Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

for

A highly unsaturated six-vertex amido-substituted silicon cluster

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Table of content

1. DFT calculations

1.1. Methods

Conformer structures of **2** were optimized without geometry constraints with density functional theory, using the resolution of the identity approximation[S1] and an atom-pairwise dispersion correction (D3).[S2] A flexible triple zeta basis set (def2-TZVP)[S3] was used in all calculations. Structure optimizations were performed with the TPSS functional.[S4] For the calculation of zero point vibrational energies and free enthalpy contributions (G^{RRHO}_{298}), a rotor approximation was applied for vibrational modes with wave numbers below 100 cm^{-1}.[S5] Single point energy calculations were performed with the PW6B95-D3 hybrid meta GGA functional.[S6] and in addition with the highly accurate DLPNO-CCSDT(T) method for comparison. NMR chemical shielding tensors were calculated with the BP86 functional.[S7]

All DFT geometry optimizations, vibrational frequency and NMR chemical shift calculations were performed with the TURBOMOLE 7.3 program.[S8] DLPNO-CCSD(T) calculations and the Mayer population analysis[S9] were conducted with ORCA.[S10] Atoms-In-Molecules[S11] analysis of the electron density taken from the TPSS-D3 DFT calculation was conducted with AIMAll.[S12] Intrinsic Bond Orbitals (IBOs)[S13] were calculated and visualized with IboView (Version 20150427)[S14] starting with the wavefunction constructed TPSS and the def2-SVP[S3] basis set.

1.2. Results

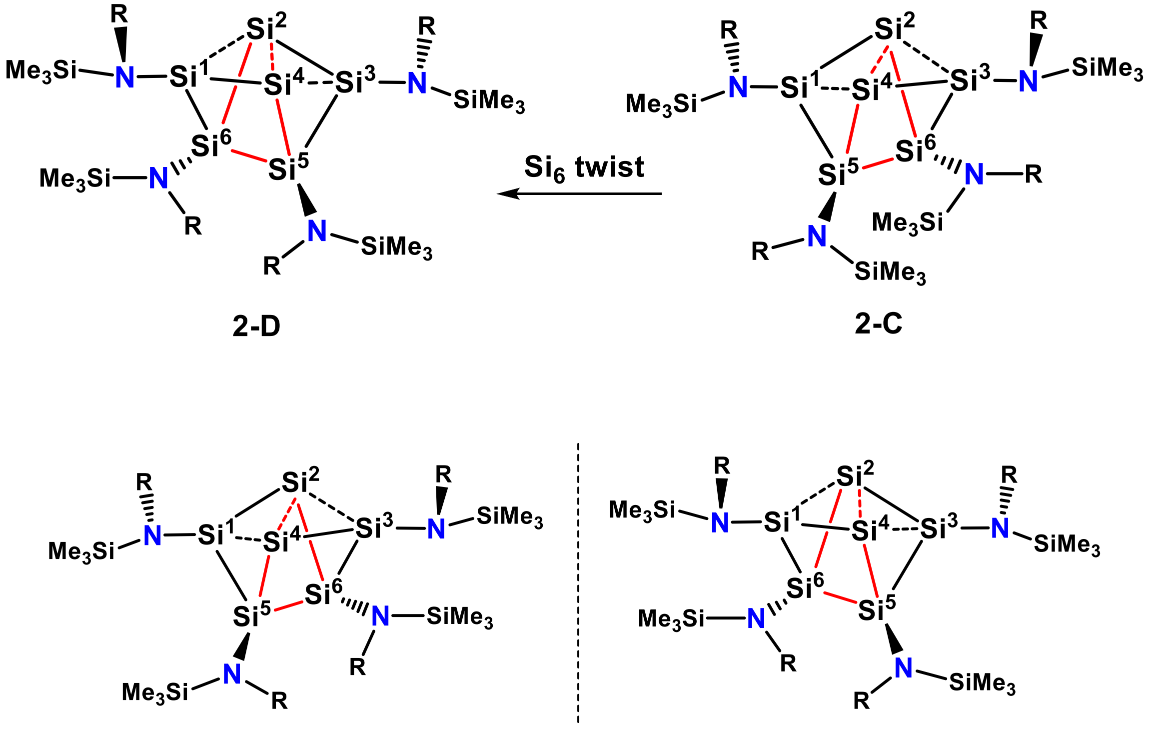
Conformers of 2

Conformational isomers of **2** (taken from the solid state structure **2-A**) were generated by rotating the ligands successively around the $Si_{Cluster}$-N single bonds in steps of 60° and optimizing the geometry. From the generated set of conformers, only the four most stable are reported here (Scheme 5), out of which one is the enantiomer of **2-A**. (**2-D** = *ent*-**2-A**). Conformers in which the substituents of Si1 and Si3 were rotated around the $Si_{cluster}$-N bond were found to have significantly higher (> 7 kcal/mol) relative free energies and are not discussed.

The relative free energies, obtained with PW6B95-D3 and DLPNO-CCSD(T) are given in Table S1. Although **2-A** and **2-D** are structurally enantiomers, the calculated free energies differ by 0.5 kcal/mol. This is presumably due to inaccuracies in the calculation of G^{RRHO}_{298}. Comparing the calculated chemical shifts of **2-C** with the ^{29}Si-NMR spectrum of **2**, we assign the minority isomer to be **2-C** (vide infra). This confirms to some extent the accuracy of the DLPNO-CCSD(T) energies ($\Delta G = +1.3$ kcal/mol), although we have used only a triple zeta basis set in the single point calculations with this correlation method.

Table S1 Relative energies of intermediates in Scheme 5 as calculated with DFT. The relative free energy is $\Delta G(298)_{solv} = \Delta E(M//TPSS\text{-}D3/def2\text{-}TZVP) + \Delta G^{RRHO}_{298} + \Delta G^{COSMO\text{-}RS}_{298}$

	E(TPSS-D3) [E_h]	E(PW6B95-D3) [E_h]	E(DLPNO-CCSD(T)) [E_h]	G^{RRHO}_{298} [kcal/mol]	$G^{COSMO\text{-}RS}_{298}$ (Toluene) [kcal/mol]	**$\Delta G(298)_{solv}$ M=PW6B95-D3 [kcal/mol]**	**$\Delta G(298)_{solv}$ M=DLPNO-CCSD(T) [kcal/mol]**
2-A	-5465.431212	-5470.524780	-5454.084805	864.44	-16.918	**0.0**	**0.0**
2-B	-5465.426151	-5470.525902	-5454.079790	866.53	-17.480	**1.4**	**5.2**
2-C	-5465.430475	-5470.529117	-5454.083904	865.15	-17.777	**-2.0**	**1.3**
2-D = *ent*-**A**	-5465.431298	-5470.525062	-5454.084836	864.92	-17.016	**0.3**	**0.5**



Scheme S1. **Top**: Illustration of the Si$_6$ twist with isomer **2-D** left and isomer **2-C** right. **Bottom**: **2-A** and enantiomer **2-D** with the Si$_6$ twist highlighted in red.

DFT-Optimized Structure of 2-A

The solid state structure **2-A** was taken as a starting point for the geometry optimization (in vacuum) with TPSS-D3/def2-TZVP. The optimized structure resembles the solid state structure closely. The optimized structure of **2-A** is depicted in Figure S1, two conformers obtained by ligand rotation (**2-B** and **2-C**) are shown in Figure S2. Structural parameters of **2-A** are listed in Table S2.

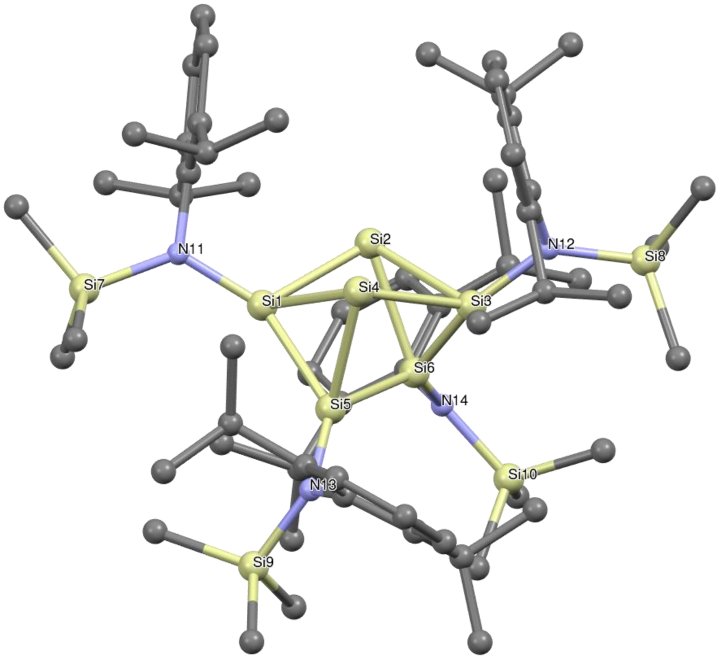


Figure S1. Gas phase (vacuum) structure of **2-A**, optimized with DFT (TPSS-D3/def2-TZVP). Bond distances and angles are given in Table S1.

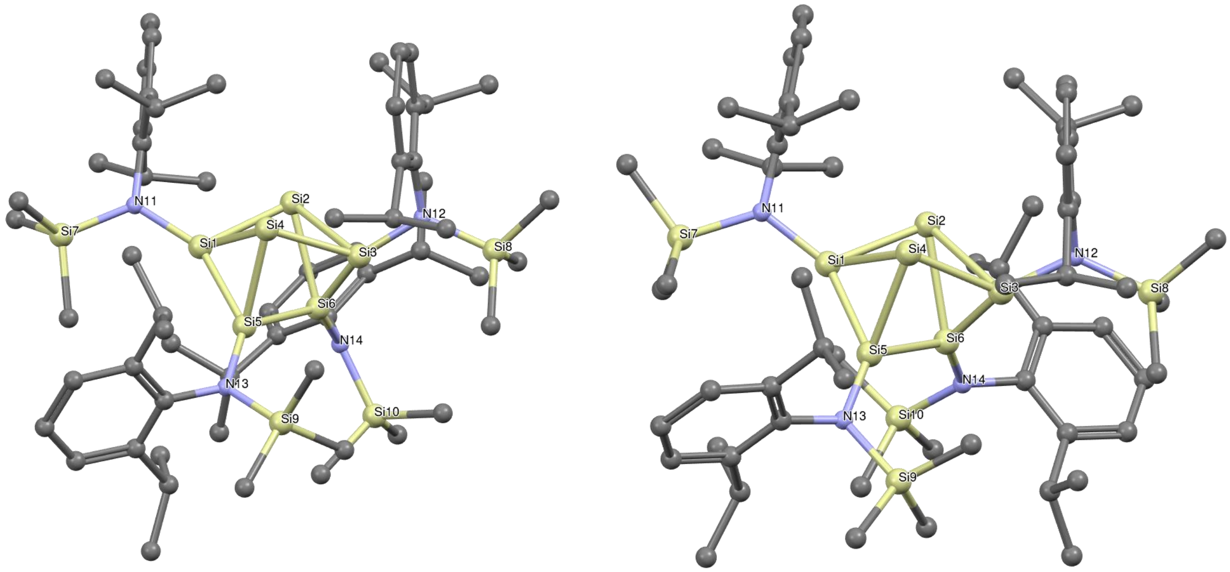


Figure S2. Gas phase (vacuum) structure of **2-B** and **2-C**, optimized with DFT (TPSS-D3/def2-TZVP).

Table S2 Structural parameters of the Si6 cluster in **2-A** after optimization with DFT (TPSS-D3/def2-TZVP). Bond lengths (> 3.0 Å) are given in [Å], dihedral angles in [°]. Atom labels are taken from Figure S1.

Parameter	Value (TPSS-D3/def2-TZVP)	Parameter	Value (TPSS-D3/def2-TZVP)
Si1-Si2	2.305	Si2-Si6	2.414
Si2-Si3	2.579	Si3-Si6	2.318
Si3-Si4	2.305	Si4-Si5	2.414
Si1-Si4	2.579	Si5-Si6	2.349
Si1-Si5	2.318	Si1-Si2-Si4-Si3	-138.9
Si2-Si4	2.789		

Electronic Structure of 2-A

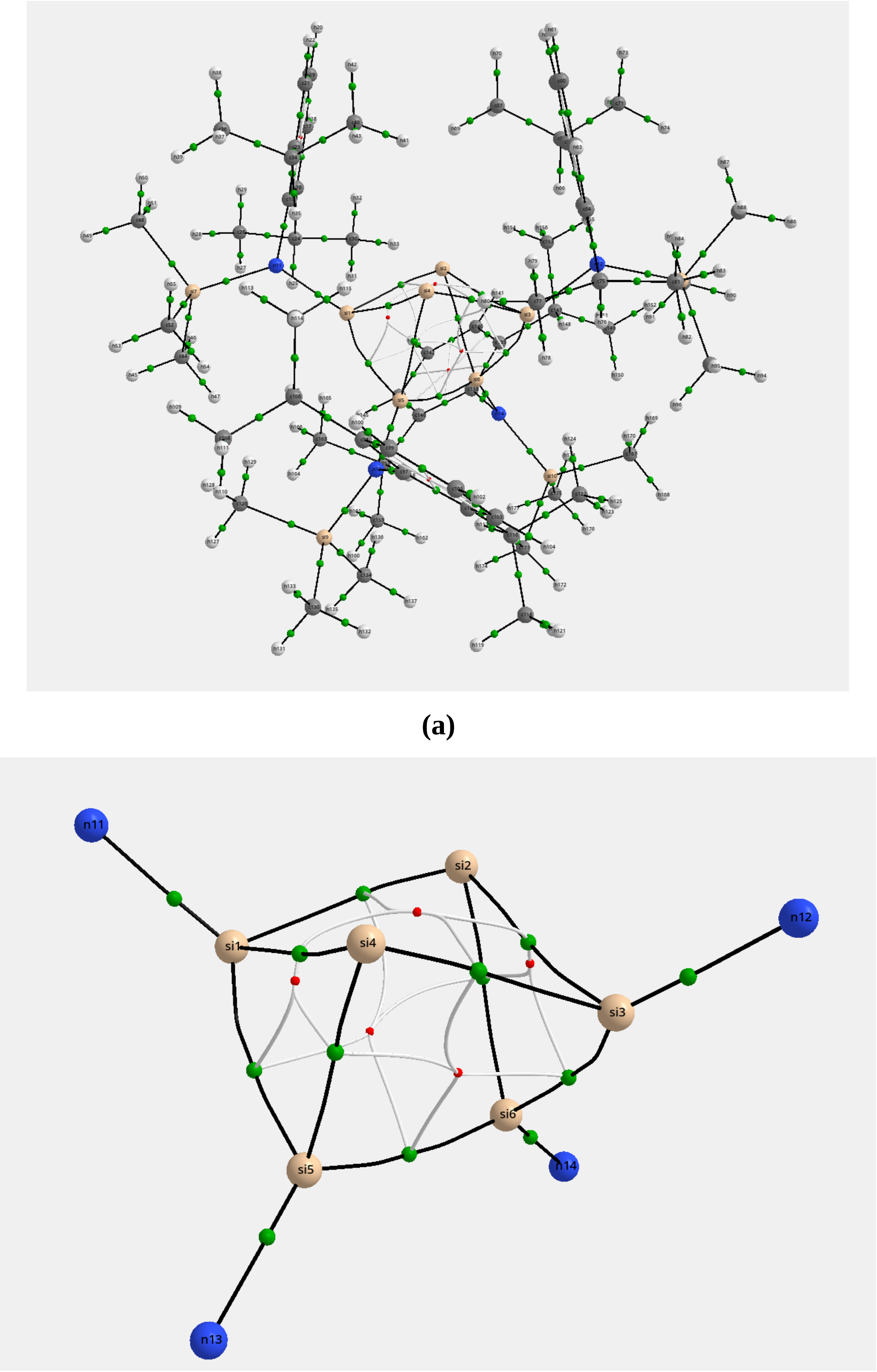
The bond orders as taken from the Mayer population analysis are reported in Table S3. The elongation of the Si1-Si4 and Si2-Si3 bonds is reflected in a reduced bond order (0.52), as is the order of the Si2-Si6 and Si4-Si5 bonds to a lesser extent (0.72). The interaction of the Si2 and Si4 has some bonding character (bond order 0.46).

The Atoms-In-Molecules (AIM) analysis (Figure S3) reveals no bond path between Si2 and Si4, but a ring critical point (rcp) of the Si1-Si2-Si3-Si4 "butterfly-shaped" ring. The bond critical points (bcps) of the two elongated Si1-Si4 and Si2-Si3 bonds lie very close to the ring critical points of the triangular faces (e.g. Si1-Si4-Si5) of the cluster. The rcps of the tetraatomic faces (e.g. Si1-Si2-Si6-Si5) are located more closely to the geometric center of the ring, corresponding to the 'stable' nature of the four Si-Si bond in this ring.

Figure S4 depicts the HOMO and the LUMO of **2**. The delocalized shape of both orbitals is indicative of the cluster nature of the Si_6 core.

Table S3 Mayer bond orders in the Si_6 cluster (**2-A**) with DFT (TPSS-D3/def2-TZVP). Bond orders > 0.40 are reported. Atom labels are taken from Figure S1.

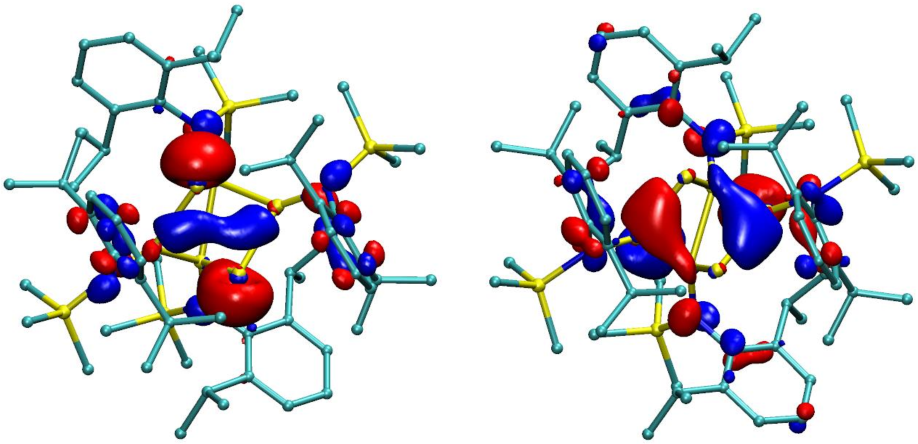
Atoms	Bond Order	Parameter	Bond Order	Parameter	Bond Order
Si1-Si2	0.862	Si2-Si4	0.461	Si1-N11	1.115
Si2-Si3	0.523	Si2-Si6	0.716	Si3-N12	1.115
Si3-Si4	0.862	Si3-Si6	0.901	Si5-N13	1.019
Si1-Si4	0.523	Si4-Si5	0.716	Si6-N14	1.019
Si1-Si5	0.901	Si5-Si6	0.886		



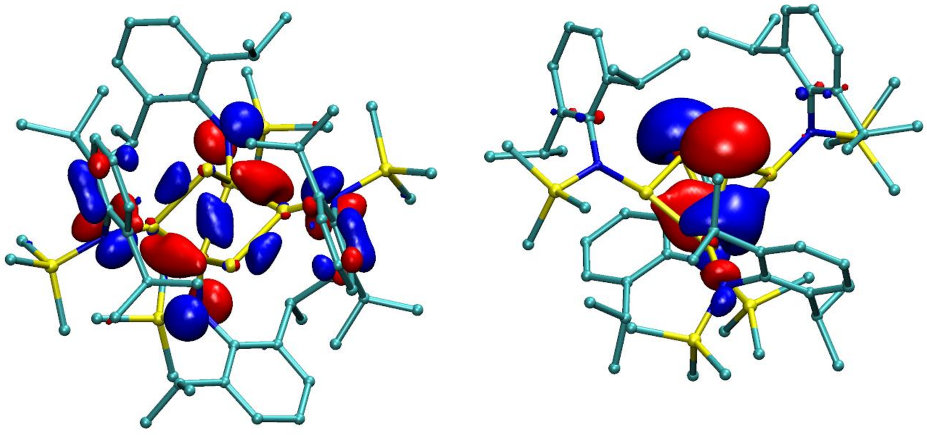
(a)

(b)

Figure S3. (a) Bond topology from the Atoms-In-Molecules analysis (TPSS-D3/def2-TZVP) of **2-A**. (b) Only the Si_6 cluster and the directly bonded N atoms are shown. (green: bond critical points, red: ring critical points).

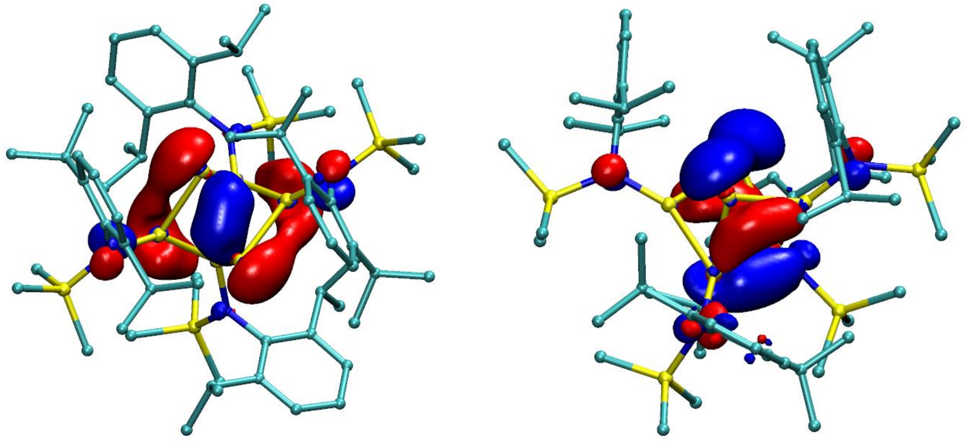


HOMO-5 (top view, -5.47 eV) HOMO-4 (top view, -5.40 eV)

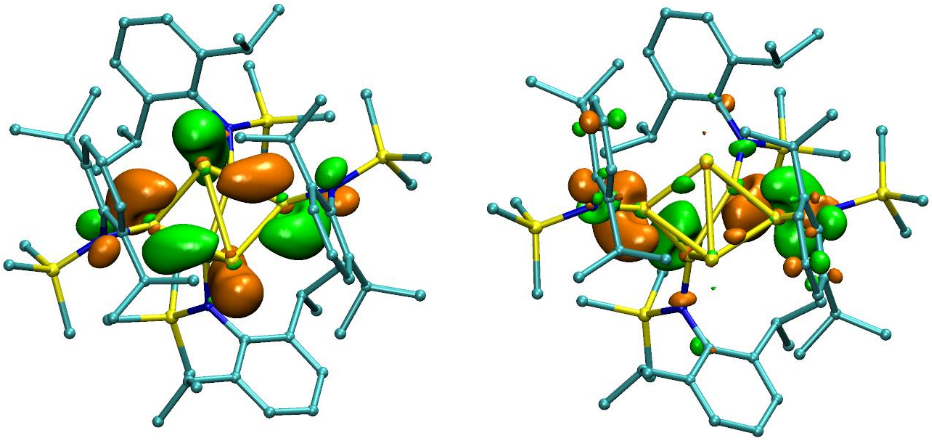


HOMO-3 (top view, -5.21 eV) HOMO-2 (side view, -4.93 eV)

Figure S4. Kohn-Sham (frontier) molecular orbitals of **2-A** (TPSS-D3/def2-TZVP).

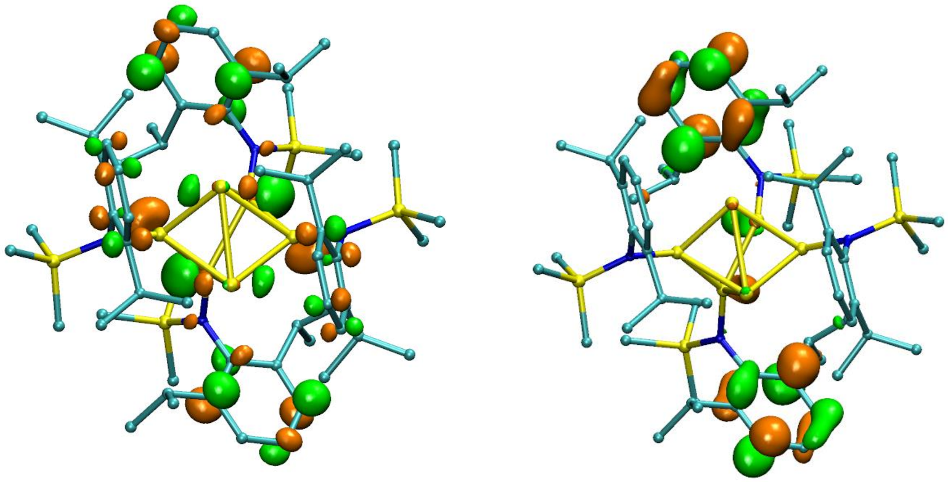


HOMO-1 (top view, -4.88 eV)   HOMO (side view, -4.84 eV)



LUMO (top view, -2.07 eV)   LUMO+1 (top view, -1.54 eV)

Figure S4 (continued). Kohn-Sham (frontier) molecular orbitals of **2-A** (TPSS-D3/def2-TZVP).



LUMO+2 (top view, -1.10 eV)

LUMO+3 (top view, -1.02 eV)

Figure S4 (continued). Kohn-Sham (frontier) molecular orbitals of **2-A** (TPSS-D3/def2-TZVP).

Intrinsic Bond Orbitals of 2-A

The intrinsic bond orbitals are unique localized molecular orbitals corresponding to chemically meaningful orbitals.[S13] The analysis of **2-A** was conducted with a double zeta basis set (def2-SVP) and gave IBOs in the Si_6 core as shown in Figure S5. We note seven single σ-bonds (IBO 291-297), lone pairs (IBO 299,300) on Si2 and Si4, and a multicenter bond (IBO 298) which explains the partial double bond character of the Si1-Si2/Si3-Si4 bonds and the partial (σ) bonding between Si2-Si4 and Si1-Si4/Si2-Si3.

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291 AB  -0.400216   SI  6  0.960  SI  5  0.959  SI  3  0.023  SI  1  0.023   (other: 0.033)
292 AB  -0.383924   SI  1  0.982  SI  2  0.826  SI  3  0.096  SI  5  0.043  SI  4  0.025   (other: 0.030)
293 AB  -0.383902   SI  3  0.982  SI  4  0.825  SI  1  0.096  SI  6  0.042  SI  2  0.024   (other: 0.030)
294 AB  -0.375821   SI  3  1.122  SI  6  0.803  SI  1  0.027   (other: 0.047)
295 AB  -0.375522   SI  1  1.123  SI  5  0.802  SI  3  0.027   (other: 0.047)
296 AB  -0.371539   SI  5  0.959  SI  4  0.783  SI  1  0.128  SI  3  0.056  SI  6  0.033   (other: 0.041)
297 AB  -0.371427   SI  6  0.960  SI  2  0.783  SI  3  0.127  SI  1  0.056  SI  5  0.033   (other: 0.042)
298 AB  -0.315759   SI  2  0.645  SI  4  0.643  SI  3  0.320  SI  1  0.317  SI  6  0.026  SI  5  0.026 (other: 0.023)
299 AB  -0.306346   SI  2  1.838  SI  5  0.045  SI  3  0.039   (other: 0.077)
300 AB  -0.306321   SI  4  1.838  SI  6  0.046  SI  1  0.040   (other: 0.077)
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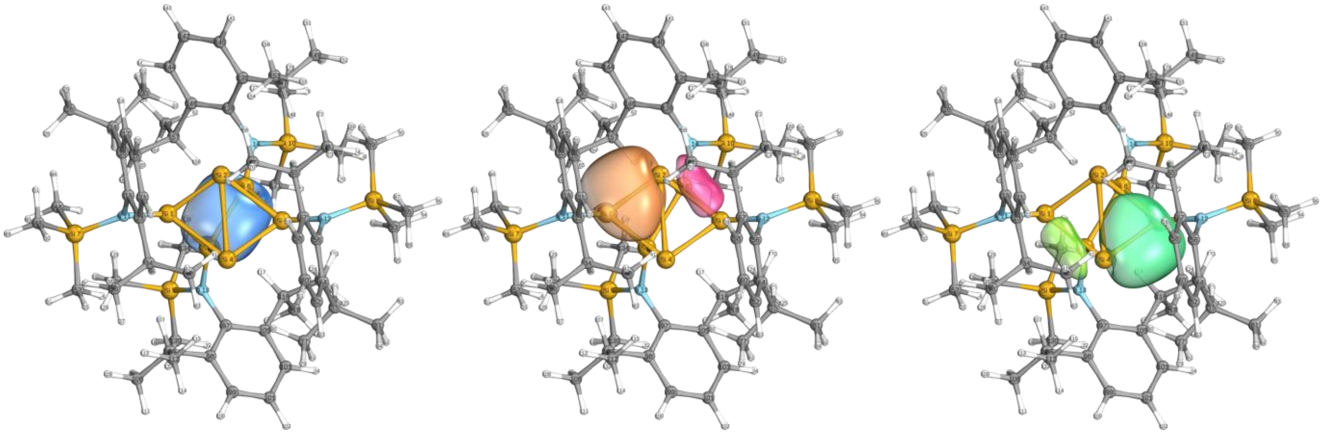
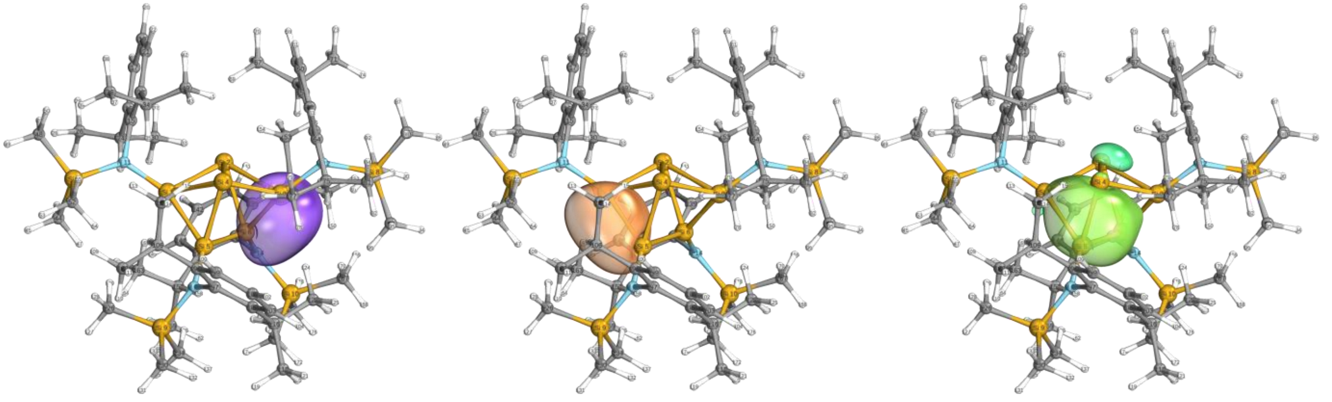


IBO 291 (σ Si5-Si6) IBO 292 (σ Si1-Si2) IBO 293 (σ Si3-Si4)



IBO 294 (σ Si3-Si6) IBO 295 (σ Si1-Si5) IBO 296 (σ Si4-Si5)

Figure S5. Intrinsic bond orbitals (IBO) of **2-A** (TPSS-D3/def2-SVP)

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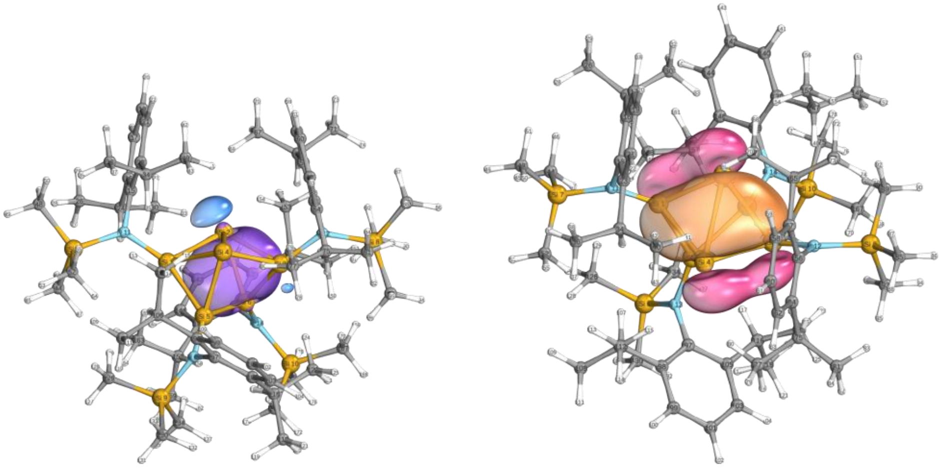
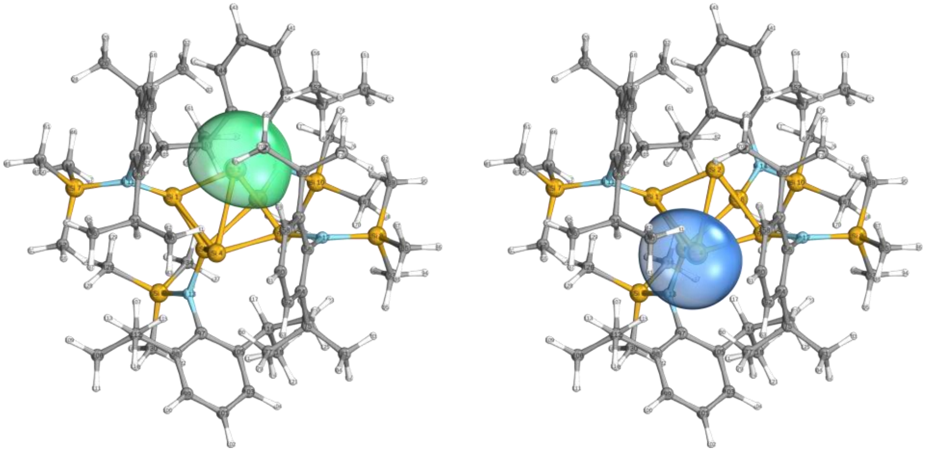


IBO 297 (σ Si2-Si6)

IBO 298 (multicenter bond)



IBO 299 (LP Si2)

IBO 300 (LP Si4)

Figure S5 (continued). Intrinsic bond orbitals (IBO) of **2-A** (TPSS-D3/def2-SVP).

Calculated ^{29}Si NMR chemical shifts of 2

Isotropic chemical shieldings of the title compound in the conformation found in the solid state (**2-A**) and of the assumed minor conformation found in solution (**2-C**) were calculated with BP86/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts (Table S4).

Table S4 ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of **2**. In brackets: chemical shift values observed in the experimental spectrum.

	2-A (Solid state conformer)		**2-C** (Minor conformer)	
Atom	σ_{iso} [ppm]	δ [ppm]	σ_{iso} [ppm]	δ [ppm]
Si(TMS)	311.566	0.0	311.566	0.0
Si1	205.891	105.7 (94.9)	254.073	57.5 (52.1)
Si2	607.037	-295.5 (-309.2)	584.976	-273.4 (-293.7)
Si3	205.854	105.7 (94.9)	254.376	57.2 (52.1)
Si4	607.204	-295.6 (-309.2)	584.697	-273.1 (-293.7)
Si5	316.187	-4.6 (7.7)	327.608	-16.0 (5.4)
Si6	316.325	-4.8 (7.7)	327.438	-15.9 (5.4)
Si7	304.614	7.0	302.996	8.6
Si8	304.594	7.0	302.993	8.6
Si9	303.199	8.4	300.228	11.3
Si10	303.198	8.4	300.143	11.4

[a] BP86//TPSS-D3/def2-TZVP

Estimation of barriers for conformer transformations (2-A → 2-C → *ent*-*2*-A)

Minimum energy path optimization with the GSM method

We conducted three optimization of the minimum energy path between conformers **2-A**, **2-B**, **2-C** and **2-D** (= *ent*-**2-A**) in order to get an estimate for the (electronic) potential energy barriers and to prove that these transformations occur as single steps. We used the growing string method (GSM)[S15] to construct these paths between the given reactant and product structure. To increase the computational efficiency, we chose the smaller def2-SVP basis set for the GSM calculations. We used 15 points for each GSM calculation. Attempts to optimize reaction paths of the synchronous (symmetric) rotation of two ligands (**2-A** → **2-C**) and eventually including the twist of the Si_6 core (**2-A** → **2-D**) gave paths with significantly higher potential energy barriers.

The three minimum energy paths were connected to a complete path as shown in Figure S6. As we find, the barriers of ligand rotation both lie well below 20 kcal/mol, the subsequent Si_6 twist has to overcome an (electronic) energy barrier of approximately 24 kcal/mol. As MD simulations with the ReaxFF force field suggest, the free energy barrier of this Si_6 transformation might be lower that the free energy barriers of the ligand rotations (see next section). This result would imply that the equilibration of the two conformers detected in the solution NMR of **2** (**2-A** and **2-C**) may occur at room temperature by two subsequent ligand rotations or by a twist of the Si_6 core.

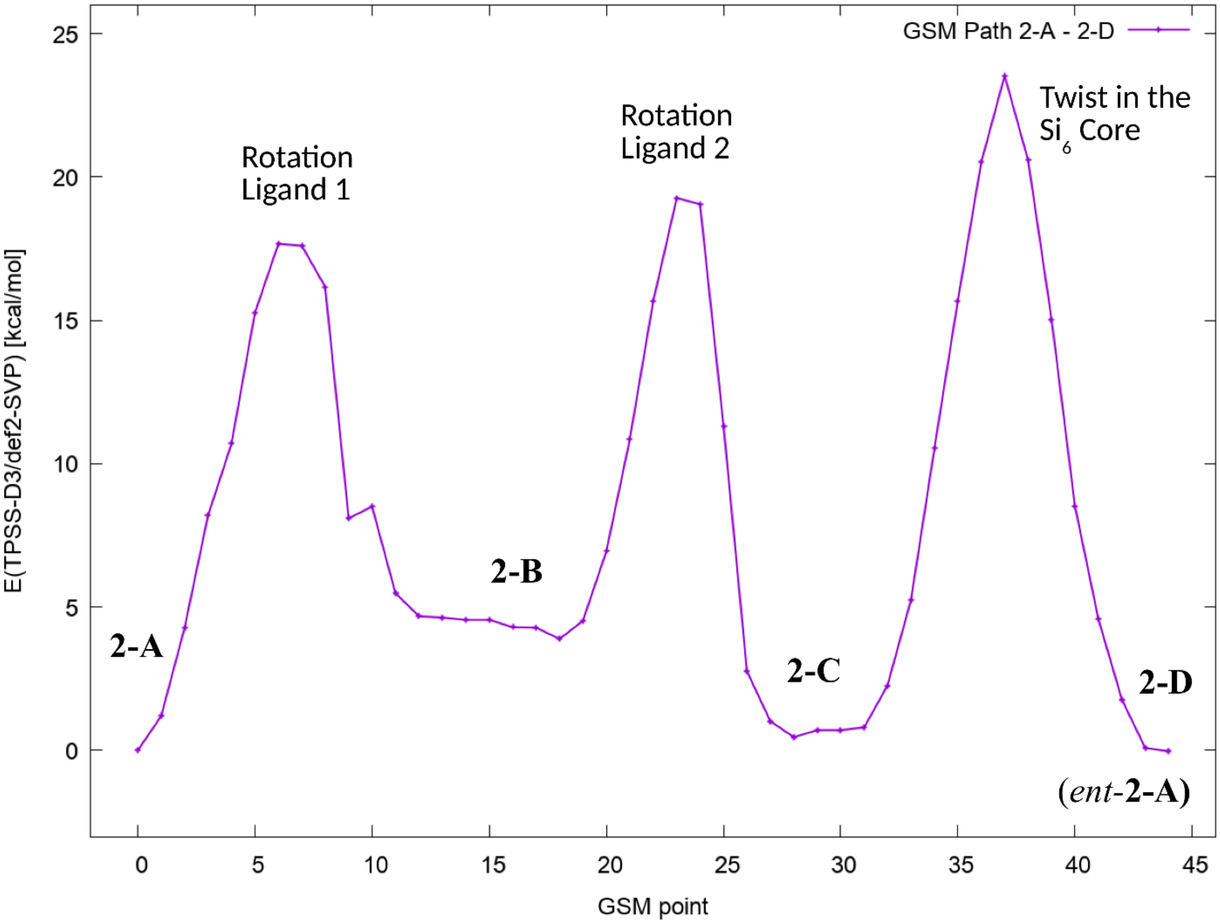


Figure S6. Energy (TPSS-D3/def2-SVP) of the minimum energy path for the stepwise transformation of **2-A** to the minority conformer **2-C** and the formation of the enantiomer of **2-A** (**2-D**).

1.3. ReaxFF MD simulation of conformational transformation (2-A→2-C→*ent*-2-A)

Computational Details

The molecular dynamics (MD) simulations were performed with the LAMMPS code (release of 7th August 2019)[S16]. The ReaxFF method was used to allow bond breaking while keeping computational cost low[S17, S18]. To our knowledge, no forcefield has been optimized for Si clusters with organic ligands so far. Therefore, we constructed a forcefield based on the forcefield of Kulkarni et al., which is parametrized for organic molecules and oxygen on silica surfaces[S19]. This forcefield is not well suited for simulations of Si clusters: optimized geometries show an opened cluster, as two Si–Si bonds break due to too weak bond parameters. This is not in line with DFT results, wherein the cluster is stable.

To adequately model the dynamics of a Si cluster as opposed to a surface, we modified the Si–Si interactions, replacing the parameters in the Kulkarni forcefield with those from the NDO0 parametrization for small Si clusters of Barcaro et al.[S20]. Specifically, we adopted all parameter values for the Si–Si bond and the Si–Si–Si angle and added an Si–Si–Si–Si dihedral angle. Optimized geometries obtained with this combined forcefield coincide well with structures obtained from DFT calculations, leaving the Si cluster itself intact (see Fig. S13, S14 and Tab. S7).

For the MD runs, a timestep of $\Delta t = 0.5$ fs was used; together with a skin distance of 2.5 Å for neighbor list builds this ensures the stability of the simulation. The temperature was fixed at $T = 300$ K with a Nosé-Hoover thermostat[S21–S23] with a time constant of 100 fs. The initial velocities were created according to a Gaussian distribution with random seed. The QEq charge equilibration method[S18,S24,S25] was applied with a Taper radius cutoff of 10 Å and a tolerance of 10^{-6}. Total linear and angular momentum of the system were removed every 100 timesteps.

Free energy profiles were calculated using the targeted MD method[26,27]. Here, we used the previously optimized structures **2-A**, **2-B**, **2-C** and **2-D** as initial and final states respectively. The reaction coordinate ξ is defined by the root-mean-squared distance (RMSD) between initial and final states. Average constraint forces are obtained from separate simulations at fixed reaction coordinate values ξ in intervals of $\Delta\xi = 0.1$ Å. Starting from the initial state, the system is allowed to relax to the defined reaction coordinate value in a 50 ps equilibration run. Subsequently the average constraint force is obtained from a 2 ns production run. An example input file is included in the SI. As the average constraint force diverges for $\xi \to 0$, for all transitions (e.g. **2-A→2-B**) the backwards path was also calculated (e.g. **2-B→2-A**). The obtained average constraint forces were interpolated and the non-diverging parts were fused to obtain the total average constraint force, which was then integrated to obtain the free energy profile.

Results

For the four DFT-optimized structures **2-A**, **2-B**, **2-C** and **2-D**, corresponding geometries were obtained with the ReaxFF forcefield. In order to qualitatively assess the formation of the enantiomer **2-D** (*ent*-**2-A**) starting from structure **2-A**, a targeted MD simulation was performed slowly pulling the system from **2-A** to **2-D** along the reaction coordinate ξ defined above, over a duration of 2 ns. A video visualizing this process is available online. In this simulation the necessary structural changes, i.e. rotation of a first ligand, rotation of a second ligand, and distortion of the Si cluster core, occur separately one after another. This suggests that the transformation **2-A→2-D** happens via a stepwise process including structures **2-B** and **2-C**. Indeed, the free energy profile in Fig. S7 shows clear minima for those structures. This also establishes the stepwise transformation **2-A→2-B→2-C** as a pathway to form the isomer **2-C** starting from **2-A**.

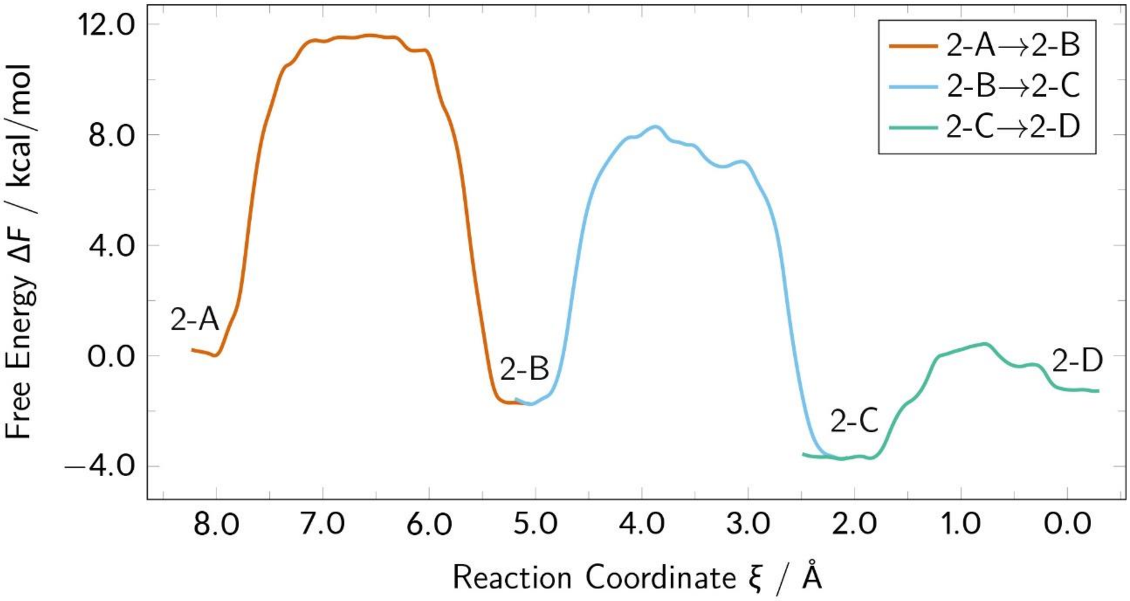


Figure S7. Free energy profiles for the transformations **2-A→2-B**, **2-B→2-C**, and **2-C→2-D**. The processes are simulated separately and the resulting curves are joined for visualization purposes. The reaction coordinate corresponds to the RMSD for each process individually and does not correspond to the actual RMSD between **2-A** and **2-D**.

The barrier heights for the individual processes are presented in Table S5 and Fig. S8. While all barriers are well below $\Delta F^{\ddagger} = 12$ kcal/mol and thus easily accessible at T = 300 K, the barrier for **2-C→2-D** is the lowest by far, with $\Delta F^{\ddagger} = 4.16$ kcal/mol. This indicates that formation of structure **2-C** starting from **2-D** would be preferred to the process starting from **2-A**. Thus, if both enantiomers **2-A** and **2-D** are present, **2-C** is most likely to form from **2-D** and a corresponding enantiomer *ent*-**2-C** would be formed from **2-A**. We note that according to the relative energies of the minima from our ReaxFF simulations, **2-C** would be more stable than **2-A** by $\Delta F = -3.74$ kcal/mol (see Tab. S6 or Fig. S9). However, this is a relatively small energy difference and a classical forcefield is not expected to exceed an accuracy of a few kcal/mol. This is exemplified in the case of **2-D**, which as an enantiomer should have the same energy as **2-A**, but is more stable by $\Delta F = -1.28$ kcal/mol in our simulations.

Table S5: Free energy reaction barriers $\Delta F^{\ddagger}$ for individual structural changes. The barrier height is given relative to the preceding minimum, i.e. the initial structure of the corresponding transformation.

Transition	$\Delta F^{\ddagger}$ / kcal/mol
2-A→2-B	11.59
2-B→2-C	10.05
2-C→2-D	4.16

Table S6: Free energy differences ΔF of structures **2-B**, **2-C** and **2-D** relative to **2-A** (which is set to zero).

Structure	ΔF / kcal/mol
2-A	0.00
2-B	−1.75
2-C	−3.73
2-D	−1.28

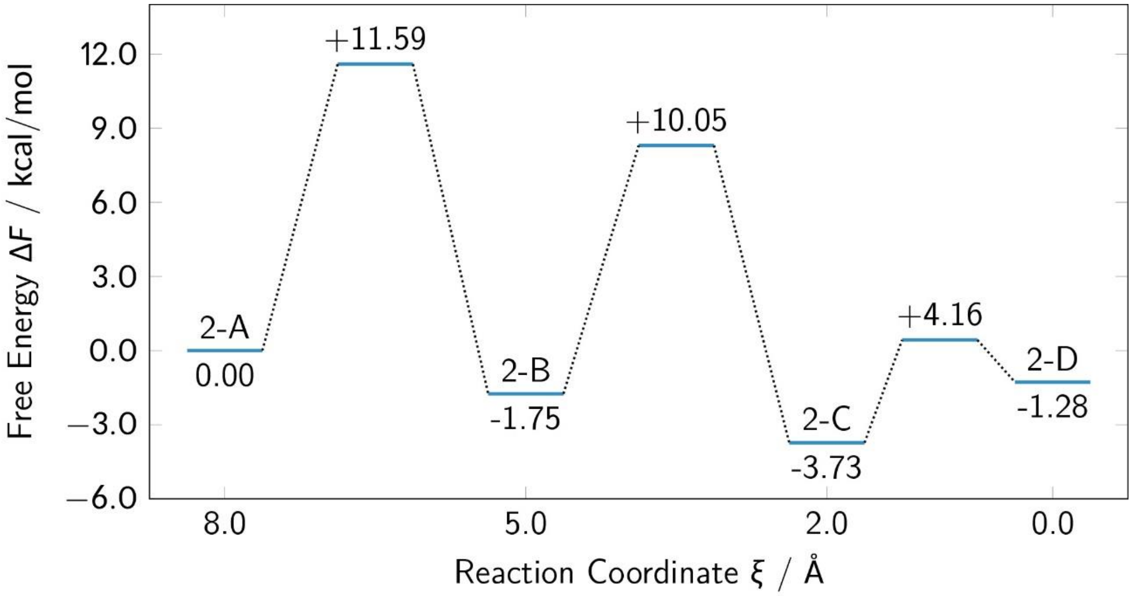


Figure S8: Scheme of the free energies ΔF of structures **2-B**, **2-C** and **2-D** relative to **2-A** (which is set to zero) as well as the barrier heights $\Delta F^{\ddagger}$ for the transformations **2-A**→**2-B**, **2-B**→**2-C**, and **2-C**→**2-D**. The barriers are labeled with their height relative to the preceding minimum, i.e. the initial structure of the individual transformation.

Computational Details of the ReaxFF simulations

Force field of Kulkarni et al.

The geometries optimized with the force field of Kulkarni et. al[S19], which was parametrized for organic molecules and oxygen on silica surfaces, exhibit opened Si clusters (see Fig. S9), which contrast DFT results (see Fig. S10).

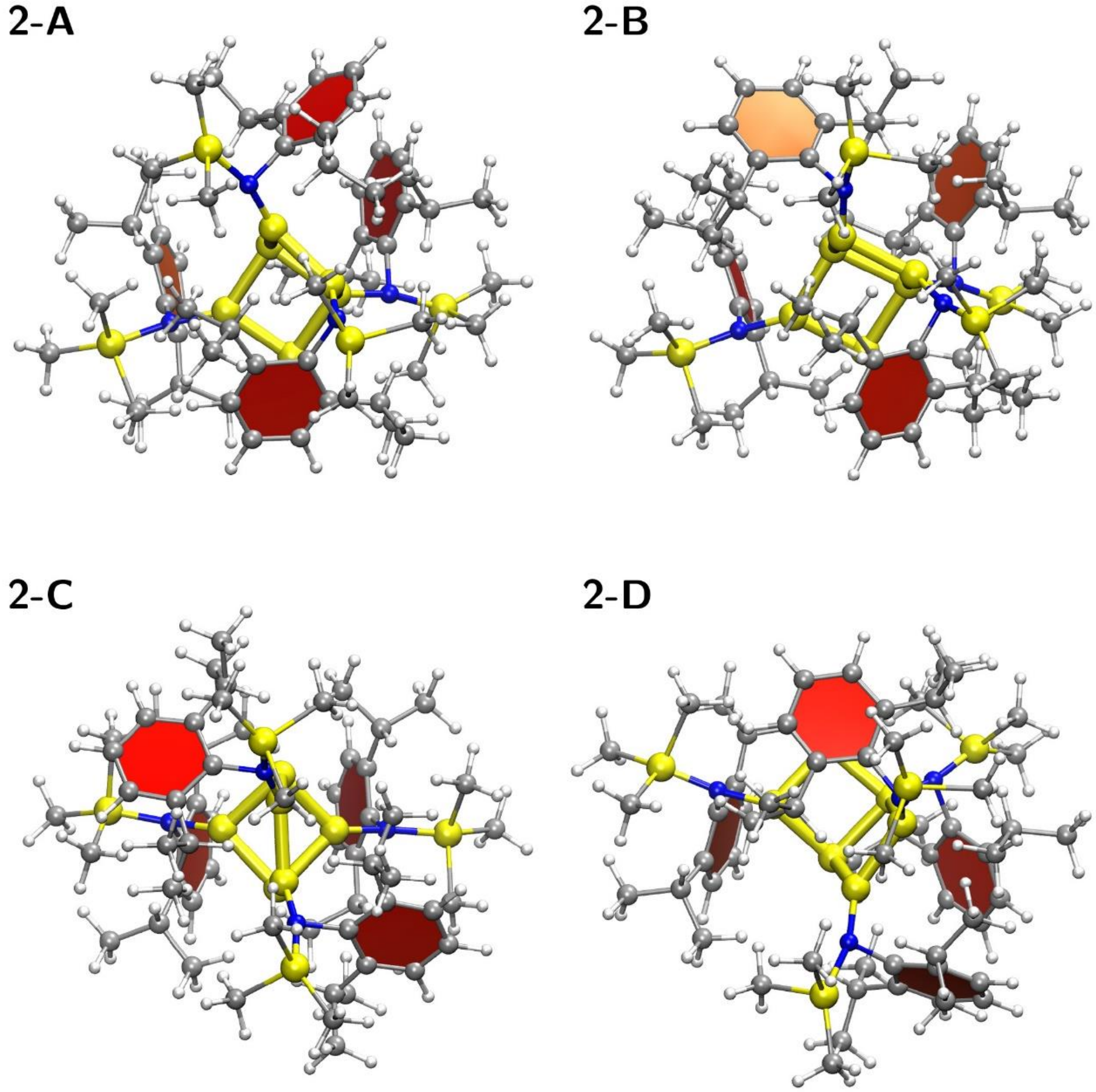


Figure S9: Structures **2-A**, **2-B**, **2-C** and **2-D**, obtained from geometry optimizations with the ReaxFF forcefield of Kulkarni et al.; Si atoms are yellow, N atoms blue, C atoms gray and H atoms white. Aromatic rings are marked with red hexagons.

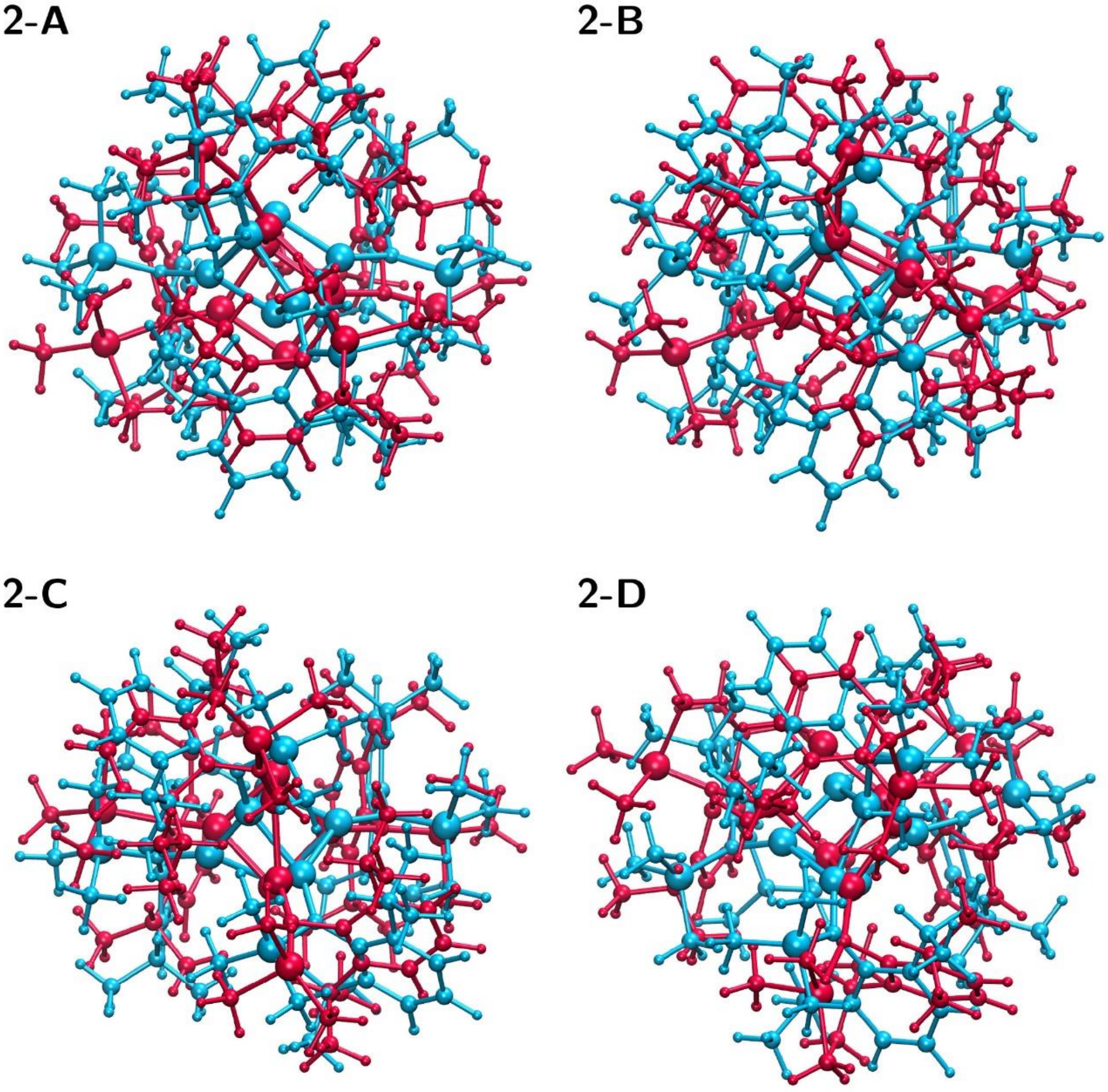


Figure S10: Structures **2-A**, **2-B**, **2-C** and **2-D**, obtained from geometry optimizations with the ReaxFF forcefield of Kulkarni et al. (red) compared to DFT optimized structures (blue).

Combined forcefield

The geometries optimized with the combined forcefield, based on the forcefield of Kulkarni et al.[S19] with parameters for Si–Si bonds, Si–Si–Si angles and Si–Si–Si–Si dihedral angles from the parametrization of Barcaro et al.[S20], exhibit intact Si clusters (see Fig. S11), which agree well with DFT results (see Fig. S12). The corresponding Root-mean-squared deviation (RMSD) calculated with respect to the DFT structures is significantly lower than the RMSD for the forcefield of Kulkarni et al. (see Tab. S7).

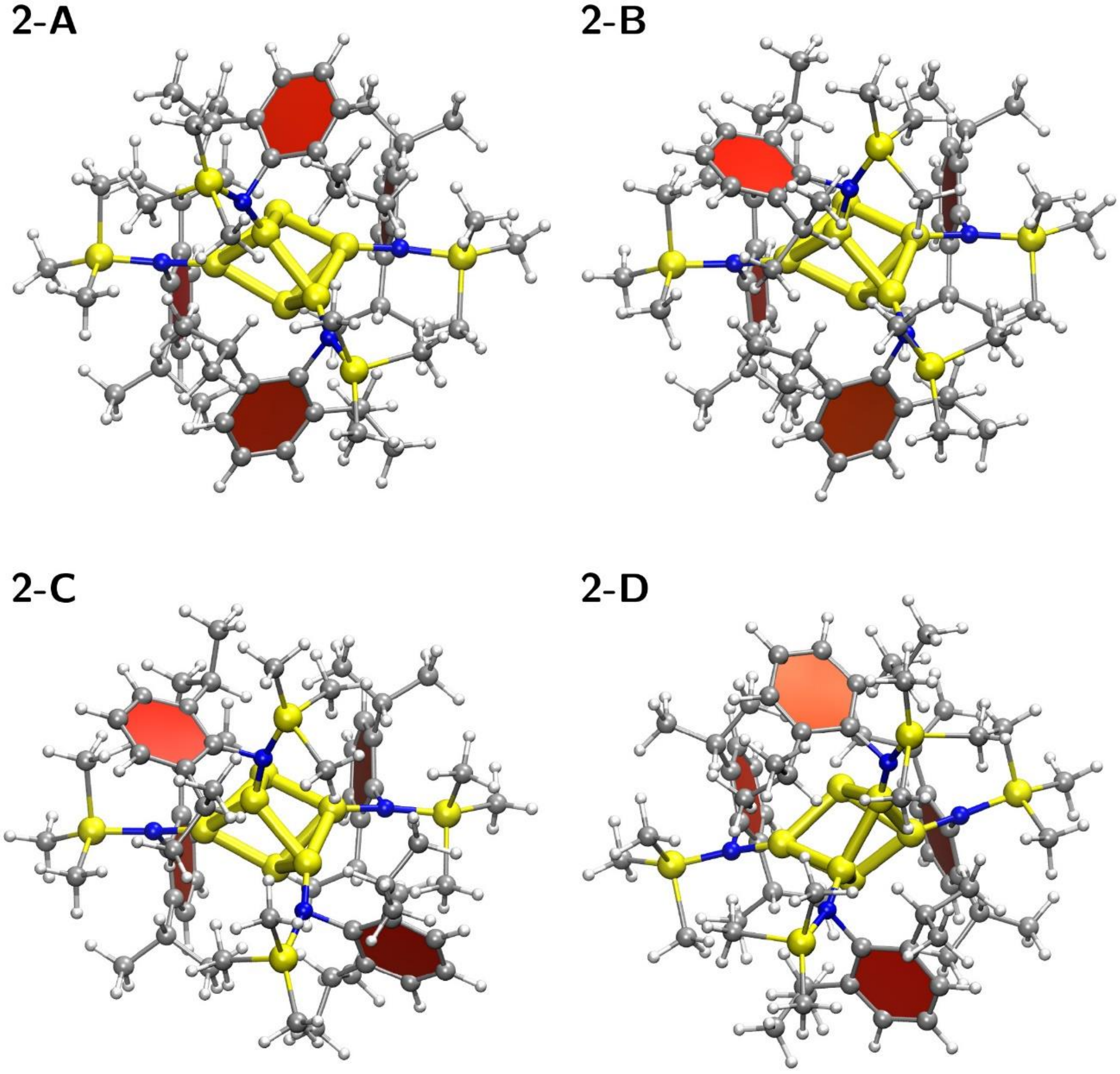


Figure S11: Structures **2-A**, **2-B**, **2-C** and **2-D**, obtained from geometry optimizations with our combined ReaxFF forcefield; Si atoms are yellow, N atoms blue, C atoms gray and H atoms white. Aromatic rings are marked with red hexagons.

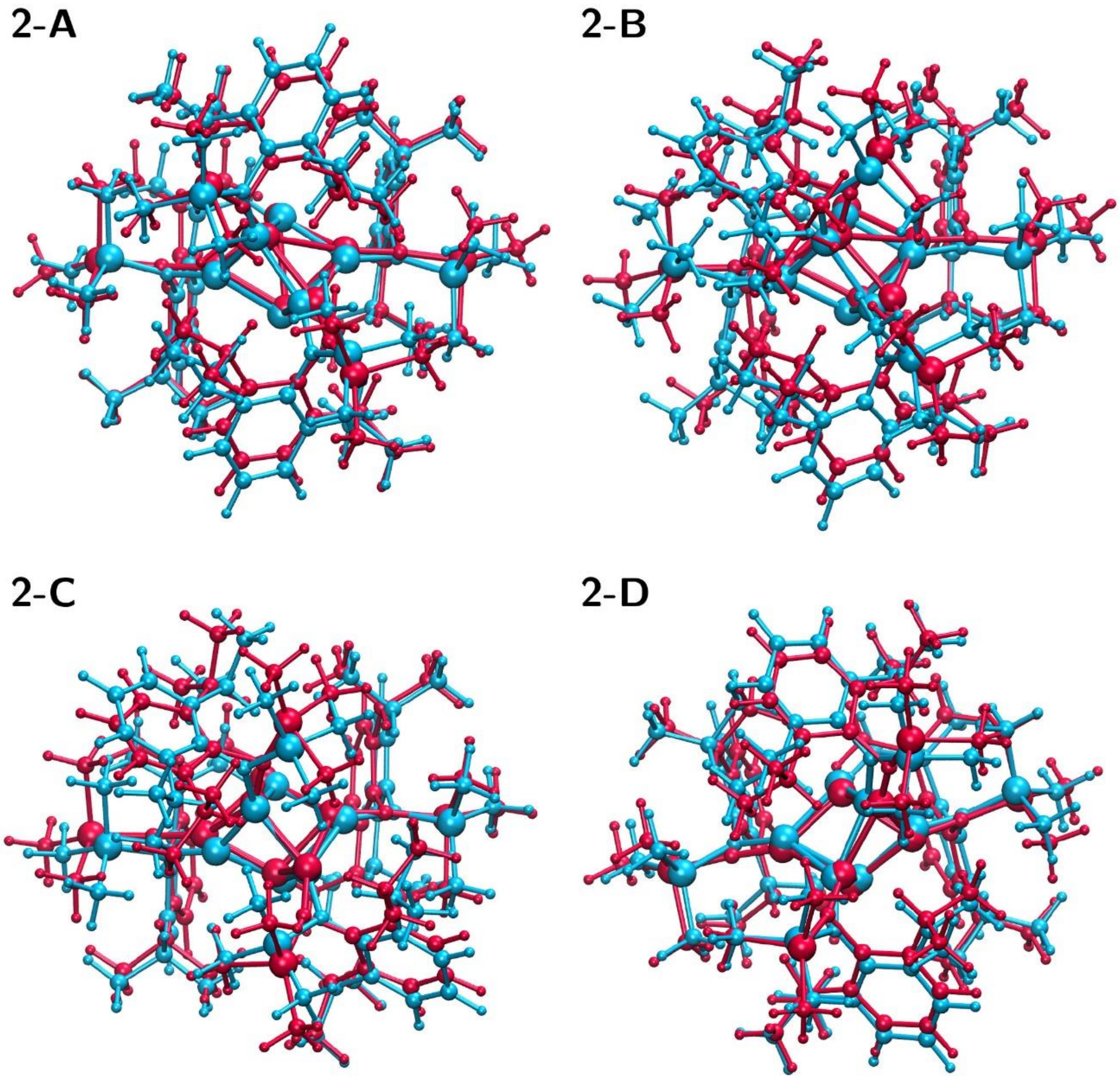


Figure S12: Structures **2-A**, **2-B**, **2-C** and **2-D**, obtained from geometry optimizations with our combined ReaxFF forcefield (red) compared to DFT optimized structures (blue).

Table S7: Root Mean Squared Deviation of structures optimized with the ReaxFF forcefield of Kulkarni et al.[S19] ("Kulkarni FF") and with our combined forcefield ("Combined FF"), with respect to DFT optimized structures. The geometries were rotated using the Kabsch algorithm as implemented by Kromann and Bratholm in order to yield the minimal RMSD[S28, S29].

	RMSD / Å	
Structure	Kulkarni FF	Combined FF
2-A	2.364	0.561
2-B	3.154	0.924
2-C	2.066	0.812
2-D	2.990	0.545

Input

This is an example input used to calculate the average force at a specific reaction coordinate ξ = `${var1}` for the transformation **2-A→2-B**.

```
units                   real
newton                  on
atom_style              charge
atom_modify             map array
read_data               data.A

pair_style              reax/c NULL
pair_coeff              * * ffield.reax.kulbar0a C H N Si
neighbor                2.5 bin
neigh_modify            every 5 delay 0 check yes

variable seed           equal round(random(10000,99999,12345))
variable var2           equal ${var1}
velocity                all create 10.0 ${seed} dist gaussian
velocity                all zero linear
velocity                all zero angular
velocity                all scale 10.0

fix                     1 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
fix                     2 all nvt temp 10.0 300.0 50.0
fix                     3 all momentum 100 linear 1 1 1 angular rescale
fix                     4 all tmd ${var2} final.B 0 relax_file

timestep                0.5
run                     100000
velocity                all zero linear
velocity                all zero angular
velocity                all scale 300.0

unfix                   4
unfix                   2
fix                     2 all nvt temp 300.0 300.0 100.0
fix                     4 all tmd ${var2} final.B 200 tmd_dump_file

dump                    1 all xyz/gz 200 SiAB_4000000_tmd_${var1}.xyz.gz
dump_modify             1 element C H N Si
thermo                  200

run                     4000000

write_data              data.tmd_${var1}
```

The input, contained in a file named `in.reax.tmd`, would be executed with the command

```
mpirun -np $NPROCS ./lmp_mpi -in in.reax.tmd -var var1 $XI
```

for the number of processors `$NPROCS` and the reaction coordinate ξ `= $XI`., the LAMMPs executable `lmp_mpi` and the forcefield file `ffield.reax.kulbar0a` are expected to be present in the current directory.

Calculation of average forces and free energies

The divergence of the average forces A(ξ) for ξ→0 is remedied by calculating the same transformation also backwards (e.g. **2-B→2-A** in addition to **2-A→2-B**, see Fig. S13). In particular, the average forces are calculated for discrete values of $\xi = \xi_{max} - n \cdot \Delta\xi$, with integer n and stepsize $\Delta\xi = 0.1$ Å. This formula is used for both backwards and forwards calculations, just with initial and final structure swapped. Thus, to obtain a common ξ axis, the reaction coordinate for the backwards calculations need to be inverted, i.e. $\xi' = \xi_{max} - \xi$. This results in grids, which are not the same for forwards and backwards calculations. Therefore, cubic splines are used to project the average forces onto a common grid with 200 evenly spaced points (see Fig. S14).

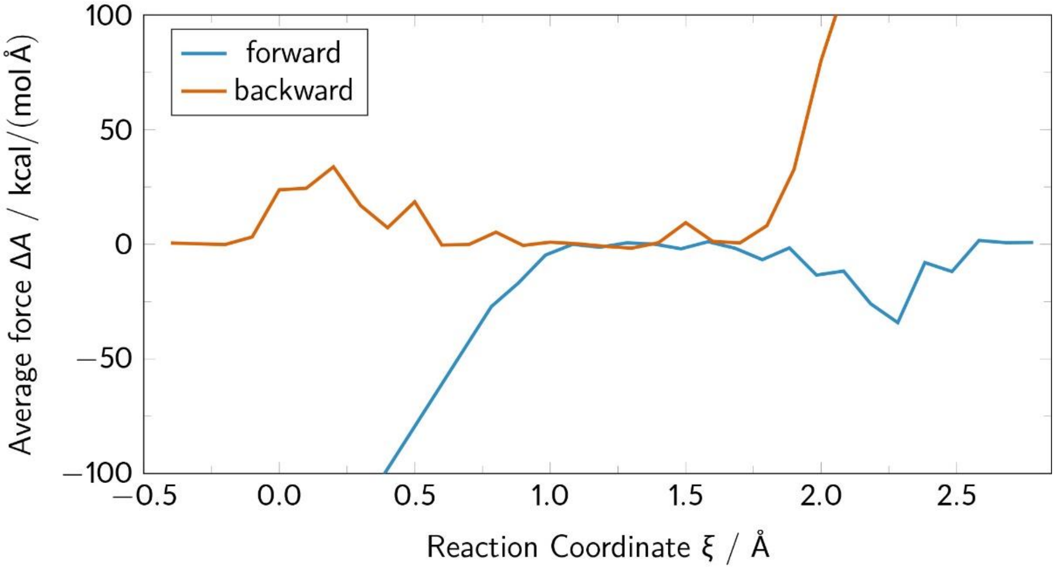


Figure S13: Average forces A(ξ) for the transformation **2-A→2-B**.

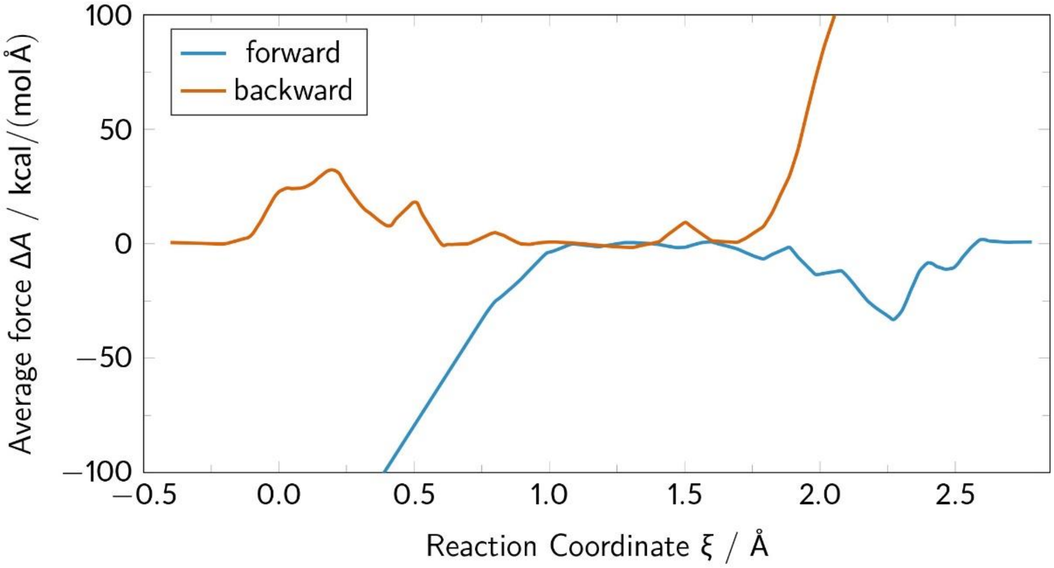


Figure S14: Interpolated average forces A(ξ) for the transformation 2-A→2-B.

The two curves for the average forces are then smoothly fused together according to the function

$$A_{total}^{\xi_{mid}}(\xi) = \frac{1}{2}\big(1 + \tanh\big(10(\xi_{mid} - \xi)\big)\big)A_{backward}(\xi) + \frac{1}{2}\big(1 + \tanh\big(10(\xi - \xi_{mid})\big)\big)A_{forward}(\xi)$$

This function ensures that A_{total} is equal to the forward/backward curve for reaction coordinates far away from ξ_{mid} and that the transition around ξ_{mid} is smooth (see Fig. S15).

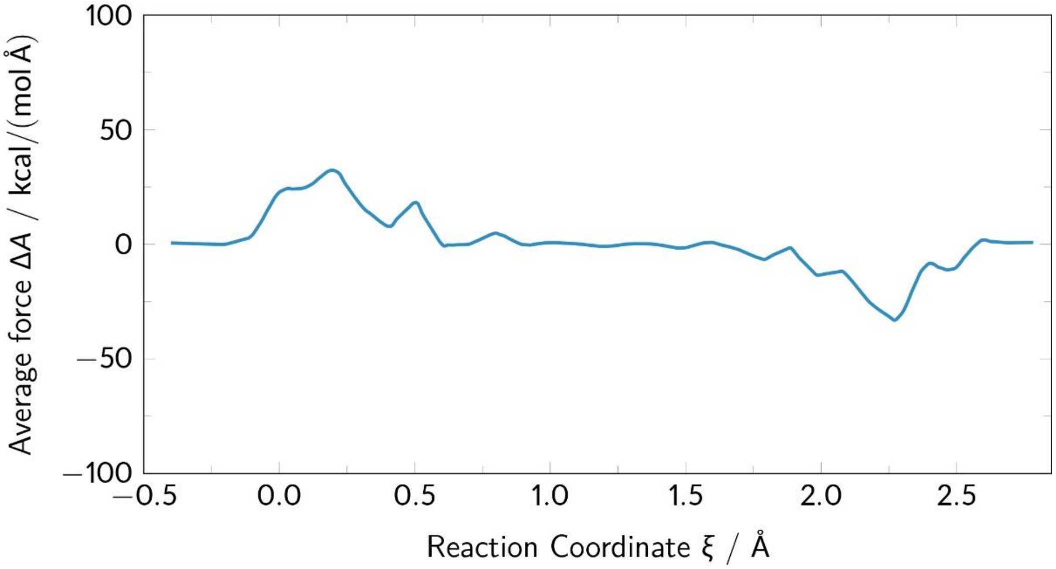


Figure S15: Total average force $A_{total}(\xi)$ for the transformation **2-A→2-B** for ξ_{mid} = 1.215 Å.

This method has one free parameter: the fusing point $_{\text{mid}}$, which could be chosen to be $\xi_{\text{mid}} = 1/2\ \xi_{\text{max}}$, i.e. the center of the axis. However, this choice is generally arbitrary. A more rigorous approach is the optimization of the total change in the free energy profile induced by varying ξ_{mid}. Thus, we choose the value of ξ_{mid}, which minimizes the functional

$$\Delta\Delta F = \int \left(\Delta F_{\xi_{mid}}(\xi) - \Delta F_{\xi_{mid}+\Delta\xi}(\xi)\right)^2 d\xi,$$

where $F_{\xi_{\text{mid}}}(\xi)$ is the free energy obtained by integrating $A^{\xi_{\text{mid}}}_{\text{total}}(\xi)$ and $\Delta\xi$ corresponds to the grid spacing. An example of the total change in free energy for the transformation **2-A→2-B** is shown in Fig. S16. In all cases investigated in this work, ξ_{mid} lies close to $\xi_{\text{max}}/2$ (see Tab. S8). A Fortran90 program which performs all these steps given the forward and backward average forces, is available on request.

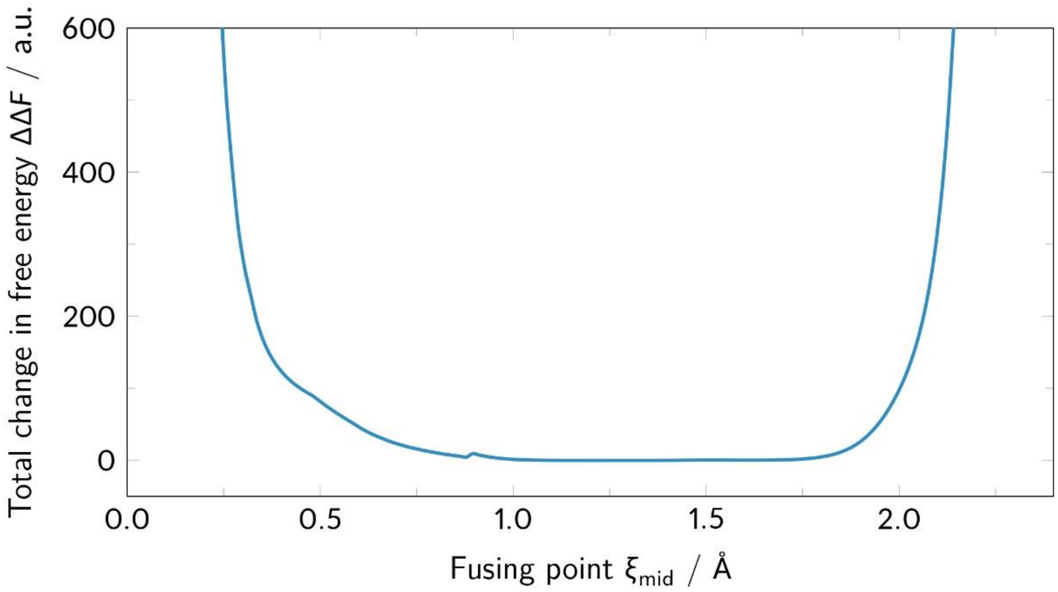


Figure S16: Total change in free energy for the transformation **2-A→2-B**.

Table S8: Optimal fusing points ξ_{mid} and half of the maximal reaction coordinate ξ_{max} for the transitions **2-A→2-B**, **2-B→2-C** and **2-C→2-D**.

Transition	ξ_{mid} / Å	$\xi_{\text{max}}/2$ / Å
2-A→2-B	1.215	1.391
2-B→2-C	1.122	1.366
2-C→2-D	1.033	1.246

2. General experimental procedures

All reactions were performed with the use of modified Schlenk techniques with additional manipulations using a MBraun Glovebox. All solvents were dried over sodium benzophenone or CaH_2, distilled and stored over 4 Å molecular sieves prior to use. Silicon tetrabromide was purchased from Aldrich and used without further purification. The starting material **1**[S30] was prepared according to a literature procedure.

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; $\delta = 0$ 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 $^{2}J_{Si\text{–}H} = 7$ 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. IR spectra were recorded using nujol oil and CsI plates on a Shimadzu IR PRESTIGE 21. UV-visible spectra were recorded as dilute PhMe solutions in 1 mL quartz cuvettes using an Agilent Cary 100 spectrometer. Mass spectrometry was performed with a Varian MAT 212 Micromass Quattro LC-Z device. CHN elemental analysis was done with a Vario EL III CHN Instrument. Melting points were measured in glass capillaries sealed under argon gas by using a Stuart Melting Point Apparatus SMP3 and are uncorrected.

2.1. Synthesis and Spectroscopic details of 2 ($Si_6\{N(SiMe_3)Dipp\}_4$·hexane)

Neat crystalline $Si_4\{N(SiMe_3)Dipp\}_4$ · 1.5 PhMe (1000 mg, 0.806 mmol, 1.0 equiv.) was heated under argon using a heatgun to about 400 °C. The red crystals liquefied and after 30 min. heating the molten mass changed the color from deep red to yellow-orange. All volatile components were removed in vacuo at 400 °C. The yellow solid residue was cooled to room temperature and was dissolved in 20 mL *n*-hexane and was filtered using a filter cannula. After several co-evaporations with about 5 mL *n*-pentane and drying for 16 h at high vacuum the obtained yellow foam was dissolved in a minimum of *n*-hexane (~ 5 mL) and was stored at −32 °C. Yellow block-like crystals of $Si_6\{N(SiMe_3)Dipp\}_4$·hexane formed after 16 h.

Yield: 230 mg (0.184 mmol, 23 %).

Melting Point: heating above 350 °C no decomposition.

MS (EI+, 20 eV, 353 K): m/z = 912 (100%, $[M-\{N(SiMe_3)Dipp\}]^+$), 1161 (31%, $[M]^+$).

CHN: $C_{60}H_{104}N_4Si_{10}$; calculated: C 62.00%, H 9.02%, N 4.82%; found: C 62.37%, H 9.24%, N 4.87%.

IR (cm-1, nujol, CsI plates): 3051-2853 (nujol), 1460 (s, medium), 1433 (s, sharp), 1402 (w, sharp), 1379 (s, sharp), 1360 (m, sharp), 1340 (w, sharp), 1311 (m, medium), 1254 (s, sharp), 1244 (s, medium), 1179 (m, sharp), 1163 (s, sharp), 1099 (s, sharp), 1080 (w, sharp), 1053 (m, sharp), 1044 (m, sharp), 965 (m, sharp), 891 (s, medium), 872 (s, sharp), 837 (s, sharp), 797 (s, sharp), 753 (m, sharp), 743 (m, sharp), 721 (w, sharp), 708 (w, sharp), 687 (m, sharp), 665 (w, sharp), 644 (m, sharp), 600 (m, sharp) 588 (m, sharp), 538 (s, sharp), 471 (w, sharp), 438 (m, sharp), 407 (m, sharp).

UV/Vis: ($2.3\cdot10^{-5}$ mol/L in PhMe at 25°C): λ_{max} = 282 nm (ε = 38166 $L\cdot mol^{-1}\cdot cm^{-1}$), 314 ($\varepsilon$ = 28125 $L\cdot mol^{-1}\cdot cm^{-1}$), 361 ($\varepsilon$ = 13233 $L\cdot mol^{-1}\cdot cm^{-1}$).

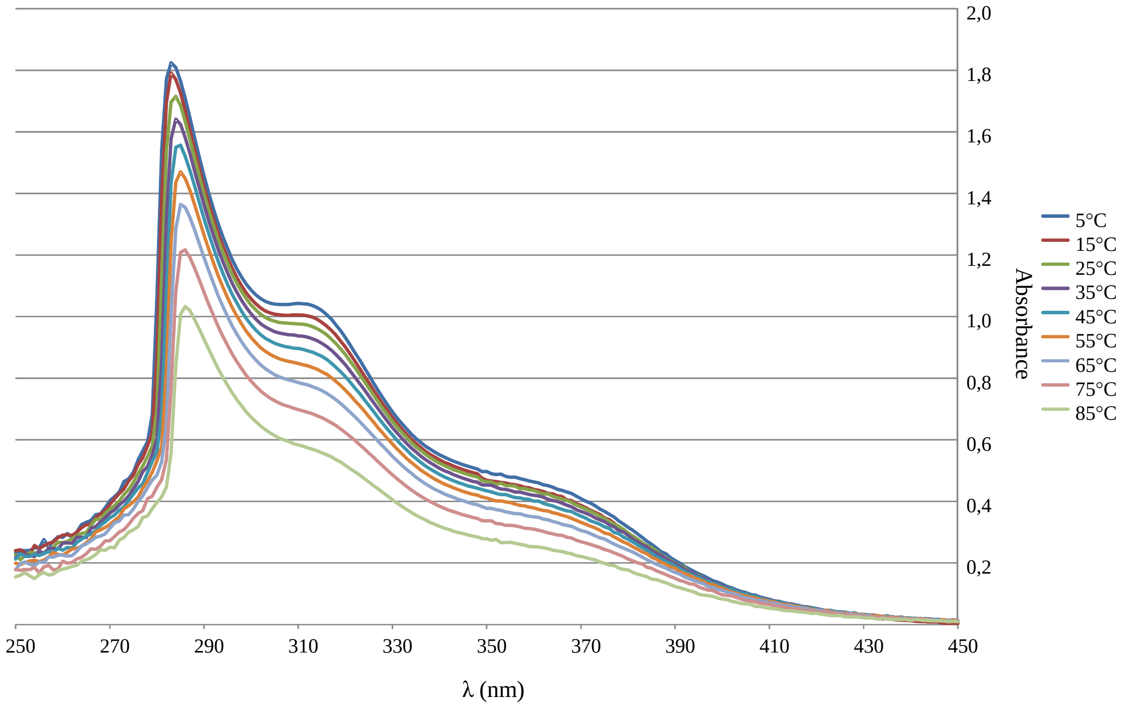


Figure S17a. UV/vis spectra of **2**·hexane in PhMe in the wavelength range from 250 to 450 nm at different temperatures (T = 5 - 85 °C).

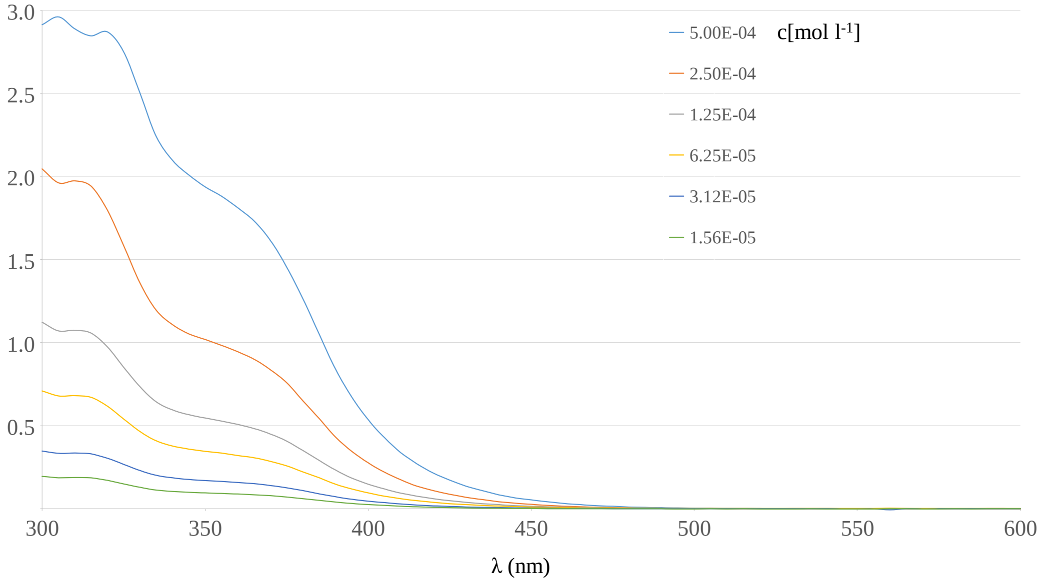


Figure S17b. UV/vis spectra of **2**·hexane in hexane in the wavelength range from 250 to 450 nm at three different concentrations.

TDDFT calculation of the electronic absorption spectrum of 2-A

We have performed a TDDFT calculation with ORCA on the optimized structure (**2-A**) of $Si_6\{N(SiMe_3)Dipp\}_4$, using the CAM-B3LYP functional, a double zeta basis set (def2-SVP) and the CPCM implicit solvent model for toluene solving for 40 excited states.

The HOMO-LUMO transition at 392 nm (State 1) is very weak and cannot be identified in the experimental spectrum. We reproduce the three major absorptions as observed in the UV/vis spectrum (Figure S17), although with a certain shift towards higher excitation energies: the most intense absorptions are found at 351 nm (State 3, mainly (HOMO-1)-LUMO), 285 nm (State 9, mainly HOMO-(LUMO+1)) and at 238 nm (State 23, mixed excitation involving several orbitals). Some other intense bands are predicted between 210 and 260 nm.

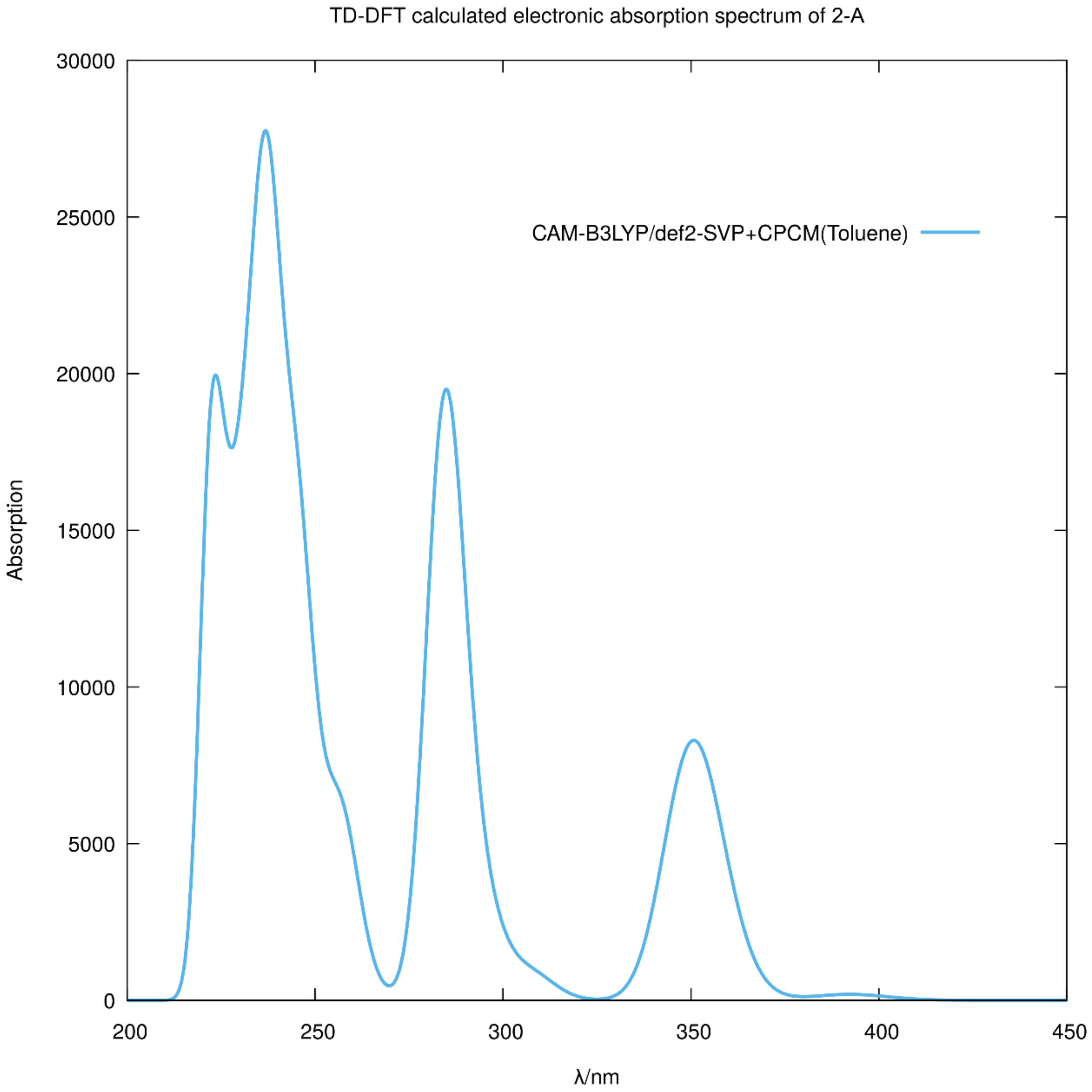


Figure S18. Calculated UV/vis spectrum of **2-A** using TDDFT calculation.

Absorption Spectrum via Transition Electric Dipole Moments

```
-----------------------------------------------------------------------------
State   Energy    Wavelength  fosc         T2        TX        TY        TZ
        (cm-1)      (nm)                 (au**2)    (au)      (au)      (au)
-----------------------------------------------------------------------------
   1   25495.2    392.2   0.001315016   0.01698   0.11319  -0.06456  -0.00018
   2   27797.4    359.7   0.001671807   0.01980   0.00048  -0.00062  -0.14071
   3   28520.5    350.6   0.056492332   0.65209   0.56312  -0.57878  -0.00011
   4   32428.1    308.4   0.003258915   0.03308   0.09931  -0.15238   0.00083
   5   32591.0    306.8   0.002404337   0.02429   0.00086  -0.00120  -0.15584
   6   33857.6    295.4   0.014846735   0.14436  -0.36342   0.11085   0.00035
   7   34251.5    292.0   0.003034991   0.02917  -0.16035   0.05881   0.00028
   8   34598.1    289.0   0.000377619   0.00359  -0.00007   0.00479   0.05975
   9   35128.9    284.7   0.131245151   1.22997   0.01440  -1.10895   0.00054
  10   37734.4    265.0   0.000960447   0.00838   0.00016  -0.00117   0.09153
  11   38100.2    262.5   0.001823739   0.01576  -0.00106  -0.00017  -0.12553
  12   38716.5    258.3   0.022738835   0.19335  -0.00125  -0.00115  -0.43971
  13   38897.6    257.1   0.001984465   0.01680   0.07822  -0.10333  -0.00073
  14   39166.0    255.3   0.009102865   0.07651   0.00048  -0.00005  -0.27661
  15   39357.4    254.1   0.007598124   0.06356   0.25206   0.00431   0.00150
  16   39736.9    251.7   0.006866458   0.05689   0.20565   0.12078  -0.00230
  17   40337.3    247.9   0.023480434   0.19164  -0.15649   0.40883  -0.00086
  18   40680.4    245.8   0.022288768   0.18038   0.18430  -0.38263   0.00174
  19   40821.2    245.0   0.032853953   0.26496  -0.21306  -0.46858   0.00005
  20   40990.4    244.0   0.015681642   0.12595   0.00001  -0.00033  -0.35489
  21   41181.4    242.8   0.007902058   0.06317   0.00145  -0.00004   0.25133
  22   41384.0    241.6   0.008514303   0.06773  -0.25139   0.06732  -0.00002
  23   42002.2    238.1   0.107671174   0.84392  -0.66133   0.63763  -0.00031
  24   42169.3    237.1   0.004306219   0.03362   0.00275  -0.00259  -0.18331
  25   42204.8    236.9   0.003579601   0.02792   0.05527   0.15769   0.00033
  26   42416.6    235.8   0.013943743   0.10822   0.28412  -0.16546   0.01109
  27   42419.7    235.7   0.002740164   0.02127  -0.02305   0.01313   0.14339
  28   42701.2    234.2   0.055397166   0.42709   0.02286   0.65312  -0.00109
  29   43268.3    231.1   0.002943430   0.02240  -0.00010  -0.00708  -0.14948
  30   43381.7    230.5   0.052187284   0.39604  -0.09272  -0.62243   0.00360
  31   43143.5    231.8   0.002725163   0.02079  -0.00059  -0.00523  -0.14411
  32   43560.3    229.6   0.000005178   0.00004   0.00151  -0.00112  -0.00597
  33   43876.1    227.9   0.003136280   0.02353   0.00012  -0.00033  -0.15340
  34   44102.7    226.7   0.037407199   0.27923   0.08665   0.52127  -0.00067
  35   44207.7    226.2   0.000173446   0.00129   0.00054   0.00319   0.03579
  36   44256.3    226.0   0.002238459   0.01665   0.00310   0.00241  -0.12898
  37   43401.7    230.4   0.000646765   0.00491   0.01368   0.06866   0.00224
  38   44741.2    223.5   0.003182914   0.02342  -0.00085  -0.00330  -0.15300
  39   44814.8    223.1   0.020671413   0.15185   0.00648  -0.00722  -0.38956
  40   45020.8    222.1   0.090803894   0.66400   0.59603  -0.55561   0.00668
```

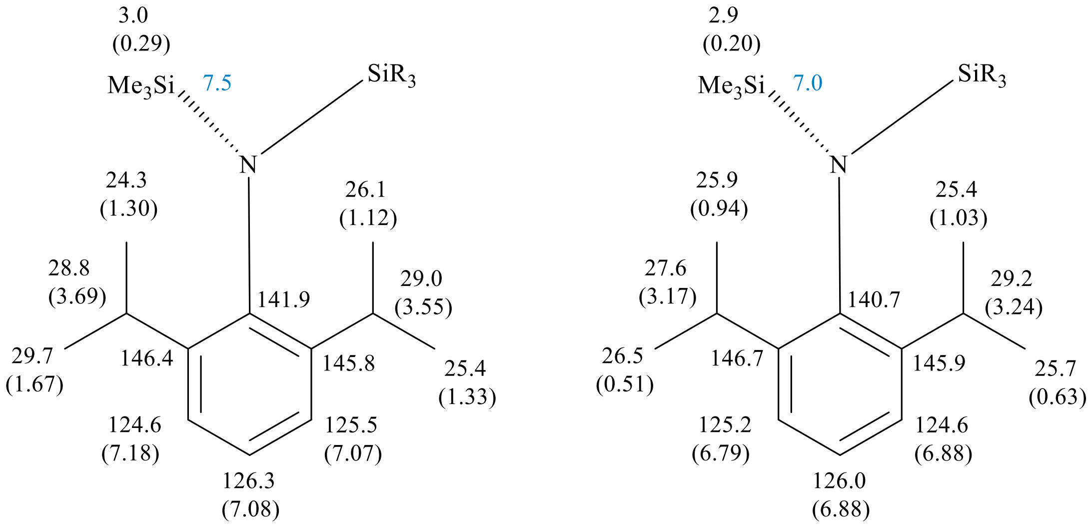
Most relevant states below 250 nm:

```
STATE  1:  E=   0.116165 au      3.161 eV    25495.2 cm**-1 (392 nm)
   314a -> 316a  :     0.256845 (c= -0.50679845)
   315a -> 316a  :     0.705241 (c= -0.83978612)           HOMO -> LUMO

STATE  2:  E=   0.126654 au      3.446 eV    27797.4 cm**-1 (360 nm)
   313a -> 316a  :     0.947775 (c=  0.97353712)           HOMO-2 -> LUMO
   313a -> 317a  :     0.010713 (c=  0.10350423)

STATE  3:  E=   0.129949 au      3.536 eV    28520.5 cm**-1 (351 nm)
   314a -> 316a  :     0.631718 (c=  0.79480694)           HOMO-1 -> LUMO
   314a -> 317a  :     0.014508 (c=  0.12044735)
   315a -> 316a  :     0.211510 (c= -0.45990177)
   315a -> 317a  :     0.044478 (c= -0.21089851)
```

```
STATE  9:  E=   0.160059 au      4.355 eV    35128.9 cm**-1 (285 nm)
   311a -> 316a  :     0.314713 (c=  0.56099308)           HOMO-4 -> LUMO
   314a -> 316a  :     0.016546 (c=  0.12863120)
   314a -> 319a  :     0.018825 (c=  0.13720543)
   314a -> 326a  :     0.014807 (c=  0.12168464)
   315a -> 316a  :     0.021978 (c= -0.14824936)
   315a -> 317a  :     0.459454 (c=  0.67783026)           HOMO -> LUMO+1
```

JanK073-THF - T=210K
major component: minor component
ca. 2:1

major component ^{29}Si: 94.2 ppm ,7.7ppm, -309.4 ppm



minor component ^{29}Si: 51.3 ppm ,-5.1ppm, -294.0 ppm

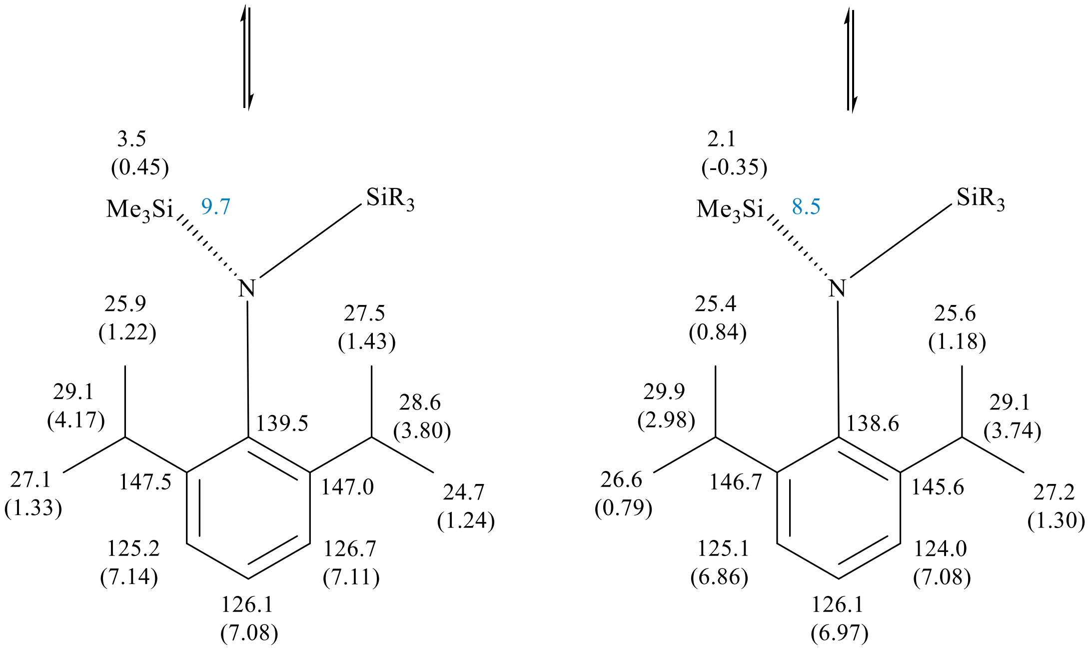


Figure S19. Assignment of the ^{1}H (in brackets), ^{13}C (black number), ^{29}Si (light blue number), NMR chemical shifts of **2**·hexane.

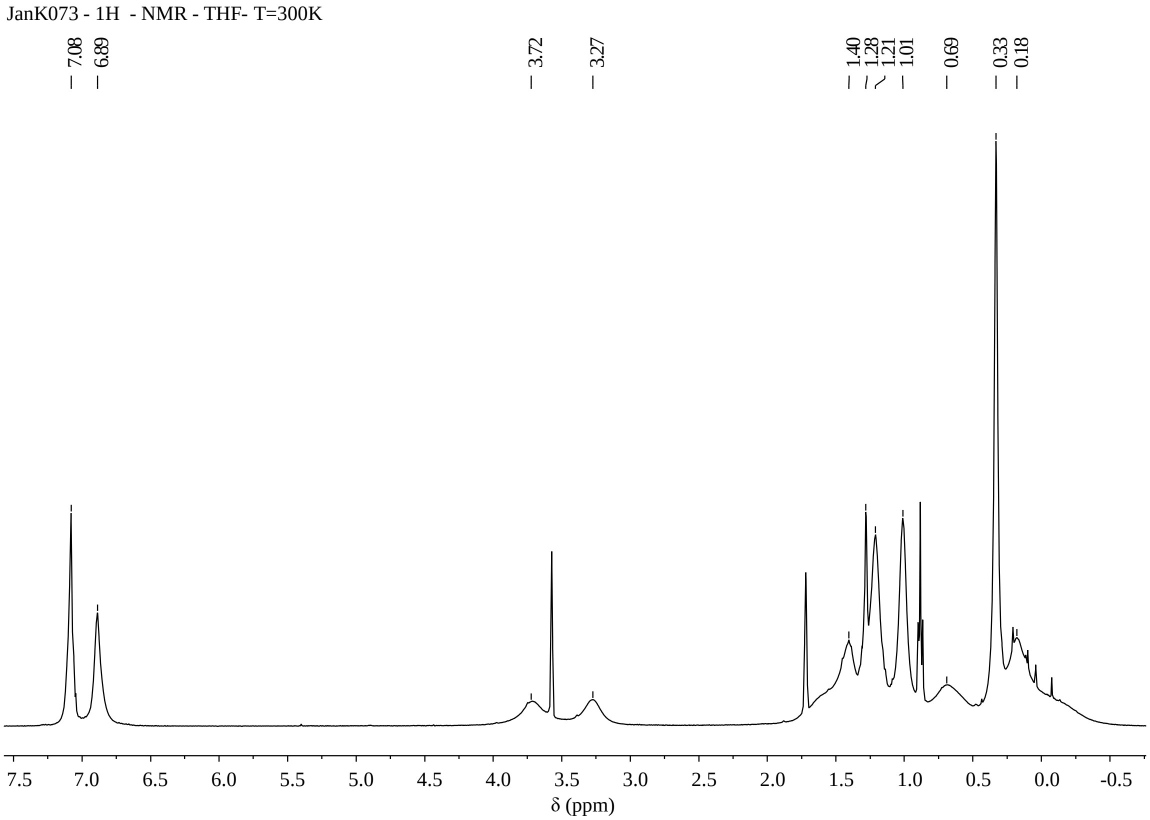


Figure S20. ^1H NMR spectrum of **2**·hexane (400 MHz, THF-d_8, 300 K).

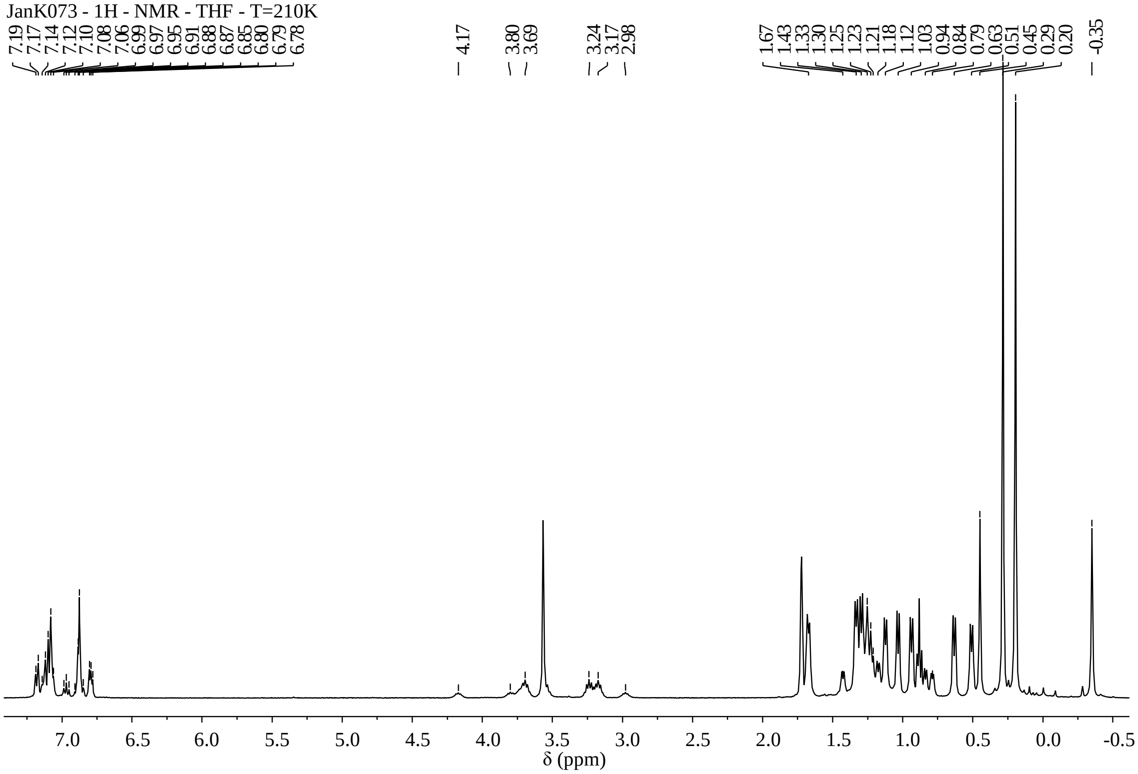


Figure S21. ^1H NMR spectrum of **2**·hexane (400 MHz, THF-d_8, 210 K).

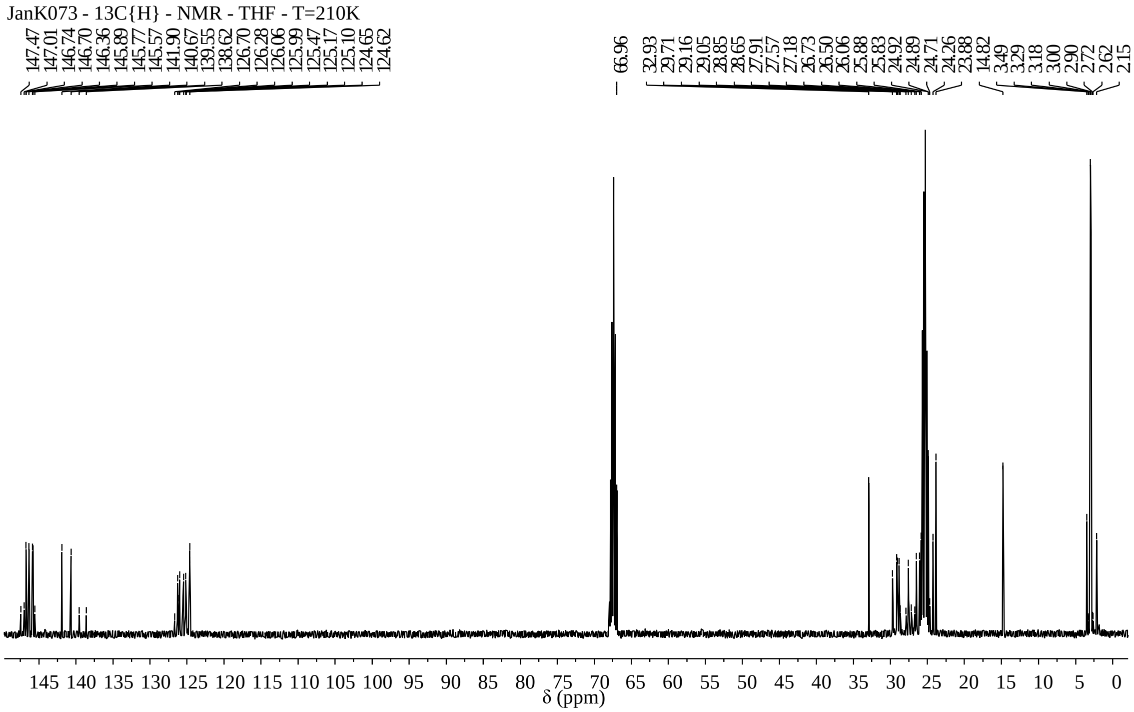


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of **2**·hexane (100.6 MHz, THF-d_8, 210 K).

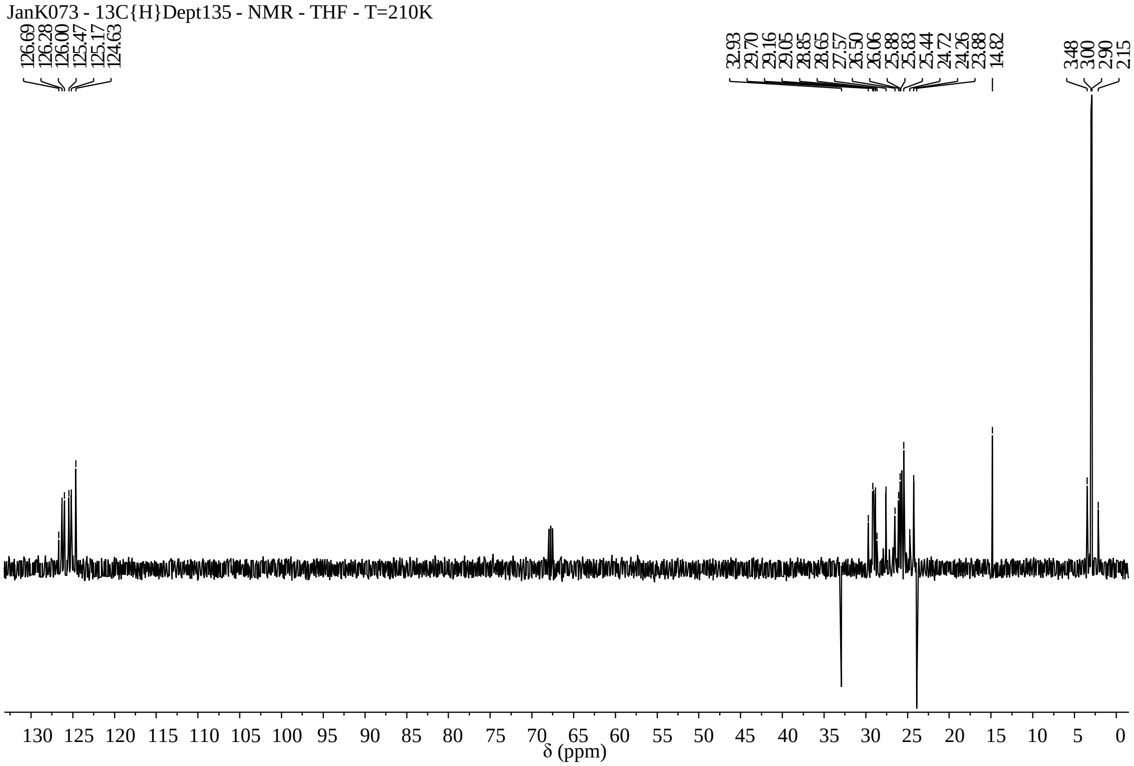


Figure S23. $^{13}C\{^{1}H\}$Dept135 NMR spectrum of **2**·hexane (100.6 MHz, THF-d_8, 210 K).

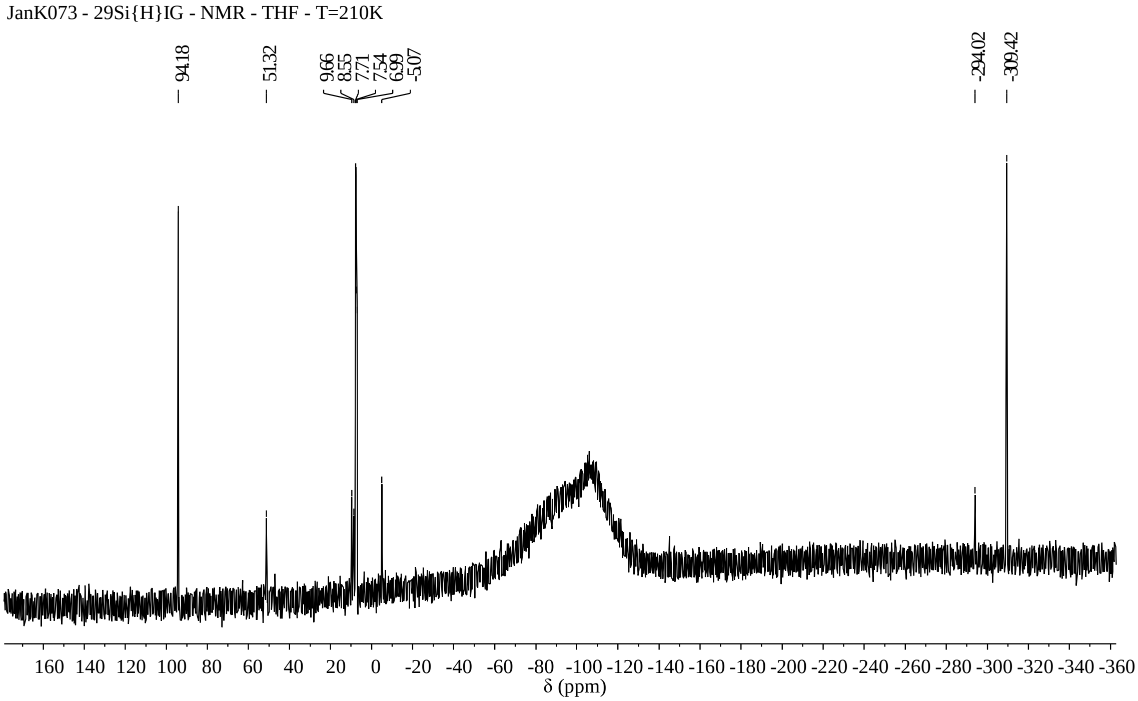


Figure S24. ^{29}Si{^{1}H} NMR spectrum of **2**·hexane (79.5 MHz, THF-d$_8$, 210 K).

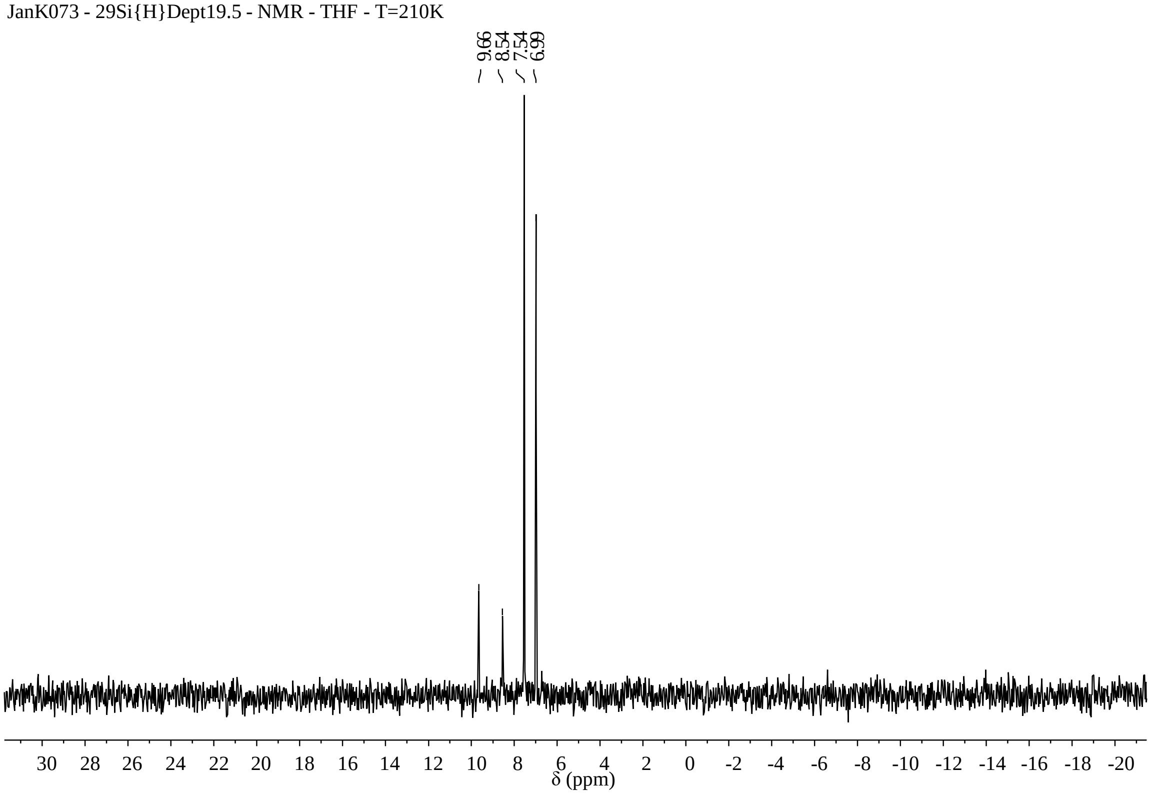


Figure S25. ^{29}Si{^{1}H}Dept19.5 NMR spectrum of **2**·hexane (79.5 MHz, THF-d$_8$, 210 K).

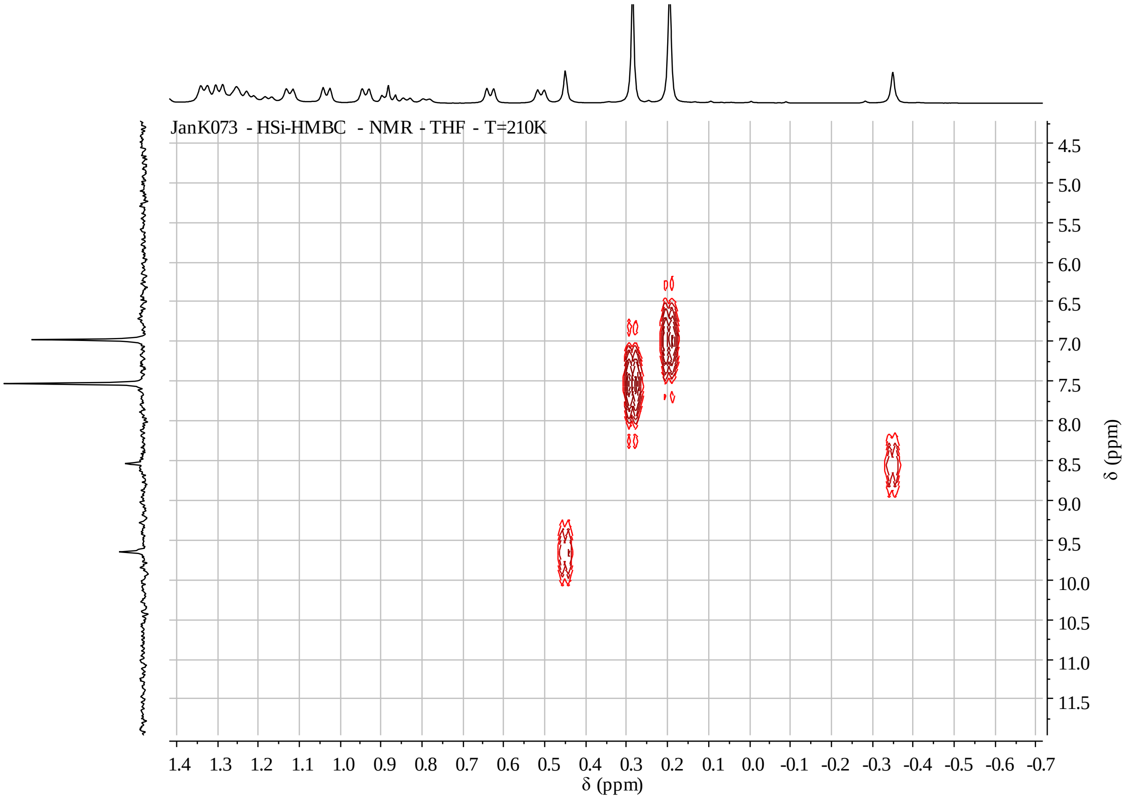


Figure S26. H,Si HMBC NMR spectrum of **2**·hexane (THF-d_8, 210 K).

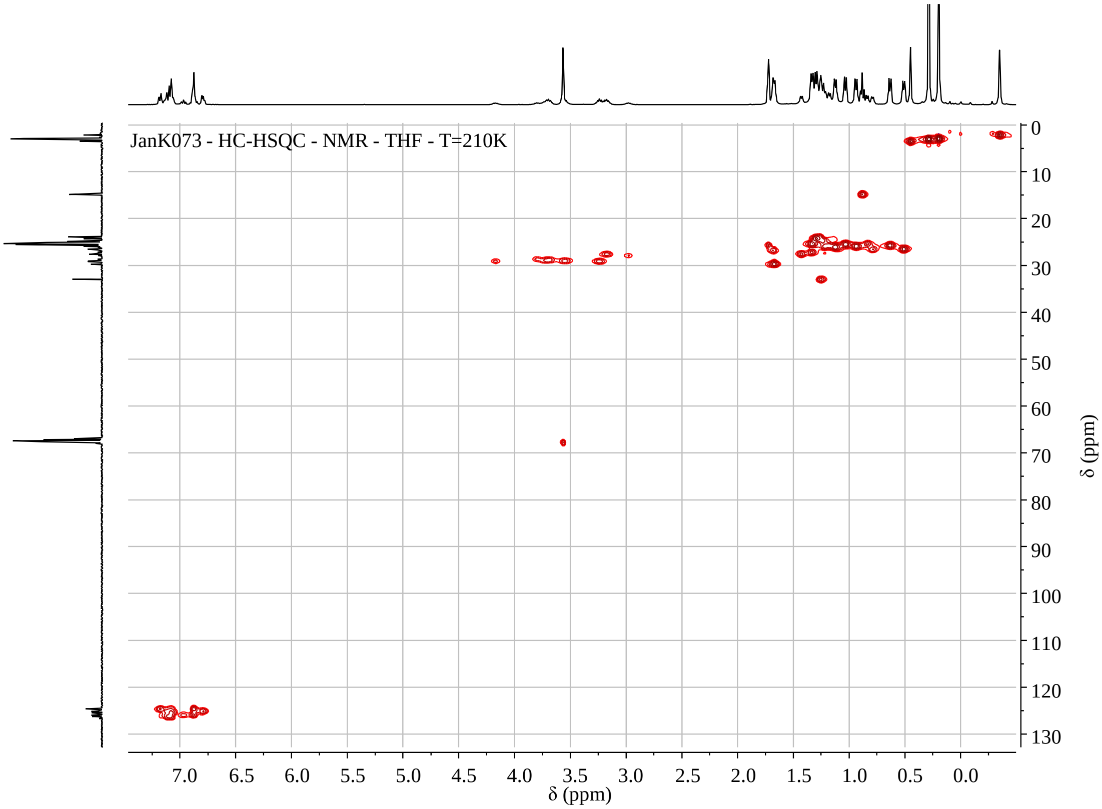


Figure S27. H,C HSQC NMR spectrum of **2**·hexane (THF-d_8, 210 K).

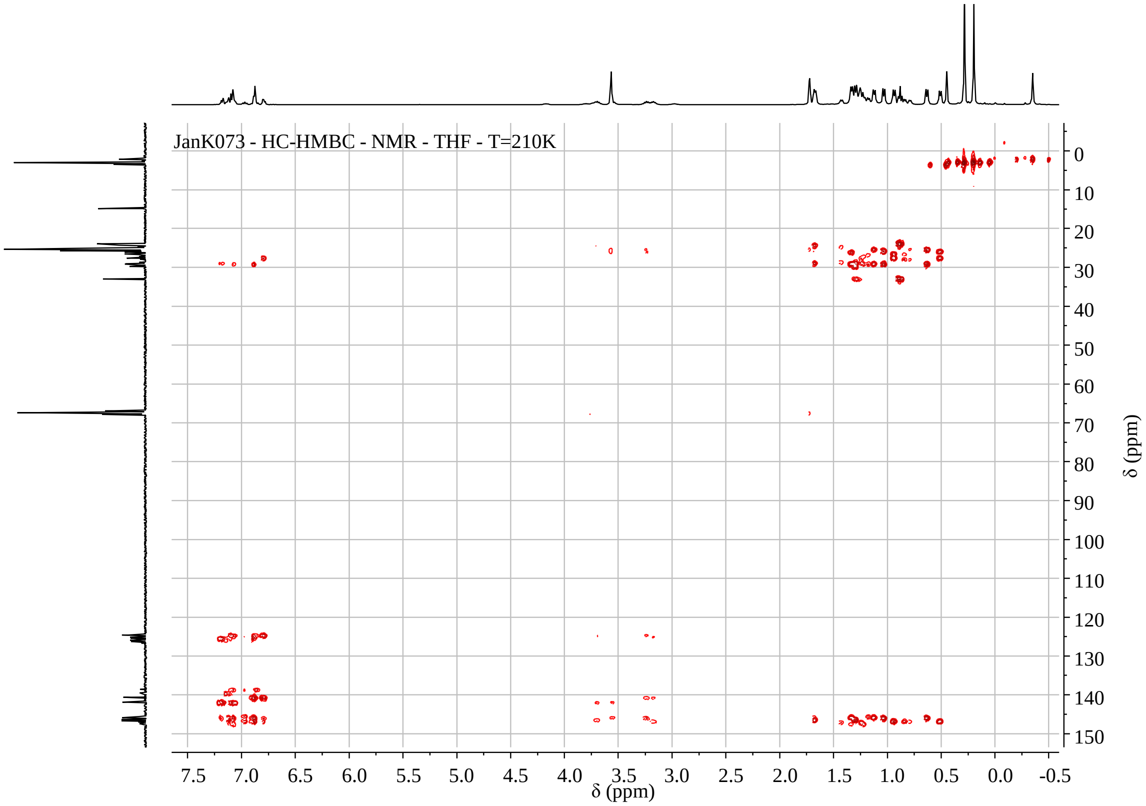


Figure S28. H,C HMBC NMR spectrum of **2**·hexane (THF-d_8, 210 K).

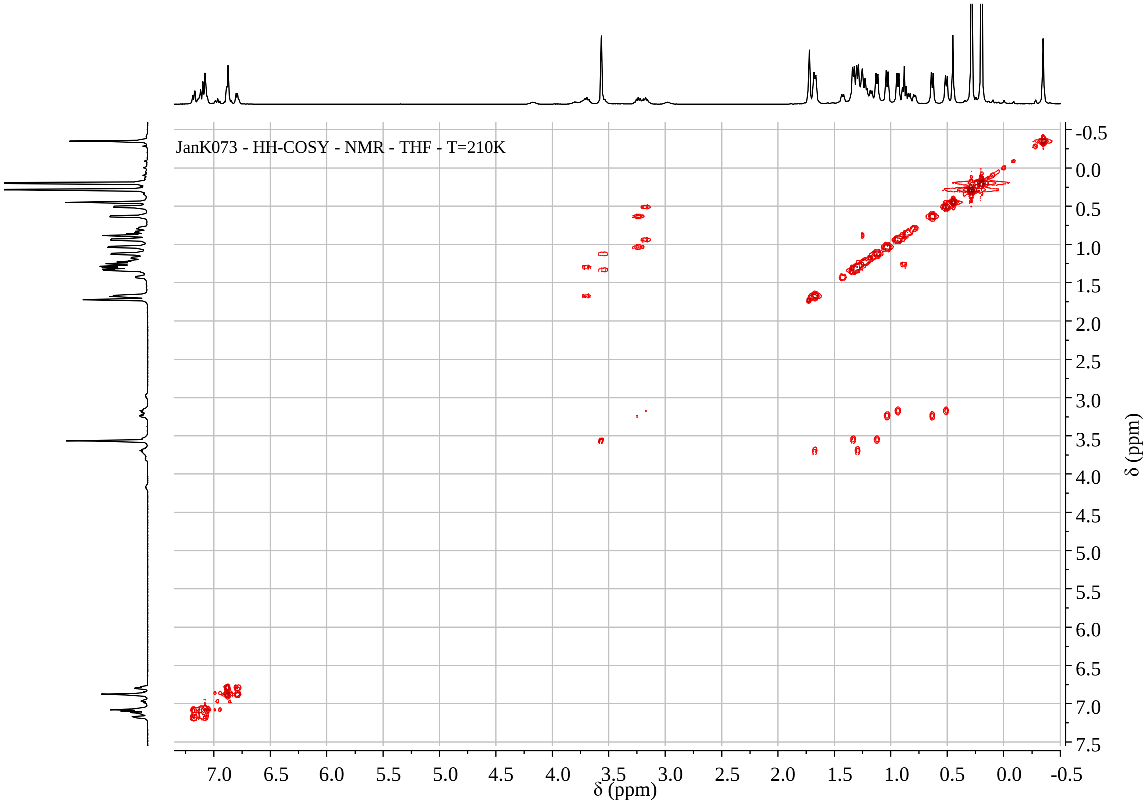


Figure S29. H,H COSY NMR spectrum of **2**·hexane (THF-d_8, 210 K).

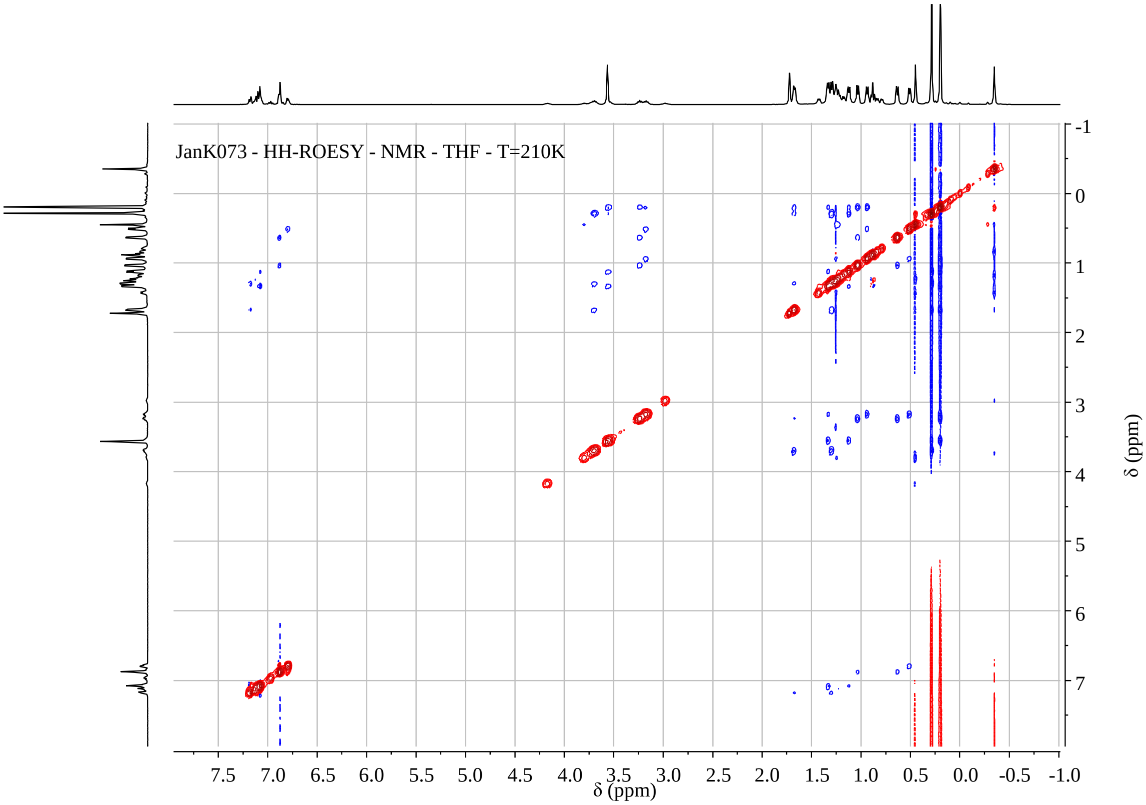


Figure S30. H,H ROESY NMR spectrum of **2**·hexane (THF-d_8, 210 K).

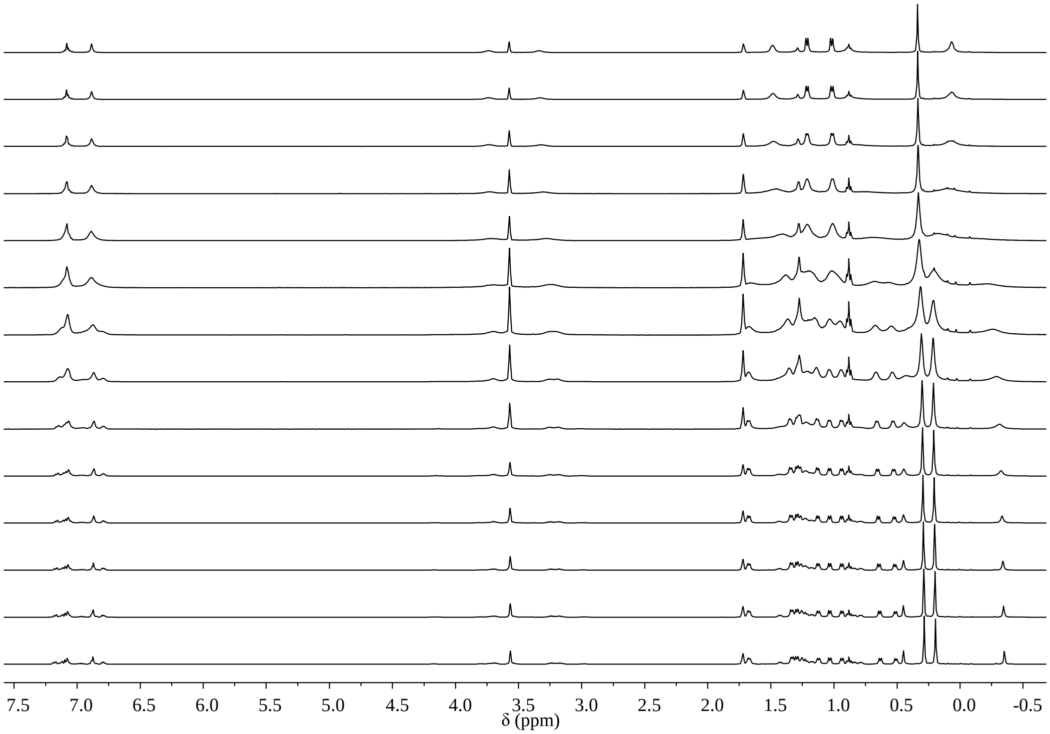


Figure S31. ^{1}H NMR spectrum of **2**·hexane in temperature range 340-210 K (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

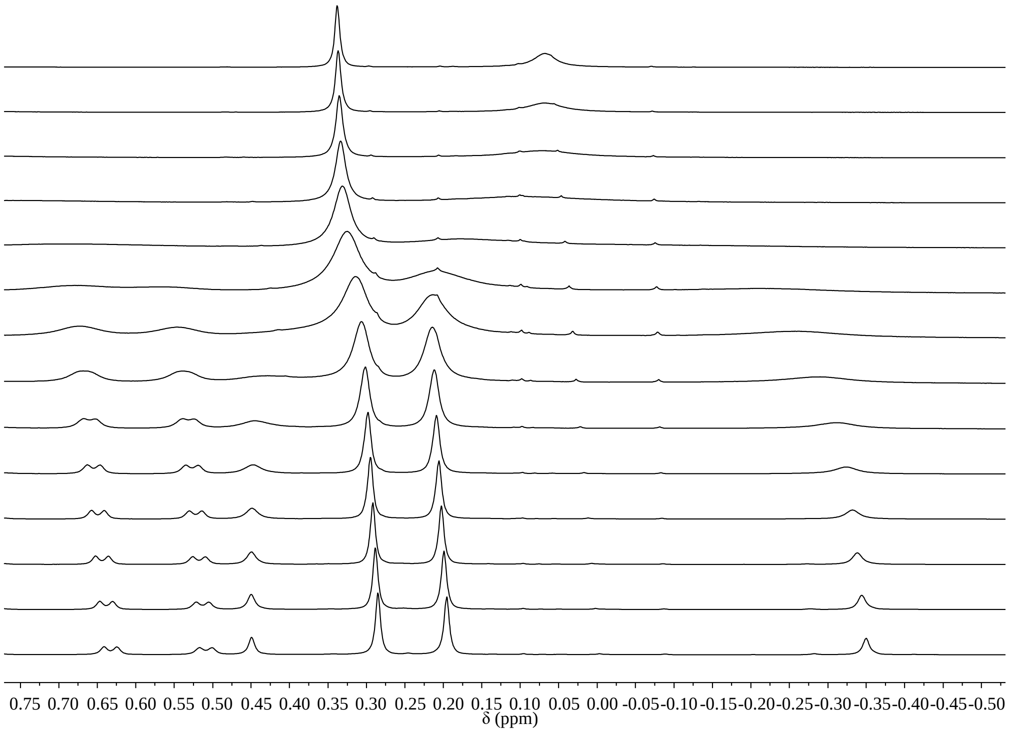


Figure S32. ^{1}H NMR spectrum of **2**·hexane in temperature range 340-210K and from -0.5 to 0.75 ppm (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

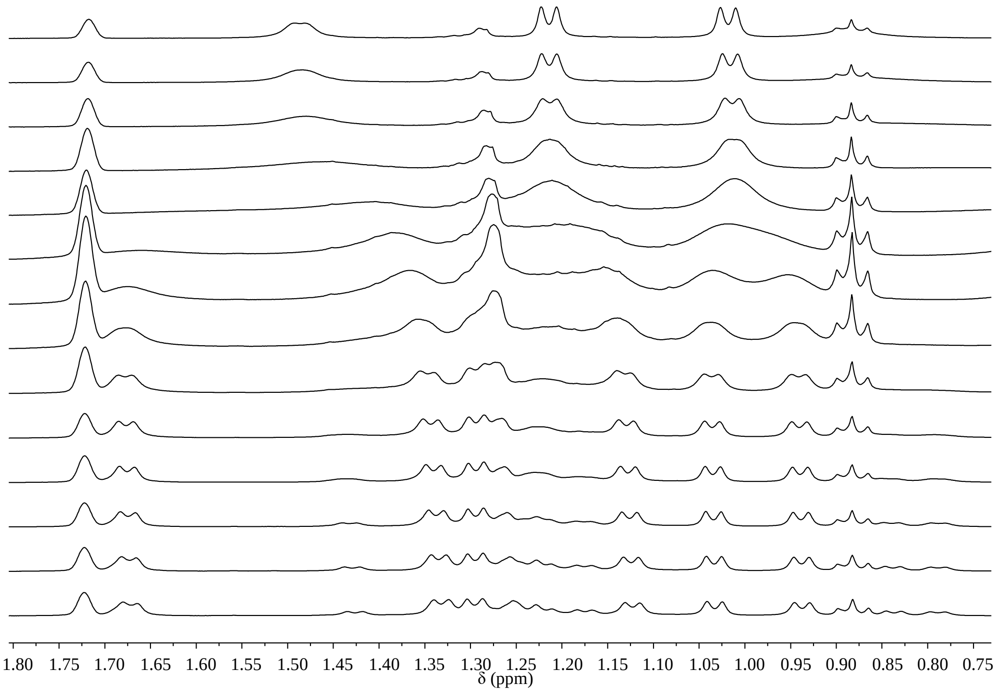


Figure S33. ^{1}H NMR spectrum of **2·**hexane in temperature range 340 K - 210 K and from 0.75 to 1.8 ppm (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

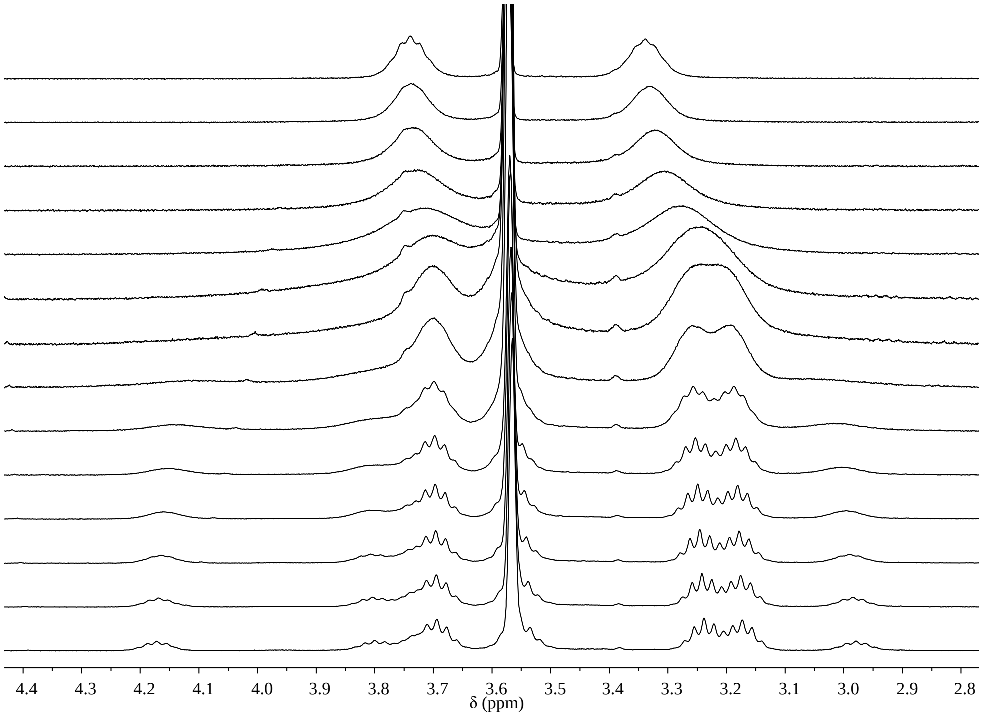


Figure S34. ^{1}H NMR spectrum of **2·**hexane in temperature range 340 K – 210 K and from 2.8 to 4.4 ppm (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

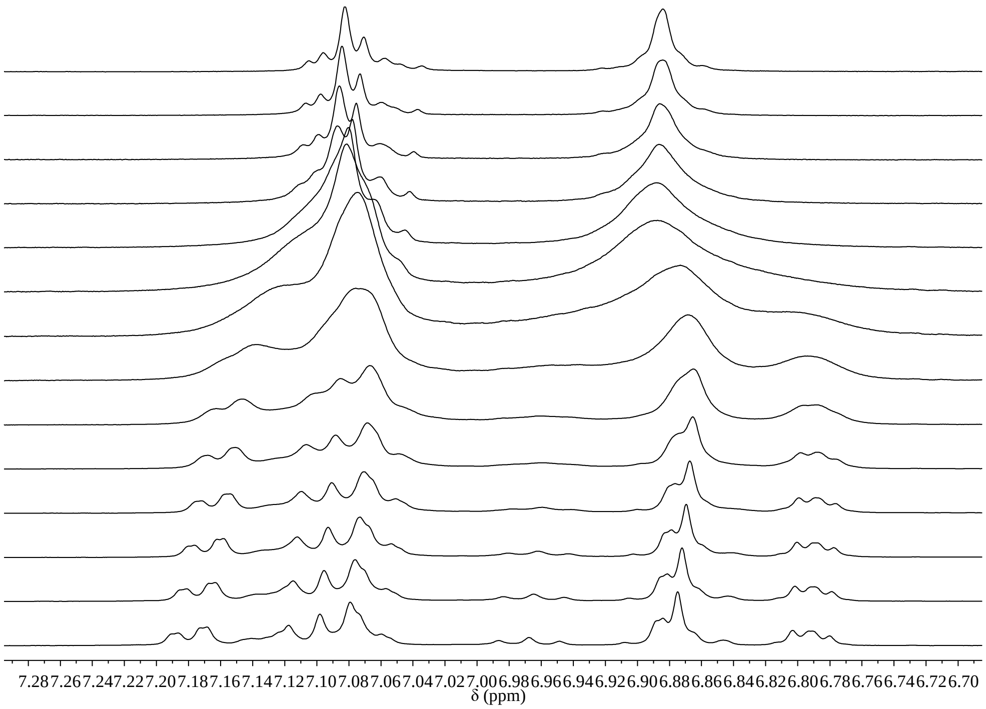


Figure S35. ^{1}H NMR spectrum of **2**·hexane in temperature range 340 K – 210 K and from 2.8 to 4.4 ppm (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

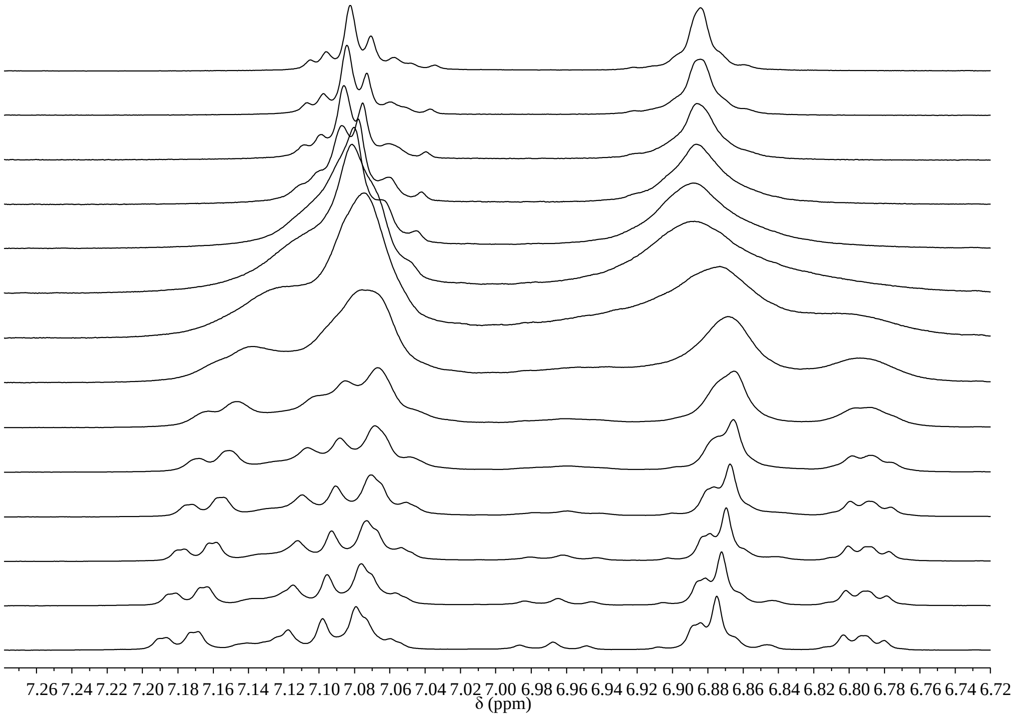


Figure S36. ^{1}H NMR spectrum of **2**·hexane in temperature range 340 K – 210 K and from 6.7 to 7.3 ppm (400 MHz, THF-d_8). Downwards from 340 K to 210 K in 10 K steps.

3. ^{29}Si CP/MAS NMR spectroscopy of 2

Experimental

All solid-state $^{29}Si\{^1H\}$ cross polarization/magic angle spinning (CP/MAS) NMR experiments were recorded on a Bruker DSX (9.4 T, $\nu_L(^{29}Si)$ = 79.5 MHz) spectrometer. A Bruker 4 mm double-resonance VTN probe was used. The sample was packed into a ZrO_2 rotor with 4.0 mm o.d. and was sealed with a Vespel cap. Tetrakis(trimethylsilyl)silane (TTMSS) was used as external reference for the chemical shift scale ($\delta(^{29}Si)$ = -9.84 ppm)[S31] and for calibration of the radio-frequency (rf) pulses. A rf-field strength of 50 kHz for ^{1}H was used for excitation and during the CP contact pulse. An 8.0 ms CP contact pulse with ramped power (70-100 %) of ^{29}Si was employed. The chemical shift anisotropy (CSA) was determined at a MAS frequency of 4.0 kHz. The free-induction decay (FID) was recorded (40 ms) with ^{1}H SW_f-TPPM[S32] decoupling. The chemical shift anisotropy (CSA) tensor from DFT calculations (Turbomole, for details see above) were obtained by matrix diagonalization which was done by a self-written Python script, following the Haeberlen-Mehring-Spiess convention.[S33,S34] The CSA parameters are defined as $\delta_{iso} = \frac{1}{3}(\delta_{xx} + \delta_{yy} + \delta_{zz})$, $\delta_\sigma = \delta_{iso} - \delta_{zz}$, $\eta_\sigma = (\delta_{xx} + \delta_{yy})/\delta_\sigma$, 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 $0 < \eta < 1$.[S33]

Data analysis, processing and plotting was done using the Bruker Topspin 4.0.7 software, dmfit2015[S35] and Python 3.7. Apodization using a Gaussian line broadening (7 Hz) was employed to the FID before Fourier Transformation.

Table S9. ^{29}Si isotropic chemical shifts (δ_{iso}) and chemical shift anisotropy parameters (δ_{aniso} , η_{σ}) obtained from ^{29}Si{^{1}H} CP/MAS NMR experiments and DFT calculations.

	Experimental			Calculated		
Site[a]	δ_{iso} / ppm	δ_{aniso} / ppm	η_{σ}	δ_{iso} / ppm	δ_{aniso} / ppm	η_{σ}
Si1/3	98.7 ± 0.2	-230 ± 20	0.10 ± 0.05	105.6	-284.7	0.14
Si2/4	-301.2 ± 0.2	96 ± 20	0.25 ± 0.05	-296.7	156.6	0.24
Si5/6	8.9 ± 0.3	-222 ± 20	0.00 ± 0.05	-4.8	-297.6	0.00
Si7/8	6.5 ± 0.2	20 ± 10	0.00 ± 0.05	6.85	-13.7	0.83
Si9/10	7.3 ± 0.2	20 ± 10	0.00 ± 0.05	8.25	-22.7	0.26

[a]The assignment follows that of Figure S37.

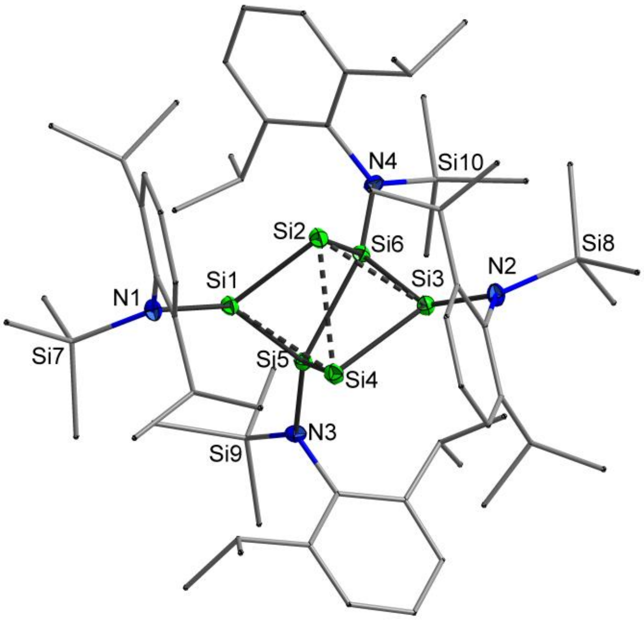


Figure S37. Molecular structure of **2** with atom labels

4. Lineshape Analysis

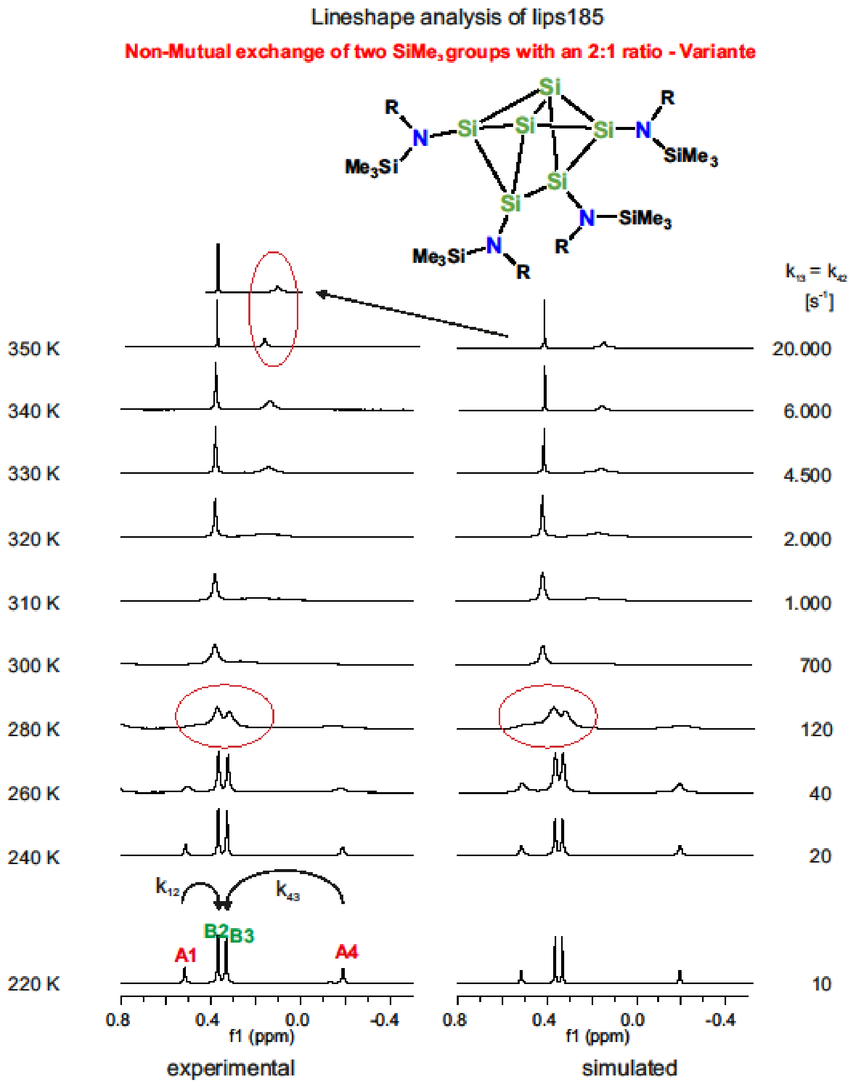
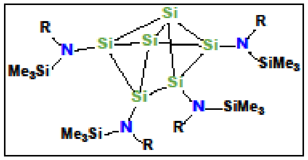


Figure S32: Experimental and simulated proton 400 MHz NMR spectra at variable temperatures. The exchanging proton pairs 1,2 and 4,3 were confirmed by 2D ROESY at 240 K. The simulation of lineshape was done with the SpinWorks program, written by K. Marat, University of Manitoba.

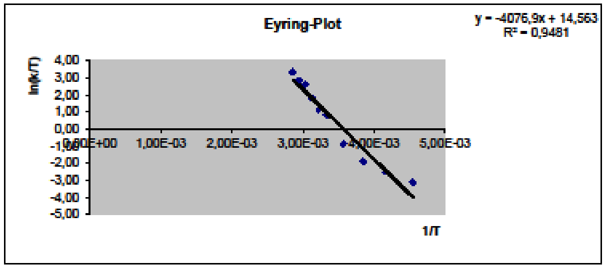
Lineshape analysis of lips185 (Non Mutual exchange)
Variante



site 1 site 2

T1/T2	T [K]	δ(A1-H)	δ(A4-H)	δ(B2-H)	δ(B3-H)	Int A	Int B	k(1,2)=k(4,3) [s-1]	K = IntB/IntA = k(12)/k(21)	k(2,1)=k(3,4) [s-1]	G# [kJ/mol]	1/T	ln(k(1,2)/T)	ln(k(2,1)/T)
0,5	350	208	-74	148	132	0,333	0,667	10000	2,003	4993	59,39	2,86E-03	3,35	2,66
0,5	340	208	-72	148	135	0,333	0,667	6000	2,003	2996	59,05	2,94E-03	2,87	2,18
0,5	330	208	-72	148	135	0,333	0,667	4500	2,003	2247	58,02	3,03E-03	2,61	1,92
0,5	320	208	-72	148	135	0,333	0,667	2000	2,003	999	58,34	3,13E-03	1,83	1,14
0,5	310	208	-72	148	135	0,333	0,667	1000	2,003	499	58,22	3,23E-03	1,17	0,48
0,5	300	208	-72	148	135	0,333	0,667	700	2,003	349	57,15	3,33E-03	0,85	0,15
0,5	280	208	-72	148	135	0,333	0,667	120	2,003	60	57,29	3,57E-03	-0,85	-1,54
0,5	260	208	-72	148	135	0,333	0,667	40	2,003	20	55,41	3,85E-03	-1,87	-2,57
0,5	240	208	-72	148	135	0,333	0,667	20	2,003	10	52,37	4,17E-03	-2,48	-3,18
0,5	220	208	-72	148	135	0,333	0,667	10	2,003	5	49,12	4,55E-03	-3,09	-3,79

Rm	8,31441		1,38E-23		4.184	6,63E-34



$$\Delta G^{\neq} = RT \cdot \left[23,76 - \ln\left(\frac{k}{T}\right)\right]$$

$$\ln\left(\frac{k}{T}\right) = -\frac{\Delta H^{\neq}}{R} \cdot \frac{1}{T} + \left(23,76 + \frac{\Delta S^{\neq}}{R}\right)$$

$$\Delta H^{\neq} = -R \cdot Steigung$$

$$\Delta S^{\neq} = (\mathrm{Achsenabschnitt} - 23,76) \cdot R$$

slope	-4577
Intercept	16,29

ΔG(320K)	58,0	kJ/mol
ΔH#	38,1	kJ/mol
ΔS#	-62,2	J/mol/K

5. Details of the single crystal X-ray diffraction analysis

Crystals of **2**·hexane were removed from a Schlenk tube under an argon atmosphere and were covered with a layer of hydrocarbon oil. A suitable crystal was selected, attached to a glass fiber and quickly placed in a low temperature Argon stream. The data were collected at 100 K on a Bruker Venture with Mo K_α radiation (λ = 0.71073 Å). The crystal structure was solved by direct methods using SHELX version 6.1 program package.[S36] Non-hydrogen atoms were refined anisotropically. Absorption corrections were applied using SADABS program (*SADABS*, an empirical absorption correction program, part of the SAINTPlus NT version 5.0 package; Bruker AXS: Madison, WI 1998). Data collected were corrected for Lorentz and polarization effects with Saint[S36] and absorption using Blessing's method and merged as incorporated with the program.[S37,S38] The SHELXTL[S39] program package was now implemented to determine the space group based upon intensity statistics. The structure was determined by direct methods with a majority of the non-hydrogen atoms from the molecule of interest being located directly using the program XT.[S40] Refinement of the structure was achieved using the program XL.[S41] Difference-Fourier least-squares refinement cycles were required to locate the remaining non-hydrogen atoms.

5.1. Refinement details

For compound **2**(·hexane) the hexane molecule is disordered over two positions with 48 and 52% occupancy, respectively.

Table S10. Crystal data and structure refinement for **2**(·hexane).

Compound	**2**(·hexane)
Empirical formula	$C_{66}H_{118}N_4Si_{10}$
Formula weight /g·mol^{-1}	1248.54
Crystal color, shape	yellow, block
Crystal size /mm^3	0.385 x 0.501 x 0.845
Crystal system	triclinic
Space group	$P\bar{1}$
a /Å b /Å c /Å	13.4808(9) 14.1304(10) 20.7309(15)
α /° β /° γ /°	81.160(2) 85.017(2) 77.197(2)
V /Å^3	3799.4(5)
Z	2
T /K	116
Completeness to θ 25.24° /%	99.4
ρ_{calc} /g·cm^{-3}	1.091
μ(Mo) /mm^{-1}	0.211
2 θ range /°	3.78-54.28
Reflections measured	39610
Independent reflections	16495
R(int)	0.0448
Ind. reflections ($I > 2\sigma(I)$)	13915
Parameters	776
Restraints	184
R_1 ($I > 2\sigma(I)$)	0.0364
wR_2 (all data)	0.0972
GooF (all data)	1.019
Max. peak/hole /e$^-$·Å^{-3}	0.35/ –0.26
Absorption correction type	Multi-scan
Min. /Max. transmission	0.6183/ 0.7455

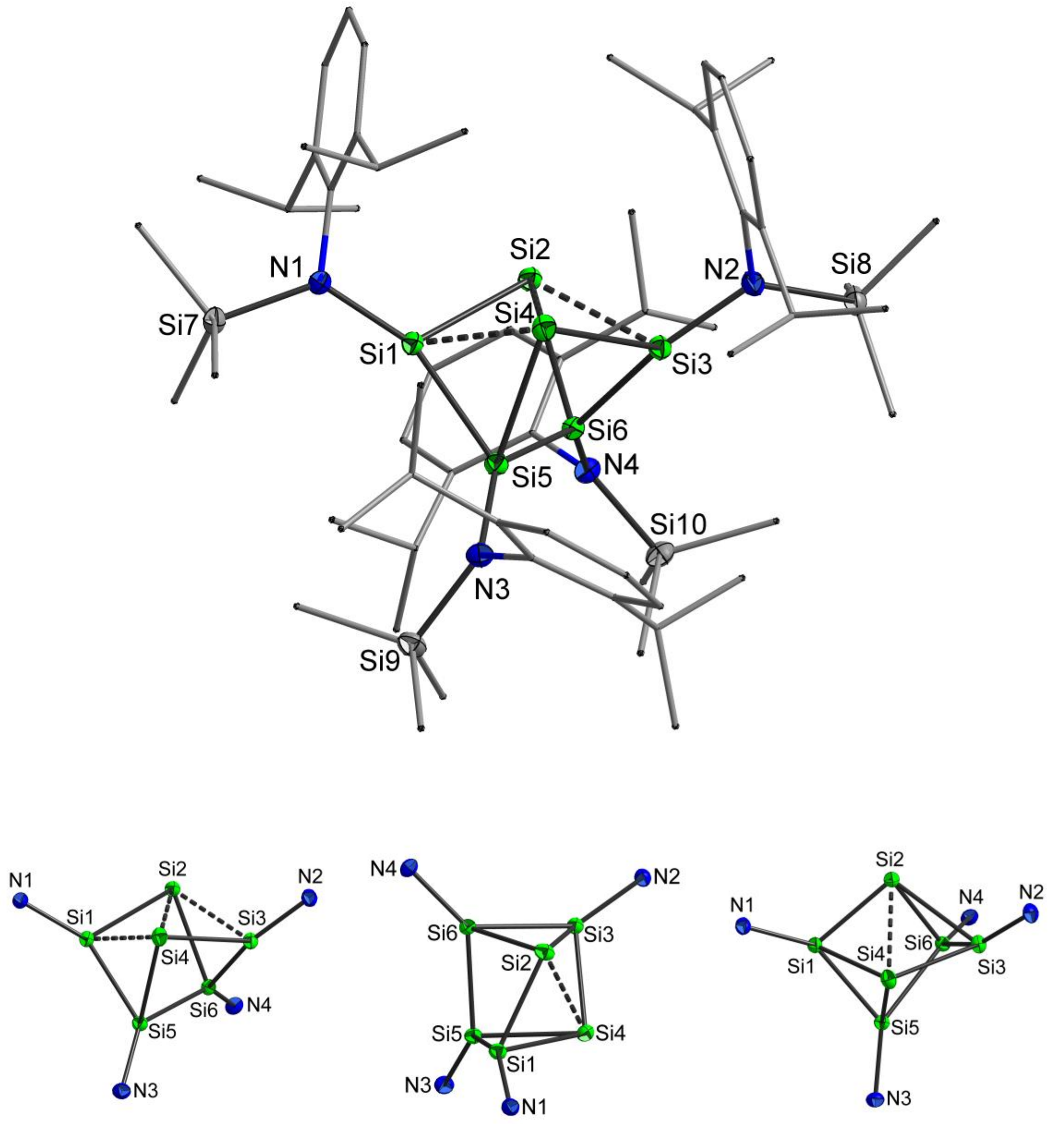


Figure S38. Molecular structure of **2**. Thermal ellipsoids are drawn at a 50% level. H atoms and co-crystallized hexane molecules are omitted for clarity. Di*iso*propyl groups of the Dipp ligand are represented in wires and sticks for clarity.

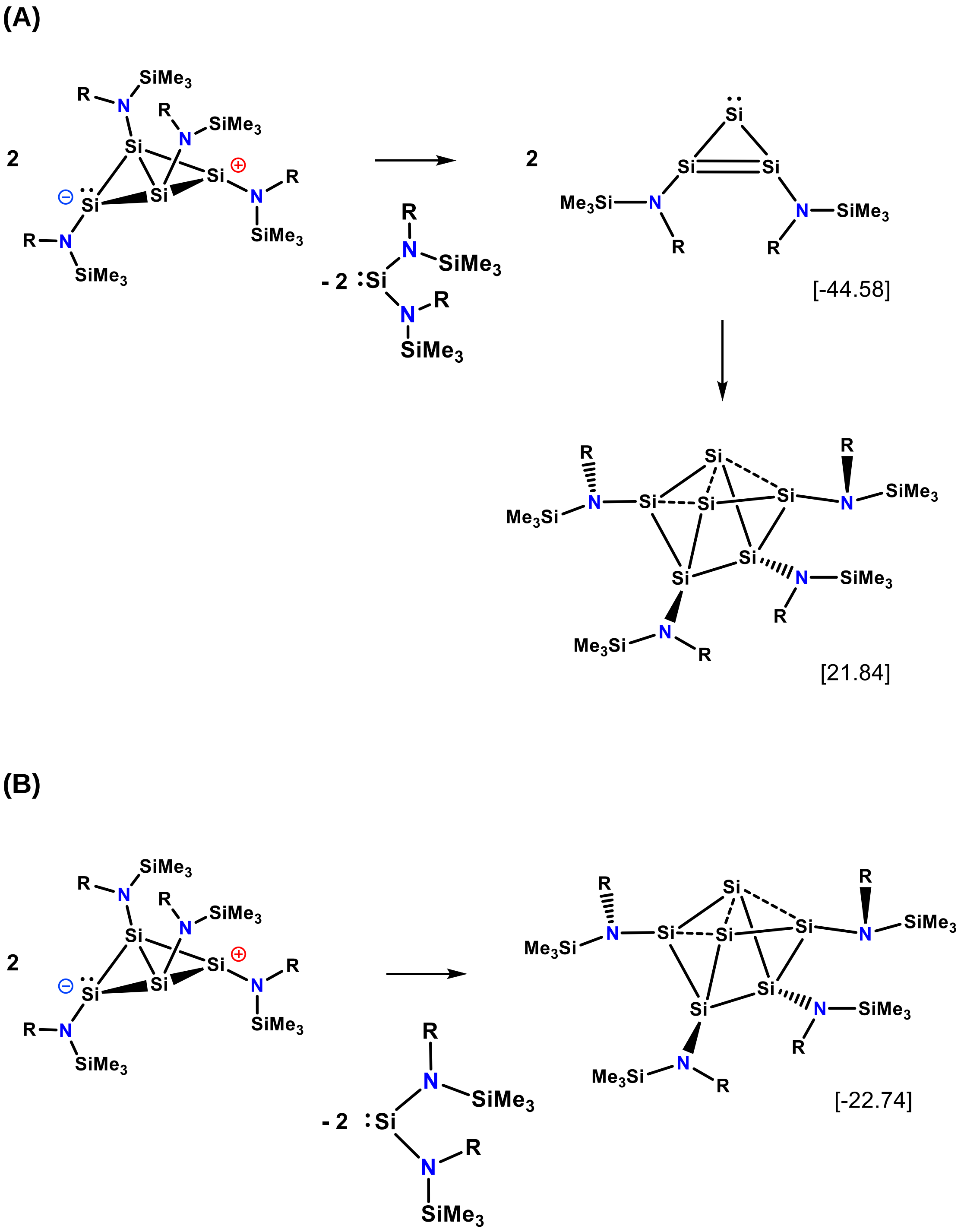
Figure S38 (continued).

Selected bond distances/Å and angles/°.

Si1−Si2 2.2813(5), Si2−Si3 2.5017(6), Si3−Si4 2.2922(5), Si1−Si4 2.5322(6), Si2−Si4 2.6356(6), Si1−Si5 2.3261(5), Si3−Si6 2.3286(6), Si2−Si6 2.4026(5), Si4−Si5 2.3890(6), Si5−Si6 2.3568(5), Si1−N1 1.7296(12), Si3−N2 1.7339(12), Si5−N3 1.7398(12), Si6−N4 1.7404(12), Si7−N1 1.7608(12), Si8−N2 1.7601(12), Si9−N3 1.7566(13), Si10−N4 1.7580(12), Si7−C13 1.8571(15), Si7−C14 1.8578(17), Si7−C15 1.8641(17), Si8−C28 1.8588(17), Si8−C29 1.8584(17), Si8−C30 1.8619(17), Si9−C43 1.8579(15), Si9−C44 1.8597(17), Si9−C45 1.8584(17), Si10−C58 1.8598(16) Si10−C59 1.8591(18), Si10−C60 1.8584(17).

N1-Si1-Si2 119.96(4), N1-Si1-Si5 146.08(4), Si2-Si1-Si5 91.154(19), N1-Si1-Si4 119.11(4), Si2-Si1-Si4 66.158(17), Si5-Si1-Si4 58.726(16), Si1-Si2-Si6 82.809(18), Si1-Si2-Si3 104.68(2), Si6-Si2-Si3 56.651(15), Si1-Si2-Si4 61.496(16), Si6-Si2-Si4 81.609(17), Si3-Si2-Si4 52.920(15), N2-Si3-Si4 120.78(4), N2-Si3-Si6 144.75(5), Si4-Si3-Si6 91.042(19), N2-Si3-Si2 116.71(4), Si4-Si3-Si2 66.538(17), Si6-Si3-Si2 59.527(16), Si3-Si4-Si5 83.345(18), Si3-Si4-Si1 103.399(19), Si5-Si4-Si1 56.324(16), Si3-Si4-Si2 60.542(16), Si5-Si4-Si2 81.666(17), Si1-Si4-Si2 52.345(14), N3-Si5-Si1 134.63(4), N3-Si5-Si6 138.31(4), Si1-Si5-Si6 82.872(18), N3-Si5-Si4 121.04(4), Si1-Si5-Si4 64.950(17), Si6-Si5-Si4 88.009(18), N4-Si6-Si3 134.58(4), N4-Si6-Si5 138.25(4), Si3-Si6-Si5 83.278(18), N4-Si6-Si2 121.69(4), Si3-Si6-Si2 63.822(17), Si5-Si6-Si2 87.478(18).

6. Postulated formation of 2



Scheme S2. Two postulated formation pathways of **2** (R = 2,6-*i*Pr$_2$C$_6$H$_3$). Values in bracket correspond to the free energies (Δ*G*) of the reactions.

Table S11. Energies *E*h and free energies *G* for the reactants and product **2** in Scheme S2.

	1	**Silylene**	**Sila-cyclopropene**	**2**
E(TPSS-D3/def2-TZVP) [Eh]	-4886.304370	-2152.8492836	-2731.8837215	-5463.9361647
G(298K) [kcal/mol]	866.186	422.774	421.122	864.088

[a] single point energy using the TPSS-D3/def2-TZVP geometry
[b] $\Delta G_{298} = \Delta E(\text{TPSS-D3/def2-TZVP}) + \Delta(G(298K))$

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[S41] Sheldrick, G. M., SHELXL2014 structure refinement program.

8. Cartesian coordinates of all compounds

2-A

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E(TPSS-D3/def2-TZVP) = -5465.431211756 (conv)
Lowest Freq. =    17.50 cm^-1
178
1-A (004-S/cx/tpss-d3.def2-TZVP)
Si    0.8540928   -1.6783347    0.3573215
Si   -1.1512836   -0.7857414    1.0597402
Si   -0.8538167    1.6779503    0.3586284
Si    1.1525958    0.7856288    1.0581510
Si    1.1732241   -0.0101963   -1.2207498
Si   -1.1754336    0.0104389   -1.2190328
Si    2.9518717   -3.9784195    0.9236326
Si   -2.9503996    3.9785191    0.9262035
Si    3.0552350   -0.4506932   -3.6620781
Si   -3.0595497    0.4494557   -3.6590561
N     1.6375902   -2.8718567    1.3614062
N    -1.6353288    2.8722662    1.3629180
N     2.4808915    0.4846900   -2.2728162
N    -2.4842990   -0.4849047   -2.2694781
C     0.9679096   -3.0685031    2.6376216
C    -0.1343627   -3.9508931    2.7185570
C    -0.7255060   -4.1654446    3.9679289
H    -1.5697462   -4.8460071    4.0427788
C    -0.2595496   -3.5207485    5.1080944
H    -0.7298451   -3.7030266    6.0705031
C     0.7964492   -2.6218643    5.0044595
H     1.1406017   -2.0956551    5.8906405
C     1.4195453   -2.3663529    3.7781946
C    -0.7111884   -4.6613673    1.5026703
H    -0.1878279   -4.2876586    0.6166177
C    -0.4974159   -6.1844437    1.5738537
H    -0.9083659   -6.6664229    0.6793930
H     0.5624524   -6.4438627    1.6463986
H    -1.0060421   -6.6047757    2.4487673
C    -2.2060296   -4.3518750    1.3216204
H    -2.5777408   -4.8044274    0.3979172
H    -2.7970180   -4.7442654    2.1569259
H    -2.3777922   -3.2727654    1.2609625
C     2.5411152   -1.3401370    3.7168546
H     2.7348065   -1.1297327    2.6600218
C     3.8416792   -1.8688413    4.3489281
H     4.6238008   -1.1025424    4.2996095
H     3.6833934   -2.1252183    5.4027861
H     4.2087233   -2.7627255    3.8376405
C     2.1354379   -0.0179856    4.3896385
H     1.1967489    0.3648662    3.9813730
H     2.0154959   -0.1394583    5.4723448
H     2.9078160    0.7400491    4.2209779
C     2.4892831   -4.9640331   -0.6088363
H     3.3303087   -5.5931498   -0.9262335
H     1.6322265   -5.6184580   -0.4192120
H     2.2297505   -4.3146436   -1.4500873
C     3.2436466   -5.1647643    2.3482192
H     4.0605380   -5.8488053    2.0848680
H     3.5204389   -4.6491527    3.2718989
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H	2.3576094	-5.7678224	2.5671263
C	4.5034080	-2.9835541	0.5787732
H	5.3206080	-3.6304266	0.2373718
H	4.3198735	-2.2404230	-0.2023608
H	4.8403406	-2.4516281	1.4742705
C	-0.9645576	3.0694945	2.6385072
C	-1.4145956	2.3671353	3.7795514
C	-0.7899326	2.6226496	5.0050497
H	-1.1328016	2.0962634	5.8916134
C	0.2659519	3.5218256	5.1073754
H	0.7374620	3.7041071	6.0691913
C	0.7302615	4.1668032	3.9666919
H	1.5743822	4.8476347	4.0405548
C	0.1376619	3.9520889	2.7180386
C	-2.5362626	1.3409199	3.7197321
H	-2.7315014	1.1305467	2.6631928
C	-2.1295540	0.0187899	4.3919319
H	-2.9022615	-0.7391984	4.2246178
H	-1.1916127	-0.3641636	3.9820371
H	-2.0077300	0.1403045	5.4744272
C	-3.8358916	1.8695660	4.3537369
H	-4.6180514	1.1032476	4.3054211
H	-3.6760523	2.1257844	5.4073986
H	-4.2036887	2.7635190	3.8430985
C	0.7126794	4.6626229	1.5014328
H	0.1877036	4.2893523	0.6161573
C	2.2071394	4.3527241	1.3178034
H	2.5776379	4.8060925	0.3940133
H	2.7995106	4.7440043	2.1526608
H	2.3783772	3.2735990	1.2557638
C	0.4995247	6.1857622	1.5734463
H	0.9079775	6.6677742	0.6778585
H	-0.5600798	6.4454124	1.6491351
H	1.0107963	6.6058622	2.4469284
C	-3.2411750	5.1649828	2.3508557
H	-4.0584305	5.8488077	2.0880803
H	-3.5169917	4.6495166	3.2749026
H	-2.3550582	5.7682911	2.5687812
C	-4.5017215	2.9829647	0.5826657
H	-5.3197405	3.6296161	0.2427686
H	-4.3186897	2.2405902	-0.1993116
H	-4.8372109	2.4501101	1.4781521
C	-2.4897266	4.9638910	-0.6069760
H	-3.3315011	5.5921229	-0.9241427
H	-1.6331347	5.6192100	-0.4182801
H	-2.2302617	4.3142313	-1.4480665
C	3.1066342	1.7650095	-2.0012384
C	4.2229578	1.8413310	-1.1380024
C	4.8741359	3.0710532	-0.9936675
H	5.7432545	3.1352687	-0.3443256
C	4.4321771	4.2087109	-1.6602340
H	4.9565779	5.1525480	-1.5389956
C	3.2980131	4.1335541	-2.4613525
H	2.9303113	5.0277808	-2.9587538
C	2.6164678	2.9254361	-2.6395009
C	4.7446568	0.6335630	-0.3777762
H	4.0066632	-0.1661621	-0.4980839

C	6.0878678	0.1454813	-0.9501026
H	6.4393057	-0.7350716	-0.4015371
H	6.0032726	-0.1206209	-2.0073122
H	6.8487910	0.9292373	-0.8617332
C	4.8884554	0.9198245	1.1261983
H	5.2049426	0.0121175	1.6508017
H	5.6400751	1.6942236	1.3149286
H	3.9373821	1.2496349	1.5556191
C	1.3525630	2.9034372	-3.4808126
H	1.0104865	1.8648487	-3.5203663
C	1.5864261	3.3846699	-4.9218295
H	2.3468337	2.7814862	-5.4267269
H	0.6573174	3.3166969	-5.4987291
H	1.9183889	4.4285825	-4.9408053
C	0.2489327	3.7326434	-2.8048360
H	-0.6803179	3.6814850	-3.3832130
H	0.0487530	3.3522088	-1.7975785
H	0.5402994	4.7853891	-2.7199410
C	3.6916704	-2.1171793	-3.0778956
H	3.9109955	-2.7758512	-3.9271158
H	4.6031546	-2.0232261	-2.4796636
H	2.9368369	-2.6130907	-2.4585758
C	4.4147331	0.5154520	-4.5219906
H	4.8112921	-0.0781857	-5.3553608
H	4.0432680	1.4606977	-4.9294415
H	5.2455972	0.7546823	-3.8518361
C	1.6455576	-0.7595054	-4.8630314
H	1.9562864	-1.4575089	-5.6503910
H	0.7828905	-1.1989946	-4.3518250
H	1.3106697	0.1643917	-5.3446608
C	-3.1095036	-1.7652186	-1.9968100
C	-4.2250717	-1.8414055	-1.1326793
C	-4.8760627	-3.0711297	-0.9874405
H	-5.7446219	-3.1352247	-0.3373602
C	-4.4345633	-4.2089238	-1.6540808
H	-4.9587914	-5.1527556	-1.5321545
C	-3.3009220	-4.1339469	-2.4559345
H	-2.9334764	-5.0283009	-2.9532899
C	-2.6196454	-2.9258150	-2.6349985
C	-4.7457754	-0.6335161	-0.3719576
H	-4.0076996	0.1660175	-0.4930087
C	-6.0893920	-0.1449836	-0.9428996
H	-6.0057093	0.1212758	-2.0001543
H	-6.8504796	-0.9285200	-0.8539368
H	-6.4400292	0.7356012	-0.3938708
C	-4.8879966	-0.9198787	1.1321475
H	-3.9364578	-1.2497640	1.5604731
H	-5.2038684	-0.0122016	1.6571815
H	-5.6394336	-1.6942727	1.3216399
C	-1.3563336	-2.9042152	-3.4772412
H	-1.0135997	-1.8658189	-3.5164295
C	-1.5917948	-3.3843915	-4.9183387
H	-0.6631421	-3.3168602	-5.4960235
H	-1.9246485	-4.4280172	-4.9376113
H	-2.3521554	-2.7803006	-5.4222108
C	-0.2526261	-3.7345325	-2.8027944
H	0.6762453	-3.6831164	-3.3817409

H	-0.0516129	-3.3552204	-1.7953068
H	-0.5442953	-4.7872585	-2.7187910
C	-3.6947772	2.1167698	-3.0758479
H	-3.9143652	2.7748414	-3.9254794
H	-4.6059229	2.0237544	-2.4769522
H	-2.9393267	2.6127974	-2.4573736
C	-1.6507318	0.7564311	-4.8614969
H	-1.9616902	1.4535854	-5.6495239
H	-0.7875541	1.1962176	-4.3514116
H	-1.3164988	-0.1681890	-5.3421588
C	-4.4204967	-0.5166563	-4.5167321
H	-4.8173573	0.0763947	-5.3503784
H	-4.0501934	-1.4626654	-4.9234854
H	-5.2509388	-0.7544690	-3.8455458

2-B

E(TPSS-D3/def2-TZVP) = -5465.426151187 (conv)
Lowest Freq. =   13.69 cm^-1
178
1-B (004-S/c3/tpss-d3.def2-TZVP)

Si	0.8091830	-1.8120994	0.2110252
Si	-1.0278776	-0.8171933	1.2338491
Si	-0.6762009	1.6633222	0.4331896
Si	1.2879877	0.6258803	1.0135424
Si	1.0448181	-0.0856254	-1.3047508
Si	-1.2753953	-0.0513894	-1.0365515
Si	2.8999881	-4.1256354	0.2583334
Si	-2.4190402	4.1615616	0.8262085
Si	2.0864630	2.2004484	-3.0819374
Si	-3.0691746	0.2302857	-3.5486858
N	1.6275551	-3.1330732	1.0044025
N	-1.3248527	2.9195677	1.4582649
N	2.1569394	0.5112493	-2.5263767
N	-2.6300886	-0.5560470	-2.0212900
C	1.1228941	-3.5102151	2.3224630
C	0.0911457	-4.4773451	2.4277540
C	-0.3320574	-4.8747713	3.7002039
H	-1.1223814	-5.6156375	3.7825179
C	0.2250528	-4.3369409	4.8534944
H	-0.1123808	-4.6659640	5.8325260
C	1.1970807	-3.3528096	4.7385804
H	1.6103934	-2.8995576	5.6355869
C	1.6507489	-2.9093143	3.4906867
C	-0.6428358	-5.0518806	1.2261891
H	-0.0754098	-4.7952846	0.3283561
C	-0.7902855	-6.5831565	1.2845910
H	-1.2007764	-6.9511940	0.3375076
H	0.1642691	-7.0832302	1.4642854
H	-1.4844138	-6.8813701	2.0779479
C	-2.0417608	-4.4199755	1.1068305
H	-2.5867166	-4.8469577	0.2607852
H	-2.6205624	-4.6039638	2.0189095
H	-1.9846022	-3.3370401	0.9595116
C	2.6382924	-1.7542633	3.4743578
H	2.8406100	-1.4967850	2.4305361
C	3.9689102	-2.1056155	4.1631533

H	4.6660737	-1.2637003	4.0844750
H	3.8097888	-2.3092119	5.2282682
H	4.4400986	-2.9844334	3.7188646
C	2.0214526	-0.5203097	4.1622678
H	1.0457936	-0.2712608	3.7358092
H	1.8891767	-0.7005654	5.2354660
H	2.6740456	0.3507494	4.0405429
C	3.0594586	-3.5863899	-1.5240421
H	3.7829575	-4.2371529	-2.0309133
H	2.1063574	-3.6720266	-2.0547144
H	3.4150689	-2.5587133	-1.6351287
C	2.4722486	-5.9533245	0.3153565
H	3.3413319	-6.5225403	-0.0394041
H	2.2564816	-6.2860161	1.3360092
H	1.6207937	-6.2144335	-0.3196788
C	4.5433405	-3.9632829	1.1531407
H	5.3154615	-4.4745809	0.5633923
H	4.8607108	-2.9280581	1.2946968
H	4.5053257	-4.4502886	2.1333366
C	-0.7447904	3.0505031	2.7819302
C	-1.3764082	2.4239642	3.8805945
C	-0.8481485	2.6223707	5.1603329
H	-1.3359837	2.1541608	6.0106531
C	0.2859216	3.3994090	5.3645030
H	0.6774897	3.5458879	6.3673582
C	0.9274299	3.9674918	4.2709803
H	1.8303460	4.5524198	4.4248162
C	0.4421616	3.7980163	2.9696436
C	-2.6100698	1.5500209	3.7241253
H	-2.7189109	1.3217976	2.6588590
C	-2.4663454	0.2184280	4.4797303
H	-3.3211791	-0.4294982	4.2597901
H	-1.5556857	-0.3082840	4.1818271
H	-2.4384309	0.3741735	5.5639982
C	-3.8783557	2.2853193	4.1954996
H	-4.7564562	1.6371928	4.0971373
H	-3.7853594	2.5726160	5.2490470
H	-4.0574390	3.1943156	3.6149358
C	1.2262418	4.4154340	1.8213365
H	0.7918648	4.0453508	0.8869275
C	2.7040101	3.9869054	1.8572642
H	3.2348066	4.3943418	0.9910885
H	3.2009973	4.3564431	2.7606880
H	2.7929824	2.8957089	1.8385961
C	1.1342154	5.9521995	1.8142159
H	1.7091600	6.3619522	0.9758036
H	0.1016699	6.2983348	1.7208521
H	1.5446527	6.3665118	2.7420051
C	-2.7076668	5.4641365	2.1450853
H	-3.3184757	6.2754475	1.7293645
H	-3.2397875	5.0534496	3.0085373
H	-1.7754607	5.8985265	2.5161954
C	-4.0468083	3.3639894	0.3465531
H	-4.7325521	4.0955449	-0.0980450
H	-3.8841745	2.5712765	-0.3899320
H	-4.5407687	2.9177592	1.2156471
C	-1.6390446	4.9200491	-0.7107081

H	-2.3342836	5.6014810	-1.2161283
H	-0.7307536	5.4809511	-0.4668619
H	-1.3612152	4.1394594	-1.4295234
C	3.3550215	-0.2320139	-2.8533930
C	3.3851815	-0.9779416	-4.0537327
C	4.5393214	-1.6974221	-4.3711021
H	4.5701086	-2.2790668	-5.2876882
C	5.6514560	-1.6811878	-3.5329985
H	6.5394430	-2.2508895	-3.7925286
C	5.6208342	-0.9239307	-2.3689772
H	6.4930140	-0.8993143	-1.7204975
C	4.4870962	-0.1827570	-2.0118103
C	2.1687663	-1.0301655	-4.9600975
H	1.6050831	-0.1052621	-4.7986477
C	2.5140572	-1.1189574	-6.4523142
H	1.6005697	-1.0228506	-7.0491233
H	3.2065593	-0.3250329	-6.7511244
H	2.9716606	-2.0811571	-6.7078706
C	1.2606489	-2.1957237	-4.5385625
H	0.3693266	-2.2425255	-5.1715650
H	1.7984391	-3.1466577	-4.6207488
H	0.9398175	-2.0773474	-3.4981421
C	4.5270105	0.6513251	-0.7435146
H	3.5578892	1.1504646	-0.6395852
C	5.6176964	1.7338466	-0.8171524
H	5.4967856	2.3626812	-1.7047388
H	5.5758932	2.3751342	0.0703332
H	6.6152111	1.2825142	-0.8616570
C	4.7212967	-0.2301024	0.4974970
H	4.6901715	0.3758949	1.4091488
H	3.9235979	-0.9758783	0.5640862
H	5.6824123	-0.7555431	0.4629954
C	0.3758108	2.5879696	-3.7435353
H	0.2746654	3.6674656	-3.9095174
H	0.1647768	2.0783812	-4.6876553
H	-0.3918804	2.2921987	-3.0200546
C	3.3774064	2.4164279	-4.4271526
H	3.3638953	3.4567237	-4.7762303
H	4.3865372	2.1943843	-4.0656944
H	3.1839966	1.7704975	-5.2898047
C	2.4078818	3.4090587	-1.6811144
H	2.1731696	4.4316521	-2.0025512
H	1.7644440	3.1723642	-0.8261614
H	3.4440030	3.3938441	-1.3334948
C	-3.3991459	-1.7200731	-1.6231035
C	-4.4529334	-1.5833833	-0.6931578
C	-5.2615632	-2.6930818	-0.4252170
H	-6.0827701	-2.5901884	0.2788388
C	-5.0438662	-3.9161424	-1.0487581
H	-5.6907004	-4.7628909	-0.8368654
C	-3.9746185	-4.0510901	-1.9262801
H	-3.7793654	-5.0148956	-2.3899033
C	-3.1307050	-2.9740482	-2.2158556
C	-4.7524864	-0.2686119	0.0044656
H	-3.9091073	0.4036634	-0.1836004
C	-6.0241866	0.3871110	-0.5628527
H	-5.9201050	0.6041719	-1.6296342

H	-6.8864204	-0.2774902	-0.4371809
H	-6.2360269	1.3269810	-0.0426906
C	-4.8759634	-0.4485295	1.5244185
H	-3.9722662	-0.9084950	1.9349948
H	-5.0193153	0.5241969	2.0050807
H	-5.7335232	-1.0776457	1.7867578
C	-1.9352702	-3.2068224	-3.1236762
H	-1.4520179	-2.2412563	-3.2927509
C	-2.3356966	-3.7939144	-4.4870831
H	-1.4529103	-3.9046153	-5.1261455
H	-2.7903920	-4.7841103	-4.3740494
H	-3.0564608	-3.1531823	-5.0041705
C	-0.9124579	-4.1195697	-2.4256990
H	-0.0610799	-4.3207856	-3.0836994
H	-0.5386027	-3.6433713	-1.5126351
H	-1.3654513	-5.0775329	-2.1477005
C	-3.3247604	2.0649557	-3.2299192
H	-3.3603905	2.6297279	-4.1691510
H	-4.2669581	2.2335919	-2.6971801
H	-2.5218959	2.4887830	-2.6182217
C	-1.7128684	-0.0313895	-4.8280489
H	-1.7633975	0.7226372	-5.6225142
H	-0.7212120	0.0279025	-4.3687050
H	-1.8040690	-1.0169738	-5.2960397
C	-4.6631104	-0.5233562	-4.1916596
H	-4.9345659	-0.0370647	-5.1375146
H	-4.5608519	-1.5959869	-4.3818447
H	-5.4962398	-0.3929530	-3.4947352

2-C

E(TPSS-D3/def2-TZVP) = -5465.430474507 (conv)
Lowest Freq. =   12.13 cm^-1
178
1-C (004-S/c8/tpss-d3.def2-TZVP)

Si	0.6822789	-1.7939532	0.3975774
Si	-1.0941288	-0.7115477	1.3924379
Si	-0.6190215	1.7552168	0.6192680
Si	1.2633729	0.6074591	1.2953122
Si	1.1008432	-0.0735950	-1.0637938
Si	-1.2253578	0.1515711	-0.9086861
Si	2.5336993	-4.2982348	0.4556954
Si	-2.4370063	4.2362943	1.1110462
Si	2.0536024	1.8629478	-3.2341112
Si	-2.4493965	-1.6087892	-3.0942158
N	1.4525589	-3.1179584	1.2265691
N	-1.2726450	3.0043213	1.6427843
N	2.2775994	0.3804883	-2.2786071
N	-2.5466279	-0.2111368	-1.9995679
C	0.9495654	-3.3635716	2.5667752
C	-0.1915595	-4.1767326	2.7532723
C	-0.6235242	-4.4359469	4.0584061
H	-1.4977078	-5.0640169	4.2106366
C	0.0370271	-3.9010402	5.1577025
H	-0.3095868	-4.1180566	6.1643401
C	1.1319996	-3.0672724	4.9582758
H	1.6310319	-2.6254918	5.8161105
C	1.6003313	-2.7716717	3.6739029

C	-0.9785881	-4.7702392	1.5950682
H	-0.5286207	-4.4134904	0.6638547
C	-0.9213352	-6.3084847	1.5968429
H	-1.4583035	-6.7110327	0.7303544
H	0.1091649	-6.6738184	1.5627025
H	-1.3886495	-6.7124402	2.5019025
C	-2.4414901	-4.2956473	1.6136149
H	-2.9805336	-4.6998418	0.7497713
H	-2.9557838	-4.6318784	2.5207909
H	-2.4923188	-3.2026861	1.5790426
C	2.7724156	-1.8172614	3.5131124
H	2.7878828	-1.5019785	2.4647345
C	4.1202660	-2.4919966	3.8244563
H	4.9371300	-1.7694569	3.7154888
H	4.1351096	-2.8723994	4.8523135
H	4.3168889	-3.3298390	3.1510092
C	2.6051979	-0.5555278	4.3759239
H	1.6331379	-0.0845620	4.2061973
H	2.6988693	-0.7841035	5.4438581
H	3.3814190	0.1739282	4.1212626
C	1.6319742	-5.1749640	-0.9470571
H	2.3436009	-5.7044019	-1.5927767
H	0.9187307	-5.9115165	-0.5633012
H	1.0770283	-4.4715853	-1.5756693
C	3.0323889	-5.5837182	1.7295570
H	3.6270787	-6.3643912	1.2381846
H	3.6330804	-5.1665278	2.5423501
H	2.1583535	-6.0626988	2.1819013
C	4.0224185	-3.3816464	-0.2104475
H	4.7031125	-4.0586371	-0.7400698
H	3.7292085	-2.5969896	-0.9163960
H	4.5844803	-2.9023006	0.5980806
C	-0.6022281	3.1446276	2.9234860
C	-1.1112274	2.4641073	4.0538456
C	-0.4819104	2.6582285	5.2877561
H	-0.8694303	2.1457014	6.1636527
C	0.6337159	3.4790013	5.4126451
H	1.1056803	3.6175322	6.3814819
C	1.1528572	4.1025830	4.2845883
H	2.0415731	4.7220798	4.3745560
C	0.5584550	3.9450747	3.0280061
C	-2.3007971	1.5216816	3.9679756
H	-2.4505260	1.2899333	2.9084318
C	-2.0350483	0.1965960	4.7012486
H	-2.8424352	-0.5125974	4.4902283
H	-1.0955238	-0.2570049	4.3738230
H	-1.9916390	0.3401943	5.7870527
C	-3.5937124	2.1660740	4.4991336
H	-4.4230015	1.4521525	4.4381921
H	-3.4758673	2.4649490	5.5470735
H	-3.8677720	3.0536776	3.9234007
C	1.1967956	4.6317737	1.8304716
H	0.6331630	4.3454541	0.9374825
C	2.6493657	4.1677368	1.6299991
H	3.0779178	4.6426273	0.7407820
H	3.2731536	4.4352600	2.4901176
H	2.6927511	3.0811889	1.5031753

C	1.1448932	6.1648458	1.9598102
H	1.5689322	6.6374819	1.0665287
H	0.1195174	6.5245696	2.0850309
H	1.7244289	6.4999751	2.8273159
C	-2.7618679	5.4160707	2.5347289
H	-3.3990562	6.2373273	2.1823190
H	-3.2675030	4.9372236	3.3775004
H	-1.8330545	5.8519569	2.9159540
C	-4.0035623	3.3678283	0.5703633
H	-4.7417760	4.0808631	0.1846667
H	-3.8071327	2.6403757	-0.2249658
H	-4.4615650	2.8261158	1.4047563
C	-1.7164112	5.2258913	-0.3212010
H	-2.5018521	5.7985389	-0.8298143
H	-0.9591224	5.9355083	0.0273850
H	-1.2460691	4.5780283	-1.0674792
C	3.5721159	-0.2667944	-2.3535696
C	3.7956186	-1.2245815	-3.3704121
C	5.0564284	-1.8163610	-3.4785976
H	5.2325197	-2.5544526	-4.2557662
C	6.0895070	-1.4735434	-2.6118632
H	7.0645025	-1.9429235	-2.7088759
C	5.8628565	-0.5266548	-1.6221022
H	6.6698602	-0.2531758	-0.9474355
C	4.6155990	0.0921050	-1.4721117
C	2.6784927	-1.6469528	-4.3069224
H	1.9464530	-0.8345162	-4.3270568
C	3.1427816	-1.8958871	-5.7483215
H	2.2736301	-2.0724727	-6.3912540
H	3.6949764	-1.0370205	-6.1440101
H	3.7893102	-2.7772282	-5.8227991
C	1.9784604	-2.8888345	-3.7300723
H	1.1775177	-3.2357639	-4.3908819
H	2.6975181	-3.7042388	-3.5980399
H	1.5434088	-2.6586355	-2.7517106
C	4.4540680	1.1341480	-0.3784545
H	3.4012494	1.4367402	-0.3541944
C	5.3052166	2.3847594	-0.6625761
H	5.0286865	2.8515071	-1.6125574
H	5.1714316	3.1234405	0.1346575
H	6.3691259	2.1269952	-0.7125869
C	4.8040418	0.5528069	1.0009971
H	4.5922455	1.2854022	1.7868314
H	4.2124076	-0.3432306	1.2059965
H	5.8651562	0.2850985	1.0602883
C	0.5715268	1.6968629	-4.3711434
H	0.3661369	2.6552535	-4.8634132
H	0.7372190	0.9466070	-5.1507477
H	-0.3246076	1.4103078	-3.8126443
C	3.5921893	2.1158976	-4.2779436
H	3.4937303	3.0465660	-4.8508965
H	4.5054611	2.1792412	-3.6795346
H	3.7235114	1.2951237	-4.9913673
C	1.7529080	3.3222343	-2.0889756
H	1.5564956	4.2377611	-2.6604813
H	0.8791527	3.1313164	-1.4524525
H	2.6047902	3.5069700	-1.4279393

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C    -3.8385352    0.4308183   -1.8585948
C    -4.1858605    1.4664629   -2.7576145
C    -5.4484340    2.0559546   -2.6573832
H    -5.7179943    2.8549353   -3.3419256
C    -6.3653970    1.6355542   -1.6990449
H    -7.3445051    2.1021455   -1.6357269
C    -6.0180041    0.6139380   -0.8254181
H    -6.7337637    0.2813606   -0.0782673
C    -4.7635518   -0.0056975   -0.8845659
C    -3.1944915    1.9739232   -3.7888360
H    -2.4707892    1.1732909   -3.9663242
C    -3.8354421    2.3340518   -5.1359547
H    -4.4337727    1.5048687   -5.5278043
H    -4.4853314    3.2125202   -5.0573589
H    -3.0534865    2.5698335   -5.8660240
C    -2.4274229    3.1717514   -3.2042367
H    -1.8727907    2.8667246   -2.3104904
H    -1.7160309    3.5795750   -3.9295289
H    -3.1241635    3.9661111   -2.9163059
C    -4.4676132   -1.1295887    0.0938528
H    -3.4210473   -1.4254751   -0.0390766
C    -5.3514633   -2.3600179   -0.1782305
H    -5.1217052   -3.1572213    0.5364484
H    -6.4125653   -2.1061786   -0.0753911
H    -5.1969152   -2.7503445   -1.1884992
C    -4.6395727   -0.6611857    1.5480940
H    -4.3329600   -1.4519439    2.2406212
H    -4.0242828    0.2200575    1.7475198
H    -5.6840264   -0.4063535    1.7610333
C    -1.1327452   -1.3350117   -4.4016619
H    -0.9998313   -2.2458667   -4.9981317
H    -1.3991688   -0.5218328   -5.0843445
H    -0.1683414   -1.0905325   -3.9467740
C    -1.9978853   -3.1504760   -2.1191784
H    -1.8719690   -4.0143857   -2.7834079
H    -1.0507645   -2.9978138   -1.5856911
H    -2.7576148   -3.3997537   -1.3725696
C    -4.1122336   -1.7966708   -3.9430701
H    -4.0894520   -2.6790976   -4.5949322
H    -4.9387296   -1.9160184   -3.2368603
H    -4.3368165   -0.9246697   -4.5666986
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2-D = ent-2-A

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E(TPSS-D3/def2-TZVP) = -5465.431298014 (conv)
Lowest Freq. =    20.86 cm^-1
178
2-D (004-S/c14/tpss-d3.def2-TZVP)
Si    1.0080671   -1.6253674    0.3258208
Si   -1.1419777   -0.5557970    1.2598337
Si   -0.8620095    1.6300160    0.5862073
Si    1.4211473    0.5246230    1.0452476
Si    0.5532644    1.0353199   -1.1496943
Si   -0.7034582   -0.9478835   -1.0826977
Si    1.8392774   -4.6498002    0.7368388
Si   -1.5913427    4.6257904    1.2985212
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Si	0.9813850	2.9128835	-3.5963276
Si	-1.5921155	-2.7082293	-3.4938847
N	1.6726946	-2.9571642	1.2368184
N	-1.3407669	2.9105236	1.6707641
N	1.5791330	1.8924977	-2.2787706
N	-1.9267871	-1.7508442	-2.0425295
C	2.3204126	-2.5355110	2.4691336
C	1.5968771	-2.5638040	3.6829332
C	2.2642446	-2.2133914	4.8614677
H	1.7218874	-2.2402216	5.8026318
C	3.5974314	-1.8182012	4.8498201
H	4.0959231	-1.5489326	5.7769765
C	4.2807162	-1.7460142	3.6412057
H	5.3140889	-1.4092062	3.6277213
C	3.6628304	-2.0917749	2.4349399
C	0.1254484	-2.9450288	3.7501480
H	-0.2543642	-2.9666531	2.7236345
C	-0.0817618	-4.3390960	4.3696194
H	-1.1506528	-4.5779998	4.4120678
H	0.4185558	-5.1200647	3.7908849
H	0.3142558	-4.3715061	5.3910820
C	-0.6933672	-1.9020531	4.5294458
H	-1.7613662	-2.1331586	4.4551797
H	-0.4248005	-1.8944591	5.5920551
H	-0.5406975	-0.8963477	4.1298945
C	4.4538892	-1.9607368	1.1415350
H	3.7732712	-2.1700281	0.3097912
C	5.6128026	-2.9720643	1.0733900
H	6.1537157	-2.8642140	0.1262952
H	6.3229623	-2.8005438	1.8902540
H	5.2580678	-4.0036665	1.1497250
C	4.9939172	-0.5343528	0.9492358
H	4.1831459	0.1997524	0.9877911
H	5.7230484	-0.2774260	1.7259938
H	5.4849133	-0.4429318	-0.0237645
C	0.1341438	-5.4034339	0.5355660
H	0.1987064	-6.4347923	0.1680317
H	-0.4094655	-5.4132920	1.4857447
H	-0.4592303	-4.8314565	-0.1832292
C	2.8067038	-5.5768478	2.0507605
H	2.9190993	-6.6240469	1.7419761
H	3.8074176	-5.1593175	2.1946247
H	2.3078141	-5.5644349	3.0237505
C	2.7649281	-4.7549790	-0.8957650
H	2.7956125	-5.7922057	-1.2521331
H	2.2871402	-4.1541756	-1.6752126
H	3.7967232	-4.4033291	-0.7932069
C	-1.7481582	2.4237271	2.9797995
C	-3.0750381	1.9749063	3.1752365

C	-3.4576887	1.5656248	4.4568090
H	-4.4766012	1.2238641	4.6197730
C	-2.5602498	1.5811285	5.5184156
H	-2.8775549	1.2631899	6.5077901
C	-1.2469272	1.9827718	5.3003136
H	-0.5381626	1.9660481	6.1237541
C	-0.8102840	2.3952514	4.0368001
C	-4.0947439	1.9037677	2.0477405
H	-3.5814036	2.1589380	1.1149422
C	-4.6652634	0.4852356	1.8885854
H	-5.3299913	0.4390057	1.0212963
H	-3.8635991	-0.2443586	1.7378063
H	-5.2367577	0.1850976	2.7741957
C	-5.2429518	2.9096870	2.2487179
H	-5.9519314	2.8462543	1.4153154
H	-5.7880577	2.6925710	3.1741890
H	-4.8770109	3.9383926	2.3094967
C	0.6492554	2.7808345	3.8473342
H	0.8308174	2.8570070	2.7703913
C	1.5949295	1.7040104	4.4055638
H	2.6313328	1.9449703	4.1459417
H	1.5289390	1.6399577	5.4977644
H	1.3663930	0.7193835	3.9899061
C	0.9739993	4.1424178	4.4883697
H	2.0332445	4.3843282	4.3441022
H	0.3785599	4.9495361	4.0533366
H	0.7743959	4.1203012	5.5658578
C	-2.2917951	5.4774504	2.8170608
H	-1.6208701	5.4137410	3.6781552
H	-2.4528733	6.5394806	2.5918457
H	-3.2510806	5.0488624	3.1212551
C	-2.8060540	4.8109393	-0.1242084
H	-2.8974801	5.8652737	-0.4137847
H	-2.4855898	4.2541622	-1.0097529
H	-3.8023818	4.4496968	0.1509069
C	0.0484660	5.3987181	0.8193021
H	-0.0803232	6.4474904	0.5253009
H	0.7615741	5.3620107	1.6490287
H	0.4930330	4.8687574	-0.0277676
C	3.0126141	1.7144204	-2.1434960
C	3.6559192	0.6881808	-2.8695751
C	5.0508427	0.5997464	-2.8227218
H	5.5514846	-0.1823944	-3.3882965
C	5.8035103	1.4909936	-2.0658975
H	6.8872562	1.4156777	-2.0470795
C	5.1555573	2.4628010	-1.3112182
H	5.7411297	3.1410837	-0.6962998
C	3.7622551	2.5875826	-1.3233637
C	2.8738048	-0.3402937	-3.6672656

H	1.8170839	-0.0646460	-3.5998794
C	3.2667353	-0.3674633	-5.1531294
H	2.6532234	-1.0971522	-5.6933853
H	3.1262712	0.6108130	-5.6222326
H	4.3170685	-0.6527064	-5.2786796
C	3.0332273	-1.7339519	-3.0391422
H	2.4325628	-2.4722951	-3.5819983
H	4.0784450	-2.0616466	-3.0618942
H	2.7027532	-1.7218494	-1.9951786
C	3.1075581	3.6619287	-0.4713807
H	2.0285086	3.4780041	-0.4943644
C	3.3727978	5.0686309	-1.0377468
H	3.0049992	5.1667550	-2.0628259
H	2.8787704	5.8277407	-0.4216826
H	4.4478154	5.2815365	-1.0456276
C	3.5668609	3.5913140	0.9943425
H	3.0300594	4.3366737	1.5904647
H	3.3676398	2.6032437	1.4208664
H	4.6387410	3.7980297	1.0871848
C	-0.1495750	1.9202060	-4.7188928
H	-0.6426914	2.5749046	-5.4481767
H	0.3991046	1.1518476	-5.2721127
H	-0.9327254	1.4179036	-4.1417572
C	2.4465915	3.5508558	-4.5797377
H	2.0899117	4.2233563	-5.3700570
H	3.1563580	4.1055295	-3.9588222
H	2.9998874	2.7356198	-5.0558211
C	-0.0129757	4.3381572	-2.8863570
H	-0.5215863	4.8988052	-3.6802498
H	-0.7801634	3.9599464	-2.2025944
H	0.6141859	5.0393483	-2.3272632
C	-3.3091473	-1.5848122	-1.6346196
C	-4.0703290	-0.5263014	-2.1773530
C	-5.4314933	-0.4446996	-1.8669064
H	-6.0241075	0.3625764	-2.2904805
C	-6.0355087	-1.3747353	-1.0279786
H	-7.0962623	-1.3037237	-0.8038355
C	-5.2645250	-2.3811928	-0.4566977
H	-5.7295309	-3.0914342	0.2218286
C	-3.8987016	-2.5009131	-0.7344646
C	-3.4448427	0.5417090	-3.0570586
H	-2.3972936	0.2629955	-3.2063271
C	-4.1127672	0.6452388	-4.4375797
H	-4.0742486	-0.3079557	-4.9733065
H	-5.1647250	0.9375794	-4.3470202
H	-3.6050646	1.4009417	-5.0473646
C	-3.4682337	1.9012202	-2.3404637
H	-2.9436383	1.8358690	-1.3812936
H	-2.9763222	2.6670884	-2.9504909

H	-4.4955134	2.2282217	-2.1454185
C	-3.1043051	-3.6159463	-0.0752375
H	-2.0473049	-3.4297998	-0.2914598
C	-3.4830524	-4.9926016	-0.6511268
H	-2.8861458	-5.7810504	-0.1799482
H	-4.5412881	-5.2074044	-0.4641481
H	-3.3185734	-5.0374905	-1.7311620
C	-3.2792180	-3.6203882	1.4523701
H	-2.6472802	-4.3956244	1.8986706
H	-2.9934943	-2.6556536	1.8829062
H	-4.3164461	-3.8316313	1.7347162
C	-0.6753067	-1.6673793	-4.7591651
H	-0.3359912	-2.2895324	-5.5967612
H	-1.3059831	-0.8704146	-5.1651771
H	0.2087477	-1.1979667	-4.3155799
C	-0.5001896	-4.1682816	-3.0474871
H	-0.1520663	-4.6902613	-3.9472025
H	0.3836496	-3.8249619	-2.4994288
H	-1.0213530	-4.8945379	-2.4164194
C	-3.2200817	-3.2947325	-4.2196937
H	-3.0218414	-3.9270829	-5.0943279
H	-3.8088581	-3.8787316	-3.5063318
H	-3.8431223	-2.4562283	-4.5458195

Silylene

E(TPSS-D3/def2-TZVP) = -2152.8492836 (conv)

Lowest Freq. = 14.00 cm^-1

Si	9.3849949	3.0384563	13.8422615
N	7.6295845	3.2652815	13.8282195
N	10.0321198	3.0660049	15.4849951
Si	6.2251028	2.8211070	14.8294026
Si	9.6202615	3.8235951	17.0397944
C	7.2730136	3.5767291	12.4402399
C	7.0031478	4.9194123	12.0967541
C	6.6439511	5.2215948	10.7809872
C	6.5642011	4.2238508	9.8130886
C	6.8536361	2.9092324	10.1567887
C	7.2088382	2.5566046	11.4646175
C	7.1665433	6.0222370	13.1286059
C	6.1647086	7.1734464	12.9728616
C	8.6157533	6.5411410	13.1007581
C	7.5407135	1.1017409	11.7638008
C	6.3928098	0.1452547	11.3961488
C	8.8358363	0.6814871	11.0435100
C	5.8080526	4.0343389	16.2103167
C	6.5227560	1.0948206	15.5185448
C	4.6889962	2.8037449	13.7461895
C	11.3908404	2.5223487	15.4277433
C	11.5918530	1.1624895	15.7485668
C	12.8878969	0.6409772	15.6983984
C	13.9669332	1.4386126	15.3304127
C	13.7554631	2.7731749	15.0033039

C	12.4774867	3.3422367	15.0463541
C	10.4139671	0.2606535	16.0769734
C	9.9411867	-0.4567948	14.7996493
C	10.7016722	-0.7414252	17.2029574
C	12.3034851	4.7988549	14.6405228
C	12.3923299	4.9467191	13.1084727
C	13.3242823	5.7350050	15.3101977
C	11.1846433	4.0751979	18.0485648
C	8.5180235	2.7446089	18.1250442
C	8.8645007	5.5044639	16.6677236
H	6.4283010	6.2504583	10.5081989
H	6.2840095	4.4733219	8.7933786
H	6.8050493	2.1339935	9.3963743
H	7.0018426	5.5685428	14.1105875
H	5.1342149	6.8032511	12.9552101
H	6.2660179	7.8706112	13.8117747
H	6.3367159	7.7425861	12.0527574
H	9.3256421	5.7217949	13.2755835
H	8.8487296	6.9735668	12.1215346
H	8.7737850	7.3052527	13.8700293
H	7.7168990	1.0139270	12.8403882
H	5.4670152	0.4016214	11.9197015
H	6.1875481	0.1676826	10.3203739
H	6.6629276	-0.8825930	11.6630175
H	9.6679245	1.3254136	11.3431411
H	9.0886895	-0.3561450	11.2896971
H	8.7148744	0.7548085	9.9566990
H	5.5662874	5.0222255	15.8015604
H	4.9053743	3.6619781	16.7134085
H	6.5771136	4.1640474	16.9715118
H	6.4053740	0.3496605	14.7234629
H	7.5322532	0.9837567	15.9244727
H	5.8091500	0.8502735	16.3145600
H	4.7781370	2.1382693	12.8841062
H	3.8329332	2.4703880	14.3474094
H	4.4607038	3.8047908	13.3640893
H	13.0530495	-0.4040998	15.9443853
H	14.9688479	1.0197192	15.2942628
H	14.5991135	3.3900679	14.7060740
H	9.5979076	0.9081741	16.4087449
H	9.6827478	0.2726244	14.0209033
H	11.0646904	-0.2329388	18.1023761
H	9.7865678	-1.2859387	17.4604995
H	11.4520741	-1.4828353	16.9077090
H	11.3006987	5.1122845	14.9491789
H	11.6399156	4.3263961	12.6119452
H	12.2360806	5.9914709	12.8158285
H	13.3819139	4.6342299	12.7554729
H	13.3318790	5.6236433	16.3985437
H	14.3394450	5.5403542	14.9476839
H	13.0846161	6.7771484	15.0720930
H	11.6989221	3.1285810	18.2445294
H	11.8960946	4.7464159	17.5612962
H	10.9137320	4.5188264	19.0157995
H	7.6266399	2.3520138	17.6339272
H	9.0948087	1.8921247	18.5029836
H	8.1895275	3.3259404	18.9967378

H	8.1399799	5.4575779	15.8512600
H	8.3629002	5.9326381	17.5434012
H	9.6596619	6.1961150	16.3652529
H	9.0606859	-1.0772558	15.0007397
H	10.7370654	-1.0950390	14.3999594

Silacyclopropene

E(TPSS-D3/def2-TZVP) = -2731.8837215 (conv)
Lowest Freq. = 8.97 cm^-1

Si	7.5874504	15.8512126	15.7792592
N	6.3585741	16.9294672	16.3361870
Si	9.4408225	14.8096166	15.9905851
Si	8.3358386	14.6277201	13.9953484
N	10.9106094	14.4539094	16.8267133
Si	6.5618771	17.9651172	17.7712746
C	4.9703448	18.9266645	18.0107337
C	8.0025309	19.1375143	17.4791555
C	6.9354063	16.8746962	19.2530903
Si	11.1609663	14.8281710	18.5491110
C	12.8768555	14.2384114	19.0208171
C	11.0173320	16.6831521	18.8079194
C	9.8274605	13.9532389	19.5432210
C	5.2159244	17.1106860	15.4568609
C	12.0082504	13.9759354	16.0040800
C	5.3243779	17.9292576	14.3152212
C	4.0107121	16.4447217	15.7701035
C	2.9111752	16.6301635	14.9290591
C	3.9359529	15.5072958	16.9637839
C	2.9985981	17.4425163	13.8002473
H	1.9743488	16.1303685	15.1558351
C	4.1959210	18.0794980	13.4991540
H	2.1336231	17.5735722	13.1560055
H	4.2626713	18.7080796	12.6148568
C	6.6081838	18.6558363	13.9487876
H	4.6510773	15.8714166	17.7088920
C	6.4163422	20.1821474	14.0118852
C	7.1285639	18.2236313	12.5675396
H	7.3713583	18.3853648	14.6860234
H	5.6811964	20.5144004	13.2704745
H	7.3620526	20.6951874	13.8042333
H	6.0610617	20.4975092	14.9983082
H	7.3012084	17.1430453	12.5369214
H	8.0751825	18.7284784	12.3445567
H	6.4134004	18.4786352	11.7775512
H	4.7203975	19.5170770	17.1228505
H	4.1216915	18.2676163	18.2204926
H	8.8888952	18.5848508	17.1447697
H	8.2710580	19.6755678	18.3964903
H	7.7650586	19.8803277	16.7101596
H	6.0934946	16.2160368	19.4936311
H	7.1569390	17.4805658	20.1400969
H	7.8070349	16.2421702	19.0539515
C	12.3284521	12.6009971	16.0187589
C	12.7254146	14.8857130	15.2009089
C	13.3956594	12.1594222	15.2328610

C	11.4924892	11.6205530	16.8239467
C	14.1220343	13.0467536	14.4416515
H	13.6599485	11.1062697	15.2340762
C	13.7828618	14.3941386	14.4257112
H	14.9474677	12.6845181	13.8351369
H	14.3466424	15.0830245	13.8018548
C	12.3962943	16.3693832	15.1546395
C	10.3041808	11.1216702	15.9787233
C	12.2984030	10.4396499	17.3814879
H	11.0738650	12.1693660	17.6735753
H	12.6496103	9.7757341	16.5840490
H	11.6681908	9.8420180	18.0487777
H	13.1720219	10.7814691	17.9467605
H	9.6909570	11.9574574	15.6247936
H	9.6661228	10.4528411	16.5675178
H	10.6648004	10.5744164	15.1007193
C	13.5627759	17.2134403	15.6991337
C	12.0044900	16.8150591	13.7353680
H	11.5311915	16.5439408	15.8033017
H	12.8342151	16.6753304	13.0335568
H	11.7330808	17.8767487	13.7332798
H	11.1466754	16.2406968	13.3720743
H	13.8290763	16.9106493	16.7171880
H	13.2923379	18.2752429	15.7134828
H	14.4544427	17.0994964	15.0727107
H	12.9841157	13.1541865	18.9163297
H	13.0826385	14.4984967	20.0665020
H	13.6455822	14.7094220	18.3985834
H	8.8351746	14.1598379	19.1246634
H	9.8260750	14.2891849	20.5871810
H	9.9680899	12.8664981	19.5382051
H	11.8134933	17.2242225	18.2853906
H	11.0763483	16.9398584	19.8728053
H	10.0579730	17.0509686	18.4284892
C	2.5522896	15.4639871	17.6255499
C	4.3909008	14.0931230	16.5538364
H	3.7154708	13.6804944	15.7961945
H	4.3938441	13.4218422	17.4202035
H	5.4009338	14.1078433	16.1285806
H	2.1992954	16.4685935	17.8818207
H	2.5984605	14.8699747	18.5446467
H	1.8051178	14.9980235	16.9738003
H	5.0781548	19.6168519	18.8566438