Stereodivergent sila-germylenation vs sila-stannylenation of an internal alkyne

V. S. Ajithkumar,[ab] Pratiksha B. Ghanwat,[ab] Sougata Saha,[c] Swapan K Pati,*[c] and Sakya S. Sen*[ab]

[a]Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India.

[b]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

[c] Theoretical Sciences Unit, School of Advanced Materials (SAMat), Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore-560064, India.

Content

General Experimental Information. All experiments were carried out under argon atmosphere using Schlenk techniques or inside a MBRAUN or VTPL glove box. THF was purified by MBRAUN solvent purification system MB SPS-800 and stored over activated 4 Å molecular sieves prior to use. Benzene-d_6 was distilled over Na/benzophenone and stored over activated 4 Å molecular sieves prior to use. The precursors, [PhC(N*t*Bu)$_2$ESi(SiMe$_3$)$_3$] [E = Ge(**1**) and E = Sn(**2**)][S1] were synthesized by previously reported literature procedures. Chemicals purchased from Sigma Aldrich and TCI Chemicals were used without further purification. The ^{1}H, ^{13}C, and ^{29}Si NMR spectra were recorded in C_6D_6 using a Bruker Advance DPX 200 or a Bruker Advance DRX 400 or 500 spectrometers. NMR spectra were referenced to external SiMe$_4$ (^{1}H, ^{13}C, ^{29}Si) and SnMe$_4$ (^{119}Sn) respectively. Melting points were measured in a sealed glass tube using Stuart SMP-30 melting point apparatus and are uncorrected. High resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific.

Synthesis of compound 3*$_{cis}$*. To a THF (5 mL) solution of **1** (0.150 g, 0.27 mmol), dimethyl acetylenedicarboxylate (0.038 g, 0.27 mmol) dissolved in THF (5 mL) was added drop by drop via a cannula at −78 °C. Upon addition, the solution turned red in color. The reaction mixture was allowed to reach room temperature slowly and stirred further for 6 hr. Subsequently the solution was filtered through a celite pad and the resulting filtrate was concentrated to get red crystals of **3*$_{cis}$*** (0.181 g, 96 %). Mp: 109 °C.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 7.52-7.51 (d, 1H, *Ph*), δ 7.10-7.09 (d, 1H, *Ph*), δ 7.03-6.96 (m, 3H, *Ph*), δ 3.51 (s, 3H, GeCCOO*Me*), δ 3.42 (s, 3H, CCOO*Me*Si), δ 1.10 (s, 18H, *tBu*), δ 0.54(s, 27H, Si*Me*$_3$) ppm;

^{13}C{^{1}H} NMR (100.5 MHz, C_6D_6, 298 K): *δ* 172.4 (GeC*C*OOMe), *δ* 169.1 (*C*OOMeCSi), *δ* 167.4 (Ge*C*=C), *δ* 164.7 (GeC=*C*), *δ* 144.6 (N*C*N), *δ* 133.4 (*Ph*), *δ* 128.3 (*Ph*), *δ* 126.5 (*Ph*), *δ* 50.5 (*C*Me$_3$), *δ* 48.5 (GeCCOO*Me*), *δ* 47.4 (CCOO*Me*Si), *δ* 28.8 (C*Me*$_3$), *δ* 0.22 (Si*Me*$_3$) ppm;

^{29}Si{^{1}H} NMR (79.49 MHz, C_6D_6, 298 K): *δ* -12.13 {s, Si(*Si*Me$_3$)$_3$}, *δ* -74.97 {s, *Si*(SiMe$_3$)$_3$} ppm.

HRMS (CH_3CN): m/z calcd for $C_{30}H_{56}N_2O_4Si_4Ge$ $[M+H]^+$, 694.25; found, 694.6173.

Elemental analysis: $C_{30}H_{56}N_2O_4Si_4Ge$; Calculated: C, 51.94; H, 8.14; N, 4.04; Found: C, 51.63; H, 7.99; N, 3.92.

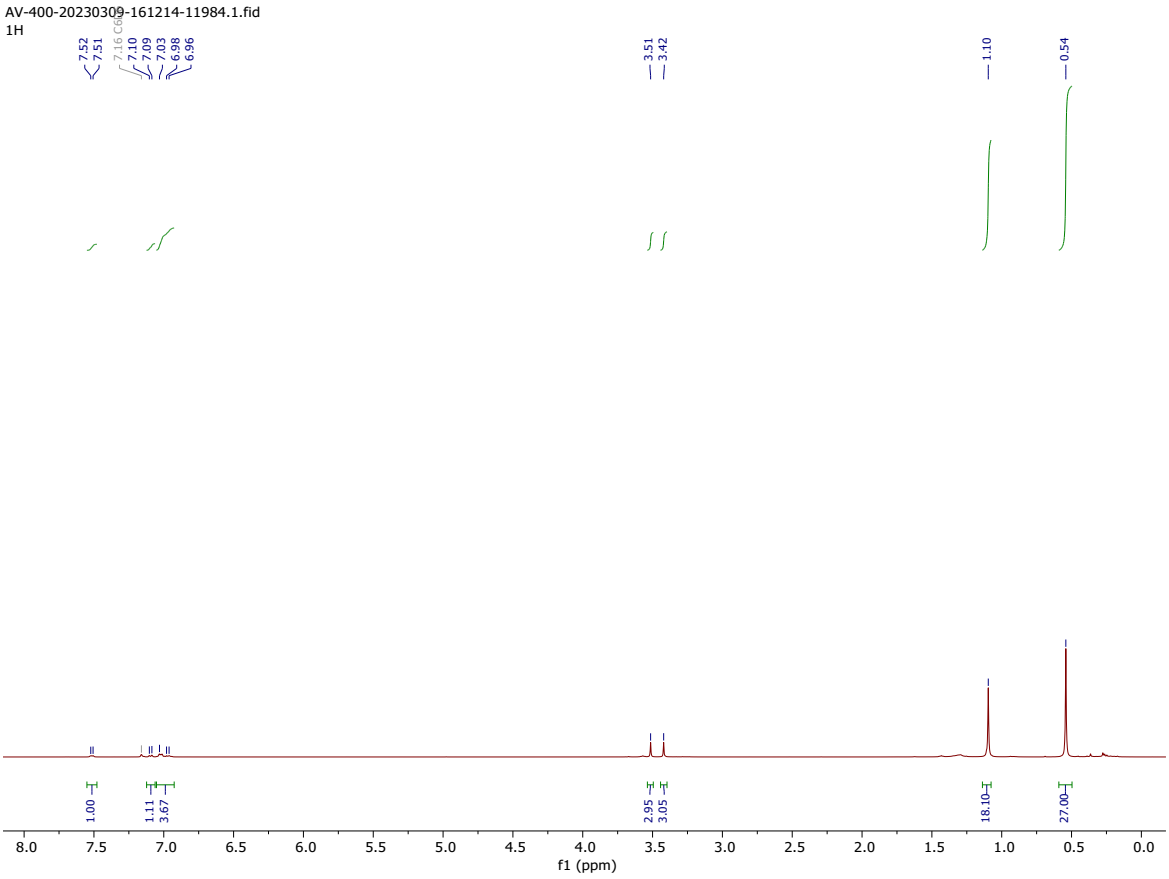


Figure S1. ^1H NMR Spectrum of $\mathbf{3}_{cis}$ (C_6D_6, 400 MHz, 298 K)

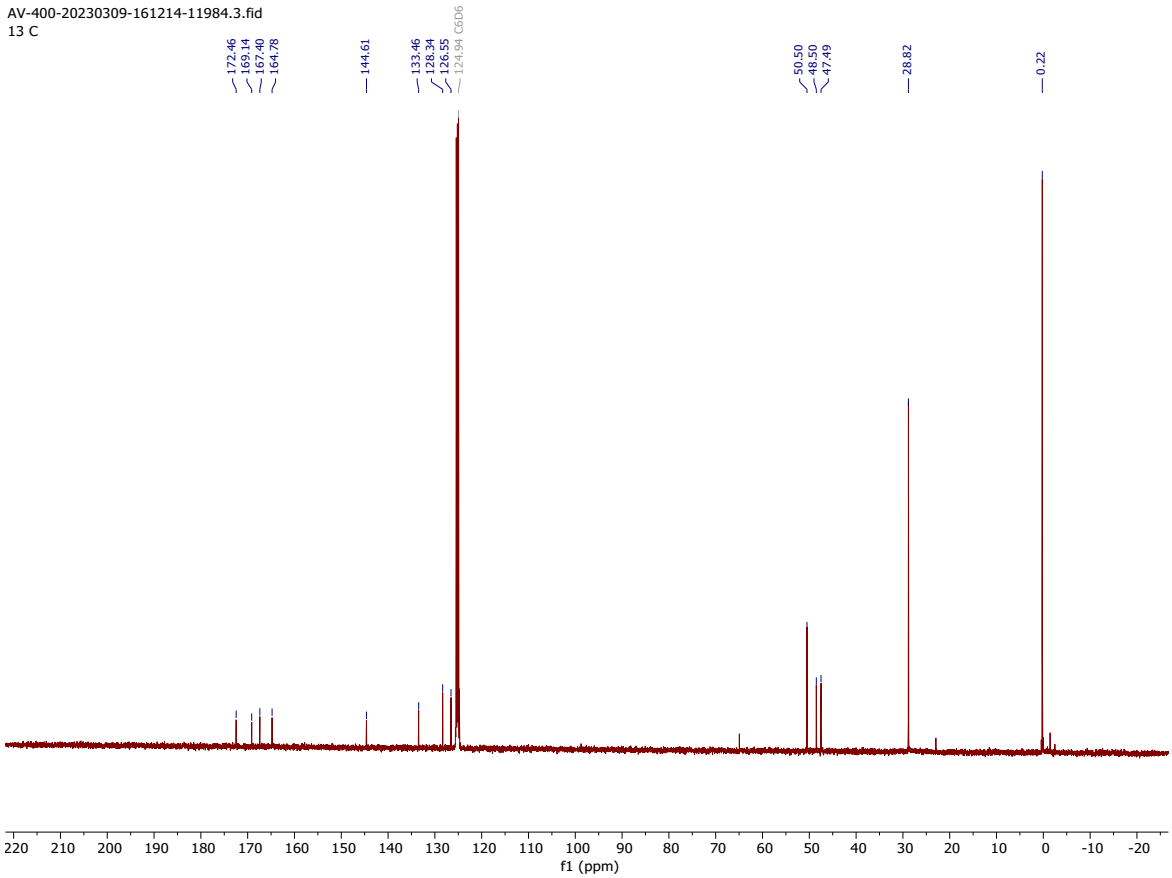


Figure S2. ^{13}C NMR Spectrum of $\mathbf{3}_{cis}$ (C_6D_6, 100.61 MHz, 298 K)

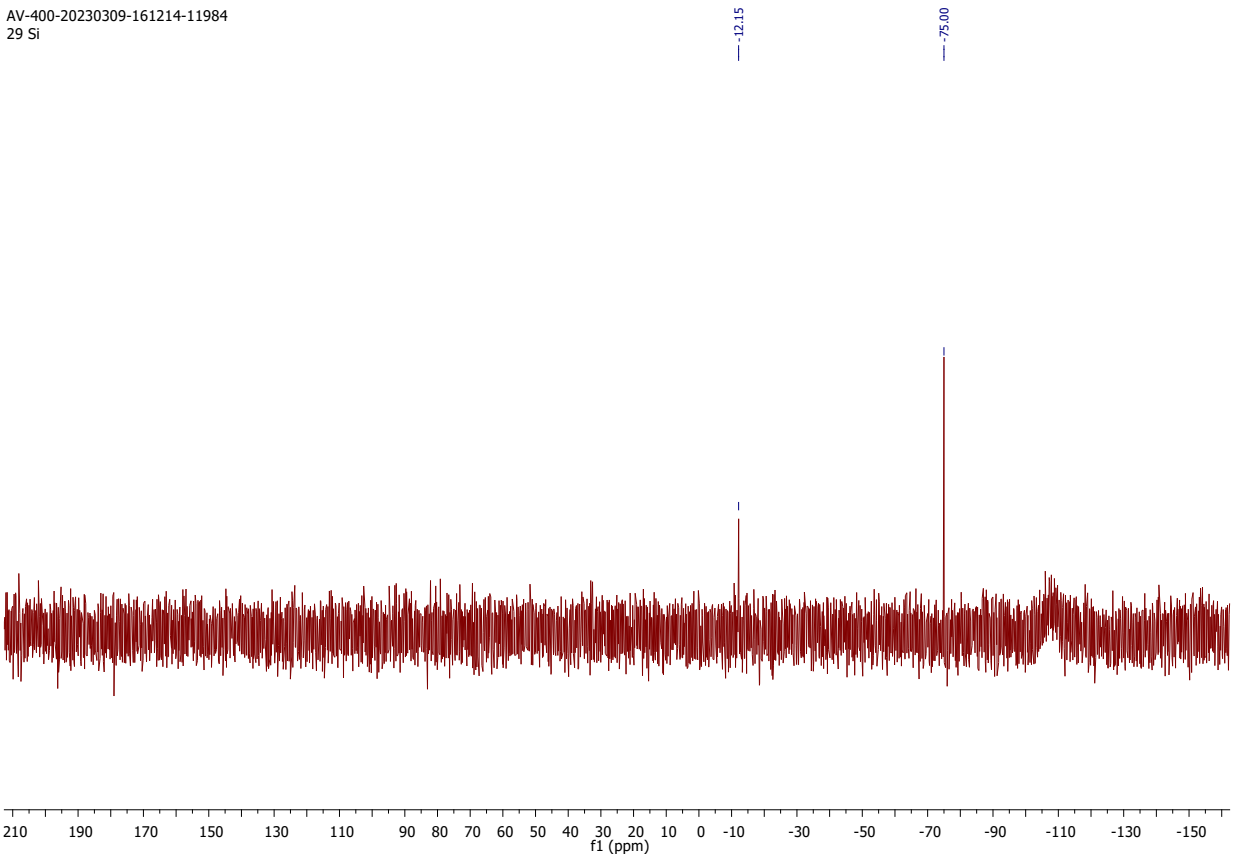


Figure S3. ^{29}Si NMR Spectrum of **3*cis*** (C_6D_6, 79.49 MHz, 298 K).

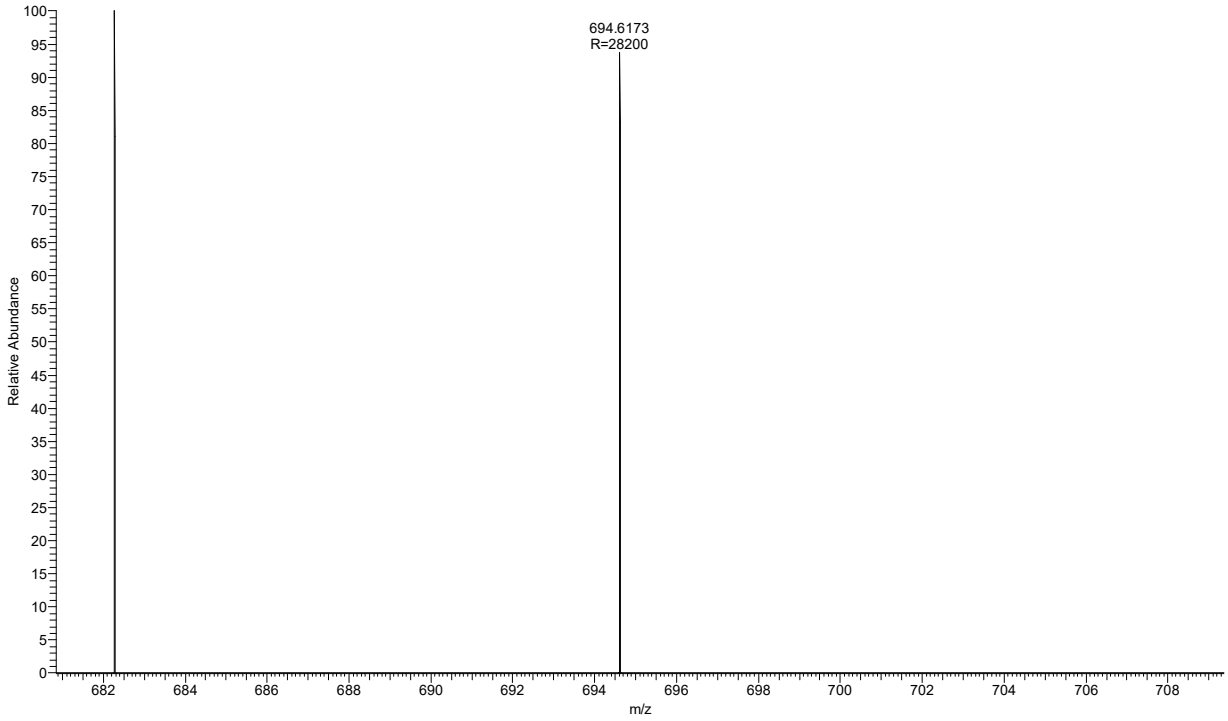


Figure S4. HRMS Spectrum of $\mathbf{3}_{cis}$

Synthesis of compound $\mathbf{4}_{trans}$. To a THF (5 mL) solution of **2** (0.150 g, 0.25 mmol), dimethyl acetylenedicarboxylate (0.035 g, 0.25 mmol) dissolved in THF (5 mL) was added drop by drop via a cannula at −78 °C. Upon addition, the solution turned dark red in color. The reaction mixture was allowed to reach room temperature slowly and stirred further for 6 hr. Subsequently the solution was filtered through a celite pad and the resulting filtrate was concentrated to get red crystals of $\mathbf{4}_{trans}$ (0.130 g, 70 %). Mp: 70 °C.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 7.66-7.64 (d, 1H, *Ph*), 7.11-7.09 (m, 1H, *Ph*), 7.03-6.96 (m, 3H, *Ph*), δ 3.74 (s, 3H, SnCCOO*Me*), δ 3.50 (s, 3H, CCOO*Me*Si), 1.06 (s, 18H, *tBu*), 0.41 (s, 27H, SiMe_3) ppm;

^{13}C{^{1}H} NMR (100.66 MHz, C_6D_6, 298 K): 174.4 (SnC*C*OOMe), δ 172.9 (*C*OOMeCSi), 171.9 (Sn*C*=C), 171.0 (SnC=*C*), 153.0 (N*C*N), 141 (Ph), 139.7 (Ph), 131.0 (Ph), 53.0 (*C*Me_3), 52.5

(*C*Me$_3$), 51.7 (*C*Me$_3$), 50.8 (SnCCOO*Me*), 50.2 (CCOO*Me*Si), 32.6 (C*Me*$_3$), 29.2 (C*Me*$_3$), 2.6 (Si*Me*$_3$), 1.4 (Si*Me*$_3$), 0.5 (Si*Me*$_3$) ppm;

^{29}Si{^{1}H} NMR (79.49 MHz, C_6D_6, 298 K): -11.4 {s, Si(*Si*Me$_3$)$_3$}, -76.9 {s, *Si*(SiMe$_3$)$_3$} ppm.

^{119}Sn{^{1}H} NMR (149.21 MHz, C_6D_6, 298 K): 0.66 ppm.

HRMS (CH_3CN): m/z calcd for $C_{30}H_{56}N_2O_4Si_4Sn$ $[M+H]^+$, 740.23; found, 741.2376.

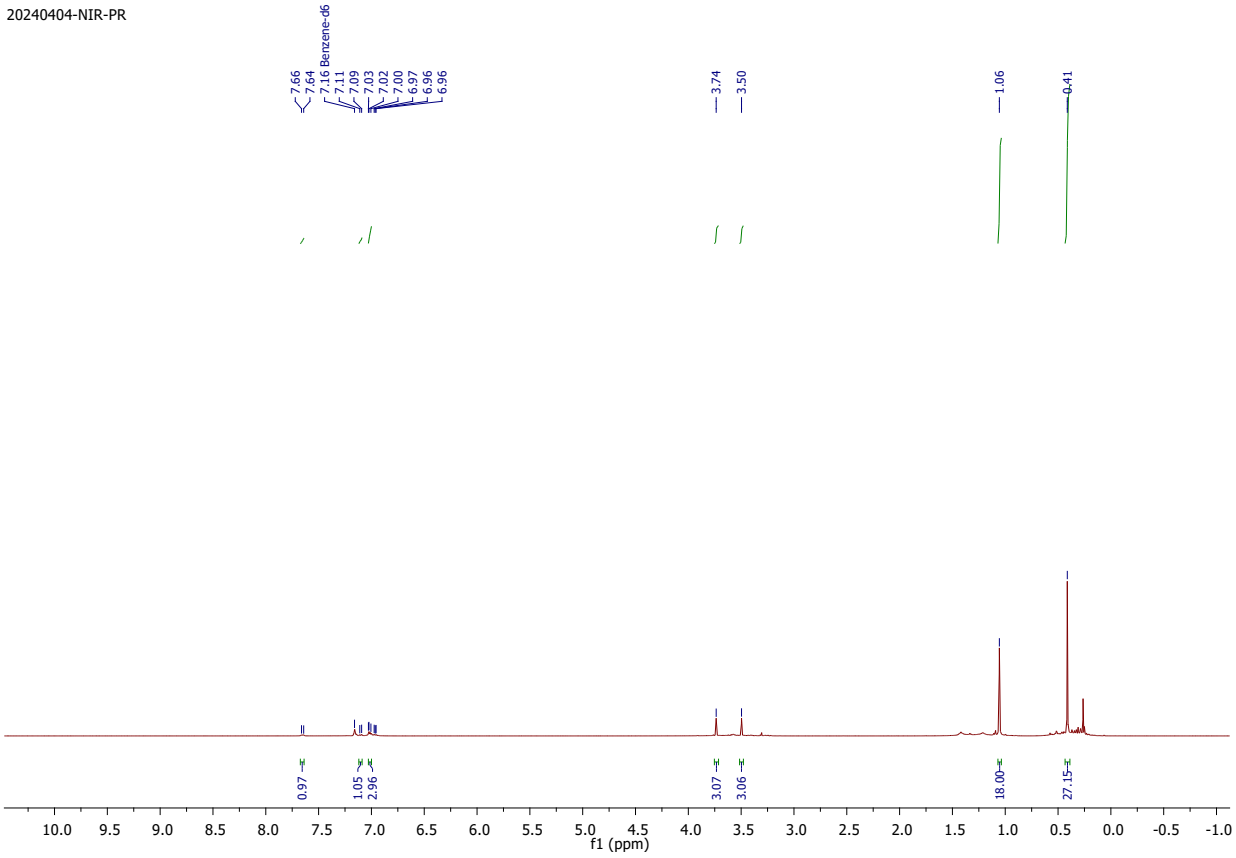


Figure S5. ^{1}H NMR Spectrum of **4*trans*** (C_6D_6, 400 MHz, 298 K)

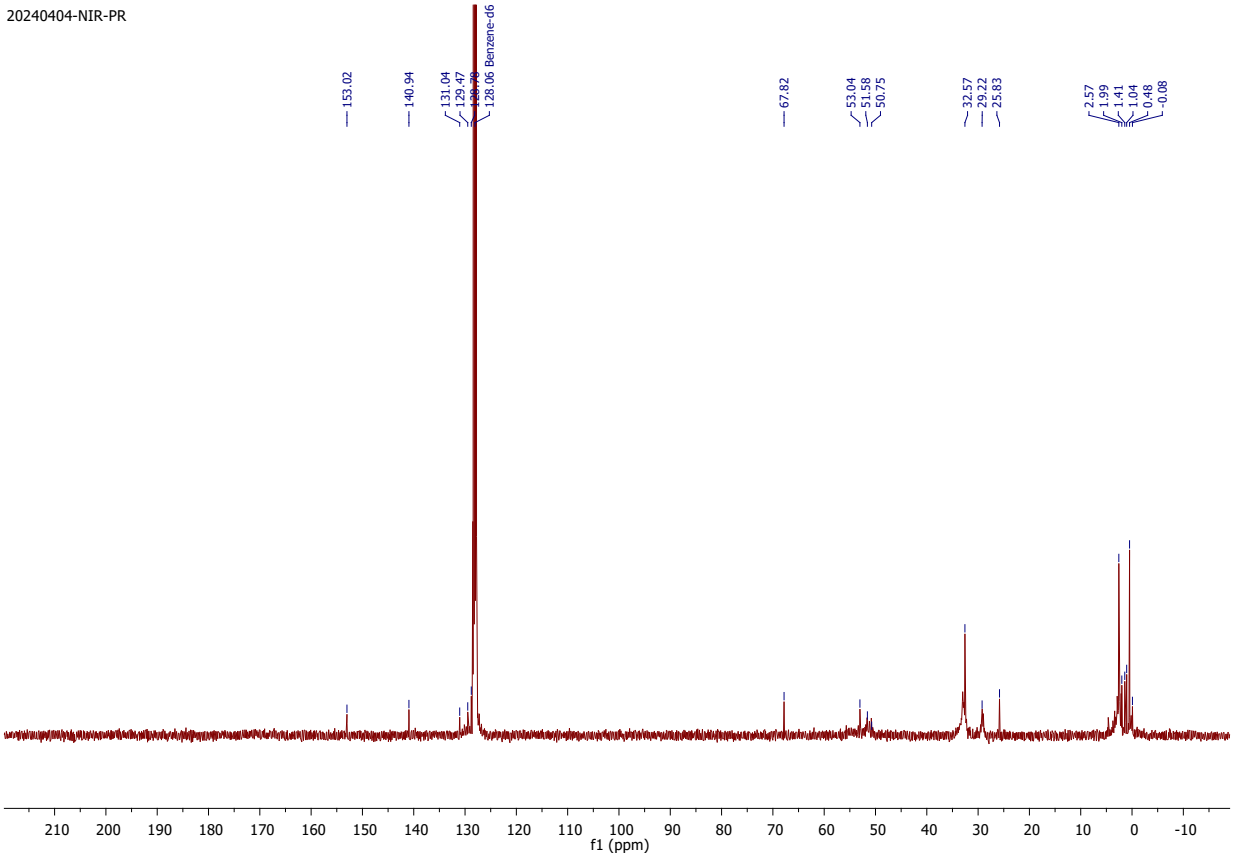


Figure S6. ^{13}C NMR Spectrum of **4*trans*** (C_6D_6, 100.61 MHz, 298 K)

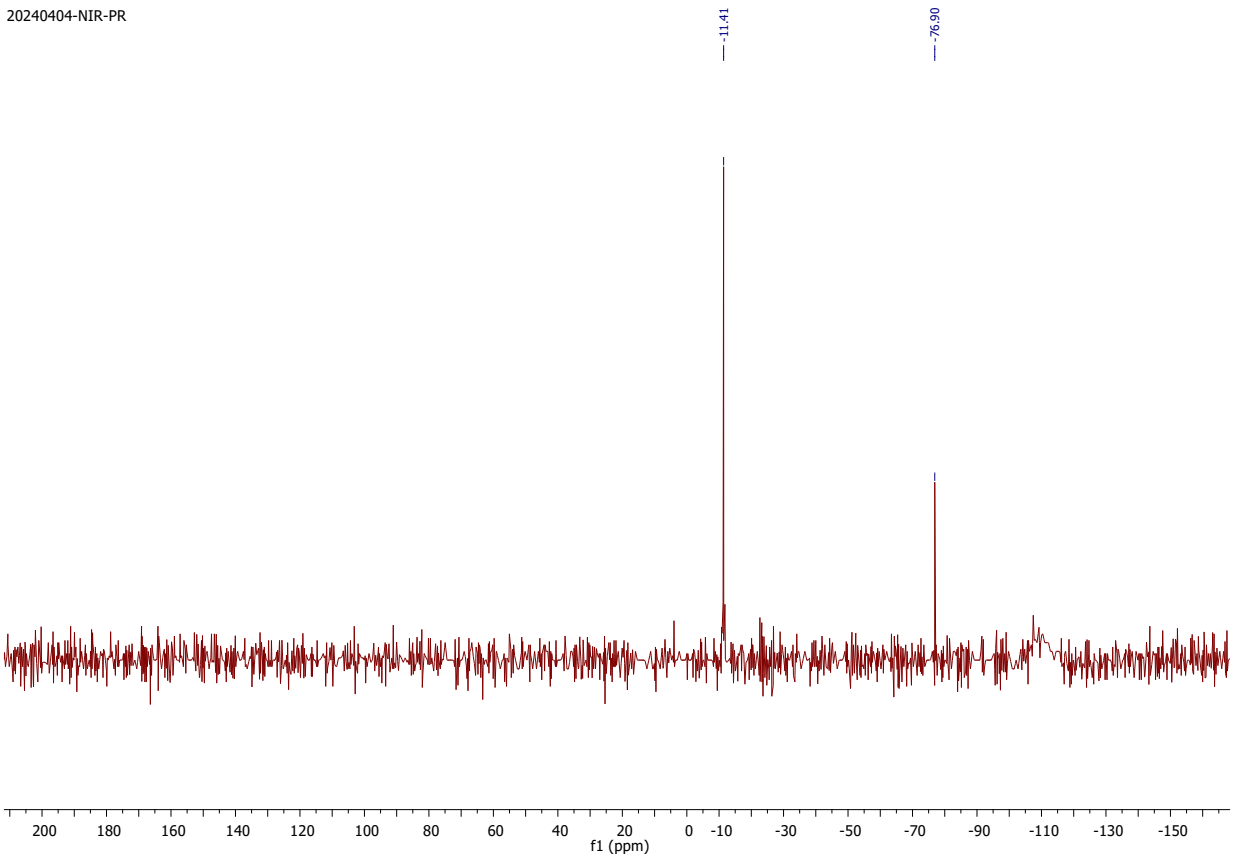


Figure S7. ^{29}Si NMR Spectrum of $\mathbf{4}_{\boldsymbol{trans}}$ (C_6D_6, 79.49 MHz, 298 K)

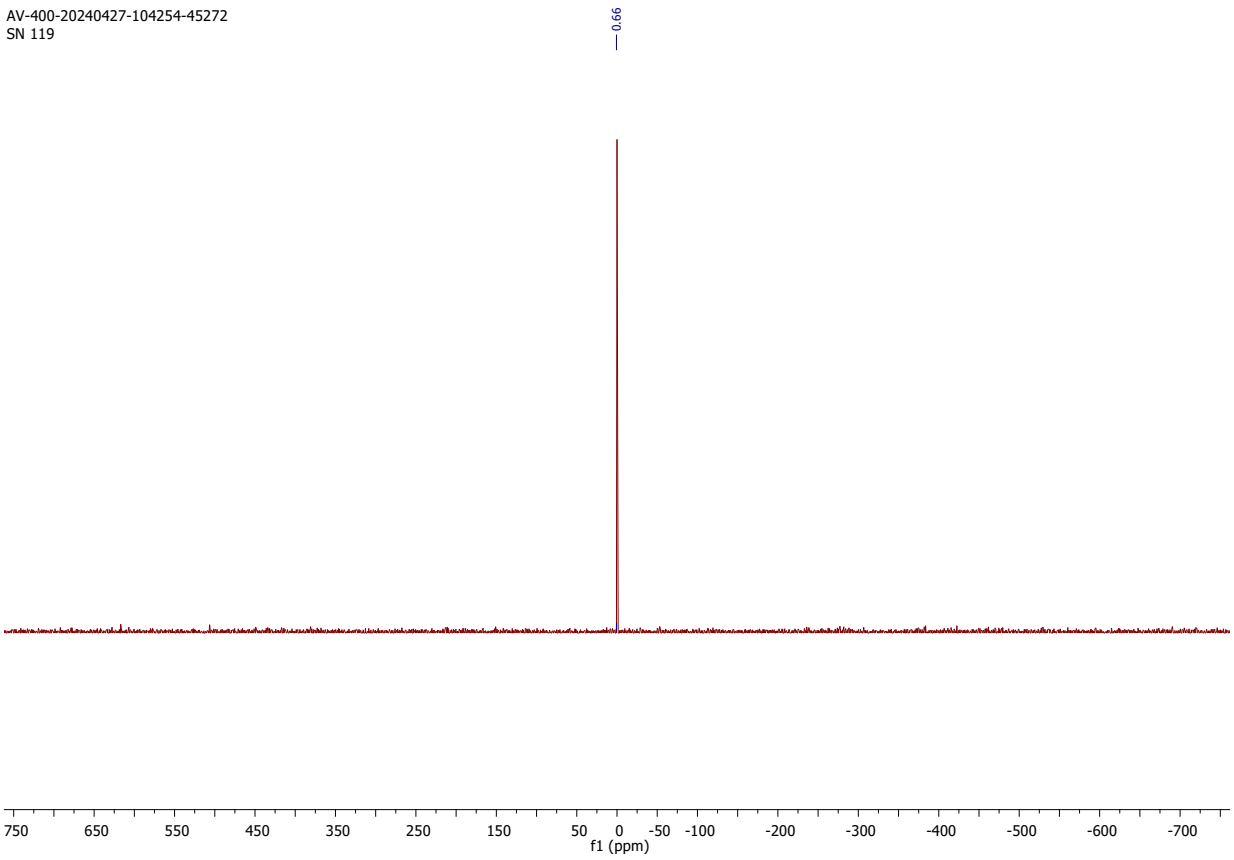


Figure S8. ^{119}Sn NMR Spectrum of $\mathbf{4}_{\boldsymbol{trans}}$ (C_6D_6, 149.21 MHz, 298 K)

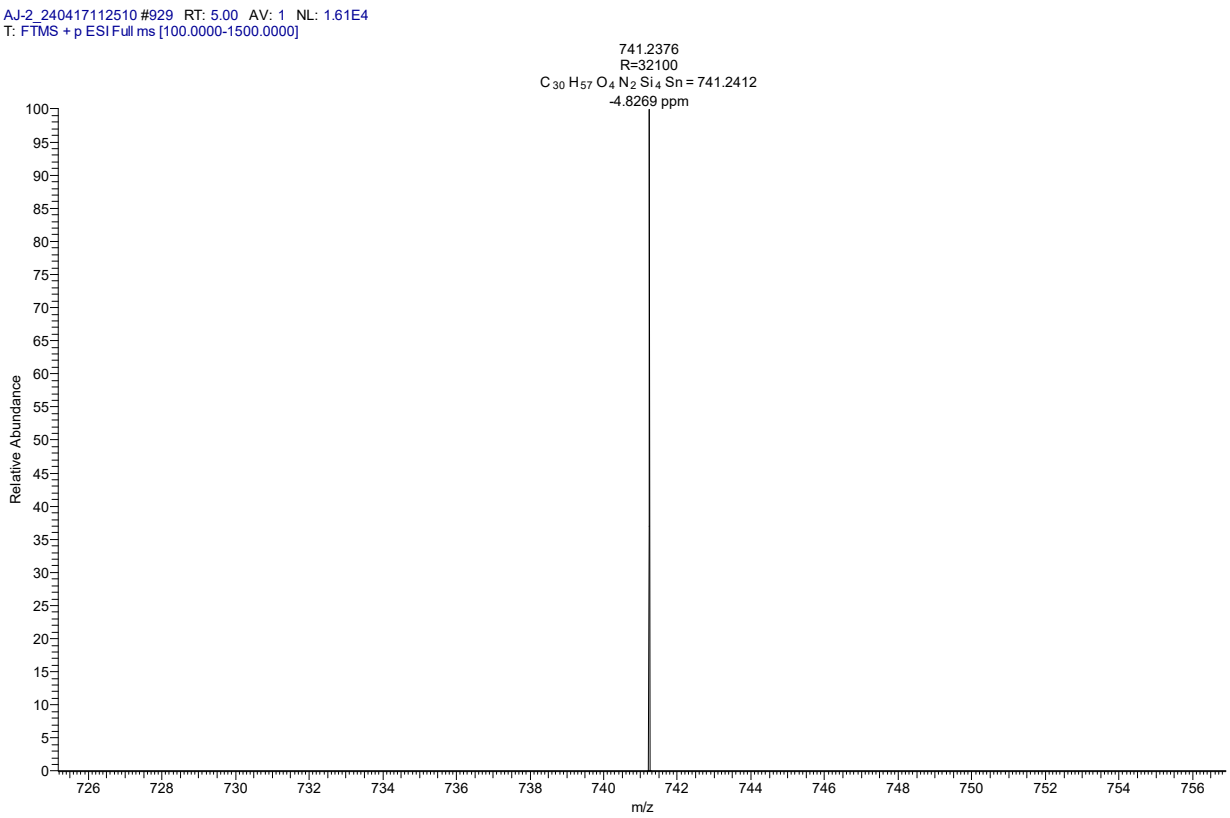


Figure S9. HRMS Spectrum of **4*trans***

Crystal Data and Structure Refinement for 3*cis* and 4*trans*

X-ray Crystallography Details. X-ray intensity data measurements were carried out on a Bruker SMART APEX II CCD diffractometer with graphite-monochromatized (MoKα= 0.71073Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX2 program (Bruker, 2006).[S2] All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full matrix least-squares refinement on

*F*2.[S3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms.

Identification code	**3**$_{cis}$	**4**$_{trans}$
Empirical formula	$C_{34}H_{64}GeN_2O_5Si_4$	$C_{30}H_{56}N_2O_4Si_4Sn$
Formula weight	765.84	739.81
Temperature/K	100(2)	100(2)
Crystal system	Triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a/Å	9.5714(9)	10.2751(10)
b/Å	13.2520(12)	15.1910(14)
c/Å	17.5019(15)	25.182(3)
α/°	97.149(3)	90
β/°	97.276(3)	99.290(3)
γ/°	102.064(3)	90
Volume/Å^3	2127.2(3)	3879.1(6)
Z	2	4
ρ_{calc}g/cm^3	1.196	1.267
μ/mm^{-1}	0.870	0.815
F(000)	820.0	1552.0
Crystal size/mm^3	0.11 × 0.07 × 0.02	0.11 × 0.1 × 0.06
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.29 to 56.814	4.576 to 56.756
Index ranges	-12 ≤ h ≤ 12, -17 ≤ k ≤	-13 ≤ h ≤ 13, -20 ≤ k ≤

	17, -23 ≤ l ≤ 23	20, -33 ≤ l ≤ 33
Reflections collected	97219	218442
Independent reflections	10635 [R_{int} = 0.0555, R_{sigma} = 0.0275]	9701 [R_{int} = 0.0683, R_{sigma} = 0.0208]
Data/restraints/parameters	10635/0/432	9701/0/387
Goodness-of-fit on F^2	1.041	1.151
Final R indexes [I>=2σ (I)]	R_1 = 0.0317, wR_2 = 0.0833	R_1 = 0.0311, wR_2 = 0.0706
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0861	R_1 = 0.0354, wR_2 = 0.0724
Largest diff. peak/hole / e $Å^{-3}$	0.70/-0.93	0.61/-0.87
CCDC No.	2347985	2347987

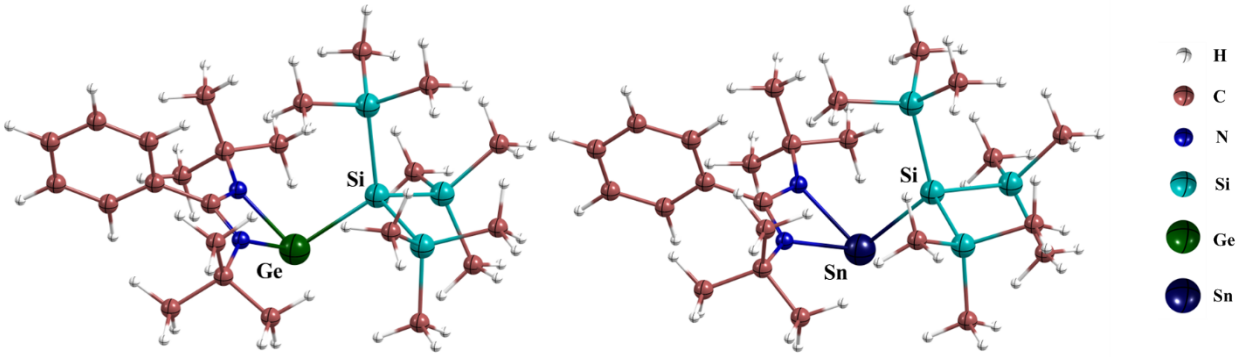
Details theoretical calculations

All DFT calculations were conducted utilizing the Gaussian 16[S4] software codes. The M062X[S5] global hybrid functional was used which comprises 54% Hartree-Fock exchange, specifically tailored for the study of main group elements. Grimme's D3[S6] dispersion model was taken into account to consider the non-covalent interactions. We used the 6-311++G(d,p) basis set for lighter elements (C, H, N, O, Si) and the Def2TZVP[S7] basis set with SDD[S8] ECP for heavy elements (Ge and Sn).

Optimized structures were confirmed as minima through harmonic vibrational frequency analysis. True minima were detected by possessing all positive frequencies, while transition state (TS) structures were distinguished by a single vibrational negative frequency. In addition, intrinsic reaction coordinate (IRC) calculations were performed on all the TS structures to elucidate the connectivity between successive minimum chemical structures (reactant and product) via the corresponding TS structure.

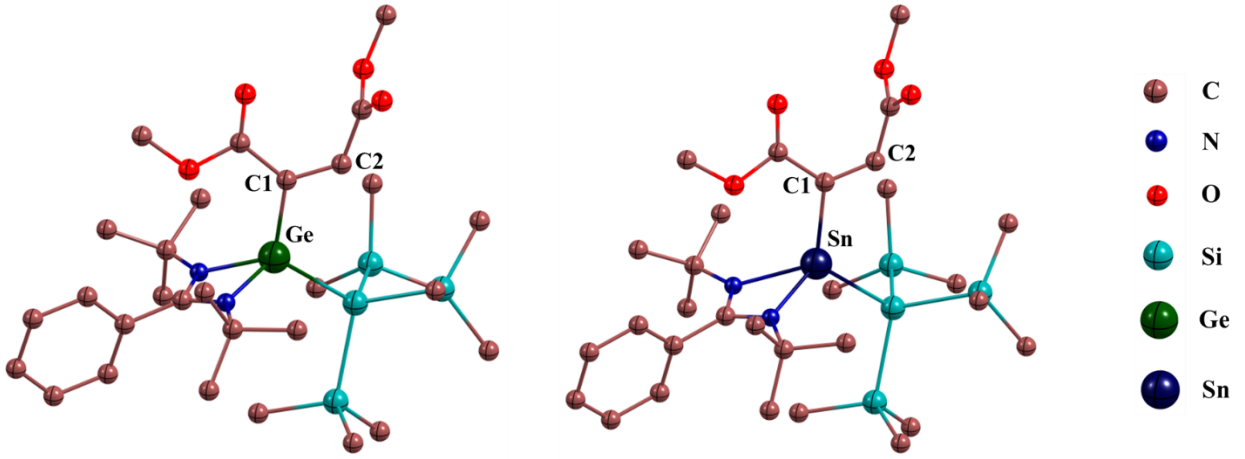
Thermochemical data were calculated employing the ideal gas rigid rotor simple harmonic oscillator approximation at 298.15K and 1atm. For the estimation of Gibbs free energy, zero-point energy corrections were included. To account for solvent effects, we employed the SMD[S9] continuum solvation model with tetrahydrofuran (THF) solvent, which was also being used experimentally. All natural bonding orbital analysis (NBO) was conducted using NBO 3.1,[S10] the built-in version in Gaussian 16.

The hypersilyl moiety stabilizes both germylene and the stannylene systems, with a Ge-Si bond length of 2.49 Å and a Sn-Si bond length of 2.68 Å (Figure S10) and. As germylene and stannylene are the heavier analogs of carbene, they contain two electrons which are not shared by other atoms. Thus, there are two possible spin states, one is singlet with S=0 and S_z=0, where electrons exhibit antiparallel alignment and the other is triplet with S=1 and three degenerate S_z states; we target S=1 and S_z=1 state, where electrons are parallel to each other. In both the systems, the singlet state is found to be more stable than the triplet state. The singlet state exhibits a stability advantage of 35.88 kcal/mol over the triplet state in the germylene system, whereas in the stannylene system, this energy difference is 33.69 kcal/mol.



1 **2**

Figure S10. Optimized structures of germylene (left) and stannylene (right)



Int-1$_{Ge}$ **Int-1$_{Sn}$**

Figure S11. Reaction intermediates for germylene and stannylene. For visual clarity hydrogen atoms are removed.

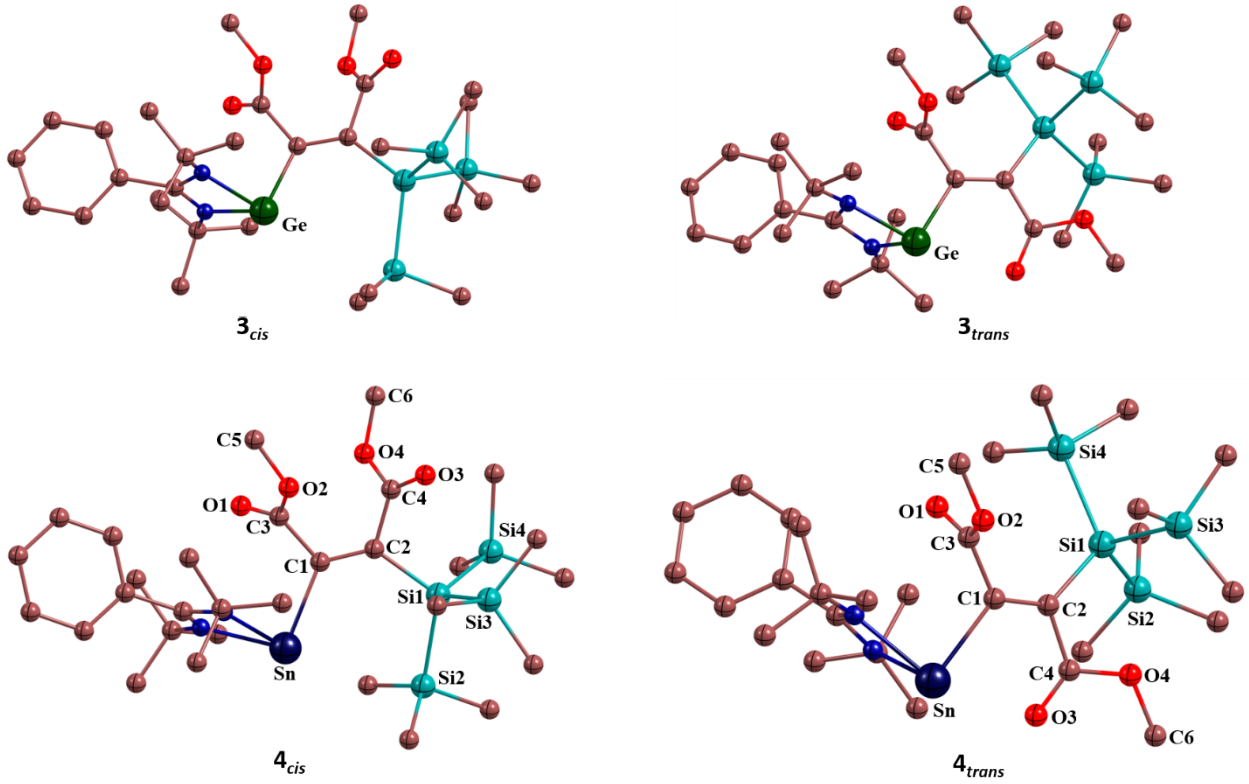


Figure S12. All possible products of the reactions are demonstrated here. Cis ($\mathbf{3}_{cis}$) and trans ($\mathbf{3}_{trans}$) products from the germylene (**1**) (above) and cis ($\mathbf{4}_{cis}$) and trans ($\mathbf{4}_{trans}$) products from the stannylene (**2**) (below). The labelled atoms indicate those involved in the electron transfer process, with similar notations applied to both systems for the same configurations (cis or trans).

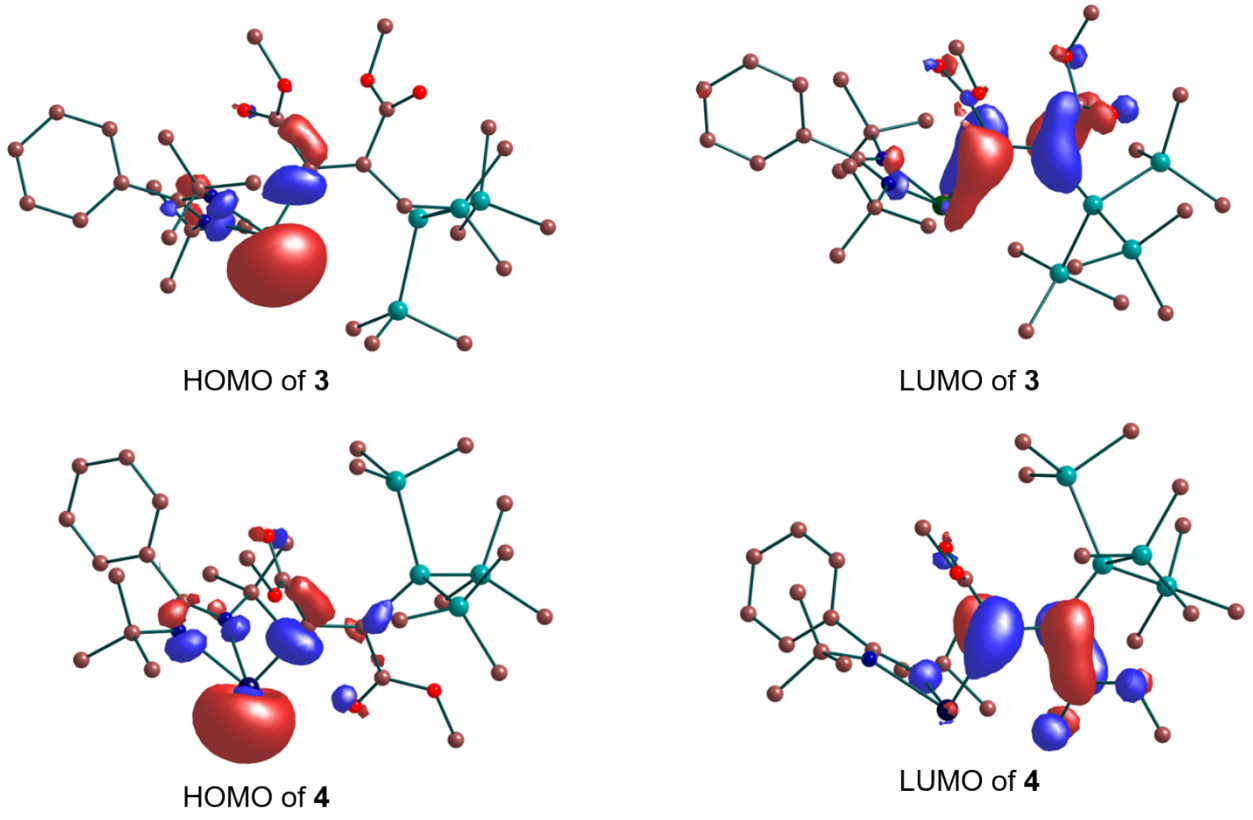


Figure S13. The molecular orbital plots of $\mathbf{3}_{cis}$ and $\mathbf{4}_{trans}$ with an isosurface value of 0.05 au. Hydrogen atoms are removed for clarity.

VT NMR

In DFT calculations, the $\mathbf{3}_{cis}$ formation requires 12.4 kcal/mol, while the $\mathbf{4}_{trans}$ requires 29.7 kcal/mol energy barrier after the formation of kinetic product $\mathbf{4}_{cis}$. Hence, we have performed a VT NMR, which indicates the formation of both $\mathbf{4}_{cis}$ and $\mathbf{4}_{trans}$ at low temperature.

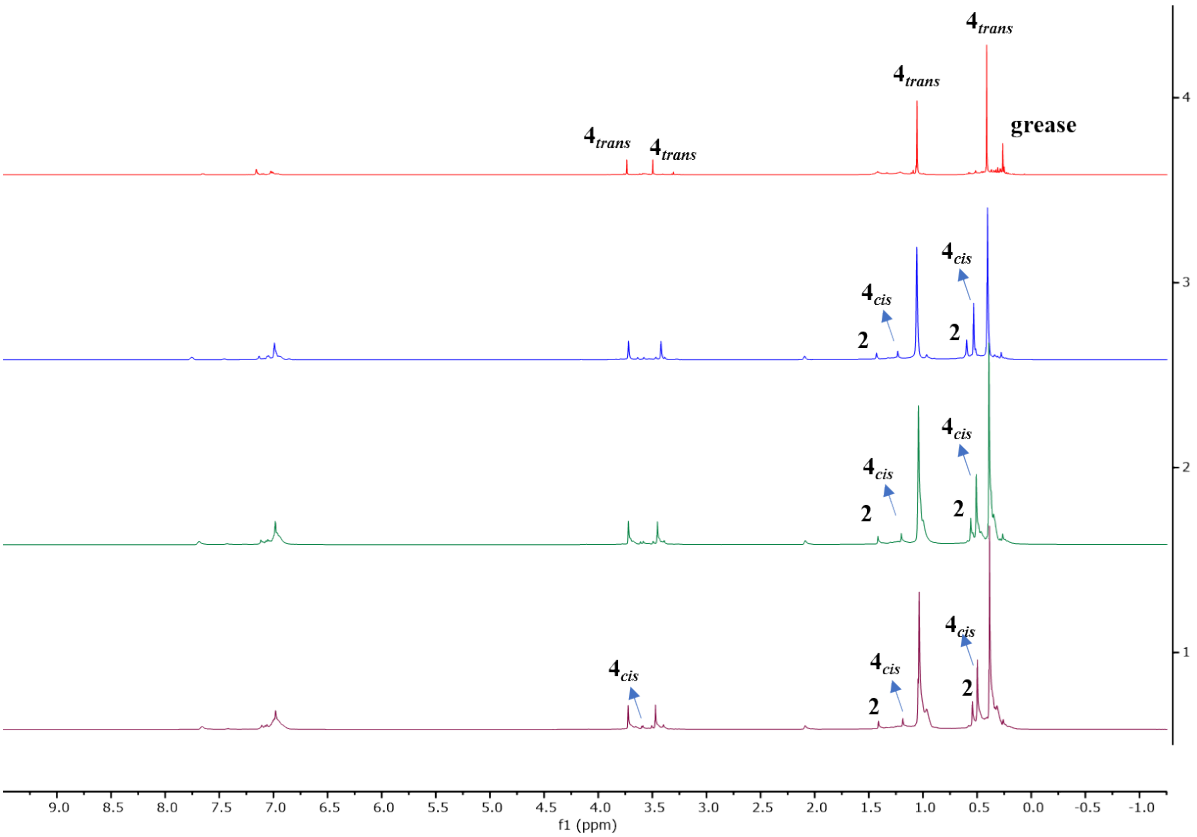


Figure S14. The full spectrum of VT NMR. The lowest set was recorded at -20 °C, followed by -10 °C, then at 0 °C, and the highest one was done at room temperature.

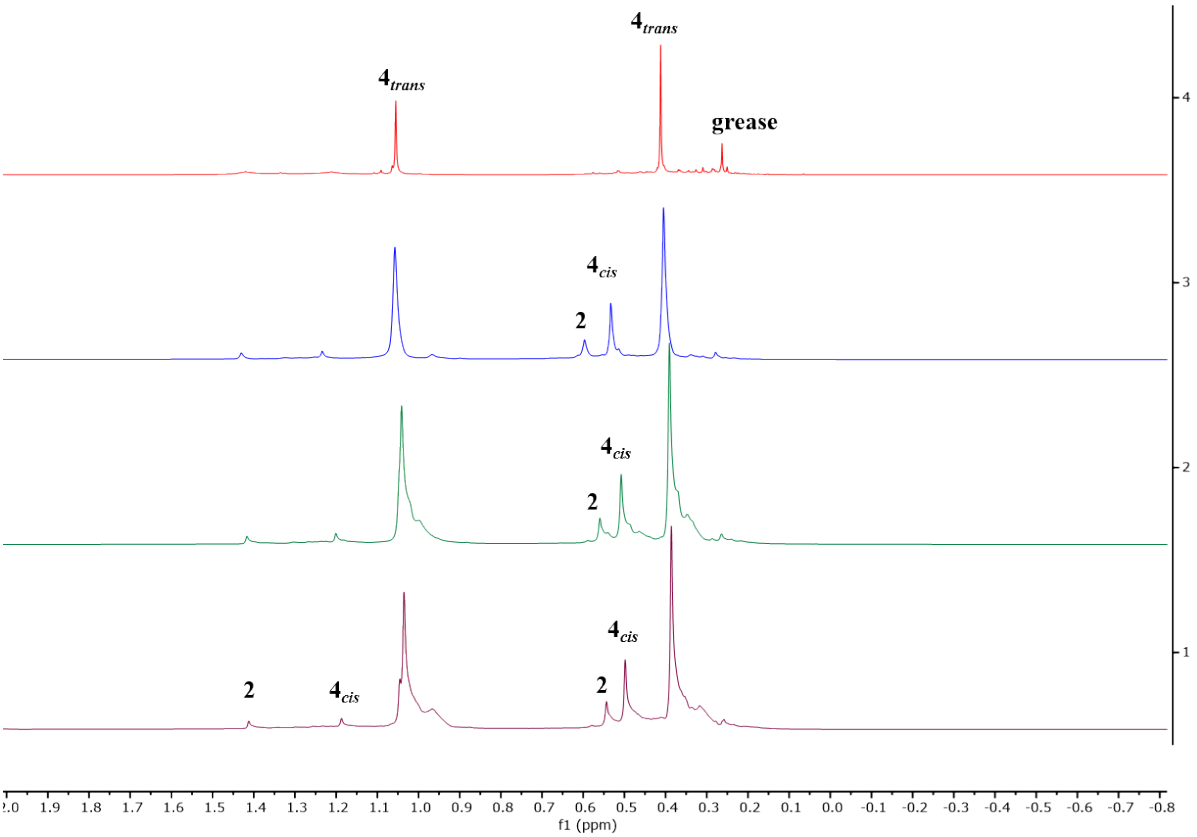


Figure S15. The enlarged version of the VT NMR for hypersilyl and *t*Bu region, which clearly indicates the formation of **4*cis*** at low temperature, but diminishes with gradual increase of the temperature. The lowest set was recorded at -20 °C, followed by -10 °C, then at 0 °C, and the highest one was done at room temperature.

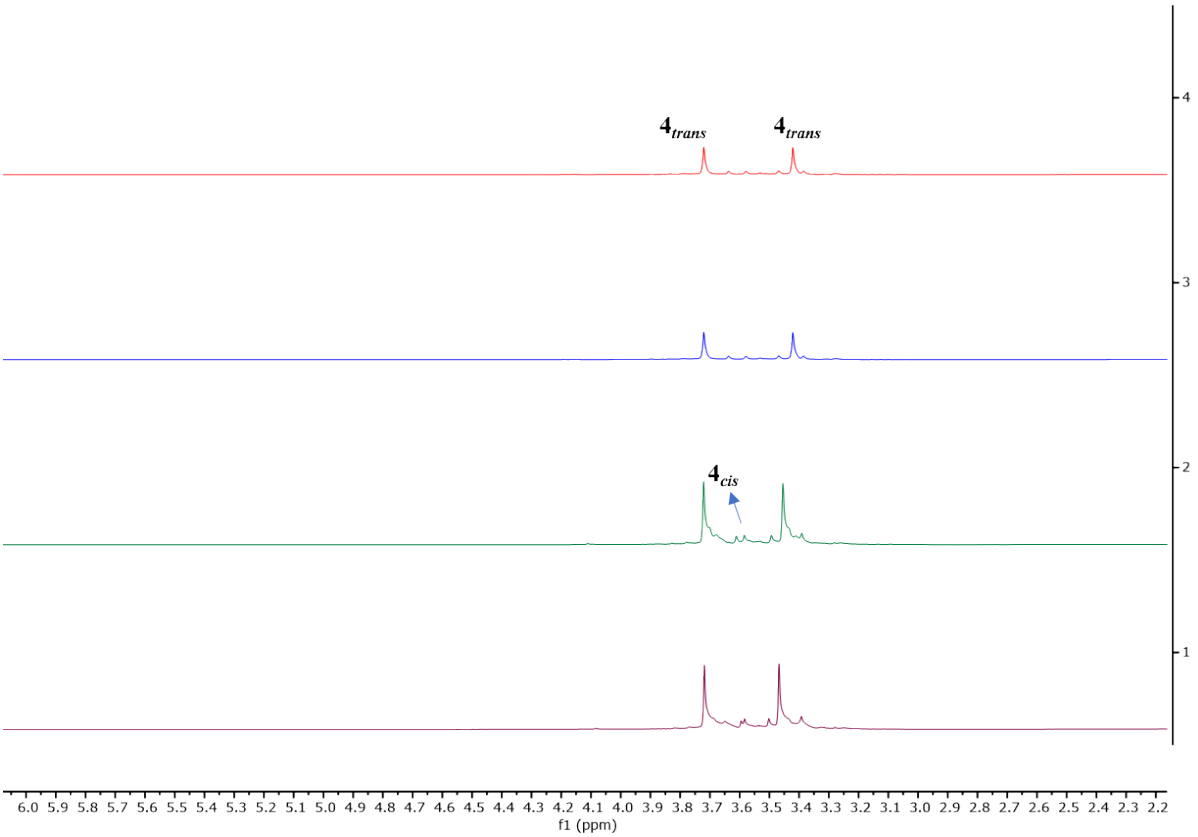


Figure S16. The enlarged version of the VT NMR for –COOMe resonances, which also indicates the formation of $\mathbf{4}_{cis}$ at low temperature as an intermediate, but diminishes with gradual increase of the temperature. The lowest set was recorded at -20 °C, followed by -10 °C, then at 0 °C, and the highest one was done at room temperature.

References:

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1

81

Si	-1.82206500	-0.05246800	0.03968500
Si	-3.52884000	-1.39210100	-0.87202700
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H	3.14765300	2.57518500	1.21941000
H	1.41526200	2.84577600	1.48419700
C	-1.94606300	3.15913500	1.45536500
H	-2.16584700	4.21575200	1.26530700

H	-2.29186500	2.92863500	2.46762800
H	-0.86168100	3.03301000	1.44186900
C	-4.63972500	1.96780400	0.78752200
H	-5.27943800	1.44368200	0.07245500
H	-4.72529000	1.46522100	1.75493400
H	-5.03290700	2.98484900	0.90273100
C	0.77831600	3.35357600	-1.17385100
H	-0.12089600	3.20714700	-0.57311800
H	1.01986700	4.41887400	-1.17403800
H	0.56722500	3.04995100	-2.20348400
C	-2.88612900	2.90634400	-1.49415800
H	-1.91105400	2.92732700	-1.98630000
H	-3.57870000	2.38123400	-2.15860300
H	-3.23816200	3.93931000	-1.39430400
C	0.19797600	-0.00382800	2.81188500
H	0.49116300	-0.35902900	3.80568000
H	0.97584100	-0.28720500	2.09801900
H	0.14494800	1.08904100	2.83743600
C	-2.82392500	-0.16709800	3.39600600
H	-2.92172200	0.92139900	3.40418100
C	5.15872500	0.01112300	2.00393600
C	4.65860000	-0.25094900	-0.72129200
H	-4.39697400	-2.35853200	1.26412600
H	-1.38636900	-2.87766600	3.51270500
H	-2.19771900	-3.12581700	1.96195900
H	2.42656300	4.12970000	0.79141200
H	-3.78779100	-0.59278500	3.10129100
H	-2.61404300	-0.49247000	4.42144000
H	5.34941800	0.11298000	3.06604100
C	6.21128400	-0.22246100	1.12329100
H	4.46292600	-0.33650900	-1.78447100
C	5.96029100	-0.34692000	-0.24082000
H	7.22526500	-0.30271700	1.49805600
H	6.77748500	-0.51742100	-0.93215300
Ge	0.06174500	0.11878000	-1.58624900

2

81

Si	-1.92877700	0.00446000	0.16380700
Si	-3.59710600	-1.45781000	-0.61543800
Si	-1.46178900	-0.62935100	2.37019800
Si	-2.99783100	2.09963200	0.16992400
N	1.62667300	1.08320600	-0.66359800
N	1.60758600	-1.11515600	-0.60437900
C	3.92500500	0.12653800	1.59697900
H	3.09112200	0.17305700	2.28820500
C	2.29942300	-0.01344600	-0.32747400
C	1.94707200	2.49958500	-0.43590600
C	1.97995800	-2.52957200	-0.45701400
C	3.36824500	2.90263700	-0.85178700
H	3.59977400	2.52773600	-1.85251100
H	3.43471500	3.99417300	-0.87149400
H	4.12388600	2.53644800	-0.15577900
C	2.36274200	-2.87192500	0.98854900
H	1.60756100	-2.49495600	1.68445900
H	2.42839300	-3.95752400	1.10458600
H	3.33014100	-2.44747300	1.26082100
C	3.10503000	-2.94011900	-1.41503500
H	4.06002100	-2.49961900	-1.12638200
H	3.22030900	-4.02801800	-1.40609500
H	2.86635700	-2.62763400	-2.43573000
C	3.69090200	0.00208000	0.22819700
C	-4.44644500	-0.74004300	-2.14355300
H	-5.14974200	-1.47007600	-2.55973400
H	-5.00910300	0.16696700	-1.90559500
H	-3.71927200	-0.49282500	-2.92341000
C	0.71374800	-3.30511100	-0.83275500
H	0.45598500	-3.12843700	-1.88269900
H	0.85745600	-4.37953200	-0.69595500
H	-0.12484700	-2.98246100	-0.21046400
C	-4.92058100	-1.78934800	0.69367700
H	-5.70692600	-2.42679000	0.27302500

H	-5.38864100	-0.86721000	1.04719300
C	-2.88700100	-3.13654900	-1.11546500
H	-2.15474500	-3.04099500	-1.92311300
H	-2.40120700	-3.63921000	-0.27413800
H	-3.69485500	-3.78557800	-1.47236500
C	-1.41036600	-2.51017500	2.55101000
H	-0.65663100	-2.97127400	1.90821100
C	1.70854400	2.85591700	1.03569600
H	2.41617000	2.33472000	1.68435800
H	0.69568700	2.57007000	1.32863300
C	-2.12243200	3.37054400	1.26361800
H	-2.78026400	4.23430400	1.41293800
H	-1.87810800	2.96378100	2.24963600
H	-1.19784500	3.73454800	0.80945200
C	-4.77217100	1.96429100	0.80921100
H	-5.38779200	1.33432200	0.16128500
H	-4.80970400	1.55081100	1.82120700
H	-5.22767600	2.96094200	0.83587100
C	0.95018100	3.27728700	-1.30058300
H	-0.07430200	2.98773900	-1.04532000
H	1.04871700	4.35257000	-1.13359200
H	1.11750900	3.07321900	-2.36240100
C	-3.09354800	2.80017900	-1.58372200
H	-2.10275000	2.95187100	-2.02186200
H	-3.65128900	2.13198900	-2.24608400
H	-3.60634600	3.76871200	-1.57525500
C	0.20970200	0.06329700	2.90875600
H	0.57039700	-0.43593400	3.81488900
H	0.94565900	-0.08375400	2.11378800
H	0.14564500	1.13560000	3.11497000
C	-2.79355700	0.00187600	3.55273700
H	-2.86473300	1.09338800	3.53207500
C	5.22947500	0.18192200	2.08005900
C	4.77174100	-0.07203500	-0.65187800
H	-4.50122800	-2.30909500	1.56010400
H	-1.16845500	-2.77116600	3.58778800
H	-2.37874900	-2.96024400	2.31368700
H	1.82933000	3.93227300	1.19208600
H	-3.77531100	-0.40642500	3.29431500
H	-2.56354500	-0.30048200	4.58084300
H	5.40349800	0.27815500	3.14563200
C	6.30513100	0.11254500	1.19942900
H	4.59010600	-0.16093600	-1.71769300
C	6.07416400	-0.01778900	-0.16798800
H	7.32023200	0.15801600	1.57702100
H	6.90780800	-0.07225300	-0.85872100
Sn	-0.00209900	-0.03228800	-1.70304500

Int-1$_{Ge}$

97

Si	-1.70414300	-1.29406000	0.02928200
Si	-3.46297400	-0.90006900	-1.50451700
Si	-0.76672800	-3.42291900	-0.35273300
Si	-2.71431800	-1.24962600	2.16474800
N	1.66089100	0.01043800	1.04921100
N	1.63694200	-0.06870300	-1.11437900
C	4.38958200	-1.63089700	0.33820000
H	3.71535100	-2.43069300	0.62272100
C	2.41497300	-0.15188300	-0.03663200
C	2.02126400	0.21349300	2.46660600
C	1.91427300	-0.21258300	-2.55531100
C	3.32089800	1.00395200	2.64617100
H	3.30928100	1.90719600	2.03138200
H	3.40071800	1.30244300	3.69464100
H	4.20462800	0.41457800	2.39888900
C	2.78239300	-1.43931600	-2.84636100
H	2.37600700	-2.32651400	-2.35242200
H	2.79667500	-1.62038700	-3.92420100
H	3.81278400	-1.29686800	-2.51566900
C	2.56679500	1.05945500	-3.10543300
H	3.58167300	1.18245900	-2.72559200
H	2.61851200	1.00195700	-4.19607000

H	1.97511800	1.93703100	-2.83142800
C	3.88169900	-0.38938100	-0.04173700
C	-4.77826500	0.27102600	-0.84342700
H	-5.59398700	0.32407800	-1.57372900
H	-5.20318900	-0.05968800	0.10721600
H	-4.36246800	1.27163100	-0.71001500
C	0.54000500	-0.37863400	-3.20509900
H	-0.08210900	0.50092000	-3.00877700
H	0.64041700	-0.48584400	-4.28729800
H	0.02877600	-1.26279100	-2.81593800
C	-4.28007400	-2.58928200	-1.74783000
H	-5.13757300	-2.48153800	-2.42188000
H	-4.65104300	-2.99546700	-0.80237600
C	-2.90408800	-0.26086200	-3.18154600
H	-2.44957200	0.72948600	-3.09338100
H	-2.19568100	-0.93186400	-3.67355400
H	-3.78498100	-0.16886400	-3.82706500
C	-0.58735500	-3.83402900	-2.18972700
H	0.36285700	-3.46503700	-2.58476800
C	2.12364100	-1.14271900	3.16749200
H	2.93819900	-1.73614600	2.74523700
H	1.19207600	-1.70119000	3.05542100
C	-1.64123000	-2.01291300	3.51696500
H	-2.27986100	-2.25930600	4.37284200
H	-1.15953800	-2.93790800	3.18624000
H	-0.86709300	-1.32996500	3.87285100
C	-4.27958600	-2.29987400	2.06573700
H	-4.99261100	-1.92824200	1.32660500
H	-4.05057900	-3.34175300	1.82565700
H	-4.77515300	-2.28388800	3.04320500
C	0.87024900	1.02637800	3.06405300
H	-0.08788600	0.52714500	2.89217900
H	1.00365000	1.13449800	4.14254400
H	0.82750600	2.02264300	2.61443900
C	-3.18424700	0.51039400	2.63744400
H	-2.31192100	1.16581200	2.70861800
H	-3.86139100	0.94474200	1.89711300
H	-3.69097200	0.51020500	3.60914200
C	0.95009000	-3.53003200	0.41484700
H	1.39520900	-4.51051500	0.21219800
H	1.59955200	-2.76721200	-0.02364200
H	0.92665000	-3.38267400	1.49768700
C	-1.88149900	-4.71924900	0.44113700
H	-1.96751900	-4.56818900	1.52095100
C	5.76488300	-1.84061200	0.33968900
C	4.74524400	0.64134200	-0.40893400
H	-3.60131500	-3.32380100	-2.18960700
H	-0.59358400	-4.92258100	-2.31388200
H	-1.39002900	-3.42454200	-2.80794400
H	2.31818600	-0.99967400	4.23408900
H	-2.88756900	-4.70525300	0.01253700
H	-1.45888400	-5.71615700	0.27391700
H	6.16008400	-2.80779900	0.62742000
C	6.62950300	-0.81188100	-0.02423000
H	4.34090100	1.60747300	-0.68630300
C	6.11922000	0.42981200	-0.39506800
H	7.70069400	-0.97706900	-0.01738500
H	6.79037400	1.23430200	-0.67212800
Ge	0.06305100	0.33132000	-0.03620300
O	0.13233200	4.48380800	-0.12150300
C	0.43521200	3.31682900	-0.06705700
O	1.71976500	2.91886000	0.09069500
C	2.67782000	3.97364800	0.20054900
H	2.69998200	4.56753900	-0.71455100
H	3.64305700	3.49799800	0.36035200
H	2.43870000	4.62151700	1.04527100
C	-1.83328300	2.29123400	-0.33289000
C	-0.50393100	2.16704100	-0.14731700
C	-2.48012200	3.56421600	-0.54012700
O	-2.94415400	4.10161000	0.61760000
O	-2.73784500	4.05703400	-1.62642300
C	-3.66281700	5.32389100	0.48063800

H	-3.02955100	6.09972500	0.04616300
H	-3.96012400	5.60982900	1.48825600
H	-4.54790000	5.19140900	-0.14416100

Int-1$_{Sn}$

97			
Si	-1.79225900	-1.50768000	0.05779200
Si	-3.51644800	-1.26068200	-1.53197000
Si	-0.68574200	-3.56574100	-0.20520000
Si	-2.75377100	-1.35894300	2.20392000
N	1.75697600	0.12869000	1.03255500
N	1.76953000	-0.06219200	-1.16007200
C	4.44720400	-1.57441600	0.43009300
H	3.74860600	-2.35159100	0.71961100
C	2.50345300	-0.08391600	-0.04816200
C	2.13393000	0.39378500	2.43301100
C	2.11720400	-0.36776200	-2.55976500
C	3.39723400	1.24998000	2.57233300
H	3.34349300	2.12187600	1.91507600
H	3.46996800	1.60227300	3.60468500
H	4.30519100	0.68955300	2.34636000
C	2.88054100	-1.69006900	-2.69280400
H	2.37510000	-2.48690700	-2.13930200
H	2.92579600	-1.97769900	-3.74665700
H	3.90431200	-1.60543600	-2.32446800
C	2.91358600	0.77624200	-3.19633000
H	3.91865200	0.84374300	-2.77911700
H	3.00642300	0.60395200	-4.27219600
H	2.39944200	1.72863300	-3.04188400
C	3.97211600	-0.33908300	-0.00957600
C	-4.83366800	-0.04836500	-0.96175600
H	-5.61201100	0.02153700	-1.73009400
H	-5.30927900	-0.37175700	-0.03213300
H	-4.40973100	0.94655200	-0.80785800
C	0.77006900	-0.48081500	-3.27957500
H	0.21919100	0.46416600	-3.20995800
H	0.91503500	-0.70848800	-4.33787000
H	0.16098000	-1.27443500	-2.83806400
C	-4.31042300	-2.96560100	-1.69054300
H	-5.15878000	-2.91193900	-2.38200100
H	-4.68856900	-3.31768400	-0.72615900
C	-2.84360200	-0.71736300	-3.20109700
H	-2.38961800	0.27582700	-3.13278500
H	-2.09705800	-1.41626700	-3.58859800
H	-3.66288200	-0.66110100	-3.92623500
C	-0.45795500	-4.04318300	-2.01393400
H	0.27985700	-3.41440300	-2.51687200
C	2.30154500	-0.92518400	3.19226100
H	3.14517500	-1.49650700	2.79913700
H	1.39881700	-1.53424200	3.10415500
C	-1.59082200	-1.99968500	3.54070700
H	-2.13946800	-2.09142500	4.48479900
H	-1.18656400	-2.98550200	3.29290800
H	-0.75443100	-1.31796400	3.71153200
C	-4.29627300	-2.44260700	2.20361200
H	-5.04165900	-2.09338000	1.48460000
H	-4.05598500	-3.48361700	1.96959000
H	-4.75606400	-2.42016000	3.19796500
C	0.95267300	1.17543000	3.01780500
H	0.01776100	0.61840900	2.88595800
H	1.09314500	1.34357000	4.08774800
H	0.85204800	2.14645000	2.52232100
C	-3.22527100	0.42406700	2.56763400
H	-2.34609400	1.07474600	2.60355000
H	-3.89447500	0.81982500	1.79859800
H	-3.73530200	0.49053600	3.53506000
C	1.00336800	-3.47524800	0.61998600
H	1.58076900	-4.38515800	0.42348000
H	1.56564600	-2.62096700	0.23297900
H	0.90978000	-3.35687700	1.70329600
C	-1.73586400	-4.89174500	0.62548800
H	-1.86937900	-4.69218600	1.69247200

C	5.81717300	-1.81047900	0.48289900
C	4.86832700	0.65860200	-0.39003700
H	-3.61174600	-3.71246400	-2.07679200
H	-0.09961200	-5.07758500	-2.06585900
H	-1.39305100	-3.98731400	-2.57743900
H	2.48543600	-0.72760000	4.25215000
H	-2.72569800	-4.96258400	0.16497900
H	-1.24873800	-5.86776700	0.52362500
H	6.18396000	-2.77359800	0.81834900
C	6.71286100	-0.81263200	0.10771000
H	4.49430400	1.62187400	-0.71742900
C	6.23733200	0.42214000	-0.32674400
H	7.78004300	-0.99667200	0.15432000
H	6.93194800	1.20273100	-0.61441500
O	-0.03559600	4.69713700	-0.07180800
C	0.24893100	3.52529400	-0.12803300
O	1.53022400	3.09416600	-0.07522000
C	2.52267800	4.11251000	0.05665900
H	2.45097600	4.82642800	-0.76495600
H	3.48473800	3.60570600	0.02600900
H	2.40585800	4.64022900	1.00505200
C	-2.02826100	2.52451600	-0.45437100
C	-0.70448500	2.39296800	-0.25515500
C	-2.66242600	3.81434500	-0.61515900
O	-3.14919300	4.29411700	0.55788400
O	-2.88473100	4.36910600	-1.67789000
C	-3.84107800	5.53626100	0.47095300
H	-3.18393700	6.32020700	0.08981600
H	-4.15342200	5.77572000	1.48606300
H	-4.71539500	5.45452700	-0.17728500
Sn	-0.06060400	0.38830400	-0.10826300

Ts-1 Ge

97

Ge	3.38113700	-0.99927600	1.06611200
Si	5.76524700	-1.78922000	0.68419600
Si	5.14184300	-4.05900100	1.12134500
Si	7.16382500	-2.06899400	-1.19429700
Si	7.04641000	-1.25266400	2.58302800
O	4.06728500	3.16513000	0.82773200
O	2.08224400	2.14591700	1.01238500
O	5.49418600	1.80344700	-1.61485900
O	6.98721300	2.18113200	0.02058000
N	1.58374700	-1.33634000	1.80405800
N	2.00141700	-1.24417300	-0.32139200
C	4.05011500	0.81458200	0.88509700
C	-1.23701100	-0.62588100	-0.02354200
H	-0.85843800	0.39013800	-0.02128800
C	1.04699100	-1.42174900	0.58520700
C	3.28720300	2.07963000	0.91589200
C	5.24530700	0.56814700	0.33571100
C	0.98258000	-1.42348600	3.14749100
C	1.96192200	-1.18554100	-1.79484100
C	6.00335700	1.60198700	-0.38077000
C	0.67533600	-2.88019400	3.50707600
H	1.56471600	-3.50334900	3.38389800
H	0.34824900	-2.94398200	4.54852900
H	-0.12229500	-3.27841300	2.87710600
C	1.53554400	0.21627300	-2.23901600
H	2.19127100	0.96982800	-1.79478900
H	1.59673100	0.29697500	-3.32786000
H	0.50755900	0.42576300	-1.93547100
C	1.04337100	-2.24927800	-2.40490400
H	-0.01265300	-2.03516000	-2.23729900
H	1.21166800	-2.27511400	-3.48453300
H	1.27405100	-3.23854800	-1.99912100
C	-0.38684200	-1.68567400	0.28883100
C	4.49318400	-4.16403000	2.90303700
H	5.30198600	-4.15706500	3.63873000
H	3.82823100	-3.32558500	3.13397400
H	3.92047700	-5.08758500	3.04527400
C	3.39549600	-1.45455700	-2.26043100

H	3.72759000	-2.43655700	-1.91342000
H	3.43933000	-1.43792800	-3.35199100
H	4.08422000	-0.69208900	-1.88172000
C	3.39006200	4.42481800	0.81452700
H	2.81965000	4.56213800	1.73401300
H	4.17056600	5.17863800	0.73984500
H	2.71929100	4.48866300	-0.04330800
C	6.45697400	-5.40914300	0.91803000
H	6.03542400	-6.38312700	1.19198700
H	7.32499700	-5.22912400	1.55864400
C	3.66498900	-4.56960100	0.03931500
H	2.82003900	-3.88298400	0.16579600
H	3.91618600	-4.60009500	-1.02497500
H	3.32206600	-5.56928400	0.33024800
C	6.46886000	-3.29608500	-2.45469700
H	5.68344900	-2.84664900	-3.06738100
C	6.20334500	2.74044800	-2.42746800
H	7.24480000	2.43785700	-2.54805800
H	6.16426500	3.73670600	-1.98368800
C	-0.28471400	-0.57075900	3.26803900
H	-1.12024500	-0.99946800	2.71317800
H	-0.10338900	0.44506100	2.90821100
C	8.24962600	0.15583900	2.25651900
H	8.86010700	0.32460000	3.15111700
H	8.92556800	-0.07637700	1.42776300
H	7.73137800	1.08296900	2.00508200
C	8.07117400	-2.73939700	3.14324700
H	7.45556600	-3.60245200	3.40655400
H	8.78229800	-3.05067900	2.37345900
H	8.64694600	-2.45816800	4.03268300
C	2.04707700	-0.87342100	4.09943300
H	2.28332000	0.16685400	3.85503100
H	1.68809200	-0.91391100	5.12982000
H	2.96451000	-1.46628600	4.03835800
C	5.91092800	-0.75934500	4.00718700
H	5.27930000	-1.59759400	4.31474200
H	6.50601500	-0.45163400	4.87434000
H	5.26393400	0.07857800	3.72939800
C	7.63196400	-0.51189700	-2.14469200
H	8.38587300	-0.77148500	-2.89665800
H	6.76899500	-0.08760800	-2.66340600
H	8.05691300	0.25456100	-1.49100700
C	8.76091000	-2.82663100	-0.51845800
H	9.42889700	-3.07396000	-1.35143000
C	-2.57189500	-0.87905500	-0.32021500
C	-0.86735500	-2.99405800	0.30634600
H	6.81041700	-5.47915300	-0.11491000
H	7.27577900	-3.60751800	-3.12794100
H	6.06279100	-4.19662300	-1.98593900
H	5.69811100	2.74006100	-3.39135200
H	-0.57471700	-0.51699000	4.32062600
H	9.28784600	-2.12664200	0.13666100
H	8.57369200	-3.74494300	0.04438700
H	-3.23482400	-0.05561100	-0.55881100
C	-3.05433200	-2.18554400	-0.30864300
H	-0.19665300	-3.81408100	0.53899400
C	-2.20252400	-3.24153700	0.00488700
H	-4.09454600	-2.38065400	-0.54272000
H	-2.57585900	-4.25889300	0.01187600

Ts-1 Sn

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Si	5.96429200	-1.84459600	0.70534300
Si	5.34523200	-4.09362100	1.20192400
Si	7.29371600	-2.11967400	-1.21580500
Si	7.18380000	-1.19489400	2.60515500
O	4.21867100	3.28654000	0.69824800
O	2.26356300	2.30773500	1.18074400
O	5.58313900	1.79373600	-1.73150800
O	7.12354100	2.16872500	-0.13978700
N	1.37944200	-1.38867300	1.85179600
N	1.85979800	-1.29991000	-0.29753000

C	4.18432900	0.93939500	0.87505300	H	7.56402500	-5.17343600	1.68406500
C	-1.34818600	-0.51257400	0.05054000	C	3.91205600	-4.64789000	0.08777400
H	-0.92497900	0.48322000	0.12518500	H	3.03069000	-4.00652700	0.20684100
C	0.89950800	-1.44143500	0.60918000	H	4.18580900	-4.64537000	-0.97123800
C	3.44658900	2.21737100	0.93638400	H	3.61148800	-5.66787400	0.35363500
C	5.32945300	0.64328700	0.26944300	C	6.54148000	-3.38163800	-2.40130700
C	0.73121400	-1.60185100	3.15533000	H	5.60233700	-3.02342900	-2.83186100
C	1.79894400	-1.16283000	-1.76310900	C	6.30591800	2.68186400	-2.58496900
C	6.10898200	1.61373200	-0.50061300	H	7.33276000	2.33855900	-2.72175300
C	0.52159900	-3.09907900	3.40582600	H	6.31363600	3.69070200	-2.16871800
H	1.46557300	-3.64039900	3.29154900	C	-0.59448500	-0.84576100	3.30331500
H	0.14916600	-3.26326300	4.42094800	H	-1.39399700	-1.29561200	2.71353900
H	-0.20585600	-3.51444200	2.70543100	H	-0.47728500	0.19865600	3.00194000
C	1.45817200	0.28388600	-2.13409500	C	8.32302400	0.26106200	2.27161200
H	2.16640800	0.97241100	-1.66428300	H	8.88465600	0.50128400	3.18155400
H	1.51042200	0.41782400	-3.21836600	H	9.04495100	0.02901500	1.48249700
H	0.44963400	0.54268800	-1.80383800	H	7.76799100	1.14661000	1.95613100
C	0.81600600	-2.13135600	-2.43115400	C	8.25550800	-2.63129100	3.20392100
H	-0.22475000	-1.85404400	-2.26093900	H	7.66448900	-3.50644800	3.48494400
H	0.99247500	-2.11855100	-3.50990700	H	8.97570200	-2.93774100	2.43976100
H	0.97261500	-3.15230000	-2.07155500	H	8.82271300	-2.31469300	4.08675400
C	-0.54422800	-1.62762700	0.28235500	C	1.72517600	-1.05363400	4.18499400
C	4.66450500	-4.18528300	2.97130600	H	1.90433600	0.01261200	4.01498500
H	5.45203600	-4.07966300	3.72250900	H	1.33913000	-1.18423900	5.19810900
H	3.91022400	-3.41527800	3.16935400	H	2.68125500	-1.58573000	4.12013900
H	4.18204700	-5.15692000	3.12807000	C	5.98150000	-0.73343300	3.98571600
C	3.21301600	-1.49222600	-2.25630400	H	5.33560200	-1.57669200	4.24851600
H	3.48751900	-2.50958800	-1.96259400	H	6.53385900	-0.44124100	4.88585200
H	3.26212200	-1.41780600	-3.34535000	H	5.34901900	0.11087900	3.69332700
H	3.94678300	-0.79384900	-1.83832400	C	7.68090500	-0.57346200	-2.21241400
C	3.55741700	4.55448600	0.71792600	H	8.40457300	-0.83312500	-2.99345400
H	3.10828000	4.73694200	1.69502900	H	6.78560500	-0.17793400	-2.69763500
H	4.32936700	5.29339200	0.51488500	H	8.11861100	0.21338700	-1.59291200
H	2.78468900	4.59425800	-0.05103600	C	8.92604300	-2.82805400	-0.57693000
C	6.70336500	-5.40407000	1.05010900	H	9.56459700	-3.10737200	-1.42275500
H	6.31195500	-6.38023800	1.35814100	C	-2.69330700	-0.68376800	-0.25939200

C	-1.08371300	-2.91015300	0.20539200
H	7.05903400	-5.49926300	0.02018900
H	7.24018800	-3.55809800	-3.22713200
H	6.35159000	-4.34271600	-1.91621600
H	5.77802500	2.67427700	-3.53667900
H	-0.89936300	-0.86900600	4.35295900
H	9.46823700	-2.08971300	0.02169500
H	8.77344300	-3.71945100	0.03730500
H	-3.31879500	0.18334300	-0.43720500
C	-3.23482500	-1.96463300	-0.33741000
H	-0.45001800	-3.77413300	0.37356700
C	-2.42963900	-3.07675300	-0.10455900
H	-4.28335200	-2.09590000	-0.57896300
H	-2.84769100	-4.07474000	-0.16783100
Sn	3.43063000	-1.03804600	1.19696400

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Ge	-0.84796800	-1.06937800	0.44065000
Si	2.81504800	-0.24735300	0.05692100
Si	2.57997400	-2.59665800	0.26928500
Si	4.37177100	0.05845100	-1.69355500
Si	3.74742700	0.49837100	2.09144900
O	-0.91704600	2.75217800	0.22468000
O	-1.78985500	1.68734000	-1.54272100
O	1.19918400	2.75425800	-1.80206500
O	2.46893800	2.93707700	0.03157000
N	-2.44549500	-0.08590700	1.15132100
N	-2.44937100	-1.10098300	-0.75886100
C	-0.01986300	0.63682200	-0.30154800
C	-5.11195000	1.01811600	-0.45723800
H	-4.38147500	1.78408200	-0.69701700
C	-3.20859700	-0.47426500	0.12453100
C	-0.99247400	1.71945000	-0.63645400
C	1.30404600	0.88123100	-0.34761600
C	-2.81482700	0.32050800	2.51596200
C	-2.71188000	-1.59461800	-2.11821600
C	1.73099700	2.28640200	-0.66689100
C	-3.42072800	-0.86148400	3.27992800
H	-2.73018500	-1.70972700	3.27737000
H	-3.62032300	-0.58066200	4.31803000
H	-4.36302800	-1.17613100	2.82421800
C	-3.76294500	-0.77649000	-2.87459100
H	-3.53052700	0.28855200	-2.81128600
H	-3.74251700	-1.07699700	-3.92570200
H	-4.77277900	-0.94746900	-2.49862100
C	-3.14142000	-3.06306100	-2.03734600
H	-4.08303500	-3.15540200	-1.48931200
H	-3.28288400	-3.47426600	-3.04084500
H	-2.37975500	-3.65587100	-1.52257800
C	-4.67092000	-0.22709000	-0.00871200
C	1.97755800	-3.18863100	1.95679600
H	1.94792100	-4.28453900	1.94964600
H	2.65803900	-2.88404500	2.75620400
H	0.97698800	-2.82687500	2.19690000
C	-1.37849900	-1.48235700	-2.86395400
H	-0.59138300	-2.03042100	-2.33656100
H	-1.46934300	-1.90734100	-3.86655200
H	-1.08221400	-0.43382100	-2.94436200
C	-1.79493200	3.84661200	-0.05184200
H	-2.83574000	3.51960000	-0.04538400
H	-1.62346600	4.57396200	0.73883200
H	-1.56333600	4.28255500	-1.02553100
C	4.34451600	-3.26304100	0.09408900
H	4.32619700	-4.33497800	0.32298200
H	5.04903700	-2.78992000	0.78171400
C	1.57998900	-3.43652600	-1.09453200
H	0.51373300	-3.46742800	-0.86142500
H	1.71027200	-2.94514100	-2.06245800
H	1.93028400	-4.47028200	-1.19395900
C	3.96572700	-1.08681000	-3.13826000
H	2.95928700	-0.88094900	-3.51702200
C	1.48406200	4.12644100	-2.09742800

H	2.55715700	4.27266400	-2.22938400
H	1.12699300	4.76826600	-1.29053400
C	-3.77764400	1.51189000	2.53381900
H	-4.77970800	1.23616900	2.20308100
H	-3.40159400	2.31526700	1.89441600
C	4.68270100	2.13142200	2.01485400
H	5.25753000	2.25824500	2.93910700
H	5.38699400	2.15213500	1.17775800
H	4.00266800	2.97517700	1.90135500
C	4.99854900	-0.77203300	2.72037800
H	4.57475900	-1.76786900	2.86433600
H	5.84858300	-0.85870700	2.03632200
H	5.38746800	-0.43265800	3.68720600
C	-1.49884700	0.74144900	3.17599400
H	-1.04701800	1.56835900	2.62129000
H	-1.67282100	1.05933500	4.20666400
H	-0.79153100	-0.09424800	3.19591400
C	2.31652100	0.62458600	3.31287800
H	1.57880300	1.35496400	2.96670400
H	1.81289600	-0.34183500	3.41916900
H	2.66569200	0.93633100	4.30313700
C	4.38324000	1.81656800	-2.37786800
H	5.19033400	1.89745300	-3.11476000
H	3.44615000	2.05819000	-2.88679700
H	4.55783200	2.56093500	-1.59713700
C	6.11181100	-0.29448400	-1.05390300
H	6.38629700	0.41790800	-0.26964600
C	-6.47200700	1.25452000	-0.61306500
C	-5.58857400	-1.23360500	0.28277100
H	4.72948000	-3.15120000	-0.92286800
H	4.67180800	-0.92053700	-3.95930700
H	4.01265200	-2.14387700	-2.86453400
H	0.95532100	4.34641400	-3.02206600
H	-3.85425200	1.89333500	3.55568600
H	6.21929900	-1.30324000	-0.64977500
H	6.83253900	-0.18109700	-1.87139400
H	-6.81525900	2.21947400	-0.96796400
C	-7.39310700	0.25048200	-0.31733700
H	-5.23958700	-2.20145300	0.62638800
C	-6.95187100	-0.99071100	0.13160100
H	-8.45416500	0.43639900	-0.43886500
H	-7.66670300	-1.77239500	0.36124400

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Si	2.99555400	-0.16914900	0.05502900
Si	2.76152200	-2.51766400	0.15669400
Si	4.59686600	0.19778100	-1.63707200
Si	3.78574000	0.61434000	2.12331300
O	-0.84947800	2.67380900	-0.07135700
O	-1.61690200	1.44575800	-1.78302900
O	1.35890100	2.71400100	-1.90866400
O	2.46825800	2.97877300	0.01756900
N	-2.49756600	-0.02826900	1.14861600
N	-2.63383600	-1.24737800	-0.67904400
C	0.12778500	0.54678200	-0.40983800
C	-4.95308600	1.18933500	-0.70198900
H	-4.11998100	1.75238800	-1.10937200
C	-3.28020000	-0.44247800	0.15142900
C	-0.86276700	1.57091300	-0.84736400
C	1.43904800	0.86449000	-0.41257700
C	-2.83992700	0.63677900	2.41415300
C	-3.07032500	-1.87811500	-1.93293700
C	1.81729600	2.28548500	-0.72681400
C	-3.55583600	-0.34273200	3.35166300
H	-2.95400800	-1.24606400	3.48791500
H	-3.71814900	0.11610600	4.33146200
H	-4.52814300	-0.63014800	2.94430900
C	-3.83122400	-0.93367000	-2.87242300
H	-3.31014100	0.02318700	-2.94648300
H	-3.87880300	-1.38736300	-3.86646700
H	-4.85499000	-0.75940900	-2.53907800

C	-3.92209400	-3.11587900	-1.62835400
H	-4.85268000	-2.83237100	-1.13099800
H	-4.17576900	-3.63965100	-2.55481400
H	-3.37484500	-3.80474300	-0.97850200
C	-4.69789300	-0.00481500	-0.02620600
C	2.13812500	-3.17093500	1.82711100
H	2.96756000	-3.65124100	2.35611300
H	1.73014900	-2.39115400	2.47355300
H	1.35444000	-3.92001400	1.68308200
C	-1.77709300	-2.31460800	-2.62803700
H	-1.21209300	-3.00240700	-1.99014700
H	-1.99715200	-2.83005200	-3.56584700
H	-1.15431900	-1.44133500	-2.84561900
C	-1.68034200	3.74874000	-0.51616200
H	-2.72742000	3.44662800	-0.55156700
H	-1.54600800	4.55020900	0.20757500
H	-1.37079100	4.07831600	-1.51007300
C	4.49051800	-3.25880800	-0.03647600
H	4.40658800	-4.34847300	0.05101100
H	5.16851900	-2.91605400	0.75058700
C	1.72458300	-3.13308300	-1.30811200
H	1.12983400	-2.33875300	-1.76776700
H	2.38915400	-3.52794900	-2.08334400
H	1.04757900	-3.93868500	-1.00855100
C	4.18099800	-0.86563100	-3.13988000
H	3.16920700	-0.64582200	-3.49587000
C	1.59235700	4.09853800	-2.19366400
H	2.66271400	4.30569100	-2.23214800
H	1.13064000	4.72386500	-1.42779200
C	-3.68272100	1.90628800	2.24334400
H	-4.71164900	1.68609800	1.95671600
H	-3.23763900	2.56217900	1.49104600
C	4.87695400	2.14401200	2.01701500
H	5.20489200	2.43121800	3.02241500
H	5.77267900	1.95355200	1.41874900
H	4.33557000	2.98072700	1.57355500
C	4.81883100	-0.75599400	2.91324400
H	4.24828500	-1.67923500	3.04729000
H	5.69728200	-0.98371400	2.30067500
H	5.17661000	-0.43643700	3.89828400
C	-1.49155200	1.03037500	3.02714000
H	-0.95487400	1.70454400	2.35371400
H	-1.63338400	1.52898900	3.98905500
H	-0.87526300	0.14098800	3.19963700
C	2.27276200	0.96909400	3.18880600
H	1.66221400	1.75333600	2.73152100
H	1.65285100	0.07283000	3.29384800
H	2.56130400	1.29990900	4.19218300
C	4.66961300	1.99070400	-2.21754400
H	5.52194300	2.10635000	-2.89654800
H	3.76801800	2.27062600	-2.76865700
H	4.79874800	2.68634600	-1.38438700
C	6.31084400	-0.24207900	-0.98030000
H	6.61001200	0.45304800	-0.19020400
C	-6.26010200	1.63008800	-0.86484600
C	-5.75418200	-0.75960700	0.47742100
H	4.94267200	-3.03798400	-1.00602700
H	4.87763800	-0.65569500	-3.95886300
H	4.23410600	-1.93506100	-2.92018200
H	1.13552600	4.28283200	-3.16342600
H	-3.70830000	2.44526400	3.19462300
H	6.36712100	-1.25587700	-0.57878800
H	7.04607100	-0.15956800	-1.78853400
H	-6.45586500	2.55665600	-1.39247700
C	-7.31830600	0.87951000	-0.35360700
H	-5.55580700	-1.69053500	0.99747200
C	-7.06479400	-0.31465400	0.31386200
H	-8.33838000	1.22422400	-0.47935000
H	-7.88551600	-0.90262600	0.70847600
Sn	-0.78127100	-1.28438900	0.53228000

Ts-2 Ge

Ge	-2.289000	-0.389000	1.341000
Si	1.079000	2.226000	1.770000
Si	0.278000	2.550000	3.954000
Si	2.646000	0.451000	1.731000
Si	1.971000	4.169000	0.726000
O	-2.105000	3.633000	-0.147000
O	-3.919000	2.432000	0.469000
O	0.240000	-0.151000	-0.792000
O	0.548000	1.916000	-1.619000
N	-4.058000	0.060000	2.158000
N	-3.847000	-0.537000	0.085000
C	-1.673000	1.620000	0.823000
C	-6.809000	1.062000	0.622000
H	-6.190000	1.949000	0.550000
C	-4.715000	-0.213000	1.035000
C	-2.692000	2.493000	0.405000
C	-0.318000	1.663000	0.598000
C	-4.550000	0.457000	3.486000
C	-4.051000	-0.846000	-1.338000
C	0.197000	1.178000	-0.733000
C	-5.634000	-0.488000	4.017000
H	-5.303000	-1.528000	3.953000
H	-5.831000	-0.254000	5.067000
H	-6.572000	-0.382000	3.470000
C	-4.991000	0.157000	-2.019000
H	-4.724000	1.176000	-1.728000
H	-4.893000	0.058000	-3.103000
H	-6.035000	-0.021000	-1.760000
C	-4.574000	-2.276000	-1.515000
H	-5.570000	-2.387000	-1.083000
H	-4.637000	-2.522000	-2.579000
H	-3.901000	-2.990000	-1.033000
C	-6.195000	-0.166000	0.868000
C	-1.290000	3.591000	3.955000
H	-1.734000	3.628000	4.956000
H	-1.049000	4.616000	3.653000
H	-2.035000	3.204000	3.256000
C	-2.668000	-0.740000	-1.983000
H	-1.963000	-1.417000	-1.490000
H	-2.724000	-1.012000	-3.039000
H	-2.286000	0.283000	-1.902000
C	-3.003000	4.662000	-0.527000
H	-3.566000	5.040000	0.330000
H	-2.380000	5.459000	-0.935000
H	-3.707000	4.321000	-1.289000
C	1.588000	3.422000	4.993000
H	1.314000	3.344000	6.051000
H	1.671000	4.483000	4.747000
C	0.038000	0.840000	4.717000
H	-0.480000	0.146000	4.052000
H	1.020000	0.414000	4.950000
H	-0.527000	0.907000	5.653000
C	1.774000	-1.175000	2.107000
H	1.030000	-1.401000	1.339000
C	0.677000	-0.722000	-2.036000
H	1.688000	-0.389000	-2.273000
H	-0.002000	-0.436000	-2.840000
C	-5.063000	1.901000	3.467000
H	-5.989000	1.987000	2.897000
H	-4.321000	2.558000	3.010000
C	3.316000	3.722000	-0.509000
H	3.712000	4.644000	-0.949000
H	4.145000	3.193000	-0.031000
H	2.924000	3.102000	-1.318000
C	2.732000	5.219000	2.094000
H	1.961000	5.629000	2.751000
H	3.443000	4.658000	2.707000
H	3.268000	6.061000	1.642000
C	-3.331000	0.388000	4.406000
H	-2.555000	1.065000	4.041000

H	-3.602000	0.691000	5.420000
H	-2.922000	-0.626000	4.443000
C	0.626000	5.161000	-0.125000
H	0.164000	4.576000	-0.921000
H	-0.160000	5.448000	0.578000
H	1.063000	6.072000	-0.551000
C	3.499000	0.305000	0.049000
H	4.484000	0.779000	0.075000
H	3.640000	-0.752000	-0.201000
H	2.935000	0.773000	-0.761000
C	3.934000	0.788000	3.064000
H	4.424000	1.755000	2.917000
C	-8.189000	1.118000	0.451000
C	-6.956000	-1.332000	0.943000
H	2.574000	2.965000	4.872000
H	2.510000	-1.987000	2.119000
H	1.272000	-1.161000	3.077000
H	0.659000	-1.799000	-1.886000
H	-5.261000	2.233000	4.491000
H	3.484000	0.781000	4.062000
H	4.707000	0.013000	3.041000
H	-8.668000	2.070000	0.254000
C	-8.952000	-0.045000	0.527000
H	-6.473000	-2.282000	1.144000
C	-8.336000	-1.269000	0.773000
H	-10.027000	0.003000	0.393000
H	-8.928000	-2.174000	0.836000

Ts-2 Sn

Sn	0.855000	-0.095000	-1.528000
Si	-3.052000	0.206000	0.289000
Si	-2.547000	2.434000	-0.422000
Si	-4.892000	-0.566000	-1.018000
Si	-3.690000	0.341000	2.592000
O	0.191000	-1.805000	2.121000
O	1.759000	-0.171000	1.772000
O	-0.982000	-2.361000	-1.876000
O	-2.671000	-2.758000	-0.209000
N	2.478000	1.150000	-0.770000
N	2.842000	-1.059000	-0.664000
C	-0.059000	-0.449000	0.259000
C	4.577000	0.806000	1.705000
H	3.620000	0.949000	2.195000
C	3.312000	0.132000	-0.363000
C	0.735000	-0.735000	1.395000
C	-1.455000	-0.832000	-0.100000
C	2.797000	2.571000	-1.022000
C	3.298000	-2.394000	-0.197000
C	-1.743000	-1.977000	-0.845000
C	4.127000	2.761000	-1.797000
H	4.143000	2.183000	-2.716000
H	4.261000	3.833000	-2.051000
H	5.004000	2.464000	-1.186000
C	3.877000	-2.400000	1.250000
H	3.236000	-1.753000	1.913000
H	3.898000	-3.439000	1.639000
H	4.902000	-2.001000	1.267000
C	4.334000	-2.959000	-1.179000
H	5.244000	-2.349000	-1.172000
H	4.613000	-3.999000	-0.902000
H	3.933000	-2.978000	-2.201000
C	4.599000	0.373000	0.361000
C	-0.996000	3.056000	0.448000
H	-0.686000	4.019000	0.023000
H	-1.175000	3.186000	1.522000
H	-0.171000	2.337000	0.322000
C	2.063000	-3.313000	-0.215000
H	1.593000	-3.304000	-1.222000
H	2.355000	-4.355000	0.011000
H	1.305000	-3.009000	0.518000
C	0.857000	-2.059000	3.379000

H	0.916000	-1.122000	3.974000
H	0.218000	-2.796000	3.905000
H	1.876000	-2.464000	3.241000
C	-3.988000	3.599000	0.062000
H	-3.735000	4.632000	-0.222000
H	-4.149000	3.567000	1.167000
C	-2.341000	2.533000	-2.301000
H	-1.541000	1.858000	-2.658000
H	-3.267000	2.280000	-2.830000
H	-2.047000	3.560000	-2.593000
C	-4.329000	-1.102000	-2.738000
H	-3.703000	-2.021000	-2.717000
C	-1.107000	-3.762000	-2.224000
H	-2.128000	-3.995000	-2.507000
H	-0.806000	-4.369000	-1.355000
C	2.838000	3.352000	0.317000
H	3.738000	3.116000	0.884000
H	1.954000	3.091000	0.921000
C	-3.605000	-1.403000	3.311000
H	-3.825000	-1.415000	4.396000
H	-4.340000	-2.048000	2.787000
H	-2.597000	-1.836000	3.157000
C	-5.449000	1.036000	2.749000
H	-5.532000	2.067000	2.363000
H	-6.195000	0.415000	2.210000
H	-5.727000	1.046000	3.814000
C	1.686000	3.128000	-1.909000
H	0.698000	2.980000	-1.431000
H	1.818000	4.205000	-2.069000
H	1.666000	2.629000	-2.893000
C	-2.552000	1.497000	3.588000
H	-1.478000	1.310000	3.393000
H	-2.746000	2.572000	3.367000
H	-2.734000	1.344000	4.672000
C	-5.831000	-1.987000	-0.181000
H	-6.254000	-1.677000	0.767000
H	-6.658000	-2.330000	-0.837000
H	-5.158000	-2.844000	-0.016000
C	-6.124000	0.853000	-1.269000
H	-6.462000	1.283000	-0.310000
C	5.781000	0.988000	2.375000
C	5.837000	0.162000	-0.282000
H	-4.935000	3.329000	-0.420000
H	-5.202000	-1.337000	-3.362000
H	-3.756000	-0.312000	-3.239000
H	-0.432000	-3.923000	-3.050000
H	2.823000	4.440000	0.128000
H	-5.697000	1.683000	-1.866000
H	-7.014000	0.463000	-1.796000
H	5.742000	1.293000	3.437000
C	6.996000	0.762000	1.762000
H	5.863000	-0.138000	-1.325000
C	7.032000	0.366000	0.422000
H	7.938000	0.916000	2.289000
H	7.986000	0.207000	-0.098000

3_{trans}

97

Si	-2.72620400	0.23705700	0.33876300
Si	-3.99795000	1.75338200	-0.93741100
Si	-2.24353800	1.28441100	2.39996000
O	0.90471100	1.20821500	1.09011500
C	0.43398700	1.25449600	-0.02222000
O	0.28054400	2.38633100	-0.72889600
C	4.29997000	2.52214500	-0.86302900
H	4.72776600	3.36254700	-1.41688200
H	5.07410100	2.12838600	-0.20259900
H	3.47706900	2.89514500	-0.24879300
C	3.79932800	1.46629900	-1.85547900
C	-1.55594900	3.03668900	2.30227400
H	-2.08816100	3.64683000	1.56617400
H	-0.49258000	3.03580300	2.06441000

H	-1.68122300	3.51342500	3.28112100
C	-3.95678800	1.43979000	3.21688400
H	-4.00580000	0.83526600	4.12701700
H	-4.77936800	1.12910100	2.56925300
H	-4.13517900	2.48223800	3.49898500
C	2.91080600	2.14067300	-2.90490000
H	2.58678700	1.41596400	-3.65814200
H	3.46397900	2.93249200	-3.41508600
H	2.02136900	2.57269900	-2.44196100
C	-2.82524200	3.05665700	-1.63113400
H	-3.38497600	3.77852400	-2.23631600
H	-2.05554100	2.60304400	-2.26107100
H	-2.31708300	3.60311300	-0.83139000
C	-4.90612000	0.94880100	-2.37956000
H	-5.54451600	0.12468800	-2.05045200
H	-4.20139200	0.55962100	-3.11779900
H	-5.54047000	1.69522300	-2.87076500
C	0.76190900	3.62181000	-0.18681300
H	-0.09365300	4.24272700	0.07827600
H	1.33974600	4.11474400	-0.96856800
H	1.38345100	3.44901500	0.69003300
C	-5.27114100	2.62507500	0.14992900
H	-4.79931400	3.16069900	0.97890400
H	-5.99907200	1.92467700	0.56991900
H	-5.82124400	3.35695600	-0.45196500
C	-1.26427800	-0.36035000	-0.76829800
Si	-3.86185900	-1.76220800	0.93474500
C	-1.11655000	0.26292700	3.51212200
C	0.00527700	0.08353700	-0.82576600
C	4.98745200	0.80939800	-2.56784400
N	2.95037200	0.44863600	-1.21021300
C	-1.59549900	-1.46618700	-1.71767100
C	-5.42213000	-2.06476400	-0.07986100
C	-2.66712900	-3.21346700	0.72512300
C	-4.40967900	-1.80471900	2.74276600
H	-1.15658500	0.65385800	4.53504900
H	-0.08601400	0.32441800	3.15683200
H	-1.40802400	-0.79068700	3.54252600
H	4.63623200	0.04080500	-3.26213400
H	5.54584100	1.55919100	-3.13596500
H	5.67128500	0.34981200	-1.85169400
C	3.25722300	-0.39886100	-0.22670900
O	-2.87836600	-1.41832100	-2.09891000
O	-0.82636600	-2.30187900	-2.13737100
H	-5.89270200	-3.00063400	0.24197300
H	-5.21667100	-2.13762800	-1.14927800
H	-6.14780300	-1.25992600	0.07449500
H	-3.10444700	-4.10427000	1.18956800
H	-2.45603100	-3.46045300	-0.31809600
H	-1.71260800	-3.01477500	1.22446200
H	-4.76293200	-2.81857000	2.96351800
H	-5.23480400	-1.11708300	2.94084100
H	-3.60014300	-1.57616000	3.44048000
N	2.42669300	-1.43371000	-0.25678500
C	4.34658000	-0.19453900	0.77237800
C	-3.30024900	-2.40395700	-3.04618100
C	2.15667900	-2.47117200	0.75700600
C	5.60856100	-0.75817000	0.59090700
C	4.07882300	0.57451600	1.90490800
H	-2.66858800	-2.37212100	-3.93419300
H	-4.32569000	-2.14887700	-3.30508000
H	-3.25714700	-3.40051900	-2.60208700
C	1.35767300	-3.55955300	0.03851600
C	3.43308200	-3.09974300	1.33032600
C	1.31030200	-1.88419200	1.89163300
H	5.80862500	-1.36895900	-0.28251600
C	6.60405400	-0.54674600	1.53925600
H	3.09232700	1.00876100	2.02821500
C	5.07499900	0.77597400	2.85528700
H	1.08484500	-4.34879800	0.74323000
H	1.94911500	-4.00276000	-0.76828400
H	0.44195400	-3.14925200	-0.39256600

H	4.11822000	-3.39114100	0.52979300
H	3.15619300	-3.99855100	1.88802500
H	3.95507100	-2.43106900	2.01559900
H	1.85220000	-1.08873900	2.40796900
H	1.06328300	-2.66765600	2.61503600
H	0.38513700	-1.45777400	1.49801400
H	7.58539200	-0.98433900	1.39631300
C	6.33803300	0.21855000	2.67238500
H	4.86513300	1.37078300	3.73688500
H	7.11410800	0.37858200	3.41216800
Ge	1.52677200	-0.78437900	-1.95075400

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97

Si	-2.80084100	0.47683800	0.08410000
Si	-4.17110100	0.49046300	-1.82919700
Si	-2.31152900	2.73334000	0.57817900
O	0.77621200	1.69392200	-0.35533800
C	0.32584000	0.87156300	-1.11957700
O	0.21235200	1.06293000	-2.44699000
C	4.17196200	1.45639300	-2.18732800
H	4.56893100	1.75412300	-3.16221800
H	4.88976300	1.76563200	-1.42607000
H	3.23470500	1.99038900	-2.01391800
C	3.93570400	-0.06038100	-2.17271800
C	-1.76467500	3.77045800	-0.89749800
H	-2.42451400	3.63088700	-1.75914900
H	-0.74059300	3.54442500	-1.19194100
H	-1.80597800	4.82893700	-0.61604500
C	-3.99322700	3.44255800	1.12038200
H	-4.18663800	4.37630200	0.58232500
H	-3.98902900	3.66957600	2.18993800
H	-4.83366700	2.77176400	0.92766700
C	3.19468700	-0.46133900	-3.45360900
H	3.06997100	-1.54811300	-3.49870900
H	3.75559400	-0.14934500	-4.33774400
H	2.20297900	-0.00312900	-3.48467600
C	-3.04895200	0.80085200	-3.31293100
H	-3.64054200	0.83297200	-4.23461900
H	-2.30169400	0.00884300	-3.41307100
H	-2.51285800	1.74949900	-3.21819500
C	-5.08747400	-1.13198500	-2.11199000
H	-5.68936700	-1.41378900	-1.24418300
H	-4.38807900	-1.94503900	-2.31962100
H	-5.75785700	-1.02810800	-2.97251400
C	0.65524900	2.29873600	-3.02010700
H	-0.21271200	2.80986000	-3.43767800
H	1.35671100	2.06083400	-3.82023400
H	1.13801500	2.92802800	-2.27518800
C	-5.44312500	1.88170100	-1.73852200
H	-4.96895200	2.86001300	-1.61682900
H	-6.14248100	1.73924500	-0.90931800
H	-6.02574700	1.90393000	-2.66615200
C	-1.35278200	-0.73435700	-0.30302800
Si	-3.81575200	-0.39785200	2.04348300
C	-1.08076800	2.96881800	1.98471800
C	-0.10914300	-0.49238600	-0.75792700
C	5.27946900	-0.79922200	-2.14140100
N	3.06243600	-0.49903100	-1.07427100
C	-1.65086100	-2.18086600	-0.08462100
C	-5.40198700	-1.35396400	1.69055800
C	-2.57150600	-1.51449500	2.92762300
C	-4.28009500	0.93874300	3.29462700
H	-1.09441000	4.01520600	2.31008600
H	-0.07194000	2.71918700	1.65154200
H	-1.32350600	2.34495700	2.84984500
H	5.11731800	-1.88075100	-2.12013600
H	5.86396400	-0.55516900	-3.03371600
H	5.86650000	-0.51613600	-1.26607700
C	3.20080200	-0.31996900	0.23432100
O	-2.94703200	-2.46173100	-0.22100000
O	-0.82615000	-3.04281600	0.15693400

H	-5.81576700	-1.74050200	2.62870100
H	-5.23636000	-2.19740100	1.01820400
H	-6.15680300	-0.70170200	1.23991400
H	-2.97404100	-1.78969900	3.90892600
H	-2.35163400	-2.44290600	2.39487000
H	-1.62612400	-0.98813900	3.09408000
H	-4.59200100	0.44439400	4.22182700
H	-5.11387500	1.55484000	2.95079400
H	-3.44371900	1.59993500	3.53580200
N	2.39056600	-1.10354300	0.94362300
C	4.15240200	0.66280000	0.84330600
C	-3.32954500	-3.83449400	-0.07770500
C	2.04333900	-1.02358200	2.37461500
C	5.43999500	0.27144400	1.20754000
C	3.74210700	1.98027100	1.04690300
H	-2.75737600	-4.46048300	-0.76243700
H	-4.38794100	-3.87564200	-0.32514300
H	-3.16586200	-4.16743500	0.94888800
C	1.28006300	-2.31458400	2.68311200
C	3.26111300	-0.95534200	3.30828000
C	1.12305700	0.17549300	2.63676000
H	5.75327700	-0.75668700	1.06236700
C	6.31518700	1.19445000	1.77155000
H	2.74287600	2.27448100	0.74482600
C	4.61658700	2.89897300	1.61929000
H	0.96132200	-2.32794200	3.72837400
H	1.91530900	-3.18756200	2.50313400
H	0.39066900	-2.39795100	2.05408900
H	4.00255400	-1.71170000	3.03622200
H	2.92991100	-1.15443500	4.33142300
H	3.73976000	0.02421000	3.29999900
H	1.64236100	1.11532200	2.44085500
H	0.79389400	0.17490100	3.68112700
H	0.24573400	0.13462500	1.98658600
H	7.31544900	0.88591200	2.05349900
C	5.90373000	2.50845700	1.98104600
H	4.29374700	3.92163900	1.77837700
H	6.58484200	3.22590100	2.42451400
Sn	1.51376100	-2.10857800	-0.85906900