413   -2.8536304   -1.3346664
N     2.6788693    0.5734380    2.4137168
C     1.0256641   -3.0756342   -2.6071730
C    -0.0585732   -3.9810545   -2.6775062
C    -0.6509436   -4.2124403   -3.9231771
```

H	-1.4815549	-4.9102447	-3.9915135
C	-0.2038559	-3.5620866	-5.0679018
H	-0.6750817	-3.7578505	-6.0271496
C	0.8331682	-2.6401638	-4.9735324
H	1.1607157	-2.1097408	-5.8634655
C	1.4563282	-2.3666086	-3.7513318
C	-0.6157635	-4.6939711	-1.4537244
H	-0.0956521	-4.3044100	-0.5724524
C	-0.3695971	-6.2124673	-1.5144292
H	0.6957678	-6.4483207	-1.5896582
H	-0.7658634	-6.6965054	-0.6145826
H	-0.8721420	-6.6506423	-2.3840621
C	-2.1154268	-4.4115712	-1.2658442
H	-2.3074908	-3.3353929	-1.2137581
H	-2.7042835	-4.8226915	-2.0936018
H	-2.4728749	-4.8620689	-0.3353951
C	2.5539874	-1.3145301	-3.6943397
H	2.7421156	-1.0949629	-2.6381848
C	3.8671791	-1.8176126	-4.3212047
H	4.6334084	-1.0355777	-4.2708753
H	4.2501722	-2.7028697	-3.8064990
H	3.7171162	-2.0796520	-5.3748164
C	2.1203581	-0.0044667	-4.3734850
H	2.8759470	0.7708644	-4.2072433
H	2.0041447	-0.1329581	-5.4557503
H	1.1728118	0.3597835	-3.9682803
C	2.5802771	-4.8424964	0.7029429
H	3.4389884	-5.4092671	1.0834297
H	2.2532203	-4.1658391	1.4988643
H	1.7653142	-5.5495455	0.5152637
C	3.3874659	-5.1101324	-2.2453817
H	4.2227596	-5.7616805	-1.9589686
H	2.5223356	-5.7457887	-2.4561211
H	3.6564851	-4.6082863	-3.1790351
C	4.5441773	-2.8298007	-0.5163727
H	5.3851133	-3.4314760	-0.1509999
H	4.8682934	-2.3011778	-1.4184739
H	4.3174799	-2.0795342	0.2475695
C	3.2155832	1.8752721	2.1279960
C	2.6682363	3.0185541	2.7555951
C	3.2732257	4.2612582	2.5434719
H	2.8639593	5.1410237	3.0344557
C	4.3828509	4.3908282	1.7147220
H	4.8468594	5.3623096	1.5678847
C	4.8757406	3.2712969	1.0518590
H	5.7227415	3.3775078	0.3789020
C	4.3017421	2.0090657	1.2308591
C	1.4169232	2.9377883	3.6130980
H	1.1383556	1.8816716	3.6819472
C	0.2578681	3.6831984	2.9299506
H	-0.6619712	3.5899059	3.5183368
H	0.4850250	4.7492501	2.8182031
H	0.0709309	3.2691789	1.9331883
C	1.6347716	3.4652678	5.0402784
H	0.7183490	3.3499760	5.6301499
H	2.4384876	2.9233012	5.5475794
H	1.8985504	4.5286752	5.0333283
C	4.8589127	0.8178920	0.4709605
H	4.1610468	-0.0109310	0.6242857
C	6.2319679	0.3909145	1.0197175
H	6.6024167	-0.4891453	0.4821758
H	6.9629872	1.1985457	0.8991194
H	6.1771830	0.1450238	2.0841695
C	4.9458841	1.0879498	-1.0400524
H	5.2894755	0.1886916	-1.5626205
H	3.9676273	1.3662727	-1.4450288
H	5.6525772	1.8948392	-1.2634107
C	4.5321064	0.6062708	4.7110199
H	4.9114973	0.0187095	5.5562921

H	5.3794505	0.8505265	4.0624785
H	4.1406360	1.5493675	5.1050645
C	3.8865527	-2.0192008	3.2175713
H	4.1056921	-2.6806416	4.0648397
H	3.1533746	-2.5284636	2.5821731
H	4.8054784	-1.9007853	2.6341354
C	1.7534696	-0.7122567	4.9402680
H	2.0296492	-1.4272392	5.7252842
H	1.3909770	0.1991274	5.4266982
H	0.9151635	-1.1433431	4.3809243
Si	-1.1242470	-0.8039781	-1.0346296
Si	-0.8833781	1.6955850	-0.3133865
Ge	-1.2483227	-0.0144235	1.3220491
N	-1.7028856	2.8527363	-1.3209390
N	-2.6588240	-0.5721589	2.4378779
Si	-3.0504043	3.8977785	-0.8312249
C	-1.0479706	3.0746436	-2.5986273
Si	-3.1774486	0.3684143	3.8277677
C	-3.1974586	-1.8743848	2.1575858
C	-2.5765683	4.8416812	0.7233267
C	-3.4074927	5.1086705	-2.2184696
C	-4.5498384	2.8283189	-0.4799293
C	0.0354795	3.9802874	-2.6775281
C	-1.4870321	2.3649184	-3.7391480
C	-4.4913680	-0.6032553	4.7518809
C	-3.8616101	2.0205982	3.2491337
C	-1.7116398	0.7176593	4.9538936
C	-2.6438966	-3.0171254	2.7807082
C	-4.2912739	-2.0091730	1.2699219
H	-3.4333021	5.4050457	1.1131921
H	-2.2389053	4.1654284	1.5151843
H	-1.7660543	5.5517763	0.5279404
H	-4.2414015	5.7593130	-1.9260414
H	-2.5445810	5.7452823	-2.4353520
H	-3.6826645	4.6065517	-3.1501849
H	-5.3875997	3.4296257	-0.1067358
H	-4.8817572	2.3004356	-1.3796252
H	-4.3164324	2.0774269	0.2813708
C	0.6185477	4.2110667	-3.9276878
C	0.6016335	4.6939277	-1.4582970
C	-0.8730442	2.6379186	-4.9661043
C	-2.5839688	1.3126043	-3.6732979
H	-4.8621259	-0.0155259	5.6008628
H	-5.3452827	-0.8473760	4.1119493
H	-4.0961643	-1.5463986	5.1420527
H	-4.0746603	2.6824987	4.0976017
H	-3.1343312	2.5302725	2.6073193
H	-4.7851330	1.9004964	2.6733537
H	-1.9806467	1.4345341	5.7396667
H	-1.3447779	-0.1925975	5.4391607
H	-0.8784061	1.1473549	4.3859222
C	-3.2495372	-4.2603858	2.5737418
C	-1.3856242	-2.9352513	3.6278773
C	-4.8656686	-3.2719167	1.0959009
C	-4.8560957	-0.8185104	0.5148920
H	1.4485257	4.9089609	-4.0025736
C	0.1630985	3.5599602	-5.0686859
H	0.0874146	4.3055271	-0.5730764
C	0.3560546	6.2125261	-1.5187058
C	2.1023756	4.4107013	-1.2805934
H	-1.2070641	2.1069056	-5.8532762
H	-2.7639676	1.0935188	-2.6156318
C	-3.9020571	1.8151159	-4.2902935
C	-2.1552252	0.0022799	-4.3550203
H	-2.8353251	-5.1397611	3.0612662
C	-4.3660283	-4.3910041	1.7544464
H	-1.1071092	-1.8789468	3.6939440
C	-0.2317612	-3.6804430	2.9357655
C	-1.5916297	-3.4621288	5.0570507

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H    -5.7183209   -3.3789148    0.4302524
H    -4.1576880    0.0109377    0.6622684
C    -6.2247579   -0.3928168    1.0755113
C    -4.9559280   -1.0885758   -0.9953279
H     0.6271792    3.7552198   -6.0315124
H    -0.7096470    6.4490053   -1.5870104
H     0.7586662    6.6970973   -0.6219696
H     0.8530352    6.6496248   -2.3920687
H     2.2940673    3.3344660   -1.2283140
H     2.6856775    4.8202041   -2.1130730
H     2.4667222    4.8622491   -0.3533357
H    -4.6677220    1.0329591   -4.2336356
H    -4.2812337    2.7005796   -3.7731037
H    -3.7601732    2.0766370   -5.3451611
H    -2.9092345   -0.7732092   -4.1824242
H    -2.0474670    0.1301186   -5.4382389
H    -1.2044402   -0.3614242   -3.9569532
H    -4.8303739   -5.3629186    1.6115816
H     0.6927976   -3.5862694    3.5165465
H    -0.4592197   -4.7466950    2.8265662
H    -0.0531720   -3.2669651    1.9372462
H    -0.6703932   -3.3464608    5.6393073
H    -2.3912064   -2.9200561    5.5707483
H    -1.8553179   -4.5255725    5.0527316
H    -6.6005155    0.4870507    0.5413502
H    -6.9561234   -1.2010193    0.9610095
H    -6.1610735   -0.1471190    2.1395222
H    -5.3051100   -0.1896973   -1.5148311
H    -3.9809036   -1.3657214   -1.4088356
H    -5.6635781   -1.8962969   -1.2125517
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(3) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

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178
Energy = -9040.392279460 Hartree
Ge    1.1608626    0.8418991   -1.0994141
Si    0.8855217   -1.7022080   -0.2715206
Si    1.1845550    0.0100563    1.2517593
Si    3.0713523   -3.9340501   -0.8152625
Si    3.0723295   -0.3696457    3.7045614
N     1.7185978   -2.8788542   -1.2622124
N     2.4754176    0.5432542    2.3091728
C     1.0435429   -3.1256968   -2.5269750
C    -0.0297317   -4.0453479   -2.5787060
C    -0.6336578   -4.2968897   -3.8151943
H    -1.4561750   -5.0056809   -3.8665673
C    -0.2073648   -3.6542344   -4.9715595
H    -0.6869530   -3.8650980   -5.9234628
C     0.8224665   -2.7224754   -4.8982397
H     1.1366441   -2.2006818   -5.7979301
C     1.4564504   -2.4290709   -3.6862560
C    -0.5620534   -4.7604482   -1.3453760
H    -0.0321670   -4.3644853   -0.4730894
C    -0.3052604   -6.2772699   -1.4088276
H     0.7598552   -6.5060059   -1.5044017
H    -0.6805669   -6.7628665   -0.5007777
H    -0.8215282   -6.7206724   -2.2677216
C    -2.0613068   -4.4936785   -1.1362443
H    -2.2637378   -3.4210100   -1.0623406
H    -2.6557743   -4.8959410   -1.9642918
H    -2.4041647   -4.9638272   -0.2102989
C     2.5495588   -1.3708785   -3.6596573
H     2.7341366   -1.1186441   -2.6101751
C     3.8674026   -1.8850904   -4.2679508
H     4.6253038   -1.0935249   -4.2485989
H     4.2608981   -2.7453133   -3.7205196
H     3.7188367   -2.1884321   -5.3106630
C     2.1154221   -0.0849175   -4.3832843
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H	2.8603998	0.7023218	-4.2253590
H	2.0223217	-0.2455138	-5.4635437
H	1.1567465	0.2811435	-4.0069834
C	2.6511002	-4.9171827	0.7311684
H	3.5232307	-5.4925136	1.0662539
H	2.3461367	-4.2708812	1.5589996
H	1.8348427	-5.6228657	0.5444538
C	3.3963951	-5.1367335	-2.2193194
H	4.2376203	-5.7870252	-1.9468463
H	2.5298799	-5.7744302	-2.4173704
H	3.6488683	-4.6340994	-3.1567384
C	4.5864466	-2.8774092	-0.4939810
H	5.4296908	-3.4867965	-0.1472433
H	4.8978456	-2.3461892	-1.3991029
H	4.3777577	-2.1299351	0.2765842
C	3.0690112	1.8399379	2.0426152
C	2.5555952	2.9845766	2.6910811
C	3.2142920	4.2071394	2.5264597
H	2.8297388	5.0886889	3.0336861
C	4.3460992	4.3127960	1.7257100
H	4.8524035	5.2676784	1.6145607
C	4.8083636	3.1913715	1.0456065
H	5.6756164	3.2793425	0.3966033
C	4.1822522	1.9473684	1.1785879
C	1.2921760	2.9304469	3.5315701
H	0.9645203	1.8866107	3.5524194
C	0.1768996	3.7558460	2.8708188
H	-0.7514050	3.6798908	3.4478893
H	0.4522869	4.8142837	2.8053920
H	-0.0173855	3.3907938	1.8566364
C	1.5184824	3.3903871	4.9808010
H	0.5894026	3.3022373	5.5550236
H	2.2848708	2.7879862	5.4774370
H	1.8383683	4.4375892	5.0170104
C	4.7304830	0.7565741	0.4099783
H	4.0021641	-0.0547879	0.5100549
C	6.0727958	0.2806164	0.9951120
H	6.4471349	-0.5850951	0.4383064
H	6.8213738	1.0784688	0.9309903
H	5.9766548	-0.0039586	2.0463424
C	4.8935029	1.0619363	-1.0883168
H	5.2140422	0.1597971	-1.6201468
H	3.9499699	1.4010582	-1.5266317
H	5.6501621	1.8358639	-1.2581383
C	4.4156834	0.6285740	4.5537964
H	4.8260065	0.0465949	5.3887971
H	5.2399278	0.8801433	3.8800363
H	4.0281575	1.5687051	4.9578218
C	3.7409931	-2.0278359	3.1339344
H	3.9682868	-2.6755905	3.9894369
H	2.9971398	-2.5415741	2.5161499
H	4.6527533	-1.9232400	2.5381465
C	1.6763969	-0.7011024	4.9151114
H	2.0072174	-1.3898839	5.7024937
H	1.3256023	0.2168388	5.3963178
H	0.8200514	-1.1601868	4.4112642
Ge	-1.1706929	-0.8432289	-1.0889015
Si	-0.8883023	1.7011984	-0.2651815
Si	-1.1749772	-0.0096481	1.2617884
N	-1.7290305	2.8782204	-1.2486500
N	-2.4559475	-0.5424146	2.3313572
Si	-3.0779575	3.9334616	-0.7903626
C	-1.0651570	3.1245839	-2.5193863
Si	-3.0428392	0.3723071	3.7297493
C	-3.0512682	-1.8395010	2.0705462
C	-2.6433812	4.9161236	0.7523777
C	-3.4147532	5.1361148	-2.1916283
C	-4.5907701	2.8774214	-0.4564546
C	0.0081135	4.0436833	-2.5804976

C	-1.4890417	2.4286958	-3.6750999
C	-4.3773106	-0.6265263	4.5922223
C	-3.7196265	2.0281694	3.1619429
C	-1.6368935	0.7083134	4.9273578
C	-2.5308344	-2.9836570	2.7142593
C	-4.1721360	-1.9480041	1.2165796
H	-3.5134162	5.4877790	1.0989493
H	-2.3258155	4.2697569	1.5754121
H	-1.8319777	5.6250103	0.5566921
H	-4.2542585	5.7858316	-1.9125743
H	-2.5502777	5.7743988	-2.3965827
H	-3.6742895	4.6331637	-3.1269527
H	-5.4298467	3.4867974	-0.0997269
H	-4.9117941	2.3489076	-1.3598030
H	-4.3752024	2.1277215	0.3100337
C	0.6010976	4.2951609	-3.8222696
C	0.5517851	4.7581811	-1.3517793
C	-0.8658687	2.7221507	-4.8926794
C	-2.5828402	1.3714801	-3.6391655
H	-4.7802053	-0.0442974	5.4306632
H	-5.2077286	-0.8789754	3.9263909
H	-3.9854734	-1.5661970	4.9931160
H	-3.9424583	2.6763338	4.0183149
H	-2.9816948	2.5432267	2.5381910
H	-4.6354083	1.9204799	2.5729044
H	-1.9611167	1.3997983	5.7150968
H	-1.2817630	-0.2078917	5.4086854
H	-0.7849914	1.1658254	4.4145746
C	-3.1894997	-4.2069614	2.5551211
C	-1.2603546	-2.9281764	3.5439872
C	-4.7980575	-3.1926676	1.0889960
C	-4.7280540	-0.7579025	0.4524658
H	1.4235696	5.0034555	-3.8808402
C	0.1639383	3.6531744	-4.9749636
H	0.0290537	4.3627649	-0.4749586
C	0.2960235	6.2752620	-1.4130749
C	2.0525171	4.4899271	-1.1556185
H	-1.1885360	2.2008722	-5.7896714
H	-2.7593151	1.1199356	-2.5881206
C	-3.9049910	1.8862759	-4.2375238
C	-2.1552385	0.0848090	-4.3654744
H	-2.7994329	-5.0881836	3.0586988
C	-4.3283810	-4.3137235	1.7646060
H	-0.9325801	-1.8843028	3.5604201
C	-0.1505123	-3.7547046	2.8755805
C	-1.4748680	-3.3857666	4.9957776
H	-5.6710192	-3.2814502	0.4477970
H	-4.0005010	0.0547039	0.5478031
C	-6.0671466	-0.2845344	1.0469510
C	-4.9009279	-1.0630709	-1.0447867
H	0.6350872	3.8640035	-5.9310783
H	-0.7696510	6.5050686	-1.4995760
H	0.6795525	6.7604824	-0.5082673
H	0.8053878	6.7181385	-2.2763472
H	2.2545886	3.4170291	-1.0840083
H	2.6402595	4.8920630	-1.9885218
H	2.4037157	4.9592581	-0.2323893
H	-4.6634254	1.0954198	-4.2113260
H	-4.2933623	2.7474704	-3.6879384
H	-3.7644304	2.1883798	-5.2816985
H	-2.8994436	-0.7019006	-4.2013589
H	-2.0704097	0.2448783	-5.4464968
H	-1.1938867	-0.2816707	-3.9964660
H	-4.8345538	-5.2691702	1.6577727
H	0.7827735	-3.6766162	3.4442326
H	-0.4257051	-4.8135048	2.8154086
H	0.0346491	-3.3922560	1.8587596
H	-0.5407122	-3.2985858	5.5618540
H	-2.2358151	-2.7813125	5.4982508

H	-1.7963972	-4.4323202	5.0360664
H	-6.4463148	0.5812386	0.4935107
H	-6.8150622	-1.0833243	0.9868418
H	-5.9645585	-0.0009633	2.0978419
H	-5.2280067	-0.1616973	-1.5739116
H	-3.9595730	-1.3992109	-1.4900239
H	-5.6564343	-1.8392516	-1.2093749

(4) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

178
Energy = -9040.338758010 Hartree

Si	1.1142921	0.8171325	-1.0483715
Ge	0.9099081	-1.7647316	-0.2069439
Si	1.2241945	0.1415615	1.2427593
Si	3.0874239	-4.0157191	-0.9125993
Si	3.0292806	-0.3122655	3.7155255
N	1.7817150	-2.9422531	-1.3947478
N	2.5063614	0.6360580	2.3095022
C	1.0698118	-3.1004019	-2.6335098
C	-0.0338734	-3.9852781	-2.7130368
C	-0.6810561	-4.1407851	-3.9431662
H	-1.5241113	-4.8236044	-4.0140603
C	-0.2725802	-3.4355150	-5.0692177
H	-0.7861932	-3.5722507	-6.0169489
C	0.7814585	-2.5328551	-4.9681801
H	1.0785492	-1.9587223	-5.8413903
C	1.4572676	-2.3345531	-3.7605516
C	-0.5518668	-4.7580153	-1.5089371
H	0.0198886	-4.4341854	-0.6331844
C	-0.3457749	-6.2752389	-1.6704784
H	0.7091189	-6.5279045	-1.8106006
H	-0.7109578	-6.8046997	-0.7829358
H	-0.8984077	-6.6499886	-2.5394212
C	-2.0337055	-4.4556407	-1.2317135
H	-2.1970686	-3.3821242	-1.0951432
H	-2.6695623	-4.7925986	-2.0582324
H	-2.3616417	-4.9639060	-0.3200737
C	2.5782096	-1.3092109	-3.6866215
H	2.7496680	-1.0974222	-2.6255195
C	3.8899605	-1.8549620	-4.2799511
H	4.6805810	-1.0984699	-4.2146889
H	4.2294008	-2.7497054	-3.7518804
H	3.7554024	-2.1176000	-5.3356032
C	2.2031707	0.0122857	-4.3762159
H	2.9737394	0.7660657	-4.1814306
H	2.1228871	-0.1077875	-5.4628121
H	1.2522742	0.4018451	-4.0031970
C	2.6008407	-4.9737400	0.6349952
H	3.4531410	-5.5413074	1.0290811
H	2.2576855	-4.3036932	1.4311892
H	1.7915224	-5.6824970	0.4286413
C	3.4464720	-5.2232281	-2.3051025
H	4.2347980	-5.9202811	-1.9940376
H	2.5621044	-5.8114814	-2.5679413
H	3.7835443	-4.7195559	-3.2157963
C	4.6075053	-2.9828013	-0.5247627
H	5.4264563	-3.6007148	-0.1369472
H	4.9672474	-2.4574989	-1.4156072
H	4.3731174	-2.2290993	0.2339255
C	3.1551332	1.9026958	2.0319683
C	2.6843956	3.0720993	2.6684254
C	3.3808504	4.2690603	2.4746444
H	3.0307329	5.1723015	2.9681791
C	4.5062459	4.3228452	1.6588804
H	5.0402140	5.2593201	1.5235622
C	4.9278771	3.1749427	0.9966974
H	5.7914158	3.2231870	0.3386379

C	4.2640246	1.9540248	1.1592170
C	1.4232170	3.0707850	3.5153215
H	1.0919480	2.0319857	3.6059849
C	0.3074394	3.8514947	2.8011028
H	-0.6190961	3.8220927	3.3851049
H	0.5892528	4.9006978	2.6585041
H	0.1059790	3.4165139	1.8162449
C	1.6501673	3.6225138	4.9316533
H	0.7248412	3.5544667	5.5145677
H	2.4283596	3.0626453	5.4590613
H	1.9528096	4.6750317	4.9048672
C	4.7653923	0.7300044	0.4108827
H	4.0262155	-0.0654316	0.5532322
C	6.1122368	0.2432749	0.9761144
H	6.4495889	-0.6516361	0.4425318
H	6.8782421	1.0187282	0.8627541
H	6.0371252	0.0006066	2.0400230
C	4.8868920	0.9918173	-1.0993875
H	5.1855705	0.0732673	-1.6152437
H	3.9316532	1.3242972	-1.5174505
H	5.6417117	1.7567601	-1.3125315
C	4.3885578	0.6326563	4.5966423
H	4.7514782	0.0427119	5.4476160
H	5.2403619	0.8399659	3.9417339
H	4.0306273	1.5927229	4.9809623
C	3.6500661	-1.9873800	3.1402311
H	3.8636949	-2.6416639	3.9943319
H	2.8947974	-2.4840019	2.5218025
H	4.5643087	-1.9010908	2.5446898
C	1.5709577	-0.5775742	4.8668682
H	1.8118748	-1.3154523	5.6419018
H	1.2748558	0.3512185	5.3647946
H	0.7017704	-0.9488210	4.3134985
Si	-1.1078416	-0.7933921	-1.0385774
Si	-0.8915912	1.6746954	-0.2791465
Ge	-1.2044506	-0.0288551	1.3558523
N	-1.6986042	2.8572386	-1.2677849
N	-2.5808344	-0.6029533	2.5092252
Si	-3.0707701	3.8792498	-0.7950113
C	-1.0364982	3.1075228	-2.5376719
Si	-3.1830006	0.3926611	3.8237254
C	-3.1288286	-1.9027786	2.2248191
C	-2.6455941	4.7999358	0.7869234
C	-3.4027339	5.1145376	-2.1669806
C	-4.5724223	2.7928073	-0.5121221
C	0.0370111	4.0260741	-2.5928947
C	-1.4627702	2.4174476	-3.6948243
C	-4.3976177	-0.6244389	4.8308263
C	-4.0173807	1.9430951	3.1641430
C	-1.7466518	0.9534078	4.8995326
C	-2.6051664	-3.0420714	2.8810085
C	-4.1961276	-2.0439207	1.3058158
H	-3.5180215	5.3455140	1.1669362
H	-2.3155873	4.1150589	1.5742301
H	-1.8402310	5.5233211	0.6207646
H	-4.2519985	5.7494591	-1.8840990
H	-2.5419401	5.7651342	-2.3475437
H	-3.6466269	4.6284399	-3.1157367
H	-5.4202469	3.3790351	-0.1377139
H	-4.8819028	2.2972855	-1.4378127
H	-4.3552792	2.0154429	0.2265364
C	0.6252943	4.2876460	-3.8343971
C	0.5892397	4.7198688	-1.3564933
C	-0.8435203	2.7203563	-4.9122513
C	-2.5504060	1.3541995	-3.6603740
H	-4.8415113	-0.0046509	5.6196969
H	-5.2110825	-1.0191203	4.2132877
H	-3.9061210	-1.4771918	5.3094607
H	-4.2955698	2.6164705	3.9846604

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H    -3.3348727    2.4917024    2.5061510
H    -4.9223967    1.7187780    2.5915634
H    -2.0749823    1.7064016    5.6266334
H    -1.3027398    0.1195494    5.4523134
H    -0.9554028    1.4060034    4.2905350
C    -3.1877265   -4.2903960    2.6419711
C    -1.4051162   -2.9503490    3.8074521
C    -4.7504291   -3.3117575    1.1039410
C    -4.7774911   -0.8548345    0.5610902
H     1.4482872    4.9955245   -3.8902950
C     0.1839716    3.6540979   -4.9906786
H     0.0690502    4.3127207   -0.4836145
C     0.3378321    6.2381782   -1.3893474
C     2.0893531    4.4381633   -1.1735434
H    -1.1671518    2.2033864   -5.8114858
H    -2.7472787    1.1195604   -2.6091463
C    -3.8616926    1.8516632   -4.2957475
C    -2.0956798    0.0573488   -4.3509324
H    -2.7904007   -5.1665089    3.1485134
C    -4.2624634   -4.4301931    1.7706316
H    -1.2021759   -1.8872140    3.9676649
C    -0.1692709   -3.5739125    3.1353536
C    -1.6538851   -3.5987713    5.1786265
H    -5.5791656   -3.4222697    0.4095089
H    -4.0989493   -0.0113676    0.7241632
C    -6.1593779   -0.4761394    1.1251500
C    -4.8729506   -1.1012177   -0.9531615
H     0.6520644    3.8724116   -5.9465639
H    -0.7284348    6.4714459   -1.4600637
H     0.7322006    6.7068274   -0.4804735
H     0.8387863    6.6947376   -2.2503689
H     2.2834542    3.3617744   -1.1348309
H     2.6762629    4.8599797   -1.9972061
H     2.4475950    4.8789993   -0.2389182
H    -4.6222176    1.0634197   -4.2577656
H    -4.2564719    2.7308725   -3.7794367
H    -3.7038954    2.1215631   -5.3462514
H    -2.8436897   -0.7286919   -4.2020955
H    -1.9699695    0.2012119   -5.4302132
H    -1.1483021   -0.3019326   -3.9415102
H    -4.7078082   -5.4066743    1.6010922
H     0.7084379   -3.4996467    3.7869257
H    -0.3412734   -4.6324161    2.9107793
H     0.0574470   -3.0621163    2.1931558
H    -0.7897006   -3.4373902    5.8328657
H    -2.5378653   -3.1770998    5.6665552
H    -1.8050178   -4.6800598    5.0876796
H    -6.5456953    0.4197708    0.6261694
H    -6.8736924   -1.2917353    0.9646911
H    -6.1133006   -0.2802318    2.2002991
H    -5.2416796   -0.2011564   -1.4566959
H    -3.8938014   -1.3516542   -1.3734173
H    -5.5652373   -1.9188429   -1.1822554
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(1) $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$

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178
Energy = -10827.84564342 Hartree
Ge    1.2232283   -0.6965658    1.1326546
Si    0.7291712    1.7556345    0.1063048
Ge    1.0521985   -0.0803519   -1.3709379
Si    2.8106884    4.1100699    0.2964992
Si    2.8184949    0.2116846   -4.0183053
N     1.5595243    3.0376419    0.9526460
N     2.4071573   -0.6625113   -2.5520777
C     0.9698964    3.3454975    2.2445983
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C	-0.1601161	4.1939790	2.3113202
C	-0.6845721	4.5069092	3.5698265
H	-1.5494877	5.1622257	3.6334185
C	-0.1267431	3.9910621	4.7338904
H	-0.5468019	4.2480708	5.7024288
C	0.9589332	3.1257881	4.6496395
H	1.3769491	2.7019760	5.5585050
C	1.5186864	2.7756595	3.4164417
C	-0.8337732	4.7688123	1.0733232
H	-0.3527858	4.3277877	0.1941093
C	-0.6642493	6.2967633	0.9887285
H	0.3895810	6.5882640	0.9711889
H	-1.1418589	6.6807870	0.0801107
H	-1.1329515	6.7855041	1.8502988
C	-2.3262513	4.4050092	1.0142926
H	-2.4692540	3.3207937	1.0533012
H	-2.8777945	4.8513506	1.8493575
H	-2.7675036	4.7679102	0.0815142
C	2.6799238	1.7929413	3.3800898
H	2.7978016	1.4660522	2.3417905
C	4.0012721	2.4425822	3.8305919
H	4.8114684	1.7048367	3.8060925
H	4.2842026	3.2790700	3.1867305
H	3.9156799	2.8203030	4.8559644
C	2.4006304	0.5468031	4.2377346
H	3.1847137	-0.2008208	4.0769122
H	2.3857415	0.7916782	5.3059399
H	1.4425240	0.0886895	3.9780703
C	2.2021370	4.8992213	-1.2973073
H	3.0039490	5.4788373	-1.7713327
H	1.8684852	4.1484070	-2.0201354
H	1.3613253	5.5757162	-1.1114888
C	3.1728068	5.4612511	1.5475683
H	3.9673150	6.1096251	1.1566489
H	2.2945621	6.0852408	1.7378413
H	3.5042796	5.0662792	2.5115938
C	4.3508862	3.1004338	-0.0542860
H	5.1236445	3.7096945	-0.5383721
H	4.7713387	2.6823988	0.8657715
H	4.1179578	2.2672041	-0.7238505
C	3.0757428	-1.8890750	-2.2129081
C	2.6027470	-3.1141574	-2.7393506
C	3.3272392	-4.2843377	-2.4936912
H	2.9721647	-5.2251083	-2.9076169
C	4.4897131	-4.2648388	-1.7301615
H	5.0471615	-5.1811194	-1.5559917
C	4.9181669	-3.0662605	-1.1695046
H	5.8116997	-3.0546504	-0.5507685
C	4.2241262	-1.8715533	-1.3855896
C	1.3068156	-3.1922754	-3.5265267
H	0.9701884	-2.1646516	-3.6917767
C	0.2306749	-3.9122088	-2.6962621
H	-0.7211408	-3.9446413	-3.2385177
H	0.5317484	-4.9413829	-2.4710820
H	0.0682507	-3.3907702	-1.7459839
C	1.4727309	-3.8638181	-4.8986148
H	0.5228591	-3.8445105	-5.4449121
H	2.2266143	-3.3522345	-5.5046575
H	1.7780710	-4.9110224	-4.7960374
C	4.7359644	-0.5890838	-0.7529087
H	3.9551988	0.1667816	-0.8869990
C	6.0123631	-0.0928398	-1.4562250
H	6.3515805	0.8508441	-1.0151023
H	6.8172508	-0.8292605	-1.3509051
H	5.8440674	0.0677375	-2.5246993
C	4.9906868	-0.7447277	0.7551604
H	5.2834408	0.2185121	1.1865380
H	4.0914835	-1.0924098	1.2731496
H	5.7984844	-1.4578798	0.9533880

C	4.1290652	-0.7602172	-4.9483418
H	4.4485031	-0.1984128	-5.8350450
H	5.0137004	-0.9534193	-4.3335461
H	3.7473025	-1.7295928	-5.2838118
C	3.4478676	1.9307029	-3.5917064
H	3.5842359	2.5382673	-4.4948967
H	2.7254764	2.4482927	-2.9510822
H	4.4022994	1.9006342	-3.0571109
C	1.2977984	0.4297061	-5.1026387
H	1.5146577	1.0983317	-5.9450535
H	0.9455465	-0.5231634	-5.5102873
H	0.4725514	0.8721465	-4.5339654
Ge	-1.2029379	0.8175712	1.1343688
Si	-0.7824262	-1.7868675	0.4870077
Si	-1.3677447	-0.2149265	-1.1098469
N	-1.4581686	-2.9519658	1.5974476
N	-2.7516750	0.1235716	-2.1206049
Si	-2.7493474	-4.1274632	1.2879123
C	-0.6880061	-3.0657701	2.8257971
Si	-3.3160576	-0.9281720	-3.4306310
C	-3.4067960	1.4028998	-1.9239740
C	-2.3225382	-5.1732556	-0.2153979
C	-2.9182360	-5.2543444	2.7790172
C	-4.3472217	-3.1958804	0.9821329
C	0.4476270	-3.9073706	2.8625346
C	-1.0697571	-2.3122616	3.9595528
C	-4.7827066	-0.1137278	-4.2711367
C	-3.8098695	-2.5941481	-2.7231921
C	-1.9315886	-1.2080591	-4.6672404
C	-3.0067154	2.5174374	-2.6930703
C	-4.4606725	1.5173555	-0.9895893
H	-3.1776051	-5.7944913	-0.5093087
H	-2.0498755	-4.5584280	-1.0783398
H	-1.4789642	-5.8395713	-0.0065258
H	-3.7180840	-5.9819663	2.5906249
H	-1.9970277	-5.8116647	2.9733872
H	-3.1671878	-4.7097704	3.6938767
H	-5.1615396	-3.8783939	0.7108669
H	-4.6528416	-2.6344999	1.8710311
H	-4.2250148	-2.4821733	0.1625541
C	1.1497912	-4.0264847	4.0665238
C	0.9468177	-4.6695755	1.6439011
C	-0.3364492	-2.4727886	5.1399422
C	-2.2327037	-1.3314304	3.9342832
H	-5.1528563	-0.7693579	-5.0694871
H	-5.6078823	0.0699039	-3.5763795
H	-4.5163531	0.8472665	-4.7209058
H	-4.0164257	-3.3147522	-3.5239530
H	-2.9994726	-3.0023279	-2.1106141
H	-4.7016841	-2.5247264	-2.0928272
H	-2.1985390	-1.9989604	-5.3791212
H	-1.7031328	-0.3033426	-5.2383884
H	-1.0131711	-1.5176831	-4.1567662
C	-3.7288567	3.7096601	-2.5762726
C	-1.7950893	2.4716324	-3.6082724
C	-5.1518394	2.7305442	-0.9069997
C	-4.8708341	0.3626270	-0.0912521
H	2.0220724	-4.6738477	4.1071972
C	0.7584917	-3.3282357	5.2029475
H	0.3198070	-4.3889447	0.7917780
C	0.8330317	-6.1928887	1.8360529
C	2.3954082	-4.2922218	1.2942749
H	-0.6238902	-1.9064054	6.0213723
H	-2.4951224	-1.1636743	2.8843334
C	-3.4743293	-1.8905245	4.6529787
C	-1.8483576	0.0267890	4.5449965
H	-3.4345862	4.5678786	-3.1755146
C	-4.8075651	3.8161416	-1.7054225
H	-1.3864247	1.4574113	-3.5569947

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C    -0.7091661    3.4349686   -3.1030992
C    -2.1431650    2.7751511   -5.0746808
H    -5.9747092    2.8235045   -0.2032474
H    -4.0891870   -0.3995977   -0.1706253
C    -6.2008969   -0.2610903   -0.5513487
C    -4.9674404    0.7822000    1.3847270
H     1.3149949   -3.4358468    6.1299396
H    -0.1966028   -6.5012897    2.0389670
H     1.1768822   -6.7143567    0.9355365
H     1.4535566   -6.5245258    2.6761501
H     2.4914385   -3.2157447    1.1239500
H     3.0840295   -4.5720123    2.0995310
H     2.7114359   -4.8042429    0.3810998
H    -4.2872370   -1.1557275    4.6286962
H    -3.8339286   -2.8109909    4.1860686
H    -3.2463333   -2.1114779    5.7020487
H    -2.6548410    0.7502319    4.3842976
H    -1.6806241   -0.0525447    5.6252003
H    -0.9416312    0.4288066    4.0853755
H    -5.3628063    4.7471423   -1.6318476
H     0.1891933    3.3614922   -3.7261733
H    -1.0569788    4.4736463   -3.1276196
H    -0.4329104    3.1912504   -2.0719579
H    -1.2452973    2.7051342   -5.6987776
H    -2.8854701    2.0730004   -5.4652290
H    -2.5494035    3.7871180   -5.1809119
H    -6.4750060   -1.0997881    0.0975953
H    -7.0057961    0.4815043   -0.5107106
H    -6.1372124   -0.6300367   -1.5787315
H    -5.1786621   -0.0932340    2.0080389
H    -4.0296287    1.2292556    1.7289117
H    -5.7734740    1.5070586    1.5437389
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(2) $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$

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178
Energy = -10827.85056364 Hartree
Ge    1.2427725   -0.7051905    1.1079551
Ge    0.7506581    1.8062863   -0.0317265
Si    1.0327069   -0.1998503   -1.3179961
Si    2.8793288    4.2174516    0.3458162
Si    2.6774895    0.1647987   -3.9353373
N     1.6532903    3.1316448    0.9812476
N     2.2539164   -0.7173997   -2.4553273
C     1.0003839    3.3710498    2.2393216
C    -0.1490158    4.1977626    2.3000976
C    -0.7516509    4.4216788    3.5424733
H    -1.6301894    5.0599366    3.5963279
C    -0.2537214    3.8406913    4.7026170
H    -0.7344343    4.0277701    5.6589784
C     0.8516282    2.9987790    4.6273546
H     1.2228432    2.5236991    5.5310739
C     1.4862866    2.7359148    3.4098033
C    -0.7580404    4.8454643    1.0650036
H    -0.2010831    4.4886316    0.1926538
C    -0.6333582    6.3796664    1.1073349
H     0.4093440    6.6984619    1.1921760
H    -1.0544299    6.8201627    0.1962338
H    -1.1796269    6.7886649    1.9647377
C    -2.2297199    4.4453596    0.8721095
H    -2.3372022    3.3594420    0.7874340
H    -2.8469992    4.7821371    1.7124242
H    -2.6279229    4.8934112   -0.0430806
C     2.6691705    1.7802000    3.3719621
H     2.7911160    1.4644195    2.3300375
C     3.9751569    2.4651415    3.8149517
H     4.8069924    1.7517500    3.7825325
H     4.2268263    3.3107267    3.1706075
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H	3.8852101	2.8380487	4.8418451
C	2.4327350	0.5236054	4.2254149
H	3.2323284	-0.2035782	4.0471868
H	2.4308669	0.7587856	5.2960424
H	1.4820610	0.0433261	3.9787047
C	2.2881025	5.0311497	-1.2473041
H	3.0948481	5.6190045	-1.7031357
H	1.9651940	4.2919188	-1.9877504
H	1.4447438	5.7052923	-1.0626908
C	3.2399814	5.5648559	1.6047664
H	4.0129405	6.2363618	1.2098609
H	2.3502247	6.1661164	1.8151320
H	3.5954281	5.1676483	2.5595514
C	4.4301154	3.2254937	-0.0284377
H	5.1916406	3.8379083	-0.5263301
H	4.8674866	2.8116182	0.8859865
H	4.1924307	2.3874250	-0.6912527
C	3.0055598	-1.9188006	-2.1448193
C	2.5782540	-3.1530493	-2.6825595
C	3.3656848	-4.2892621	-2.4735023
H	3.0466998	-5.2405553	-2.8920984
C	4.5452461	-4.2211614	-1.7395283
H	5.1508523	-5.1109986	-1.5916499
C	4.9321693	-3.0098583	-1.1772061
H	5.8425355	-2.9614007	-0.5857405
C	4.1767355	-1.8457726	-1.3580126
C	1.2722505	-3.2785241	-3.4473807
H	0.8909278	-2.2651025	-3.6018981
C	0.2376913	-4.0404880	-2.6031665
H	-0.7219368	-4.1005407	-3.1288174
H	0.5770772	-5.0603288	-2.3905925
H	0.0750375	-3.5306109	-1.6470320
C	1.4409093	-3.9373732	-4.8252471
H	0.4822565	-3.9493296	-5.3558653
H	2.1659235	-3.3962263	-5.4408430
H	1.7846961	-4.9734834	-4.7335262
C	4.6599608	-0.5479071	-0.7307502
H	3.8589224	0.1904372	-0.8466593
C	5.9170227	-0.0196223	-1.4467068
H	6.2452100	0.9231305	-0.9964476
H	6.7360293	-0.7428362	-1.3616987
H	5.7334807	0.1536726	-2.5104906
C	4.9446901	-0.7032556	0.7725268
H	5.2093198	0.2676101	1.2040464
H	4.0680942	-1.0863036	1.3035541
H	5.7812314	-1.3880712	0.9503776
C	4.0293459	-0.7817009	-4.8284369
H	4.3487600	-0.2119399	-5.7102515
H	4.9081337	-0.9552989	-4.2007791
H	3.6748905	-1.7590064	-5.1706996
C	3.2471249	1.8981037	-3.4951111
H	3.3865640	2.5068176	-4.3968790
H	2.4955603	2.3937914	-2.8712206
H	4.1899488	1.8962201	-2.9403100
C	1.1824748	0.3179300	-5.0581405
H	1.4077668	0.9804007	-5.9031234
H	0.8737970	-0.6509159	-5.4626190
H	0.3281255	0.7430428	-4.5226535
Ge	-1.1752714	0.8055147	1.1259949
Si	-0.7797558	-1.7739087	0.4555345
Si	-1.3312143	-0.2138317	-1.1497913
N	-1.4351458	-2.9582297	1.5576828
N	-2.7086753	0.1375354	-2.1685320
Si	-2.7457095	-4.1220926	1.2782673
C	-0.6591803	-3.0820004	2.7826600
Si	-3.3320843	-0.9359465	-3.4311713
C	-3.3637827	1.4164743	-1.9631087
C	-2.3674940	-5.1772816	-0.2308727
C	-2.8861447	-5.2506129	2.7712576

C	-4.3441316	-3.1778620	1.0170348
C	0.4706190	-3.9311211	2.8091793
C	-1.0347882	-2.3380441	3.9247279
C	-4.7800723	-0.0981506	-4.2815771
C	-3.8731748	-2.5642353	-2.6715783
C	-1.9802554	-1.3105836	-4.6779456
C	-2.9562084	2.5367606	-2.7203332
C	-4.4261452	1.5270248	-1.0376680
H	-3.2311003	-5.8035327	-0.4869214
H	-2.1282014	-4.5717447	-1.1095692
H	-1.5153979	-5.8395338	-0.0446368
H	-3.7003682	-5.9671572	2.6026358
H	-1.9670566	-5.8204779	2.9370788
H	-3.1016412	-4.7069206	3.6949070
H	-5.1676063	-3.8533732	0.7560625
H	-4.6272211	-2.6262302	1.9192902
H	-4.2369113	-2.4546502	0.2039876
C	1.1767714	-4.0641111	4.0092459
C	0.9593480	-4.6876726	1.5831682
C	-0.2977199	-2.5125800	5.1009531
C	-2.1937291	-1.3520074	3.9167088
H	-5.1903151	-0.7717238	-5.0446617
H	-5.5845665	0.1493140	-3.5826581
H	-4.4837049	0.8310042	-4.7772041
H	-4.1104803	-3.2997102	-3.4500136
H	-3.0682613	-2.9800873	-2.0567946
H	-4.7549590	-2.4517564	-2.0337971
H	-2.3011685	-2.0969894	-5.3722816
H	-1.7117608	-0.4287568	-5.2672410
H	-1.0733447	-1.6624651	-4.1745553
C	-3.6809971	3.7273545	-2.6061938
C	-1.7381210	2.4958127	-3.6265739
C	-5.1176636	2.7402806	-0.9547191
C	-4.8456429	0.3719296	-0.1439486
H	2.0453235	-4.7169687	4.0413977
C	0.7935479	-3.3731550	5.1528390
H	0.3259156	-4.4020830	0.7377127
C	0.8456220	-6.2118374	1.7677348
C	2.4054332	-4.3086956	1.2261711
H	-0.5798663	-1.9527201	5.9882502
H	-2.4717029	-1.1816910	2.8711923
C	-3.4267297	-1.9042335	4.6554174
C	-1.7927870	0.0034049	4.5229641
H	-3.3815684	4.5883834	-3.1988348
C	-4.7677788	3.8294882	-1.7451564
H	-1.3024096	1.4961363	-3.5336932
C	-0.6829399	3.5119495	-3.1612858
C	-2.0913490	2.7302920	-5.1047144
H	-5.9462700	2.8294253	-0.2571453
H	-4.0777722	-0.4027883	-0.2378140
C	-6.1938893	-0.2242893	-0.5874875
C	-4.9185078	0.7855720	1.3355366
H	1.3530067	-3.4909430	6.0767751
H	-0.1828103	-6.5201996	1.9768807
H	1.1816238	-6.7285307	0.8614735
H	1.4722764	-6.5493779	2.6008669
H	2.4984661	-3.2323170	1.0532222
H	3.0978729	-4.5849146	2.0293115
H	2.7188069	-4.8228852	0.3134060
H	-4.2361753	-1.1653518	4.6421493
H	-3.7985477	-2.8241398	4.1970601
H	-3.1834298	-2.1235427	5.7013871
H	-2.5970309	0.7320280	4.3753431
H	-1.6093938	-0.0788870	5.6004107
H	-0.8908843	0.4016667	4.0514991
H	-5.3240443	4.7598678	-1.6721491
H	0.2232530	3.4302422	-3.7713228
H	-1.0554779	4.5389287	-3.2427959
H	-0.4118731	3.3331051	-2.1155761

H	-1.1888397	2.6789072	-5.7239606
H	-2.7994266	1.9819915	-5.4719498
H	-2.5429811	3.7184781	-5.2462249
H	-6.4691607	-1.0668650	0.0561092
H	-6.9858151	0.5302300	-0.5203504
H	-6.1578780	-0.5799749	-1.6207117
H	-5.1366956	-0.0891674	1.9574182
H	-3.9707673	1.2173957	1.6713274
H	-5.7116764	1.5221981	1.5050292

(3) $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$

178
Energy = -10827.79496294 Hartree

Si	1.1582946	-0.6600803	1.0628344
Ge	0.7514907	1.8013915	-0.0292189
Ge	1.0579162	-0.2224331	-1.4130791
Si	2.8627007	4.1864409	0.3595724
Si	2.8062201	0.1735590	-4.0479616
N	1.6153932	3.1222671	0.9991873
N	2.3804488	-0.7750869	-2.6306228
C	0.9736764	3.3529963	2.2646314
C	-0.1759960	4.1776356	2.3359782
C	-0.7617939	4.4049858	3.5853290
H	-1.6411783	5.0410781	3.6489697
C	-0.2464486	3.8288924	4.7406667
H	-0.7141358	4.0189768	5.7028168
C	0.8574615	2.9865498	4.6533582
H	1.2406474	2.5133363	5.5531096
C	1.4756069	2.7193724	3.4280958
C	-0.8050989	4.8126534	1.1046621
H	-0.2576359	4.4529765	0.2273834
C	-0.6886944	6.3475521	1.1316946
H	0.3537501	6.6720161	1.1975818
H	-1.1261342	6.7777757	0.2234473
H	-1.2235961	6.7612473	1.9939456
C	-2.2760213	4.3979707	0.9367416
H	-2.3742935	3.3090803	0.8820394
H	-2.8863737	4.7505289	1.7756736
H	-2.6878773	4.8204189	0.0153325
C	2.6554031	1.7604681	3.3778041
H	2.7850432	1.4642363	2.3311427
C	3.9587399	2.4326846	3.8474509
H	4.7909077	1.7207074	3.8002209
H	4.2142965	3.2969446	3.2292664
H	3.8623768	2.7765469	4.8838219
C	2.4037396	0.4867173	4.2008335
H	3.2060362	-0.2372601	4.0222836
H	2.3807699	0.6998039	5.2758176
H	1.4582844	0.0115682	3.9262175
C	2.2779032	4.9655758	-1.2518120
H	3.0816227	5.5507150	-1.7159690
H	1.9659465	4.2066283	-1.9775294
H	1.4264415	5.6345236	-1.0858807
C	3.2171284	5.5455570	1.6057072
H	4.0295214	6.1824758	1.2337341
H	2.3406416	6.1807474	1.7664922
H	3.5167704	5.1526277	2.5813643
C	4.4063894	3.1737214	0.0135374
H	5.1753816	3.7730979	-0.4887785
H	4.8349314	2.7722150	0.9374074
H	4.1684471	2.3267293	-0.6382988
C	3.0901154	-1.9758153	-2.2789541
C	2.6492138	-3.2167450	-2.7971041
C	3.3847702	-4.3701481	-2.5101032
H	3.0542084	-5.3247351	-2.9119163
C	4.5283653	-4.3169776	-1.7196292
H	5.0923971	-5.2217725	-1.5104824

C	4.9320814	-3.1000004	-1.1816399
H	5.8139118	-3.0618302	-0.5474639
C	4.2265243	-1.9196563	-1.4377519
C	1.3774570	-3.3262621	-3.6209032
H	1.0597020	-2.3071949	-3.8597798
C	0.2637099	-3.9836665	-2.7863757
H	-0.6711073	-4.0373348	-3.3557428
H	0.5454590	-5.0005879	-2.4914382
H	0.0761251	-3.4088291	-1.8720923
C	1.5807272	-4.0810417	-4.9438793
H	0.6541302	-4.0710770	-5.5288716
H	2.3719455	-3.6232868	-5.5456496
H	1.8535408	-5.1278647	-4.7708573
C	4.7178411	-0.6165427	-0.8297735
H	3.9472061	0.1397777	-1.0144676
C	6.0209723	-0.1499111	-1.5045687
H	6.3432753	0.8122144	-1.0913577
H	6.8210450	-0.8796890	-1.3360098
H	5.8950942	-0.0367742	-2.5852231
C	4.9184420	-0.7249950	0.6907577
H	5.2065309	0.2486693	1.1007464
H	3.9973636	-1.0460353	1.1870769
H	5.7103654	-1.4404192	0.9384129
C	4.0828111	-0.7857685	-5.0343263
H	4.4184753	-0.1910106	-5.8928514
H	4.9618459	-1.0379859	-4.4327162
H	3.6670583	-1.7236852	-5.4164987
C	3.4723435	1.8563946	-3.5386666
H	3.6172312	2.5047104	-4.4117781
H	2.7595679	2.3552535	-2.8718083
H	4.4273682	1.7855681	-3.0093701
C	1.2729847	0.4782900	-5.0908489
H	1.4926614	1.1780678	-5.9067440
H	0.8885891	-0.4465694	-5.5322869
H	0.4706915	0.9171369	-4.4870062
Si	-1.1354802	0.7829495	1.0584776
Ge	-0.8091502	-1.8428177	0.3912086
Si	-1.3807067	-0.1007880	-1.1588448
N	-1.4959642	-3.0243403	1.6811564
N	-2.7529071	0.2109883	-2.1786984
Si	-2.7737251	-4.1945675	1.3717009
C	-0.6863447	-3.0675710	2.8699016
Si	-3.3132843	-0.8890988	-3.4518247
C	-3.4395412	1.4705724	-1.9645742
C	-2.3558112	-5.2296551	-0.1451626
C	-2.9432166	-5.3280251	2.8587094
C	-4.3729566	-3.2618237	1.0565108
C	0.4683710	-3.8854752	2.9123467
C	-1.0334843	-2.2547897	3.9765714
C	-4.7776857	-0.1005864	-4.3182756
C	-3.8031952	-2.5308633	-2.6869095
C	-1.9138015	-1.1985272	-4.6630156
C	-3.0511784	2.6058492	-2.7090673
C	-4.4975263	1.5461777	-1.0321179
H	-3.2011742	-5.8702838	-0.4255514
H	-2.1182766	-4.6033186	-1.0118375
H	-1.4914412	-5.8761691	0.0410861
H	-3.7491398	-6.0509928	2.6799543
H	-2.0224714	-5.8906248	3.0414718
H	-3.1782855	-4.7816757	3.7766608
H	-5.1823073	-3.9376858	0.7551809
H	-4.6954601	-2.7182627	1.9506002
H	-4.2362029	-2.5296490	0.2543154
C	1.2171717	-3.9266175	4.0928048
C	0.9384764	-4.6965247	1.7144846
C	-0.2558700	-2.3391522	5.1354760
C	-2.2144544	-1.2971042	3.9327255
H	-5.1548409	-0.7813661	-5.0916869
H	-5.5986473	0.1113772	-3.6264494

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H    -4.5076358    0.8427202   -4.8022852
H    -4.0245755   -3.2742910   -3.4625077
H    -2.9848527   -2.9243775   -2.0743660
H    -4.6853622   -2.4390845   -2.0458785
H    -2.1745850   -1.9984401   -5.3669858
H    -1.6733294   -0.3024406   -5.2432033
H    -1.0044230   -1.5051897   -4.1342130
C    -3.7937979    3.7829205   -2.5718086
C    -1.8331620    2.5947779   -3.6177043
C    -5.2071584    2.7471590   -0.9267590
C    -4.8866650    0.3696823   -0.1520086
H     2.1030784   -4.5554692    4.1353644
C     0.8552399   -3.1738898    5.2040334
H     0.2595970   -4.4867038    0.8820211
C     0.8892206   -6.2099923    1.9908862
C     2.3524163   -4.2837762    1.2733304
H    -0.5181323   -1.7276116    5.9942354
H    -2.4806623   -1.1617387    2.8786589
C    -3.4427536   -1.8720879    4.6616912
C    -1.8633943    0.0836804    4.5091735
H    -3.5113765    4.6584446   -3.1513597
C    -4.8766512    3.8537131   -1.7018739
H    -1.3957803    1.5928682   -3.5634523
C    -0.7763702    3.5915889   -3.1139191
C    -2.1860323    2.8812450   -5.0865551
H    -6.0326150    2.8134965   -0.2229331
H    -4.1182769   -0.3998527   -0.2799133
C    -6.2405920   -0.2281344   -0.5751049
C    -4.9182914    0.7558545    1.3363499
H     1.4481268   -3.2205071    6.1133830
H    -0.1194247   -6.5391865    2.2574789
H     1.2102313   -6.7683357    1.1040145
H     1.5577597   -6.4759611    2.8173588
H     2.3957831   -3.2146176    1.0437485
H     3.0889224   -4.4910334    2.0579205
H     2.6478439   -4.8329400    0.3744460
H    -4.2787952   -1.1647766    4.6125098
H    -3.7687694   -2.8171100    4.2198087
H    -3.2128924   -2.0555292    5.7176531
H    -2.6880468    0.7824298    4.3320651
H    -1.6923997    0.0379078    5.5908898
H    -0.9683160    0.4980084    4.0381372
H    -5.4458085    4.7745924   -1.6103215
H     0.1318984    3.5291502   -3.7233915
H    -1.1472095    4.6214772   -3.1595114
H    -0.5079613    3.3754209   -2.0746266
H    -1.2840281    2.8425992   -5.7074871
H    -2.9001611    2.1503100   -5.4767803
H    -2.6299079    3.8768686   -5.1965396
H    -6.4914668   -1.0877688    0.0556480
H    -7.0382692    0.5161637   -0.4719760
H    -6.2257594   -0.5602572   -1.6171238
H    -5.1267524   -0.1286121    1.9474687
H    -3.9572725    1.1726160    1.6533597
H    -5.6998701    1.4962890    1.5397377
```

(4) $Si_3Ge_3\{N(SiMe_3)Dipp\}_4$

```
178
Energy = -10827.79330323 Hartree
Si    1.1741811   -0.6685401    1.0759504
Ge    0.7448373    1.8208444    0.0019559
Ge    1.0976732   -0.2257935   -1.3739728
Si    2.8542623    4.1951661    0.3815016
Si    2.7997210    0.1446675   -4.0303947
N     1.6308605    3.1187997    1.0433371
N     2.4412210   -0.7676109   -2.5696136
C     0.9952623    3.3362159    2.3132854
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C	-0.1569258	4.1565090	2.3993596
C	-0.7397091	4.3639365	3.6537404
H	-1.6205260	4.9967899	3.7289829
C	-0.2202270	3.7719437	4.7991267
H	-0.6860461	3.9467370	5.7651039
C	0.8857000	2.9335142	4.6969186
H	1.2720228	2.4481201	5.5888071
C	1.5013917	2.6868474	3.4663655
C	-0.7921611	4.8071510	1.1790205
H	-0.2444814	4.4649383	0.2948531
C	-0.6850523	6.3421900	1.2309152
H	0.3552675	6.6719391	1.3035553
H	-1.1241221	6.7843018	0.3292506
H	-1.2236582	6.7385885	2.0989896
C	-2.2612708	4.3872898	1.0051575
H	-2.3544233	3.2992306	0.9316931
H	-2.8728848	4.7226372	1.8502846
H	-2.6758867	4.8224644	0.0907912
C	2.6845693	1.7336688	3.3944827
H	2.7974826	1.4421383	2.3444083
C	3.9923312	2.4125388	3.8415051
H	4.8279836	1.7058424	3.7779748
H	4.2305117	3.2787640	3.2192162
H	3.9129293	2.7549597	4.8797900
C	2.4554490	0.4556867	4.2173832
H	3.2588636	-0.2625772	4.0213162
H	2.4511587	0.6640767	5.2935151
H	1.5075322	-0.0237099	3.9579283
C	2.2266584	4.9735118	-1.2150514
H	3.0180945	5.5546853	-1.7045855
H	1.8913443	4.2128808	-1.9292059
H	1.3822321	5.6456688	-1.0274921
C	3.2314366	5.5504447	1.6251475
H	4.0290114	6.1958320	1.2361893
H	2.3549098	6.1780613	1.8131470
H	3.5599640	5.1536695	2.5900339
C	4.3948318	3.1932706	-0.0079374
H	5.1490731	3.7996558	-0.5240108
H	4.8471531	2.7863405	0.9022234
H	4.1447252	2.3502665	-0.6605693
C	3.1568631	-1.9644940	-2.2238285
C	2.7198250	-3.2089477	-2.7359708
C	3.4725611	-4.3543529	-2.4611336
H	3.1472761	-5.3123145	-2.8591969
C	4.6269447	-4.2888804	-1.6868430
H	5.2049109	-5.1873502	-1.4886853
C	5.0225520	-3.0689610	-1.1485754
H	5.9110302	-3.0224938	-0.5242155
C	4.2997321	-1.8967903	-1.3928183
C	1.4317586	-3.3297189	-3.5326276
H	1.0990574	-2.3146698	-3.7682769
C	0.3412574	-3.9877875	-2.6688360
H	-0.6056113	-4.0485140	-3.2174706
H	0.6338751	-5.0021425	-2.3752647
H	0.1709902	-3.4073318	-1.7547847
C	1.6096786	-4.0888596	-4.8565457
H	0.6689450	-4.0902483	-5.4185303
H	2.3812224	-3.6263573	-5.4799222
H	1.8965689	-5.1322911	-4.6857452
C	4.7727165	-0.5881705	-0.7824491
H	3.9872146	0.1542435	-0.9589195
C	6.0606705	-0.0917201	-1.4643590
H	6.3725565	0.8692134	-1.0407821
H	6.8742495	-0.8111506	-1.3174052
H	5.9185556	0.0364259	-2.5414468
C	4.9816791	-0.7006080	0.7365368
H	5.2558446	0.2755307	1.1500924
H	4.0672405	-1.0380062	1.2345956
H	5.7850785	-1.4050351	0.9787047

C	4.1114893	-0.7859000	-4.9974820
H	4.4052385	-0.2085131	-5.8828424
H	5.0096244	-0.9678296	-4.3987258
H	3.7416463	-1.7586480	-5.3374372
C	3.3942020	1.8685301	-3.5736129
H	3.5046568	2.5006492	-4.4633477
H	2.6685051	2.3542424	-2.9109180
H	4.3565176	1.8477036	-3.0523984
C	1.2389485	0.3351842	-5.0603976
H	1.4058907	1.0212719	-5.9000150
H	0.8992618	-0.6220812	-5.4686342
H	0.4219995	0.7457621	-4.4562385
Si	-1.1217538	0.7691812	1.0879947
Si	-0.7744456	-1.7686767	0.4969544
Ge	-1.4178678	-0.2049542	-1.1876723
N	-1.4115255	-2.9339941	1.6148597
N	-2.9280995	0.1546766	-2.2474361
Si	-2.7242997	-4.0862316	1.2930427
C	-0.6468561	-3.0437400	2.8459590
Si	-3.4822484	-0.9371747	-3.5070447
C	-3.5222779	1.4460796	-2.0325305
C	-2.3080692	-5.0956312	-0.2363523
C	-2.8908002	-5.2341300	2.7667959
C	-4.3067630	-3.1210644	1.0122436
C	0.4924431	-3.8793098	2.8845419
C	-1.0401588	-2.2948597	3.9778501
C	-4.9185806	-0.1318213	-4.4083785
C	-4.0241220	-2.5653821	-2.7418620
C	-2.0727880	-1.3081581	-4.6959404
C	-3.0883436	2.5602154	-2.7884660
C	-4.5462033	1.5966494	-1.0673413
H	-3.1498775	-5.7396806	-0.5188011
H	-2.0801253	-4.4551713	-1.0941440
H	-1.4369264	-5.7359992	-0.0621440
H	-3.7106919	-5.9404384	2.5844928
H	-1.9782919	-5.8147083	2.9328171
H	-3.1081803	-4.6973629	3.6943951
H	-5.1312485	-3.7817915	0.7189364
H	-4.6059551	-2.5804009	1.9159584
H	-4.1713054	-2.3857023	0.2131583
C	1.1864367	-4.0006928	4.0926594
C	1.0062894	-4.6232672	1.6610737
C	-0.3142967	-2.4574540	5.1627141
C	-2.2035818	-1.3147733	3.9458837
H	-5.3016580	-0.8109709	-5.1802001
H	-5.7429509	0.1034859	-3.7275325
H	-4.6230197	0.8015188	-4.8969827
H	-4.2426470	-3.3128197	-3.5145444
H	-3.2294221	-2.9712730	-2.1064053
H	-4.9182595	-2.4483630	-2.1211503
H	-2.3480762	-2.1052869	-5.3977622
H	-1.7890297	-0.4270414	-5.2801612
H	-1.1830678	-1.6424506	-4.1488473
C	-3.7526428	3.7809175	-2.6332161
C	-1.8958599	2.4785036	-3.7265298
C	-5.1796997	2.8370271	-0.9461876
C	-4.9722184	0.4456952	-0.1725138
H	2.0623099	-4.6429454	4.1364961
C	0.7830287	-3.3094455	5.2296179
H	0.3809153	-4.3399144	0.8086926
C	0.9063917	-6.1496226	1.8331684
C	2.4517728	-4.2216226	1.3251634
H	-0.6094362	-1.8945487	6.0439121
H	-2.4785628	-1.1656324	2.8964075
C	-3.4356847	-1.8606469	4.6904680
C	-1.8087494	0.0548582	4.5231528
H	-3.4334039	4.6368478	-3.2231595
C	-4.8049089	3.9203348	-1.7345227
H	-1.5276457	1.4482348	-3.6933506

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C    -0.7641641    3.3980347   -3.2364792
C    -2.2607265    2.8055703   -5.1837703
H    -5.9791097    2.9551168   -0.2191795
H    -4.2336331   -0.3506131   -0.3062664
C    -6.3472663   -0.1093994   -0.5842090
C    -4.9745107    0.8399911    1.3135170
H     1.3335889   -3.4186143    6.1599110
H    -0.1224634   -6.4697383    2.0225993
H     1.2632516   -6.6564412    0.9293793
H     1.5221748   -6.4861141    2.6747721
H     2.5332642   -3.1398119    1.1812430
H     3.1405737   -4.5102051    2.1271391
H     2.7781475   -4.7091313    0.4021748
H    -4.2521829   -1.1303950    4.6557542
H    -3.7953316   -2.7948042    4.2507905
H    -3.1966850   -2.0541971    5.7424649
H    -2.6195777    0.7744348    4.3678485
H    -1.6146711   -0.0047896    5.6001923
H    -0.9139242    0.4506108    4.0360184
H    -5.3142611    4.8744777   -1.6310659
H     0.1217118    3.2931873   -3.8727263
H    -1.0727294    4.4491564   -3.2525042
H    -0.4806406    3.1449297   -2.2091904
H    -1.3780585    2.7097373   -5.8262146
H    -3.0342455    2.1317291   -5.5632938
H    -2.6343993    3.8315693   -5.2746266
H    -6.6225272   -0.9596581    0.0499037
H    -7.1202526    0.6604361   -0.4794905
H    -6.3466439   -0.4439438   -1.6256505
H    -5.2100718   -0.0327871    1.9322072
H    -3.9951059    1.2218947    1.6188113
H    -5.7248744    1.6103850    1.5232608
```

(1) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

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178
Energy = -12615.30772502 Hartree
Ge    1.1377178    0.6772554    1.2334739
Ge    0.1746654   -1.8897920    0.6585115
Si   -1.2481933   -0.0545674    1.2115967
Si    0.8914852   -4.4145060    2.5588317
Si   -3.6790875   -0.7617490    3.0283875
N     1.3312790   -3.2140922    1.3506934
N    -2.3249988    0.2752109    2.5444639
C     2.5438612   -3.3178794    0.5833554
C     2.5643845   -4.0745156   -0.6136523
C     3.7621607   -4.1672833   -1.3298900
H     3.7856174   -4.7500892   -2.2474375
C     4.9151100   -3.5243190   -0.8953024
H     5.8369580   -3.6086506   -1.4642815
C     4.8751432   -2.7527045    0.2618722
H     5.7703894   -2.2290014    0.5848714
C     3.7017360   -2.6209177    1.0105165
C     1.3291515   -4.7756906   -1.1582675
H     0.4930631   -4.5434882   -0.4914827
C     1.5032875   -6.3051804   -1.1795533
H     1.7233793   -6.7003235   -0.1836149
H     0.5890486   -6.7859667   -1.5461039
H     2.3258454   -6.5936510   -1.8435719
C     0.9596880   -4.2681693   -2.5616586
H     0.7720461   -3.1897321   -2.5555630
H     1.7630206   -4.4672693   -3.2797557
H     0.0526381   -4.7640164   -2.9195194
C     3.6992557   -1.7389218    2.2498926
H     2.6522551   -1.5143171    2.4819092
C     4.3087696   -2.4597173    3.4665318
H     4.2957995   -1.8010356    4.3428172
H     3.7573528   -3.3694422    3.7163319
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H	5.3491898	-2.7402117	3.2657395
C	4.4302917	-0.4064537	2.0200574
H	4.2724097	0.2577891	2.8765417
H	5.5108067	-0.5538181	1.9090990
H	4.0615676	0.1056964	1.1274739
C	-0.6854706	-5.3147184	2.0597796
H	-1.0229101	-5.9775907	2.8664506
H	-1.5032196	-4.6195870	1.8446307
H	-0.5280188	-5.9275644	1.1655956
C	2.2735288	-5.6780037	2.7092697
H	2.0263457	-6.3984158	3.4994132
H	2.4058653	-6.2363652	1.7774643
H	3.2375737	-5.2246993	2.9559112
C	0.6004588	-3.5401151	4.1955429
H	0.2119085	-4.2266846	4.9573522
H	1.5244207	-3.0932306	4.5766219
H	-0.1303055	-2.7347817	4.0703246
C	-2.0491717	1.4653261	3.3279031
C	-2.6937424	2.6761380	2.9918709
C	-2.5148477	3.7870530	3.8220704
H	-3.0191963	4.7186099	3.5769777
C	-1.6991897	3.7209821	4.9464392
H	-1.5738405	4.5914984	5.5842810
C	-1.0220716	2.5404954	5.2324004
H	-0.3615345	2.4977255	6.0942645
C	-1.1730037	1.4009523	4.4346627
C	-3.5446565	2.8112571	1.7408401
H	-3.5529593	1.8333233	1.2503053
C	-2.9129110	3.8183359	0.7661130
H	-3.4907580	3.8685346	-0.1633297
H	-2.8778209	4.8236664	1.2002075
H	-1.8878175	3.5223061	0.5188864
C	-4.9990289	3.2011093	2.0513942
H	-5.5816703	3.2602827	1.1252540
H	-5.4774183	2.4697678	2.7094444
H	-5.0476860	4.1786177	2.5437132
C	-0.4050599	0.1389277	4.7935521
H	-0.5312750	-0.5663131	3.9649397
C	-0.9586996	-0.5125297	6.0740064
H	-0.4040454	-1.4280681	6.3061818
H	-0.8599007	0.1717490	6.9243041
H	-2.0166094	-0.7692535	5.9726180
C	1.1003717	0.4097446	4.9561802
H	1.6332658	-0.5323399	5.1222743
H	1.5149567	0.8849396	4.0620741
H	1.2964472	1.0617627	5.8145855
C	-4.5384917	0.0219598	4.5007231
H	-5.3495263	-0.6351029	4.8393413
H	-3.8602512	0.1835533	5.3435915
H	-4.9762567	0.9917782	4.2452204
C	-3.0402509	-2.4730928	3.4585106
H	-3.8693147	-3.1722403	3.6230203
H	-2.4334942	-2.8645973	2.6347501
H	-2.4174329	-2.4708798	4.3578630
C	-4.8909956	-0.9434044	1.6079339
H	-5.6553985	-1.6924522	1.8493232
H	-5.4008590	-0.0018932	1.3818774
H	-4.3804225	-1.2729031	0.6969599
Ge	1.1079972	-0.6648045	-1.2617109
Ge	0.1406457	1.8937144	-0.6605032
Si	-1.2833193	0.0461594	-1.1694543
N	1.2688571	3.2204650	-1.3941946
N	-2.3983506	-0.2931319	-2.4679037
Si	0.7808003	4.4205191	-2.5840821
C	2.5063100	3.3315047	-0.6688774
Si	-3.7767306	0.7322497	-2.9064962
C	-2.1390881	-1.4800214	-3.2616346
C	-0.7833273	5.3104048	-2.0292315
C	2.1494072	5.6922931	-2.7807355

C	0.4376619	3.5477472	-4.2115368
C	2.5626494	4.0848050	0.5292325
C	3.6543744	2.6462223	-1.1391550
C	-4.6730089	-0.0554498	-4.3544813
C	-3.1684241	2.4510389	-3.3508882
C	-4.9460619	0.8977446	-1.4489728
C	-2.7663929	-2.6951334	-2.9087951
C	-1.2980952	-1.4081939	-4.3948115
H	-1.1492339	5.9765199	-2.8207061
H	-1.5907392	4.6099844	-1.7929471
H	-0.6004988	5.9183535	-1.1366314
H	1.8679804	6.4152947	-3.5569395
H	2.3152389	6.2466645	-1.8519383
H	3.1055056	5.2455260	-3.0669701
H	0.0196516	4.2338010	-4.9580850
H	1.3498788	3.1058654	-4.6253739
H	-0.2845132	2.7386700	-4.0626037
C	3.7847002	4.1873690	1.2018082
C	1.3415762	4.7739492	1.1195401
C	4.8528744	2.7876716	-0.4332743
C	3.6149648	1.7657389	-2.3790460
H	-5.5001047	0.5947319	-4.6665385
H	-4.0188040	-0.2081604	-5.2177301
H	-5.0935923	-1.0301599	-4.0889238
H	-4.0094417	3.1416002	-3.4889149
H	-2.5414455	2.8473782	-2.5447898
H	-2.5728649	2.4571655	-4.2684982
H	-5.7247402	1.6400169	-1.6642117
H	-5.4395707	-0.0494013	-1.2106029
H	-4.4108521	1.2292787	-0.5530620
C	-2.6080493	-3.8028628	-3.7472710
C	-3.5754894	-2.8380022	-1.6312250
C	-1.1661493	-2.5449876	-5.1998859
C	-0.5488149	-0.1410323	-4.7744533
H	3.8358859	4.7680835	2.1194895
C	4.9273845	3.5571124	0.7236209
H	0.4822555	4.5279695	0.4879809
C	1.4977986	6.3056007	1.1253858
C	1.0339935	4.2711657	2.5393615
H	5.7408183	2.2734898	-0.7899801
H	2.5621410	1.5333656	-2.5741491
C	4.1758830	2.4917874	-3.6157421
C	4.3639850	0.4387500	-2.1767204
H	-3.0995901	-4.7377169	-3.4890646
C	-1.8281934	-3.7296092	-4.8963604
H	-3.5771487	-1.8601690	-1.1404460
C	-2.9023894	-3.8387963	-0.6777814
C	-5.0353398	-3.2417561	-1.8942947
H	-0.5330820	-2.4965563	-6.0818422
H	-0.6529367	0.5618335	-3.9407238
C	-1.1460675	0.5098687	-6.0354429
C	0.9522121	-0.4031851	-4.9845984
H	5.8684971	3.6494161	1.2588329
H	1.6714029	6.6976681	0.1191913
H	0.5939065	6.7776341	1.5272633
H	2.3439133	6.6072108	1.7530020
H	0.8630007	3.1900025	2.5475770
H	1.8605525	4.4878905	3.2252693
H	0.1334489	4.7557172	2.9278588
H	4.1375681	1.8332689	-4.4914281
H	3.6089189	3.3970855	-3.8457005
H	5.2204712	2.7804088	-3.4513312
H	4.1815450	-0.2256489	-3.0281946
H	5.4464861	0.5947352	-2.1034027
H	4.0308161	-0.0774161	-1.2725583
H	-1.7184942	-4.5977229	-5.5403234
H	-3.4494435	-3.8952033	0.2697558
H	-2.8709387	-4.8434842	-1.1136729
H	-1.8729305	-3.5323068	-0.4634390

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H    -5.5871306   -3.3052304   -0.9497267
H    -5.5415234   -2.5155797   -2.5371325
H    -5.0910286   -4.2202600   -2.3838675
H    -0.6038693    1.4286926   -6.2834060
H    -1.0708520   -0.1724667   -6.8897150
H    -2.2015259    0.7608768   -5.8999166
H     1.4744080    0.5421496   -5.1655011
H     1.3971432   -0.8776477   -4.1048003
H     1.1249555   -1.0525669   -5.8500018
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(2) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

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178
Energy = -12615.29988917 Hartree
Ge    1.1802457    0.6754641    1.2354343
Si    0.3258235   -1.8466020    0.6265110
Ge   -1.2413440   -0.1664255    1.2685051
Si    0.8445209   -4.3086360    2.5038999
Si   -3.7355745   -0.8032938    3.1591838
N     1.3279764   -3.1097287    1.2882693
N    -2.3504066    0.1966332    2.7483070
C     2.5844661   -3.2747020    0.5779954
C     2.6181656   -4.0428189   -0.6091277
C     3.8468842   -4.2150310   -1.2551460
H     3.8862085   -4.8069586   -2.1659499
C     5.0106516   -3.6381263   -0.7598370
H     5.9561472   -3.7858615   -1.2744104
C     4.9536913   -2.8513804    0.3858826
H     5.8593215   -2.3785866    0.7555078
C     3.7502065   -2.6417245    1.0672107
C     1.3734686   -4.6711383   -1.2191293
H     0.5109382   -4.3549371   -0.6236568
C     1.4341128   -6.2091370   -1.1839697
H     1.5480088   -6.5876646   -0.1641481
H     0.5169508   -6.6335855   -1.6077354
H     2.2810704   -6.5765360   -1.7742638
C     1.1406089   -4.1880670   -2.6600858
H     1.0687775   -3.0969840   -2.7027795
H     1.9567666   -4.5013300   -3.3208143
H     0.2063399   -4.5999990   -3.0520473
C     3.7345848   -1.7382305    2.2913875
H     2.6874100   -1.5039024    2.5102420
C     4.3367385   -2.4316957    3.5273184
H     4.3200390   -1.7520393    4.3870376
H     3.7828874   -3.3345490    3.7970626
H     5.3778525   -2.7183818    3.3398068
C     4.4694474   -0.4117925    2.0336126
H     4.3193799    0.2684938    2.8787409
H     5.5480335   -0.5673227    1.9167857
H     4.0957832    0.0841976    1.1336186
C    -0.7298968   -5.1711153    1.9466330
H    -1.1254977   -5.8119480    2.7442132
H    -1.5122099   -4.4523365    1.6831328
H    -0.5493046   -5.7986558    1.0675748
C     2.2130705   -5.5800889    2.6790539
H     1.9316998   -6.3100509    3.4487525
H     2.3797731   -6.1253087    1.7452572
H     3.1683231   -5.1349077    2.9701430
C     0.5382903   -3.4231017    4.1276681
H     0.1590509   -4.1111899    4.8926400
H     1.4546363   -2.9601591    4.5076105
H    -0.2056290   -2.6314164    3.9957986
C    -2.0692829    1.4179446    3.4518790
C    -2.7222828    2.6155687    3.0776385
C    -2.5189144    3.7658045    3.8464740
H    -3.0305083    4.6850445    3.5710181
C    -1.6720878    3.7549153    4.9498106
H    -1.5316016    4.6550867    5.5419154
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C	-0.9829246	2.5898964	5.2714827
H	-0.2963717	2.5897451	6.1140510
C	-1.1542254	1.4159649	4.5317419
C	-3.5979045	2.6947785	1.8388868
H	-3.6556399	1.6863418	1.4178858
C	-2.9430799	3.6042752	0.7856062
H	-3.5444407	3.6298067	-0.1302242
H	-2.8426407	4.6302996	1.1567472
H	-1.9436309	3.2354731	0.5303808
C	-5.0287982	3.1654681	2.1447968
H	-5.6294271	3.1693791	1.2282339
H	-5.5184396	2.5105485	2.8716071
H	-5.0318295	4.1821613	2.5531102
C	-0.3735934	0.1696380	4.9114258
H	-0.4989154	-0.5453612	4.0922167
C	-0.9320782	-0.4729653	6.1936146
H	-0.3789915	-1.3869911	6.4368776
H	-0.8419592	0.2179684	7.0395924
H	-1.9890322	-0.7307561	6.0825544
C	1.1299847	0.4494535	5.0663631
H	1.6668664	-0.4861524	5.2567774
H	1.5414844	0.9012721	4.1583821
H	1.3288228	1.1244695	5.9061723
C	-4.6276786	-0.0227668	4.6155771
H	-5.4776620	-0.6510039	4.9100767
H	-3.9725421	0.0879544	5.4854161
H	-5.0129702	0.9715683	4.3696567
C	-3.1555618	-2.5363397	3.5957677
H	-4.0056965	-3.2152347	3.7364319
H	-2.5370939	-2.9445130	2.7889753
H	-2.5565138	-2.5493066	4.5118241
C	-4.8965503	-0.9487233	1.6866582
H	-5.6724693	-1.7019738	1.8720156
H	-5.3948609	-0.0003959	1.4616185
H	-4.3473766	-1.2542402	0.7886625
Ge	1.1487660	-0.6654342	-1.2683570
Si	0.2933026	1.8494770	-0.6350868
Ge	-1.2796320	0.1571637	-1.2285689
N	1.2659497	3.1174907	-1.3306145
N	-2.4307037	-0.2145456	-2.6736360
Si	0.7331653	4.3128587	-2.5289172
C	2.5445647	3.2909784	-0.6632386
Si	-3.8371986	0.7740221	-3.0374294
C	-2.1650421	-1.4341584	-3.3859315
C	-0.8270074	5.1648991	-1.9178598
C	2.0860053	5.5936119	-2.7515672
C	0.3769173	3.4245185	-4.1408908
C	2.6131702	4.0591621	0.5223286
C	3.6975612	2.6669342	-1.1924158
C	-4.7672913	-0.0100602	-4.4678264
C	-3.2860768	2.5132612	-3.4865247
C	-4.9522691	0.9052069	-1.5285575
C	-2.7991307	-2.6355436	-2.9917330
C	-1.2856332	-1.4264063	-4.4949492
H	-1.2549487	5.8016985	-2.7018688
H	-1.5945923	4.4410088	-1.6262756
H	-0.6203124	5.7950123	-1.0464318
H	1.7705142	6.3249082	-3.5066175
H	2.2855428	6.1360751	-1.8225994
H	3.0319924	5.1557604	-3.0813657
H	-0.0330042	4.1097204	-4.8925398
H	1.2825285	2.9672814	-4.5521397
H	-0.3568084	2.6280971	-3.9831058
C	3.8619788	4.2405913	1.1259122
C	1.3855713	4.6788644	1.1744233
C	4.9220834	2.8855607	-0.5526694
C	3.6467200	1.7636588	-2.4158225
H	-5.6312436	0.6116751	-4.7341795
H	-4.1380677	-0.1126100	-5.3575373

H	-5.1363289	-1.0084167	-4.2134351
H	-4.1460934	3.1851594	-3.5976462
H	-2.6455215	2.9243549	-2.6987275
H	-2.7169627	2.5340462	-4.4213025
H	-5.7396181	1.6528076	-1.6865764
H	-5.4356203	-0.0477919	-1.2911143
H	-4.3771355	1.2120762	-0.6474755
C	-2.6162240	-3.7835832	-3.7688998
C	-3.6315706	-2.7207509	-1.7240217
C	-1.1336023	-2.5983848	-5.2420126
C	-0.5230049	-0.1760201	-4.8971695
H	3.9280437	4.8328766	2.0349077
C	5.0123873	3.6725901	0.5907258
H	0.5051238	4.3541566	0.6104632
C	1.4323834	6.2172321	1.1333956
C	1.2075042	4.1979102	2.6238548
H	5.8180494	2.4197378	-0.9533677
H	2.5945185	1.5209619	-2.5982748
C	4.1999195	2.4620443	-3.6716512
C	4.4008687	0.4431615	-2.1845967
H	-3.1139931	-4.7056754	-3.4780877
C	-1.8068474	-3.7669136	-4.8999704
H	-3.6788830	-1.7133683	-1.2991825
C	-2.9372895	-3.6294019	-0.6955248
C	-5.0702528	-3.1965277	-1.9815415
H	-0.4752766	-2.5938149	-6.1068189
H	-0.6249104	0.5369157	-4.0729654
C	-1.1251687	0.4665864	-6.1593803
C	0.9759795	-0.4492151	-5.1006522
H	5.9738654	3.8274907	1.0725304
H	1.5066628	6.5939147	0.1092537
H	0.5275222	6.6354566	1.5886626
H	2.2969366	6.5929530	1.6920958
H	1.1473479	3.1063378	2.6718630
H	2.0431281	4.5206623	3.2550009
H	0.2835773	4.6024464	3.0469384
H	4.1592249	1.7821720	-4.5304083
H	3.6294410	3.3600655	-3.9218663
H	5.2444701	2.7574732	-3.5202490
H	4.2272292	-0.2378903	-3.0245886
H	5.4815216	0.6075836	-2.1051626
H	4.0627351	-0.0563960	-1.2726019
H	-1.6822508	-4.6653933	-5.4981601
H	-3.5067404	-3.6588638	0.2403352
H	-2.8455757	-4.6543840	-1.0717620
H	-1.9312096	-3.2569361	-0.4739424
H	-5.6390462	-3.2045128	-1.0448716
H	-5.5870992	-2.5420874	-2.6897080
H	-5.0833858	-4.2124388	-2.3915813
H	-0.5838369	1.3831716	-6.4188507
H	-1.0600015	-0.2225927	-7.0090770
H	-2.1788981	0.7201306	-6.0134441
H	1.5023924	0.4889665	-5.3070344
H	1.4183381	-0.9002153	-4.2068652
H	1.1507168	-1.1224328	-5.9472430

(3) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

178
Energy = -12615.24965525 Hartree

Si	1.1353708	0.6605860	1.1414828
Ge	0.2087097	-1.8918935	0.6796014
Ge	-1.2719964	0.0000438	1.2919142
Si	0.8946829	-4.3901764	2.5498781
Si	-3.7408078	-0.7351255	3.1488134
N	1.3850948	-3.1931344	1.3556705
N	-2.4130512	0.3436560	2.7406027
C	2.6022123	-3.2895295	0.5971609

C	2.6313433	-4.0381729	-0.6048726
C	3.8361944	-4.1265587	-1.3093497
H	3.8686743	-4.7030306	-2.2305524
C	4.9844275	-3.4844517	-0.8603162
H	5.9115084	-3.5653947	-1.4211850
C	4.9329365	-2.7156817	0.2984894
H	5.8238677	-2.1902343	0.6305167
C	3.7526000	-2.5895327	1.0368650
C	1.3970300	-4.7242395	-1.1710504
H	0.5531318	-4.4876496	-0.5153197
C	1.5538609	-6.2553313	-1.2001196
H	1.7478937	-6.6607265	-0.2028505
H	0.6423296	-6.7226384	-1.5899460
H	2.3871133	-6.5479066	-1.8488231
C	1.0525225	-4.2019325	-2.5759251
H	0.9081193	-3.1169605	-2.5687596
H	1.8506338	-4.4311536	-3.2909855
H	0.1283994	-4.6620313	-2.9382964
C	3.7300771	-1.7115526	2.2785430
H	2.6791199	-1.4940283	2.4992745
C	4.3282720	-2.4377669	3.4974519
H	4.2902311	-1.7911957	4.3818889
H	3.7849086	-3.3587018	3.7242360
H	5.3757496	-2.7018567	3.3118029
C	4.4523911	-0.3725162	2.0618734
H	4.2884194	0.2827906	2.9239766
H	5.5340507	-0.5104764	1.9501565
H	4.0800064	0.1448989	1.1736204
C	-0.7054771	-5.2167104	1.9978871
H	-1.1196308	-5.8461005	2.7952428
H	-1.4692412	-4.4758142	1.7349928
H	-0.5446757	-5.8494014	1.1181530
C	2.2422405	-5.6864065	2.7160692
H	1.9427429	-6.4361792	3.4591646
H	2.4197626	-6.2049400	1.7689971
H	3.1962434	-5.2577289	3.0367292
C	0.5959383	-3.5192438	4.1866021
H	0.1838022	-4.2040032	4.9376189
H	1.5225794	-3.0927805	4.5842009
H	-0.1190646	-2.6999620	4.0581615
C	-2.1015234	1.5180299	3.5094880
C	-2.7536924	2.7379544	3.2107370
C	-2.4890749	3.8566300	4.0059859
H	-2.9919909	4.7951508	3.7866644
C	-1.5906973	3.7913560	5.0663726
H	-1.3990860	4.6698833	5.6762601
C	-0.9241299	2.5991182	5.3269982
H	-0.2081230	2.5533179	6.1433294
C	-1.1560079	1.4530154	4.5596934
C	-3.6909557	2.8693395	2.0218123
H	-3.8908543	1.8596152	1.6515108
C	-2.9998169	3.6550471	0.8924142
H	-3.6514153	3.7316729	0.0147108
H	-2.7459336	4.6686089	1.2222861
H	-2.0712684	3.1588605	0.5871251
C	-5.0363299	3.5177853	2.3836093
H	-5.6998254	3.5173323	1.5116354
H	-5.5342931	2.9778977	3.1948609
H	-4.9074487	4.5580130	2.7022822
C	-0.4120355	0.1711764	4.8931469
H	-0.6122160	-0.5405012	4.0851296
C	-0.9332144	-0.4402406	6.2066398
H	-0.4313669	-1.3922055	6.4126436
H	-0.7413729	0.2366468	7.0469097
H	-2.0114587	-0.6205068	6.1627543
C	1.1086384	0.3837338	4.9670890
H	1.6126979	-0.5726683	5.1415903
H	1.4913887	0.8069987	4.0331804
H	1.3781822	1.0588424	5.7868392

C	-4.7222169	0.0467953	4.5437994
H	-5.5272771	-0.6269432	4.8620932
H	-4.0922783	0.2562489	5.4145596
H	-5.1776401	0.9924213	4.2327911
C	-3.0819205	-2.4194210	3.6605856
H	-3.9013697	-3.1331085	3.8120396
H	-2.4323046	-2.8254585	2.8767148
H	-2.4987751	-2.3745490	4.5855588
C	-4.8195638	-0.9892940	1.6308774
H	-5.5575023	-1.7828678	1.8020141
H	-5.3601572	-0.0768264	1.3599482
H	-4.2121858	-1.2839133	0.7669233
Si	1.1030596	-0.6528364	-1.1782022
Ge	0.1734496	1.8927702	-0.6870730
Ge	-1.3129548	-0.0097072	-1.2511789
N	1.3193449	3.2004758	-1.4019444
N	-2.4978869	-0.3619497	-2.6621243
Si	0.7830510	4.3953347	-2.5785653
C	2.5598378	3.3053403	-0.6834785
Si	-3.8464587	0.7066215	-3.0270825
C	-2.2028775	-1.5337858	-3.4413949
C	-0.8019665	5.2143767	-1.9740948
C	2.1178839	5.6982003	-2.7893583
C	0.4338696	3.5232242	-4.2046332
C	2.6226119	4.0533850	0.5176757
C	3.7006011	2.6148750	-1.1615102
C	-4.8656457	-0.0832302	-4.3900816
C	-3.2180299	2.3963156	-3.5591623
C	-4.8782911	0.9532957	-1.4756229
C	-2.8385026	-2.7578075	-3.1242478
C	-1.2903571	-1.4621923	-4.5199713
H	-1.2424281	5.8446492	-2.7565509
H	-1.5550720	4.4702858	-1.6903899
H	-0.6163068	5.8450529	-1.0978945
H	1.7856439	6.4525435	-3.5136662
H	2.3322340	6.2099645	-1.8462054
H	3.0595241	5.2757700	-3.1520056
H	-0.0047559	4.2065257	-4.9418589
H	1.3484565	3.0996815	-4.6321965
H	-0.2738970	2.7016013	-4.0529759
C	3.8496760	4.1522486	1.1812366
C	1.4018814	4.7281403	1.1254174
C	4.9039545	2.7511570	-0.4631796
C	3.6437201	1.7356932	-2.4012453
H	-5.6848796	0.5846304	-4.6836208
H	-4.2617071	-0.2893097	-5.2798625
H	-5.3046679	-1.0316346	-4.0642455
H	-4.0480455	3.1027093	-3.6851446
H	-2.5480551	2.8083425	-2.7958522
H	-2.6635235	2.3562882	-4.5018038
H	-5.6284114	1.7399183	-1.6244159
H	-5.4017520	0.0365950	-1.1860145
H	-4.2462292	1.2550285	-0.6321221
C	-2.5913968	-3.8743161	-3.9280979
C	-3.7380001	-2.8954815	-1.9072392
C	-1.0748473	-2.6064236	-5.2948750
C	-0.5655643	-0.1753489	-4.8757030
H	3.9080847	4.7286894	2.1011256
C	4.9877780	3.5205259	0.6933315
H	0.5377955	4.4805032	0.5007342
C	1.5431567	6.2609332	1.1441406
C	1.1127066	4.2069582	2.5430563
H	5.7876810	2.2333291	-0.8250950
H	2.5876154	1.5109944	-2.5876443
C	4.1974487	2.4641803	-3.6396187
C	4.3814964	0.4016761	-2.2066371
H	-3.0818096	-4.8159792	-3.6945233
C	-1.7258540	-3.8028797	-5.0151041
H	-3.9370310	-1.8868773	-1.5334542

```
C    -3.0041587   -3.6706427   -0.7976559
C    -5.0869238   -3.5589059   -2.2258068
H    -0.3843938   -2.5556783   -6.1326443
H    -0.7439224    0.5344012   -4.0608691
C    -1.1331588    0.4337559   -6.1709389
C     0.9531935   -0.3781341   -4.9992694
H     5.9325406    3.6097532    1.2225524
H     1.6966097    6.6649395    0.1393119
H     0.6413376    6.7198466    1.5652828
H     2.3961666    6.5644390    1.7613996
H     0.9805649    3.1203893    2.5441813
H     1.9323985    4.4477288    3.2292963
H     0.1964774    4.6577881    2.9358372
H     4.1353865    1.8160722   -4.5215712
H     3.6408003    3.3810112   -3.8499270
H     5.2485642    2.7355814   -3.4881554
H     4.1943140   -0.2557172   -3.0624134
H     5.4652190    0.5470378   -2.1298422
H     4.0413004   -0.1171901   -1.3064016
H    -1.5474318   -4.6798299   -5.6312228
H    -3.6276567   -3.7521290    0.0998066
H    -2.7494171   -4.6821751   -1.1330258
H    -2.0721309   -3.1636744   -0.5220914
H    -5.7236608   -3.5615295   -1.3341093
H    -5.6146529   -3.0273787   -3.0236606
H    -4.9573645   -4.5991501   -2.5441375
H    -0.6444092    1.3890405   -6.3924126
H    -0.9645674   -0.2413737   -7.0175819
H    -2.2105246    0.6070293   -6.0916911
H     1.4452595    0.5817163   -5.1884962
H     1.3687209   -0.8002752   -4.0789505
H     1.2003156   -1.0503211   -5.8284217
```

(4) $Si_4Ge_2\{N(SiMe_3)Dipp\}_4$

```
178
Energy = -12615.30377130 Hartree
Ge    1.1644756    0.6831048    1.2458231
Ge    0.2093686   -1.9035468    0.6571625
Si   -1.1988709   -0.0483122    1.2465862
Si    0.9067860   -4.4169143    2.5584247
Si   -3.6597828   -0.7437161    3.0073891
N     1.3804166   -3.2021545    1.3799991
N    -2.2684676    0.2736911    2.5835732
C     2.5928290   -3.2990287    0.6136128
C     2.6182079   -4.0475622   -0.5891292
C     3.8170696   -4.1269955   -1.3055101
H     3.8450689   -4.7043619   -2.2263567
C     4.9648035   -3.4767537   -0.8679522
H     5.8871003   -3.5508112   -1.4376953
C     4.9189419   -2.7104192    0.2928140
H     5.8097997   -2.1802389    0.6173422
C     3.7449118   -2.5933635    1.0424729
C     1.3878604   -4.7535608   -1.1397492
H     0.5454896   -4.5184960   -0.4814855
C     1.5646350   -6.2830400   -1.1501512
H     1.7728849   -6.6730058   -0.1497035
H     0.6560154   -6.7674293   -1.5257693
H     2.3961303   -6.5726988   -1.8024968
C     1.0262126   -4.2571921   -2.5493320
H     0.8485196   -3.1773099   -2.5553319
H     1.8281966   -4.4722317   -3.2644506
H     0.1143510   -4.7474256   -2.9029779
C     3.7296819   -1.7191496    2.2870104
H     2.6800260   -1.4915644    2.5039025
C     4.3137655   -2.4537337    3.5076345
H     4.2891753   -1.8033994    4.3899245
H     3.7511181   -3.3616556    3.7377894
```

H	5.3556249	-2.7397842	3.3228068
C	4.4707570	-0.3886694	2.0800353
H	4.3044194	0.2674347	2.9412552
H	5.5520098	-0.5398384	1.9824276
H	4.1160385	0.1339847	1.1873740
C	-0.6628649	-5.2989370	2.0024316
H	-1.0574911	-5.9349064	2.8047294
H	-1.4517940	-4.5901661	1.7287198
H	-0.4755044	-5.9356128	1.1310081
C	2.2796371	-5.6867660	2.7371451
H	1.9685978	-6.4645714	3.4461036
H	2.5022737	-6.1733031	1.7825835
H	3.2127686	-5.2509450	3.1051121
C	0.5719620	-3.5618803	4.1969059
H	0.1760053	-4.2597312	4.9445249
H	1.4832661	-3.1082610	4.6002682
H	-0.1653793	-2.7636600	4.0644883
C	-2.0010675	1.4558011	3.3798482
C	-2.6607879	2.6638294	3.0640488
C	-2.4779073	3.7682593	3.9020845
H	-2.9900783	4.6992503	3.6718875
C	-1.6499123	3.6958429	5.0174161
H	-1.5229763	4.5610810	5.6621405
C	-0.9655939	2.5156544	5.2875171
H	-0.2992376	2.4673607	6.1445814
C	-1.1172147	1.3836369	4.4794036
C	-3.5255284	2.8031870	1.8225941
H	-3.5969848	1.8131869	1.3624976
C	-2.8476086	3.7373116	0.8069527
H	-3.4435160	3.8069896	-0.1099077
H	-2.7291702	4.7468929	1.2160393
H	-1.8544479	3.3582491	0.5429081
C	-4.9504654	3.2871764	2.1353515
H	-5.5446963	3.3272113	1.2157031
H	-5.4551363	2.6187764	2.8394456
H	-4.9417465	4.2914244	2.5730011
C	-0.3502611	0.1169777	4.8226344
H	-0.4732238	-0.5765639	3.9838944
C	-0.9162445	-0.5516880	6.0887492
H	-0.3664191	-1.4719517	6.3129644
H	-0.8250368	0.1203950	6.9495584
H	-1.9738539	-0.8040314	5.9720002
C	1.1545471	0.3817622	4.9957208
H	1.6834387	-0.5632737	5.1575760
H	1.5752508	0.8614094	4.1067132
H	1.3493764	1.0269755	5.8594997
C	-4.5263362	0.0186354	4.4861333
H	-5.3651474	-0.6220928	4.7861120
H	-3.8603132	0.1285600	5.3471632
H	-4.9266259	1.0104191	4.2548659
C	-3.0658053	-2.4781090	3.4069597
H	-3.9129268	-3.1612800	3.5444442
H	-2.4534637	-2.8685253	2.5871330
H	-2.4593991	-2.5051267	4.3173715
C	-4.8385290	-0.8453003	1.5511863
H	-5.6080801	-1.6072734	1.7260652
H	-5.3432952	0.1081434	1.3673719
H	-4.3028587	-1.1188757	0.6360317
Ge	1.1442964	-0.6642043	-1.2489737
Si	0.2653249	1.8273920	-0.6436344
Ge	-1.3136375	0.1439500	-1.1922768
N	1.2253287	3.1189147	-1.3132105
N	-2.4851941	-0.2418105	-2.6191409
Si	0.7177063	4.3068505	-2.5315272
C	2.4984385	3.3053281	-0.6367856
Si	-3.8402588	0.7897506	-3.0458812
C	-2.2101662	-1.4569064	-3.3382547
C	-0.8560293	5.1637056	-1.9651160
C	2.0714332	5.5914236	-2.7257762

C	0.4081009	3.4118016	-4.1493626
C	2.5521608	4.0808228	0.5443065
C	3.6615474	2.6928167	-1.1570917
C	-4.7952078	-0.0227207	-4.4437613
C	-3.2297914	2.4878850	-3.5707392
C	-4.9570671	1.0395497	-1.5540769
C	-2.8481941	-2.6600517	-2.9544748
C	-1.3222488	-1.4472587	-4.4407346
H	-1.2534289	5.8069212	-2.7599087
H	-1.6378611	4.4451546	-1.7013518
H	-0.6718635	5.7889695	-1.0851311
H	1.7682535	6.3215372	-3.4870939
H	2.2500502	6.1344589	-1.7929408
H	3.0255052	5.1572359	-3.0362660
H	0.0048026	4.0910160	-4.9099586
H	1.3294719	2.9687013	-4.5403785
H	-0.3165267	2.6043687	-4.0079031
C	3.7949413	4.2787979	1.1548463
C	1.3140942	4.6907614	1.1848061
C	4.8796622	2.9279493	-0.5106871
C	3.6321070	1.7835956	-2.3768458
H	-5.6161104	0.6318847	-4.7623402
H	-4.1608063	-0.2170377	-5.3142477
H	-5.2278955	-0.9796296	-4.1361596
H	-4.0678740	3.1817128	-3.7116375
H	-2.5780886	2.9105996	-2.7984236
H	-2.6589970	2.4537332	-4.5037521
H	-5.7216457	1.7984985	-1.7620510
H	-5.4682777	0.1152716	-1.2665798
H	-4.3786359	1.3820661	-0.6883514
C	-2.6514755	-3.8086116	-3.7270220
C	-3.7059350	-2.7451058	-1.7042224
C	-1.1554995	-2.6208559	-5.1826574
C	-0.5672591	-0.1944395	-4.8499851
H	3.8489379	4.8763941	2.0611823
C	4.9547206	3.7206762	0.6296361
H	0.4419728	4.3577194	0.6133700
C	1.3471282	6.2293784	1.1431161
C	1.1296636	4.2086917	2.6327770
H	5.7829145	2.4701435	-0.9042088
H	2.5838608	1.5371908	-2.5762979
C	4.2064836	2.4759080	-3.6265545
C	4.3850879	0.4663275	-2.1245764
H	-3.1513033	-4.7313183	-3.4417655
C	-1.8257456	-3.7920930	-4.8458814
H	-3.7640544	-1.7353073	-1.2875041
C	-3.0347319	-3.6516357	-0.6583217
C	-5.1380901	-3.2240313	-1.9909337
H	-0.4880354	-2.6143104	-6.0403874
H	-0.6862763	0.5296985	-4.0374377
C	-1.1593027	0.4202277	-6.1311904
C	0.9365474	-0.4550224	-5.0350281
H	5.9114768	3.8879254	1.1166130
H	1.4268077	6.6060965	0.1193825
H	0.4342722	6.6394355	1.5899261
H	2.2029212	6.6139228	1.7092096
H	1.0724433	3.1168210	2.6797482
H	1.9612381	4.5329922	3.2683533
H	0.2029797	4.6111904	3.0515514
H	4.1806808	1.7914270	-4.4821745
H	3.6410468	3.3729051	-3.8916540
H	5.2483467	2.7718517	-3.4586084
H	4.2267764	-0.2215519	-2.9619580
H	5.4638890	0.6343241	-2.0286848
H	4.0343724	-0.0279330	-1.2148334
H	-1.6881106	-4.6917063	-5.4394173
H	-3.6229712	-3.6789776	0.2657060
H	-2.9361357	-4.6772902	-1.0307969
H	-2.0315805	-3.2827007	-0.4173951

H	-5.7267300	-3.2302009	-1.0665387
H	-5.6406131	-2.5725903	-2.7119245
H	-5.1411394	-4.2412108	-2.3979676
H	-0.6319772	1.3444896	-6.3926425
H	-1.0623157	-0.2782824	-6.9701342
H	-2.2210167	0.6524179	-6.0105043
H	1.4564266	0.4860655	-5.2445206
H	1.3742870	-0.8949180	-4.1336046
H	1.1248162	-1.1337343	-5.8743029

9.2 Cartesian coordinates of the most stable isomers of mixed silicon germanium clusters with {N(SiH$_3$)CH$_3$} substituents

$Si_4Ge_2\{N(SiH_3)CH_3\}_4$

```
42
Energy = -6856.550918193 Hartree
Ge     1.0327686     0.5430757    -1.5407714
Si     0.7541642    -1.9904201    -0.5007549
Si     1.0773345    -0.1971660     0.8785983
Si     3.4708962    -3.3134745    -0.6717935
Si     1.8516911     0.3160593     3.7584725
N      1.8806335    -3.0216430    -1.3270225
N      2.2437026     0.2908325     2.0640564
C      1.5710590    -3.5171976    -2.6868798
C      3.6152190     0.6550293     1.6426540
Ge    -1.2570733    -1.0093927    -1.4286853
Si    -0.8381123     1.5748477    -0.4830275
Si    -1.2390895    -0.1499440     0.9240629
N     -1.7526737     2.9364696    -1.0277635
N     -2.3986058    -0.4576152     2.1765921
Si    -3.2177814     3.4278160    -0.2096273
C     -1.3467953     3.6748527    -2.2456570
Si    -2.6073187     0.6537263     3.4972547
C     -3.2168844    -1.6906297     2.1444345
H      0.5190208    -3.3213349    -2.9186569
H      2.1854174    -3.0078710    -3.4392904
H      1.7489355    -4.5966449    -2.7551977
H      3.7730144    -4.7690484    -0.6908385
H      4.5209066    -2.6219388    -1.4666166
H      3.4794454    -2.8010519     0.7180406
H      0.4634793    -0.1819681     3.8973501
H      2.7813090    -0.5527799     4.5298424
H      1.9577235     1.6904362     4.3171770
H      3.8871076     1.6479466     2.0212516
H      4.3479454    -0.0742643     2.0091174
H      3.6714189     0.6813470     0.5496675
H     -1.6712396     1.7803782     3.2736520
H     -4.0075180     1.1544994     3.5518769
H     -2.3171298     0.0052355     4.8044953
H     -0.4098988     3.2604586    -2.6315040
H     -2.1108530     3.5844754    -3.0267275
H     -1.1931182     4.7371235    -2.0226675
H     -3.1149347     4.8441813     0.2297236
H     -4.3846514     3.3177322    -1.1236669
H     -3.3964297     2.5369332     0.9582013
H     -2.9697187    -2.3512429     2.9847291
H     -4.2858838    -1.4484169     2.1912400
H     -3.0302254    -2.2340670     1.2129953
```

$Si_3Ge_3\{N(SiH_3)CH_3\}_4$

```
42
Energy = -8644.008645231 Hartree
Ge     0.8576120     0.0222886     1.6426595
Ge     0.3628207     2.4165329     0.1972595
Si     0.7554739     0.3074277    -0.8704180
Si     3.3031605     3.4049150     0.4949329
Si     1.4695496    -0.6579666    -3.6438678
N      1.6706300     3.4455049     1.0706501
N      1.9110141    -0.3263196    -1.9927128
C      1.3683320     3.9516906     2.4200930
C      3.3000191    -0.5944045    -1.5550002
Ge    -1.5773954     1.2451092     1.3770114
Si    -0.8111815    -1.3532050     0.6687120
Si    -1.5687913     0.1343562    -0.8524026
N     -1.2573698    -2.9474080     1.1535376
N     -2.7490434     0.0566542    -2.1189949
Si    -2.6056067    -3.7755488     0.4056892
C     -0.5160873    -3.6503968     2.2266167
Si    -2.8334140    -1.2960509    -3.2091503
C     -3.6743648     1.1950397    -2.3225869
H      0.2656969    -2.9950923     2.6229769
H     -1.1906850    -3.9229983     3.0463084
H     -0.0436228    -4.5613223     1.8404062
H     -2.1444539    -4.9611722    -0.3627384
H     -3.5418390    -4.2471769     1.4587995
H     -3.2810707    -2.8148738    -0.4935441
H     -1.7605372    -2.2425267    -2.8241009
H     -4.1585080    -1.9677403    -3.1292710
H     -2.6416285    -0.8562553    -4.6170925
H     -3.5058521     1.6708716    -3.2964775
H     -4.7179404     0.8615816    -2.2697005
H     -3.5167703     1.9451935    -1.5412760
H      0.2836101     4.0253474     2.5598746
H      1.7594615     3.2845528     3.2011203
H      1.7984179     4.9505842     2.5655091
H      3.9244529     4.7557717     0.5685190
H      4.1725258     2.4765440     1.2735252
H      3.2587299     2.9403911    -0.9142510
H      3.4128196    -0.3268129    -0.4996722
H      3.5471269    -1.6572165    -1.6675848
H      4.0139878    -0.0017100    -2.1388758
H      2.3966151     0.0340372    -4.5783271
H      1.5306582    -2.1135094    -3.9438583
H      0.0862286    -0.1639402    -3.8361254
```

$Si_2Ge_4\{N(SiH_3)CH_3\}_4$

```
42
Energy = -10431.46006112 Hartree
Ge     1.4701329     0.5528377     1.2349105
Ge     0.4131678    -1.9850564     0.4875562
Si    -0.9312464    -0.1682834     1.1656306
Si     0.5873325    -4.1049503     2.7727127
Si    -3.7646546    -0.5567712     2.1191871
N      1.2716985    -3.3985580     1.3408397
N     -2.1570457     0.0662120     2.3650715
C      2.5746839    -3.8642629     0.8324033
C     -1.8195136     0.6770104     3.6707601
Ge     1.4290621    -0.5662376    -1.2928541
Ge     0.3891087     1.9686960    -0.5070793
Si    -0.9697622     0.1492844    -1.1458055
N      1.2039205     3.3997735    -1.3730345
N     -2.2348196    -0.0845646    -2.3039672
Si     0.4630961     4.1150463    -2.7722536
C      2.5179546     3.8748627    -0.9031328
Si    -3.8322214     0.5422145    -2.0066501
C     -1.9414255    -0.6967139    -3.6196645
H     -4.2121849     1.5221850    -3.0592409
H     -4.8503520    -0.5410754    -2.0076314
H     -3.7977443     1.2085138    -0.6836905
H      0.2515959     5.5767338    -2.5867135
H      1.3073555     3.9400832    -3.9856866
H     -0.8405349     3.4354948    -2.9663360
H     -4.1129912    -1.5357648     3.1835039
H     -4.7797091     0.5288809     2.1525769
H     -3.7740376    -1.2231566     0.7958478
H      0.3847569    -5.5708034     2.6114967
H      1.4711283    -3.9072436     3.9540972
H     -0.7159072    -3.4364136     3.0043323
H      2.8349617    -3.3217412    -0.0830188
H      3.3696355    -3.6848598     1.5679476
H      2.5484890    -4.9367935     0.6012457
H      2.8148272     3.3252359    -0.0032520
H      3.2896154     3.7129469    -1.6669861
H      2.4874635     4.9443853    -0.6589585
H     -0.8995854    -1.0307339    -3.6471741
H     -2.5856741    -1.5670419    -3.7930113
H     -2.0953873     0.0230230    -4.4330548
H     -0.7767491     1.0092577     3.6641273
H     -2.4561988     1.5483384     3.8657285
H     -1.9478187    -0.0429901     4.4883406
```

$Si_6\{N(SiH_3)CH_3\}_4$

```
42
Energy = -3281.588214406 Hartree
Si     1.0275316     0.5903401    -1.3996232
Si     0.7866177    -1.8918225    -0.4885007
Si     1.1088482    -0.1300545     0.9388431
Si     3.4135722    -3.3777138    -0.6759634
Si     1.9289096     0.2890458     3.8216677
N      1.8512719    -2.9659476    -1.3349960
N      2.2866452     0.3376769     2.1199010
C      1.5208886    -3.4083987    -2.7090164
C      3.6453652     0.7352435     1.6857739
Si    -1.1678449    -0.9131014    -1.3265626
Si    -0.8360115     1.5873116    -0.4588934
Si    -1.2029434    -0.1286321     0.9760053
N     -1.7583314     2.9108004    -1.0741384
N     -2.3853674    -0.4777510     2.1937695
Si    -3.2194174     3.4368169    -0.2713045
C     -1.3732621     3.5683485    -2.3444540
Si    -2.5987502     0.5843540     3.5542183
C     -3.2346779    -1.6855184     2.0860796
H      0.4866128    -3.1369529    -2.9430179
H      2.1757455    -2.9239080    -3.4432125
H      1.6271535    -4.4954771    -2.8006011
H      3.6071664    -4.8514107    -0.6957159
H      4.5122954    -2.7645370    -1.4686104
H      3.4538128    -2.8686527     0.7146581
H      0.5429377    -0.2140071     3.9657237
H      2.8715115    -0.6117722     4.5383956
H      2.0482326     1.6394526     4.4333285
H      3.9200372     1.7066585     2.1144678
H      4.3916426    -0.0081481     1.9916196
H      3.6736242     0.8247611     0.5951815
H     -1.6425274     1.7036252     3.3850420
H     -3.9918820     1.1043082     3.6055008
H     -2.3371327    -0.1172571     4.8396192
H     -0.4249235     3.1532314    -2.6997222
H     -2.1342563     3.3983834    -3.1151541
H     -1.2506173     4.6479407    -2.1996579
H     -3.1367587     4.8861730     0.0476574
H     -4.4031707     3.2286055    -1.1454614
H     -3.3534902     2.6408605     0.9693607
H     -3.0319395    -2.3842756     2.9070990
H     -4.2979080    -1.4163614     2.1088419
H     -3.0319530    -2.1968951     1.1401879
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$Ge_6\{N(SiH_3)CH_3\}_4$

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42
Energy = -14006.36171674 Hartree
Ge    1.4754214    0.5528144    1.2060113
Ge    0.4036549   -2.0181201    0.4969654
Ge   -1.0121307   -0.1728753    1.2469566
Si    0.7176858   -4.1021024    2.7980908
Si   -3.9162379   -0.5553860    2.3027148
N     1.3627285   -3.3532045    1.3678060
N    -2.3056804    0.0325987    2.5621145
C     2.7106588   -3.7109307    0.8892857
C    -1.9065015    0.5900924    3.8680012
Ge    1.4342646   -0.5753941   -1.2674219
Ge    0.3791477    1.9925855   -0.5176020
Ge   -1.0529735    0.1460723   -1.2278491
N     1.2909452    3.3509467   -1.4018806
N    -2.3914815   -0.0532433   -2.4983290
Si    0.5892600    4.1082295   -2.8010202
C     2.6463001    3.7266295   -0.9592805
Si   -3.9864000    0.5524317   -2.1883592
C    -2.0406273   -0.6178493   -3.8149717
H    -4.3690031    1.6041748   -3.1707710
H    -5.0097384   -0.5250761   -2.2717980
H    -3.9674672    1.1279052   -0.8223098
H     0.4993628    5.5833862   -2.6272042
H     1.4024678    3.8521343   -4.0209123
H    -0.7658032    3.5306950   -2.9694207
H    -4.2782037   -1.6039672    3.2961898
H    -4.9248144    0.5328563    2.4197089
H    -3.9472645   -1.1294826    0.9363042
H     0.6484080   -5.5809691    2.6478834
H     1.5625073   -3.8144930    3.9891773
H    -0.6416207   -3.5454534    2.9998917
H     2.9310847   -3.1801217   -0.0432866
H     3.4756137   -3.4311228    1.6252186
H     2.7871933   -4.7887663    0.6979013
H     2.9050295    3.1861888   -0.0422659
H     3.3929037    3.4721712   -1.7227333
H     2.7091316    4.8027422   -0.7537795
H    -1.0108469   -0.9904534   -3.8037612
H    -2.7001468   -1.4588462   -4.0651305
H    -2.1209231    0.1367121   -4.6085944
H    -0.8737736    0.9520015    3.8242090
H    -2.5487079    1.4372441    4.1414077
H    -1.9690001   -0.1657560    4.6619644
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10. References

[S1] a) P. v. d. Sluis, A. L. Spek, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **1990**, *46*, 194–201; b) A. L. Spek, *Acta Cryst.* **2015**, C*71*, 9–18.