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Supporting Information

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Conversion of a Singlet Silylene to a stable Biradical**

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Content:

(S1) Synthesis

All reactions and handling of reagents were performed under an atmosphere of dry nitrogen or argon using standard Schlenk techniques or a glove box where the O_2 and H_2O levels were usually kept below 1 ppm. Ligand L^1: and L:$SiCl_2$ were prepared according to literature methods.[S1,S2] Solvents were purified with the M-Braun solvent drying system. Solution NMR spectra were recorded on Bruker Avance 200, Bruker Avance 300, and Bruker Avance 500 MHz NMR spectrometers. Deuterated NMR solvent C_6D_6 was dried by stirring for 2 days over Na/K alloy followed by distillation in vacuum and degassed. EI-MS spectra were obtained with a Finnigan MAT 8230 or a Varian MAT CH5 instrument (70 eV) by EI-MS methods. Elemental analyses were performed by the Analytisches Labor des Instituts für Anorganische Chemie der Universität Göttingen. Melting points were measured in sealed glass tubes on a Büchi B-540 melting point apparatus.

Synthesis of polymorph II of **L^1:$_2$SiCl$_2$ (2)**: A molar mixture (3:1) of L^1: (6 mmol) and L:$SiCl_2$ (**1**) (2 mmol) was given into a 50 mL round bottom flask. After addition of THF (10 mL) at room temperature to the colorless mixture, an immediate color change to dark blue was observed. Stirring continued for two to five minutes and microcrystalline blue-black crystals of **2** were formed. From the filtrate dark blue-black blocks of **2** were grown after storing the solution for one week in a freezer. Yield is 91%. Elemental analysis found % (cal.) for $C_{40}H_{62}Cl_2N_2Si$; C 70.05 (71.71), H 9.32 (9.33), N 3.94 (4.18). Melting point 179-181 °C, decomposition point 185-186 °C, UV λ_{ab} = 569 nm. ^{1}H (298 °C, THF-d_8, δ ppm, 500.133 MHz): 7.12 (m, 2H, *m*-H_{ar}), 7.09 (m, 2H, *m*-H_{ar}), 7.04 (m, 2H, *p*-H_{ar}), 3.59 (m, 2H, $CHMe_2$), 3.43 (m, 2H, $CHMe_2$), 1.89 (S, 6H, $NCMe_2$), 1.85 (d, 2H, CH_2), 1.69 (S, 6H, $NCMe_2$), 1.65 (d, 2H, CH_2), 1.57 (s, 6H, CMe_2), 0.85 (s, 6H, CMe_2), 1.50 (d, 6H, $CHMe_2$), 1.39 (d, 6H, $CHMe_2$), 1.29 (d, 6H, $CHMe_2$), 1.14 (d, 6H, $CHMe_2$); ^{13}C (δ ppm): 210.0 (C), 143.3, 127.5, 127.1, 125.5, 124.1, 73.5, 67.7, 58.4, 30.2, 29.1, 28.5, 27.7, 27.3, 26.3, 26.0, 25.4, 25.1; ^{29}Si NMR (δ ppm) 4.13.

Synthesis of **L^1:$_2$SiCl$_2$ (2)** enriched with polymorph I: The reaction mixture of L:$SiCl_2$ (**1**) (488 mg, 1 mmol) and L^1: (855 mg, 3 mmol) in 1:3 molar ratio in THF (5 mL) at room temperature turns immediately to a drak blue solution which was stirred for 2-3 minutes. This solution was stored at 0 °C in a freezer. After two days very small dark blue-black crystals were obtained. Then this small amount of mall dark blue-black crystals was seperated by carefully turning the flask horrizonetally. After 7-10 days blue blocks of **2** enriched with polymorph I were obtained. NMR data is identical as obtained for polymorph II. Melting point 167-168 °C, decomposition point 172-173 °C.

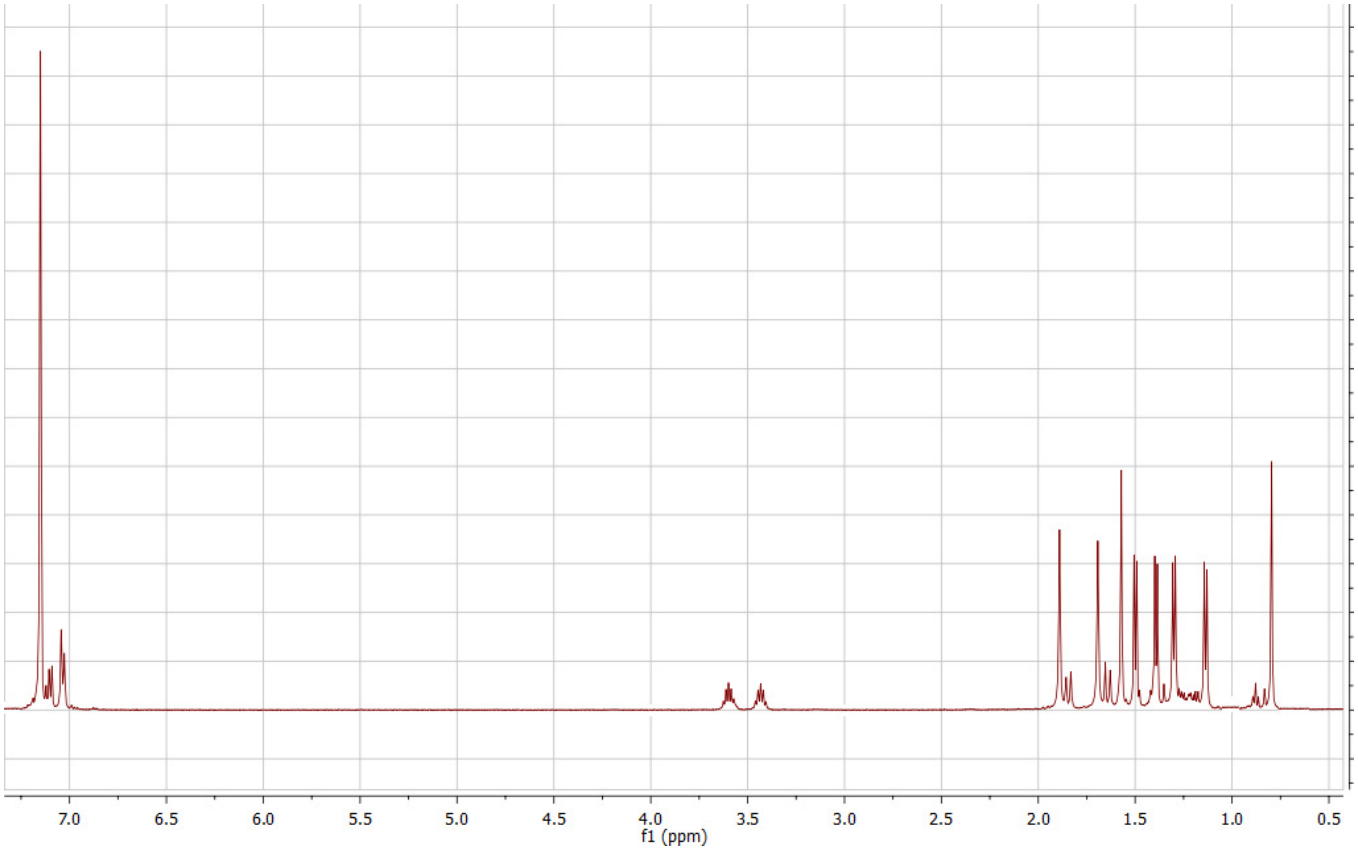


Figure S1. ^{1}H spectra of compound **2** in C_6D_6.

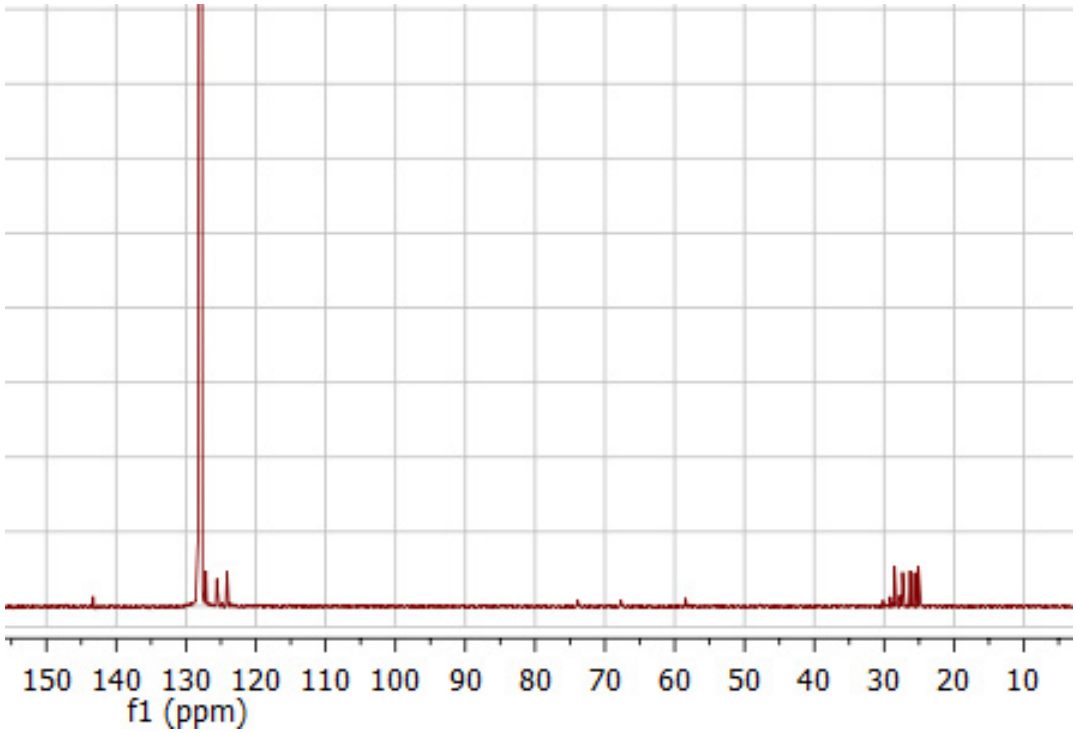


Figure S2. ^{13}C spectra of compound **2** in C_6D_6.

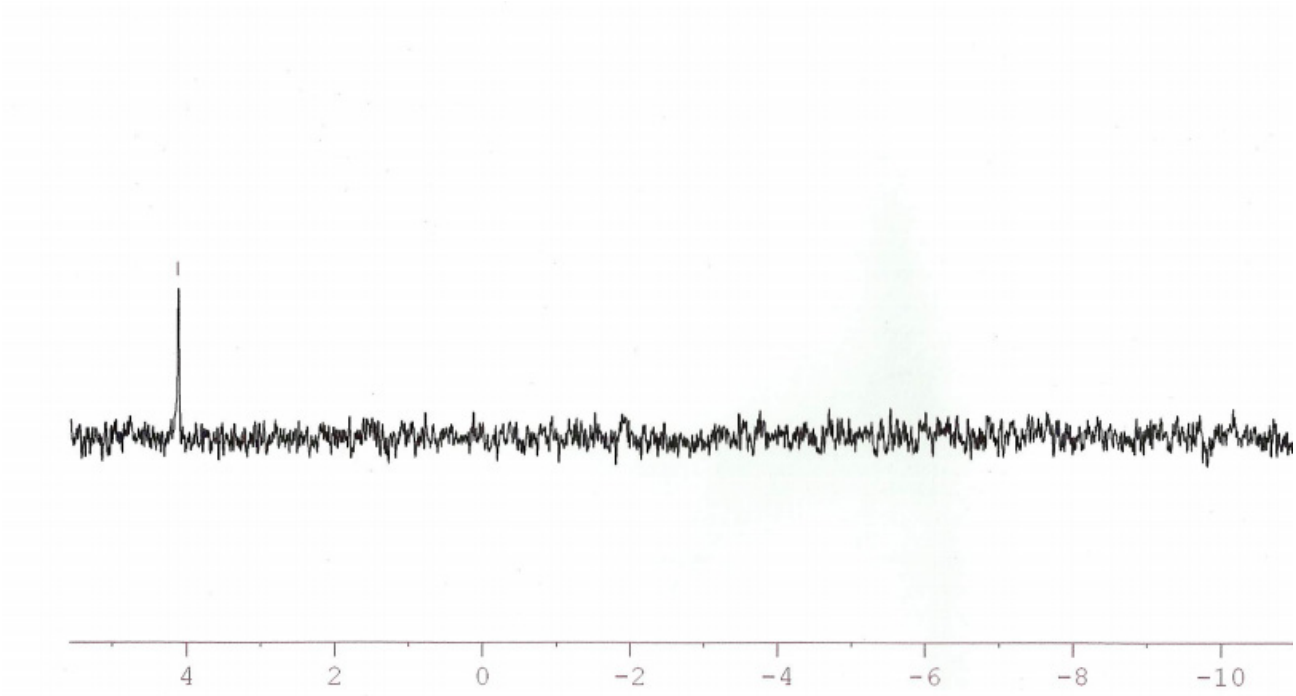


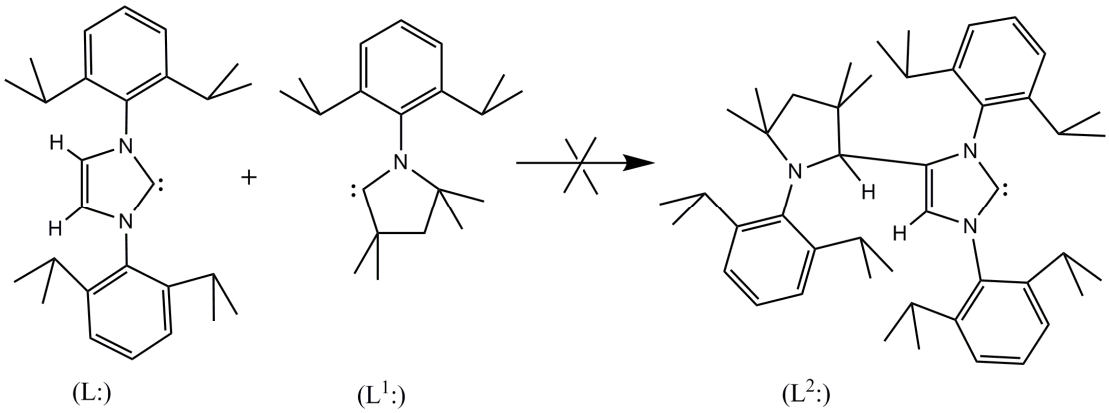
Figure S3. ^{29}Si spectra of compound **2** in THF-d_8.

Synthesis of **3**: After the separation crystals of **2** through filtration, the filtrate was dried and extracted with *n*-hexane (30 mL) and the resulting volume was reduced to 5-7 mL which produced colorless crystals of **3**.

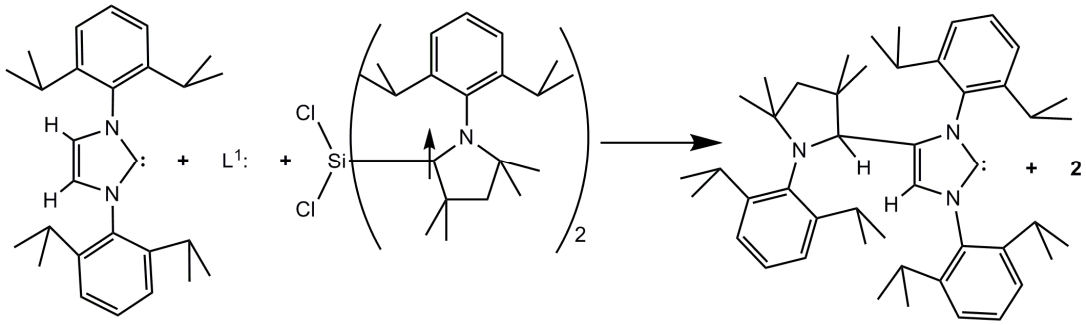
Alternative synthesis of **3**: When the mixture of **2** and L: was reacted in THF-d_8 in molar ratios of 1:1 and 1:2 it produces **3** after a week. For the former ratio 50% conversion into **3** and for latter complete conversion were observed in the NMR tube.

^{1}H (298 °C, C_6D_6, δppm, 300.13 MHz): 7.36-7.31 (m, 3H, H_{ar}), 7.30 (s, 1H, $H_{imidazole}$), 7.18-7.12 (m, 3H, H_{ar}), 7.15-6.98 (m, 3H, H_{ar}), 4.32 (s, 1H, C-H of L^1:H), 3.89 (m, 2H, $CHMe_2$ of L^1:H), 3.59 (m, 2H, $CHMe_2$ of NHC), 3.01 (m, 2H, $CHMe_2$ of NHC), 1.52 (d, 6H, $CHMe_2$), 1.46 (s, 2H, CH_2), 1.40 (d, 6H, $CHMe_2$), 1.34 (d, 6H, $CHMe_2$), 1.26 (d, 3H, $CHMe_2$), 1.22 (s, 6H, $NCMe_2$), 1.19 (d, 3H, $CHMe_2$), 1.12 (d, 3H, $CHMe_2$), 1.07 (d, 3H, $CHMe_2$), 0.95 (d, 3H, $CHMe_2$), 0.91 (d, 3H, $CHMe_2$) 0.74 (s, 3H, CMe_2), 0.57 (d, 3H, CMe_2); ^{13}C (δppm): 220.0 (C), 151.6, 148.1, 147.1, 146.7, 146.0, 143.6, 139.2, 138.7, 137.7, 128.9, 128.6, 128.3, 127.6, 127.0, 125.8, 124.4, 124.1, 124.1, 123.7, 123.1, 121.6, 73.0, 67.7, 63.5, 59.9, 43.6, 33.2, 31.9, 30.4, 29.6, 29.3, 28.5, 28.4, 27.95, 27.93, 27.9, 27.0, 25.7, 25.5, 25.4, 24.9, 24.7, 23.8, 23.1, 21.8, 20.0; EI MS 673.53.

Compound **3** plausibly resulted from the C-H activation of one of the ring protons imidazole carbene by CAAC carbene. To prove that, an independent reaction of L: and L^1: in benzene was carried out which does not produce **3**. Thus it could be proposed that the compound **2** reacts with L: to produce L^2 (**3**) as shown in Scheme S2.



Scheme S1. The reaction between L: with L^1: does not produce L^3: (**3**).



Scheme S2. Proposed reaction for the formation of L^2: (**3**).

(S2) UV-visible spectroscopy

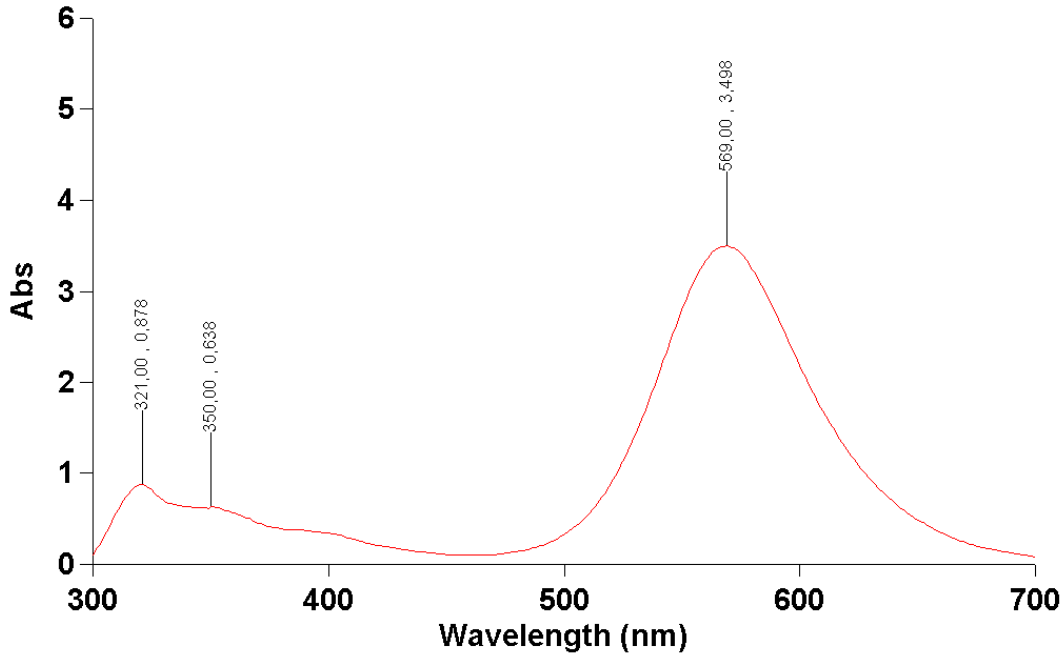


Figure S1. UV-visible spectrum of compound **2** in *n*-hexane (of 3.36 mM solution). The molar extinction coefficient ε = 10411 L mol^{-1} cm^{-1}.

(S3) Magnetic Measurements

Magnetic susceptibility measurements. Temperature-dependent magnetic susceptibility measurements on compound **2** were carried out with a *Quantum-Design* MPMS-XL-5 SQUID magnetometer equipped with a 5 Tesla magnet in the range from 295 to 2.0 K at a magnetic field of 0.5 T. The powdered sample was contained in a gel bucket and fixed in a non-magnetic sample holder. Each raw data file for the measured magnetic moment was corrected for the diamagnetic contribution of the sample holder and the gel bucket. The molar susceptibility data were corrected for the diamagnetic contribution. Both the samples were prepared under an atmosphere of dry nitrogen using standard Schlenk techniques or a glove box where the O_2 and H_2O levels were usually kept below 1 ppm. Temperature-independent paramagnetism (*TIP*) and a Curie-behaved paramagnetic contribution (*PI*) with spin $S = 1/2$ were included according to $\chi_{calc} = (1 - PI)\cdot\chi + PI\cdot\chi_{mono} + TIP$.[S3]

(a) Magnetic measurement was performed on 29.0 mg powder sample of polymorph II of **2** which was synthesized at room temperature in 1:2 molar ratio of **1** and L^1:. Paramagnetic contribution was found to be 0.9 % using above equation suggesting 0.45 % of polymorph I as a paramagnetic component.

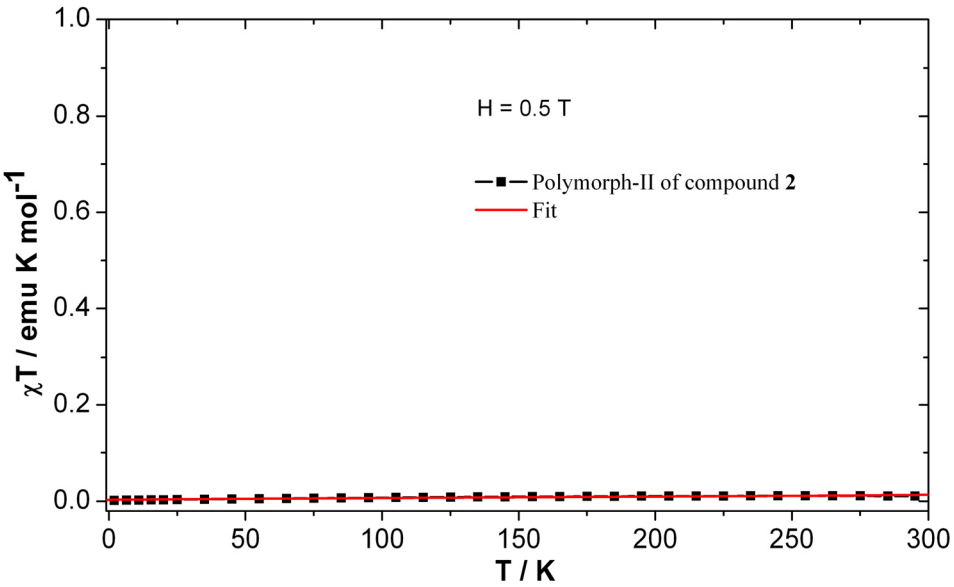


Figure S1. χT vs T plot of polymorph II of compound **2**. Red line (paramagnetic contribution) represents fitting with above mentioned equation.

```
Spin 1 = 0.0
_var_____________value__ifit_________
   g1                   0.000
   D1                   0.000
E/D1                    0.000
-----------------------------------------
PI [%] (S=0.5)           0.9
TIP [1e-6 emu]          32.4   (subtracted)
T_W [K]                 0.000   TW_TIP [K]=      0.000
-------------------------------   fsum =    0.1018E-02
m[mg]=29.00;   M[g/mol]= 669.00;   chi(dia)= -335.0;   B-fields:  1
B[T]=    0.500
powder average: Lebedev grid  16pts   high_precission
efil:   C:\julx_v141\12_KM4.rso.dat
-----------------------------------------
holder:     _file: none
Kapsel       25.60mg,  d:-0.120E-03,  s:  0.000E+00,  p:  0.000E+00
-----------------------------------------
```

(b) Magnetic measurement was performed on 12.9 mg powder sample enriched with polymorph I of **2** which was crystallized at 0 °C refrigerator in 1:3 molar ratio of **1** and L^1:. Paramagnetic contribution was found to be 16.4 % using above equation.

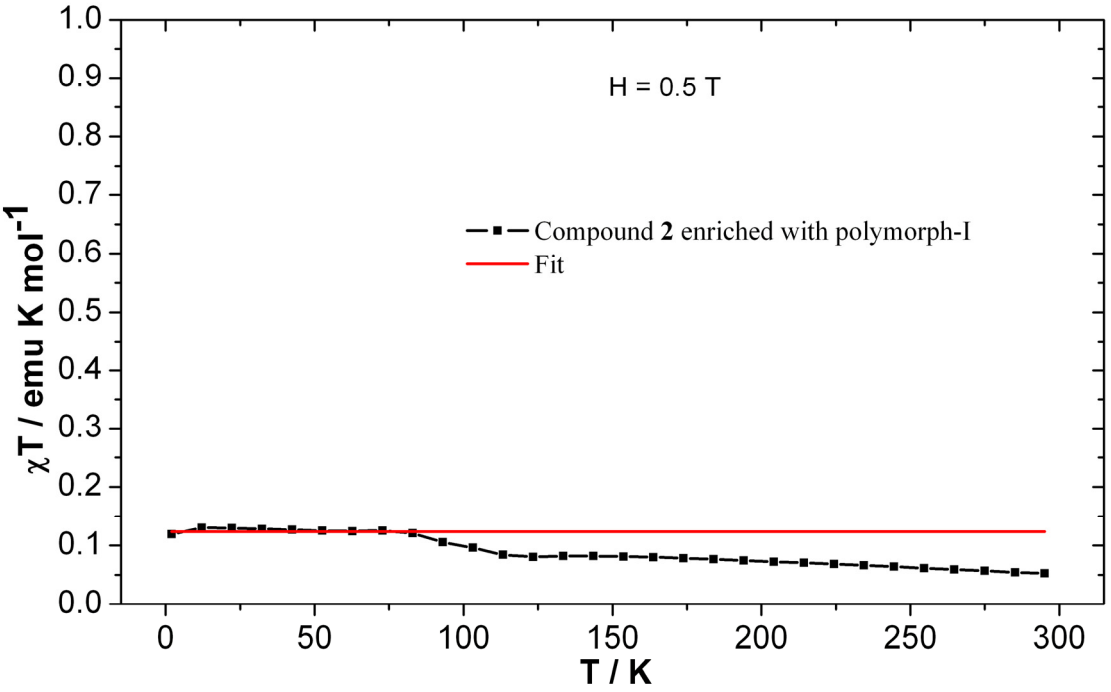


Figure S2. χT vs T plot of compound **2** enriched with polymorph I. Red line (paramagnetic contribution) represents fitting with above mentioned equation.

```
Spin 1 = 0.0
_var_____________value__ifit_________
   g1                   2.000    0
   D1                   0.000    0
E/D1                    0.000    0
-----------------------------------------
PI [%] (S=1.0)           12.3
TIP [1e-6 emu]           0.0   (subtracted)
T_W [K]                 0.000   TW_TIP [K]=      0.000
-------------------------------   fsum =    0.5127E-02
 powder average: Lebedev grid  16 pts
efil:   C:\Dokumente und Einstellungen\serhiyd\Desktop\Magnetm
m[mg]=12.90 /M[g/mol]= 669.00 /chi(dia)= -335.0 /B-fields:  1
B[T]=    0.500
-----------------------------------------
holder:     _file: none
Kapsel       27.40mg,  d:-0.129E-03,  s:  0.000E+00,  p:  0.000E+00
-----------------------------------------
```

Discussion of magnetic properties of both polymorph I and II:

Since Cu^{II} ion has S = 1/2 spin thus some hetero atom bridged Cu^{II}_2X (X = O^{2-}, Cl^- etc.) is taken as an example for comparison.[S4] These kinds of complexes were well studied in the literature. Generally metal ions with unpaired spins have d-orbitals which are more diffused around the nuclei and they couple (and/or super exchange) to other metal ions through the filled nonbonding-orbitals on bridging anions (X = O^{2-}, Cl^- etc.). In contrast two spins of **2** are bridged by the saturated tetrahedral $SiCl_2$ unit. Thus, exchange magnetic coupling through such $SiCl_2$ is unexplored till now. But two spins in polymorph II of **2** can interact through dipolar interactions. These two spins are on the p-orbital of each carbene carbon center. Apparently the $SiCl_2$ bridge is unlikely to mediate a moderate magnetic exchange between them. In the literature there are some reports[S5] of stable radical anions of several trimethylsilyl substituted polyenes, benzenes and naphthalenes. EPR investigation showed coupling constant of ^{29}Si nuclei in trimethylsilyl substituents are of the same order of magnitudes as the corresponding values of protons attached to centers of π-spin population, suggesting $C_\pi \rightarrow Si$ electron delocalization.[S5] Similarly some spin delocalizations from each carbene radical center to $SiCl_2$ unit are expected. But the EPR spectrum does not show an evident observation since no further splitting of the hyperfine line occurred due to chlorine. How the $SiCl_2$ bridge mediates strong antiferromagnetic coupling leading to diamagnetic closed-shell configuration of polymorph II of **2** is not clear.

It is less likely to think of the same compound with two spins (two S = 1/2), the conformer is very strongly antiferromagnetically coupled (S_{eff} = 0) and the other one very ferromagnetically coupled (S_{eff} = 1). Thus, slight perturbation can cause two spins to couple very weakly while one is strongly antiferromagnetically coupled. Thus polymorph I can be compared with the weakly coupled Cu^{II}_2X dimer. For this kind of compound magnetic behaviour is usually like a paramagnetic sample.

Observation: When the powdered samples of polymorph II and samples of enriched with polymorph I are exposed to air after the magnetic measurements, major amount of the powder turned colorless in 2-3 days and 30 minutes respectively.

(S4) EPR spectroscopy

Continuous-wave (CW) EPR spectra were recorded at X-band microwave frequencies (9 GHz) using a Bruker ElexSys E500 spectrometer with a Bruker SuperX CW bridge. The spectrometer was equipped with the Bruker SHQ rectangular microwave cavity (Bruker 4122SHQ) and a helium flow cryostat (Oxford Instruments) for low temperature experiments.

The sample used for recording the EPR spectra of Figures S1 to S7 which was prepared from the reaction of L:$SiCl_2$ (**1**) and L^1: in 1:3 molar ratio at room temperature and separated by filtration followed by washing with cold THF. On our course to the X-ray structure determination we found that this crystal contains polymorph-II as major component and polymorph-I as minor component. EPR spectra recorded on crystals enriched with polymorph-I as major component showed similar results when ten to fifteen times more diluted solutions were used. More concentrated solutions produced unresolved EPR spectra. Polymorph II of compound **2** has diamagnetic close-shell spin ground in the temperature range of 2-300 K. Thus polymorph II is EPR silent but polymorph I is EPR active. Polymorph I (magnetic) is weakly coupled and susceptibility slightly increases below 100 K indicating weak coupling between two radical centers.

The X-band EPR spectrum on a powdered sample of polymorph I of **2** at room temperature shows a broad resonance close to g = 2.0035 which splits into hyperfine signals upon lowering the power (Figure S1, Supporting Information). However, an unresolved multiplet was observed with the same g value of a 5 mM solution of polymorph I of **2** in C_6D_6, which was further resolved into a sextet upon dilution to a 0.1 mM concentration (Figure S1). This pattern suggests that the splitting is due to the nitrogen hyperfine coupling (nuclear spin I = 1). The sextet might result from a dipole-dipole interaction of two coupled radicals and their hyperfine interaction with the closest ^{14}N neighbour nuclei, respectively. The data of the EPR spectrum of polymorph I of **2** given in Figure S1 can be fitted with the use of the EasySpin simulation package[S6] considering two different models (see Figures S1 and S7). Firstly, it could be simulated as two weakly coupled electrons (two S_{eff} = 1/2), each electron interacts with the closest ^{14}N nucleus. The principal values of the electron-electron interaction tensor (which includes isotropic exchange, anisotropic exchange and anisotropic magnetic dipolar interaction) are: J_{xx}= 3.3 MHz, J_{yy}= -8.7 MHz, J_{zz} = 61 MHz. Secondly, the effective electronic spin S_{eff} = 1 (2 coupled electrons) interacts with two N nuclei. The simulation parameters for the fit are: S_{eff} = 1, g = 2.0035, |D| = 24.5 MHz, |E|= 5.1 MHz. The calculated distance between the two unpaired electrons, following a simple dipole-dipole approximation,[S7] produced ~15 Å (assuming D = 24.5 MHz), which is far from the C1-C21 distance of 3.25 Å found in the X-ray structure. The failure of point-dipole approximation for **2** might be due to delocalization of the electron density.[S7] The dipolar interaction is not completely averaged in the solution under investigation. The isotropic part of the hyperfine tensor, a (α-^{14}N), was determined to 5.7 G (16 MHz), which is in agreement with values for similar pyridine derivatives known from the literature.[S8] The EPR spectrum of a powdered sample of **2** exhibits satellite lines with likely anisotropic hyperfine interactions, which were assigned to the coupling with the central α-^{29}Si-isotope and the neighbour ^{13}C-isotope, respectively (Figure S3). Double integrals of the satellite lines are in a reasonable agreement with the natural abundance of the magnetic isotopes (4.68% and 1.07% for ^{29}Si and ^{13}C, respectively). These satellites were observed only in solid state not in solution. This might be due to the slight differences between molecules in solid and solution phase. However, both the satellites were not observed in the solid measured with low power (Figure S2). The a(α-^{29}Si) of 140 G is far larger than the values of typical persilyl-substituted silyl radicals (55.6−62.8 G).[S9] An a(α-^{29}Si) of about 193 G was reported for the trialkyl-substituted silyl radical with a pyramidal geometry.[S10] The observed characteristic splitting pattern indicates the presence of a hyperfine interaction of the unpaired electrons with the nitrogen nuclei of each carbene (L^1:). The half field Δm_s = ±2 forbidden transition was not observed neither in the solid state nor in solution of polymorph I of **2**, which excludes a genuine triplet state of polymorph I of **2** which might be due to weak magnetic interactions. Roques et al.[S11] reported the exchange in silole-bridged biradicals and most of the compounds show Δm_s = ±2 forbidden transition (characteristic of triplet) . The half-field signal is not observed for **7a**[S11] and **12**[S11] of this report even when large signal amplification and high concentrations are used. The magnetic susceptibility measurements showed that more than 50% of molecules of **7a** and **12** are in singlet ground states (0.36 cm^3 K mol^{-1} (**7a**) and 0.35 cm^3 K mol^{-1} (**12**) at room temperature). Similar situation is faced for compound **2**.[S11] EPR spectrum recorded in frozen

solution at 200 K of compound **2** shows loss of hyperfine coupling (signal broadening, Figure S6) like that reported for compounds **7a** and **12** at 4 K.[S11]

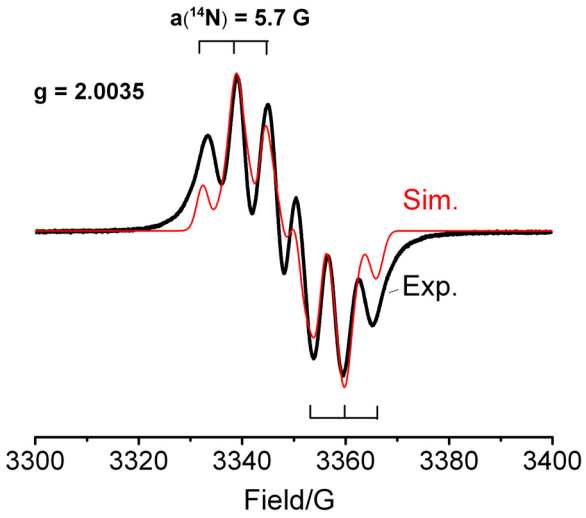


***Figure* S1**. X-band EPR spectrum of 0.1 mM C_6D_6 solution of **2** at 298 K ($\nu_{\mu W}$ = 9.3921 GHz, B_{mod} = 0.5 G at 100 kHz) together with the simulated spectrum based on the fitting parameters given in the text (simulation model with two S_{eff} = 1/2).

EPR intensity vs 1/T plot of polymorph I of **2** follows a straight line (see Figure S4). In the solid state the EPR intensities of **2** decrease with decreasing temperature. However the solution of **2** shows abrupt and inconsistent (300 K to 25 K) when the solution was cooled from room temperature to 4.3 K. But it is steady when wormed from 4.3 K to 100 K. EPR intensity does not appreciably change much above 100 K to room temperature which is consistent with our magnetic susceptibility from 300-2K. Rajca et al.[S12] have described the same problem when they measured the solvent specific susceptibility in solution and stated they are consistent when cooled steadily at a fixed cooling rate and waiting at low temperatures for a long time. There is some similarities between reported 1,3-phenylene-based bis(aminoxyl) biradical and our compound **2**.[S12] Thus, bistability between two polymorphs of **2** are also expected in solution but their interconversion is not clearly observed. EPR intensity of the reported biradical[S12] is also scattered.

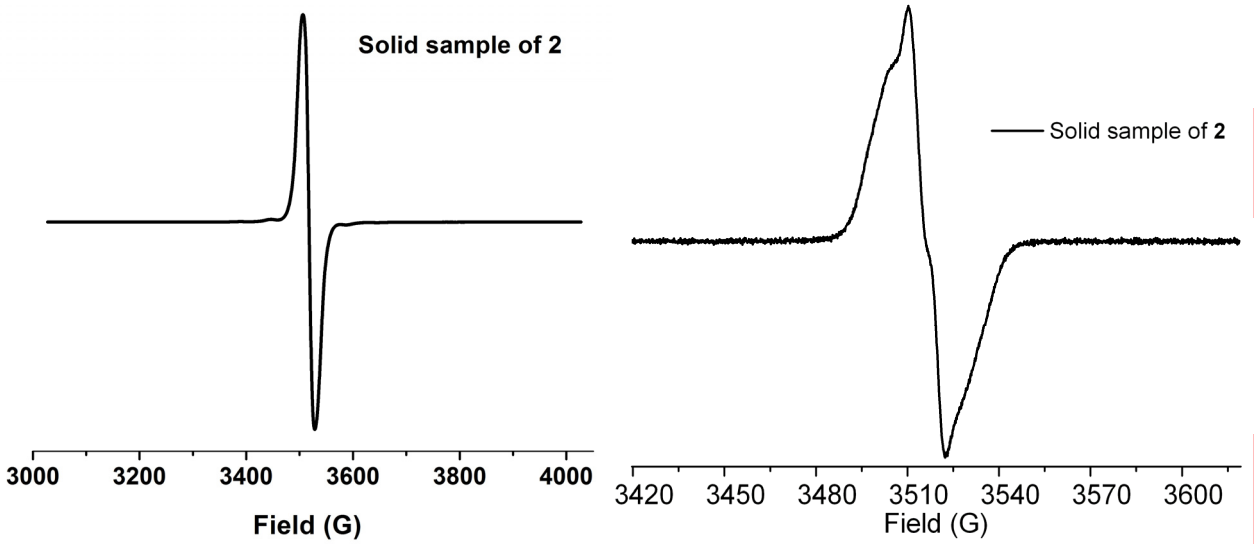


Figure S2. X-band EPR spectra of the powdered solid sample of **2** recorded at room temperature under high power (5dB) (left) with the applied microwave frequency of 9.8596 GHz and under low power (33 dB) (right) with the applied microwave frequency of 9.8589 GHz. This indicates the splitting due to dipole-dipole interactions between two electrons.

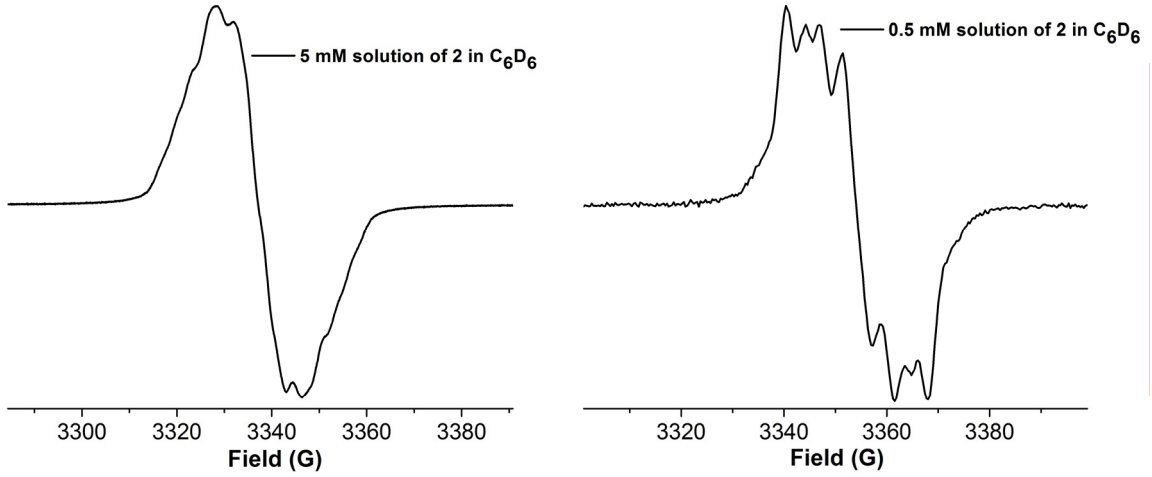


Figure S3. X-band EPR spectra of 5 mM (left) and 0.5 mM (right) C_6D_6 solution of **2** recorded at room temperature. Microwave frequencies were 9.3585 GHz and 9.3971GHz for left and right, respectively.

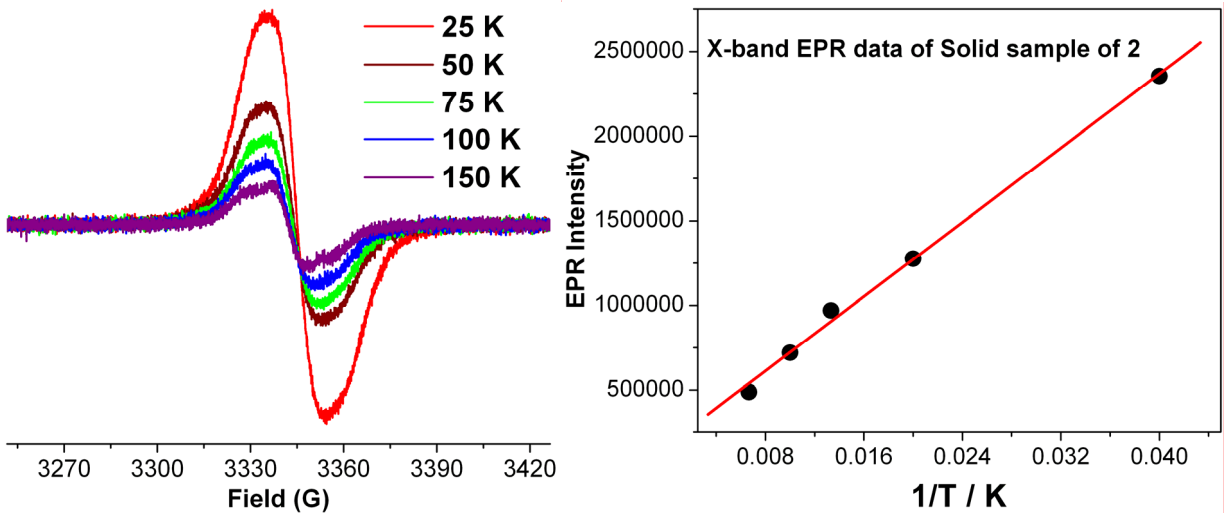


Figure S4. EPR spectra of the powdered sample of compound **2** recorded at indicated temperatures in the temperature range from 25 K up to 150 K. (left). EPR intensity vs 1/T plot (right). Red line represents the linear fit to the experimental data.

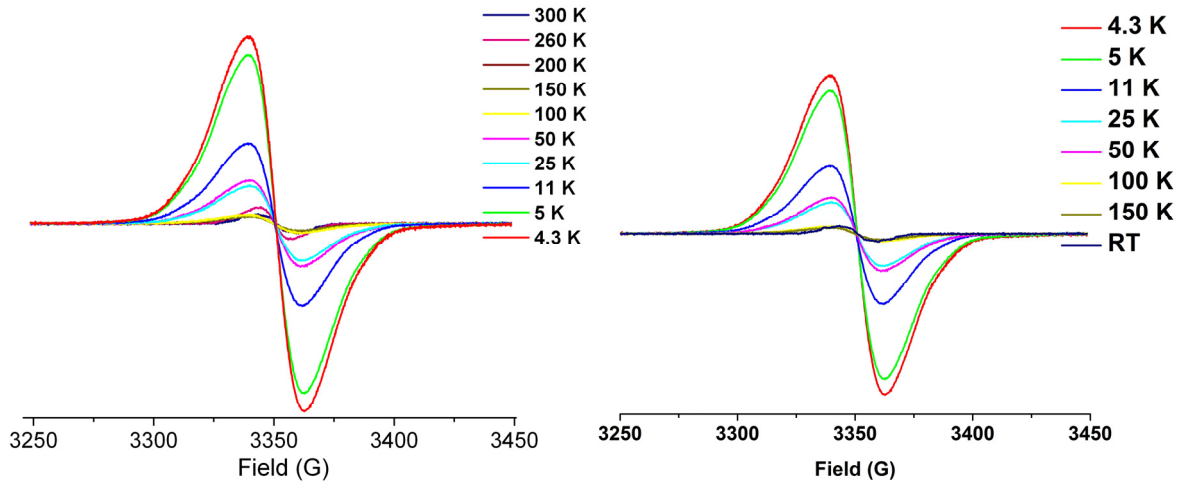


Figure S5. EPR spectra of 0.3 mM C_6D_6 solution of **2** at different temperatures when cooled from 300-4.3 K (left) and wormed from 4.3-300 K (right). Vanishing of the hyperfine splitting indicates a broadening of the hyperfine lines due to anisotropy of the hf-tensor resolved in a frozen solution. Likewise, powder averaging over all possible orientations of the dipolar component of the inter spin interaction tensor in respect to the static magnetic field leads to the increase of the total spectrum width.

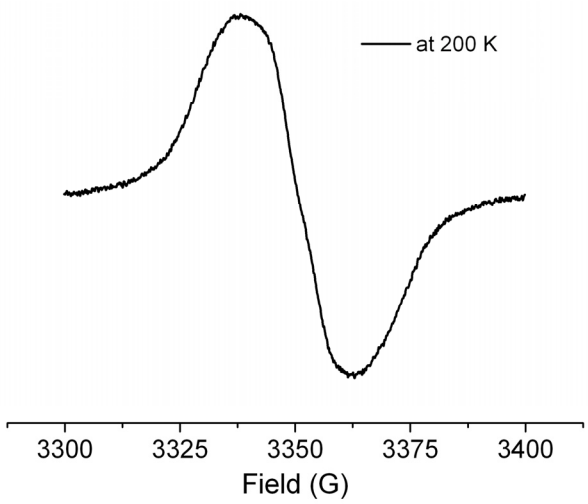


Figure S6. X-band EPR spectrum of 0.5 mM C_6D_6 solution of **2** recorded at 200 K. Microwave frequencies were 9.3976 GHz.

The simulation of the EPR spectrum is ambiguous. The 6-line spectrum of 0.1 mM solution of **2** in C_6D_6 can be simulated considering two different models:

a) 2 weakly coupled electrons (two $S_{eff} = ½$), each electron interacts with the closest ^{14}N nucleus. To fit the EPR spectrum, the magnetic dipolar (anisotropic) interaction must be included:

Simulation parameters for the fit (see Figure S1 of the main text) are:

The principal values of the electron-electron interaction tensor (which includes isotropic exchange, anisotropic exchange and anisotropic magnetic dipolar interactions) are:

J_{xx}= 3.3 MHz, J_{yy}= -8.7 MHz, J_{zz} = 61 MHz.

the principal values of the hyperfine interaction are:

$A(e_1\_^{14}N1)$= [15.12, 15.20, 16.43] (MHz)

$A(e_1\_^{14}N2)$= [0, 0, 0] / no interaction

$A(e_2\_^{14}N1)$= [15.15, 15.23, 15.87] (MHz)

$A(e_2\_^{14}N2)$= [0, 0, 0] / no interaction

Here, the same isotropic g-value for both electrons was assumed: $g(e_1,e_2) = 2.0035$.

b) Effective electron spin $S_{eff} = 1$ (2 coupled electrons) which interacts with two ^{14}N nuclei:

Simulation parameters for the fit (see Figure S7) are:

$S_{eff} = 1$, g = 2.0035, |D| = 24.5 MHz, |E| = 5.1 MHz.

the principal values of the hyperfine interaction are:

$A(^{14}N1) = [A_{xx}, A_{yy}, A_{zz}]$ = [15.12 , 15.20 , 16.43] (MHz),

$A(^{14}N2_{)} = [A_{xx}, A_{yy}, A_{zz}]$ = [15.15 , 15.23 , 15.87] (MHz).

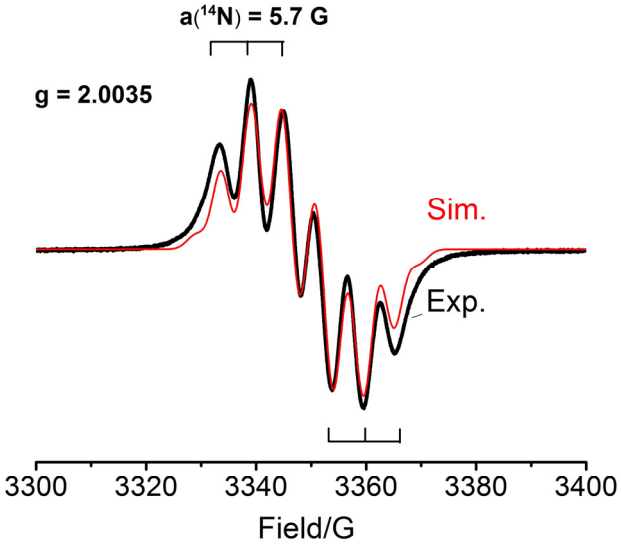


Figure S7. X-band EPR spectrum of 0.1 mM C_6D_6 solution of **2** at 298 K ($\nu_{\mu W}$ = 9.3921 GHz, B_{mod} = 0.5 G at 100 kHz) together with the simulated spectrum based on the fitting parameters given in the text below. In this simulation S_{eff} = 1 was assumed. This model, however, was not supported by spin echo nutation experiment at room temperature, which shows that the effective spin of **2** is close to 1/2 which is expected for a weakly coupled system (polymorph-I) at room temperature.

As additional measurements spin counting in solution and SQID magnetic susceptibility experiments have been carried out on polymorph-II of compound **2**. It has been found that 0.45% contribution comes from polymorph-I as minor component (0.9 % paramagnetic contribution from magnetic susceptibility measurements, spin counting shows 0.42% molecules have two spins per molecule). The ratio of polymorph I/II slightly varies from batch to batch. The similar experiment on compound **2** crystallized at 0 °C in a freezer showed 16.4% (fitting magnetic susceptibility by given equation and calculated with two S = 1/2 spins; spin counting at room temperature shows 17.3% molecules have two spin per molecule) of molecules containing two unpaired electrons per molecule. This shows a mixture of both phases. We were not able to obtain polymorph-I in a pure state. The crystallographic data given in this manuscript were recorded on a single crystal of **2** crystallized at 0 °C (polymorph-I). (see Single-crystal structural analysis).

(S5) Single-crystal structural analysis

Table S1. Crystal data and structure refinement for **2** and **3**:

Compound	L^1:$_2SiCl_2$ (L^1: = :C(CH_2)(CMe_2)$_2$N-2,6-*i*$Pr_2C_6H_3$) (**2**) Polymorph I	L^1:$_2SiCl_2$ (L^1: = :C(CH_2)(CMe_2)$_2$N-2,6-*i*$Pr_2C_6H_3$) (**2**) Polymorph II	L^2: **(3)**
Empirical formula	$C_{40}H_{62}Cl_2N_2Si$	$C_{40}H_{62}Cl_2N_2Si$	$C_{47}H_{67}N_3$
CCDC no.	885692	-	885693
Molecular weight	669.91	669.91	674.04
Crystal size [mm]	0.18 x 0.15 x 0.10	0.10 x 0.08 x 0.05	0.2 x 0.15 x 0.05
Wavelength [pm]	71.073	154.178	71.073
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*C*2/*c*	*C*2/*c*	$P2_1/c$

a [pm]	3435.2(10)	3520.2(2)	1307.8(2)
b [pm]	984.4(3)	994.3(2)	1482.2(2)
c [pm]	2294.7(7)	2268.0(3)	2186.6(3)
β [°]	101.02(2)	106.00(2)	104.810(10)
V [nm^3]	7.62(1)	7.6308(19)	4.0977(10)
Z	8	8	4
Temperature [K]	173(2)	100(2)	111(2)
ρ [Mgm^{-3}]	1.168	1.166	1.093
μ [mm^{-1}]	0.231	2.037	0.063
F (000)	2912	2912	1480
θ-area [°]	1.21 to 26.79	2.611 to 58.743	1.61 to 26.41
Total number reflect.	132336	24072	101802
Unique reflections	8123	5209	8403
R_{int}	0.0659	0.0703	0.0781
Number of restraints	0		55
Parameters	422	422	485
$R1$ [$I>2\sigma(I)$]	0.0374	0.0639	0.0418
$wR2$ [$I>2\sigma(I)$]	0.0949	0.1388	0.0958
$R1$ [all data]	0.0449	0.0968	0.0606
$wR2$ [all data]	0.0990	0.1559	0.1064
GooF	1.104	1.059	1.023
Extinction coefficient	-		0.0019(3)
Largest diff. peak / hole max. / min. [10^3·e·nm^{-3}]	0.562 and -0.270	0.480 and -0.398	0.287 and -0.274

The data collection for structure **2** was very challenging. Several data sets of different polymorphs were collected. The two first batches of crystals were not sensitive to air and did not need low temperature mounting (polymorph-II). The diffraction pattern showed additional spots due to a second species with a slightly different cell (a = 3522.7(3) pm, b = 995.2(2) pm, c = 2267.6(3) pm, β = 105.96(2)°, V = 7.643(2) nm^3). Trials to segregate the effect of overlapping spots were not completely satisfying. In a second batch the diffraction pattern again showed spots of two different species. But now the main component (polymorph I) showed the cell of the former minor one. The structure was nearly identical to the first one (Si1-C1 184.6 to 184.0 pm, Si1-C21 184.8 to 183.0 pm, Si1-Cl1 206.6 to 206.4 pm, Si1-Cl2 206.9 to 205.4 pm), but the quality was poor. Therefore the data are not deposited in the CCDC. For comparison purposes the data are listed in table S1. In a third approach, when the crystals (polymorph-I) were grown at 0 °C we again got crystals of the previous low temperature phase with only a very small amount of the high temperature phase, which could be ignored. The color of these crystals was a bit lighter blue than the other stable ones. All mentioned values refer to this data collection on the low temperature phase (polymorph-I).

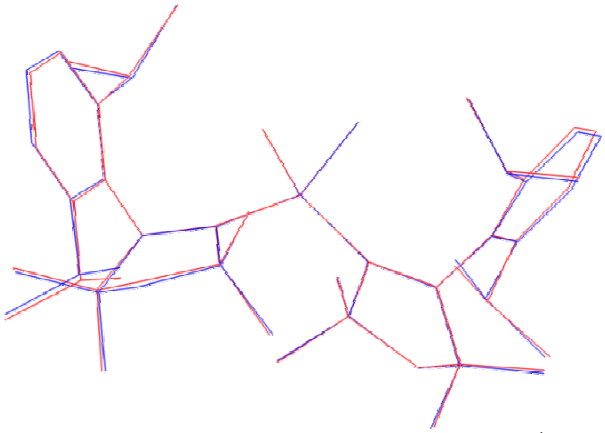


Figure S1. Superposition of the crystal structures from the two polymorphs of **2**. $L^1{}_2SiCl_2$ (**2**), (L_1: = :C(CH$_2$)(CMe$_2$)$_2$N-2,6-*i*Pr$_2$C$_6$H$_3$).

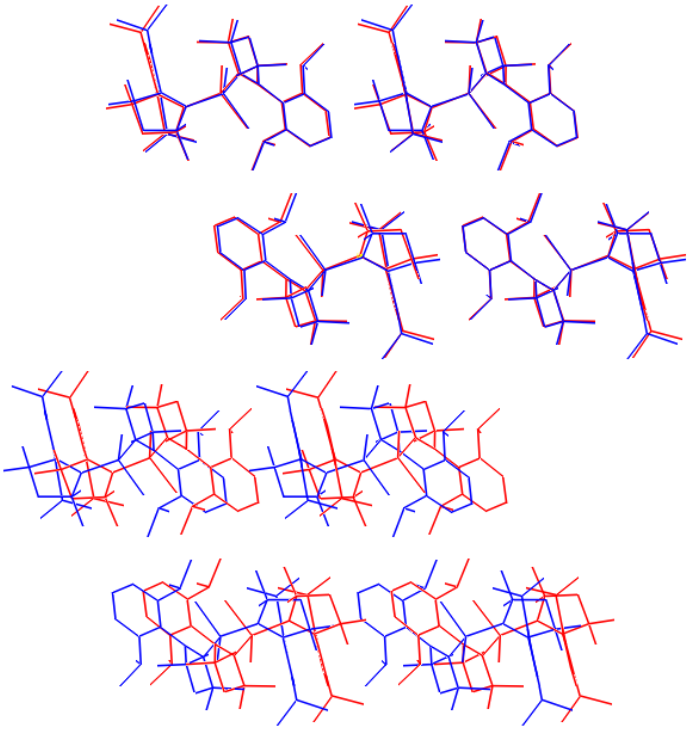


Figure S2. Superposition of the crystal structures from the two polymorphs of **2**. L^1:$_2SiCl_2$ (**2**) view along a-axes, (L_1: = :$C(CH_2)(CMe_2)_2$N-2,6-*i*$Pr_2C_6H_3$).

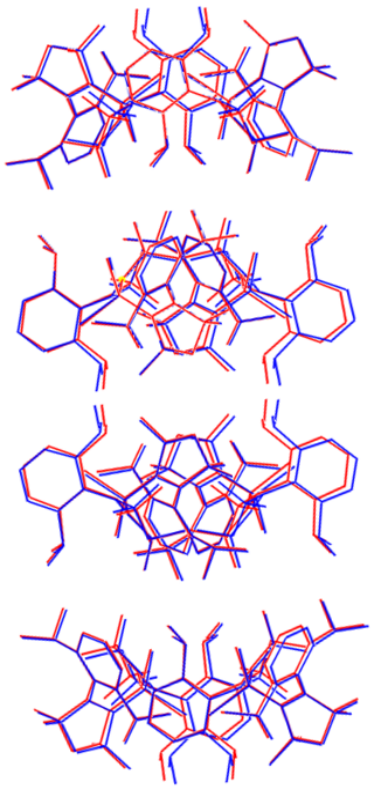


Figure S3. Superposition of the crystal structures from the two polymorphs of **2**. L^1:$_2SiCl_2$ (**2**) view along c-axes, (L_1: = :$C(CH_2)(CMe_2)_2$N-2,6-*i*$Pr_2C_6H_3$).

Synthesis of X-ray quality crystals of **2**, first batch: The reaction mixture of L:$SiCl_2$ (**1**) (488 mg, 1 mmol) and L^1: (570 mg, 2 mmol) in 1:2 molar ratio in 10 mL THF at room temperature was stirred for 10 minutes to get a dark blue solution which was dried to get dark blue-black solid mass which was extracted with 30 mL *n*-hexane. Large dark blue-black crystals were grown under slow evporation of solvent in 1 hour.

Synthesis of X-ray quality crystals of **2**, second batch: The reaction mixture of L:$SiCl_2$ (**1**) (488 mg, 1 mmol) and L^1: (570 mg, 2 mmol) in 1:2 molar ratio in 5 mL THF at room temperature to get a dark blue solution which was stirred for 2-3 minutes. Small dark blue-black crystals were grown after one day.

Synthesis of X-ray quality crystals of **2**, third batch: The reaction mixture of L:$SiCl_2$ (**1**) (488 mg, 1 mmol) and L^1: (570 mg, 2 mmol) in 1:2 molar ratio in 4 mL of THF at room temperature to get a drak blue solution which was stirred for 2-3 minutes. The solution was stored at 0 °C freezer. After two days very small dark blue-black crystals were obtained. Then this small amount of mall dark blue-black crystals were seperated by carefully turning the flask horrizonetally. After 7-10 days blue blocks of **2** were obtained.

Synthesis of X-ray quality crystals of **2**, fourth batch: The reaction mixture of L:$SiCl_2$ (**1**) (488 mg, 1 mmol) and L^1: (855 mg, 3 mmol) in 1:2 molar ratio in 5 mL of THF at room temperature to get a dark blue solution which was stirred for 2-3 minutes. The solution was stored at 0 °C in a freezer. After two days very small dark blue-black crystals were obtained. Then this small amount of mall dark blue-black crystals were seperated by carefully turning the flask horrizonetally. After 7-14 days blue blocks of **2** were obtained.

Polymorphs I and II do not differ in the molecular structural geometry nor in the arrangement in the cell but only in the distance of the different molecules relative to each other. However, due to the wide intermolecular distances any long-range interaction can be excluded in any case.

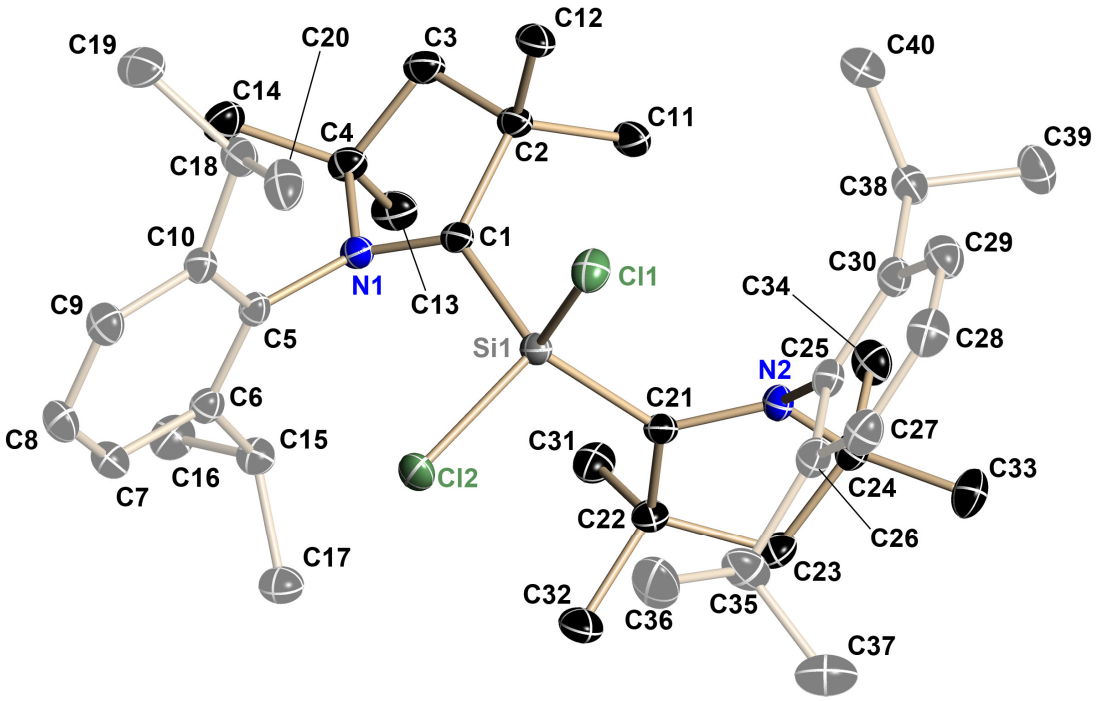


Figure S4. Molecular structure of L^1:$_2SiCl_2$ (L_1: = :$C(CH_2)(CMe_2)_2N$-2,6-$iPr_2C_6H_3$) (**2**) in the crystal. Anisotropic displacement parameters are depicted at the 50 % probability level.

Table S2. Bond lengths [pm] and angles [°] for **2**.

Cl(1)-Si(1)	206.62(7)	Si(1)-C(1)	184.55(16)
Cl(2)-Si(1)	206.90(8)	Si(1)-C(21)	184.82(17)

N(1)-C(1)	139.94(19)	C(35)-C(37)	153.6(2)
N(1)-C(5)	144.8(2)	C(38)-C(40)	153.4(2)
N(1)-C(4)	151.31(19)	C(38)-C(39)	153.7(2)
N(2)-C(21)	139.5(2)		
N(2)-C(25)	144.94(19)	C(1)-Si(1)-C(21)	122.99(7)
N(2)-C(24)	151.4(2)	C(1)-Si(1)-Cl(1)	106.31(5)
C(1)-C(2)	154.3(2)	C(21)-Si(1)-Cl(1)	107.33(5)
C(2)-C(3)	153.4(2)	C(1)-Si(1)-Cl(2)	107.00(5)
C(2)-C(11)	153.6(2)	C(21)-Si(1)-Cl(2)	106.52(5)
C(2)-C(12)	154.1(2)	Cl(1)-Si(1)-Cl(2)	105.51(3)
C(3)-C(4)	152.9(2)	C(1)-N(1)-C(5)	123.41(13)
C(4)-C(14)	152.4(2)	C(1)-N(1)-C(4)	111.81(12)
C(4)-C(13)	153.8(2)	C(5)-N(1)-C(4)	120.26(12)
C(5)-C(6)	141.4(2)	C(21)-N(2)-C(25)	122.72(12)
C(5)-C(10)	141.6(2)	C(21)-N(2)-C(24)	112.14(12)
C(6)-C(7)	139.5(2)	C(25)-N(2)-C(24)	120.41(12)
C(6)-C(15)	152.1(2)	N(1)-C(1)-C(2)	108.69(12)
C(7)-C(8)	138.0(3)	N(1)-C(1)-Si(1)	126.77(11)
C(8)-C(9)	138.3(3)	C(2)-C(1)-Si(1)	122.88(11)
C(9)-C(10)	139.5(2)	C(3)-C(2)-C(11)	112.38(14)
C(10)-C(18)	152.2(2)	C(3)-C(2)-C(12)	108.25(13)
C(15)-C(17)	153.6(2)	C(11)-C(2)-C(12)	107.47(14)
C(15)-C(16)	153.6(2)	C(3)-C(2)-C(1)	102.15(12)
C(18)-C(19)	153.2(3)	C(11)-C(2)-C(1)	112.55(13)
C(18)-C(20)	153.6(3)	C(12)-C(2)-C(1)	114.00(13)
C(21)-C(22)	154.4(2)	C(4)-C(3)-C(2)	107.42(12)
C(22)-C(31)	153.7(2)	N(1)-C(4)-C(14)	112.65(13)
C(22)-C(23)	153.9(2)	N(1)-C(4)-C(3)	100.26(12)
C(22)-C(32)	154.3(2)	C(14)-C(4)-C(3)	111.26(14)
C(23)-C(24)	153.0(2)	N(1)-C(4)-C(13)	112.46(13)
C(24)-C(33)	152.6(2)	C(14)-C(4)-C(13)	108.90(14)
C(24)-C(34)	153.5(2)	C(3)-C(4)-C(13)	111.15(14)
C(25)-C(30)	140.9(2)	C(6)-C(5)-C(10)	120.18(15)
C(25)-C(26)	141.6(2)	C(6)-C(5)-N(1)	119.96(14)
C(26)-C(27)	139.5(2)	C(10)-C(5)-N(1)	119.84(14)
C(26)-C(35)	151.9(2)	C(7)-C(6)-C(5)	118.61(15)
C(27)-C(28)	138.1(2)	C(7)-C(6)-C(15)	117.76(15)
C(28)-C(29)	138.1(2)	C(5)-C(6)-C(15)	123.57(14)
C(29)-C(30)	139.7(2)	C(8)-C(7)-C(6)	121.55(16)
C(30)-C(38)	151.9(2)	C(7)-C(8)-C(9)	119.60(16)
C(35)-C(36)	153.3(3)	C(8)-C(9)-C(10)	121.47(16)

C(9)-C(10)-C(5)	118.56(15)
C(9)-C(10)-C(18)	117.52(15)
C(5)-C(10)-C(18)	123.92(15)
C(6)-C(15)-C(17)	110.90(14)
C(6)-C(15)-C(16)	112.66(14)
C(17)-C(15)-C(16)	108.90(14)
C(10)-C(18)-C(19)	111.70(15)
C(10)-C(18)-C(20)	112.10(16)
C(19)-C(18)-C(20)	109.58(16)
N(2)-C(21)-C(22)	109.10(13)
N(2)-C(21)-Si(1)	127.17(11)
C(22)-C(21)-Si(1)	121.49(11)
C(31)-C(22)-C(23)	111.70(13)
C(31)-C(22)-C(32)	107.55(13)
C(23)-C(22)-C(32)	108.84(13)
C(31)-C(22)-C(21)	112.83(12)
C(23)-C(22)-C(21)	102.49(12)
C(32)-C(22)-C(21)	113.39(13)
C(24)-C(23)-C(22)	107.97(13)
N(2)-C(24)-C(33)	112.33(13)
N(2)-C(24)-C(23)	101.01(12)
C(33)-C(24)-C(23)	110.68(13)
N(2)-C(24)-C(34)	112.08(13)
C(33)-C(24)-C(34)	109.36(14)
C(23)-C(24)-C(34)	111.19(13)
C(30)-C(25)-C(26)	119.84(14)
C(30)-C(25)-N(2)	120.76(13)
C(26)-C(25)-N(2)	119.40(13)
C(27)-C(26)-C(25)	118.72(14)
C(27)-C(26)-C(35)	117.22(14)
C(25)-C(26)-C(35)	124.06(14)
C(28)-C(27)-C(26)	121.62(15)
C(29)-C(28)-C(27)	119.25(15)
C(28)-C(29)-C(30)	121.63(15)
C(29)-C(30)-C(25)	118.78(14)
C(29)-C(30)-C(38)	117.38(14)
C(25)-C(30)-C(38)	123.84(14)
C(26)-C(35)-C(36)	111.39(14)
C(26)-C(35)-C(37)	111.48(14)
C(36)-C(35)-C(37)	109.86(14)
C(30)-C(38)-C(40)	111.45(13)
C(30)-C(38)-C(39)	111.17(13)
C(40)-C(38)-C(39)	109.51(14)

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kt48 (compound **2**, **polymorph I**))

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kt48 (compound 2)

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Bond precision:  C-C = 0.0023 A          Wavelength=0.71073

Cell:            a=34.352(10)     b=9.844(3)          c=22.947(7)
                 alpha=90         beta=101.02(2)      gamma=90
Temperature:     173 K
```

	Calculated	Reported
Volume	7617(4)	7617(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C40 H62 Cl2 N2 Si	C40 H62 Cl2 N2 Si
Sum formula	C40 H62 Cl2 N2 Si	C40 H62 Cl2 N2 Si
Mr	669.91	669.91
Dx,g cm-3	1.168	1.168
Z	8	8
Mu (mm-1)	0.231	0.231
F000	2912.0	2912.0
F000'	2915.81	
h,k,lmax	43,12,29	43,12,29
Nref	8155	8123
Tmin,Tmax	0.959,0.977	0.623,0.745
Tmin'	0.959	

```
Correction method= MULTI-SCAN

Data completeness= 0.996          Theta(max)= 26.790

R(reflections)= 0.0374( 7090)     wR2(reflections)= 0.0990( 8123) S = 1.104

                           Npar= 422
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW .gt. 10 Outliers . 2

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.08
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3
PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L= 0.600 31

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 10.49

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) new (compound **2 polymorph II, not deposited**)

No syntax errors found. CIF dictionary Interpreting this report

Datablock: new (compound 2, polymorph II)

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Bond precision:  C-C = 0.0069 A          Wavelength=1.54178

Cell:            a=35.202(2)     b=9.943(2)          c=22.680(3)
                 alpha=90        beta=106.00(2)      gamma=90
Temperature:     100 K

                 Calculated                Reported Volume
                 7631(2)                   7630.8(19) Space group
                 C 2/c                     C 2/c
Hall group       -C 2yc                    -C 2yc
Moiety formula   C40 H62 Cl2 N2 Si         C40 H62 Cl2 N2 Si Sum formula
C40 H62 Cl2 N2 Si           C40 H62 Cl2 N2 Si Mr                669.91
669.90
Dx,g cm-3        1.166                     1.166
Z                8                         8
Mu (mm-1)        2.037                     2.037
F000             2912.0                    2912.0
F000'            2925.82
h,k,lmax         38,11,25                  38,10,25
Nref             5444                      5209
Tmin,Tmax        0.822,0.903               0.562,0.752
Tmin'            0.816

Correction method= MULTI-SCAN

Data completeness= 0.957          Theta(max)= 58.743

R(reflections)= 0.0639( 3779)     wR2(reflections)= 0.1559( 5209) S = 1.059

                           Npar= 422
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
          Calculated sin(theta_max)/wavelength =    0.5545
```

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0069 Ang
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.431
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.554        230
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        107
```

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 48.63
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 55 Perc.

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

L^2: **(3):**

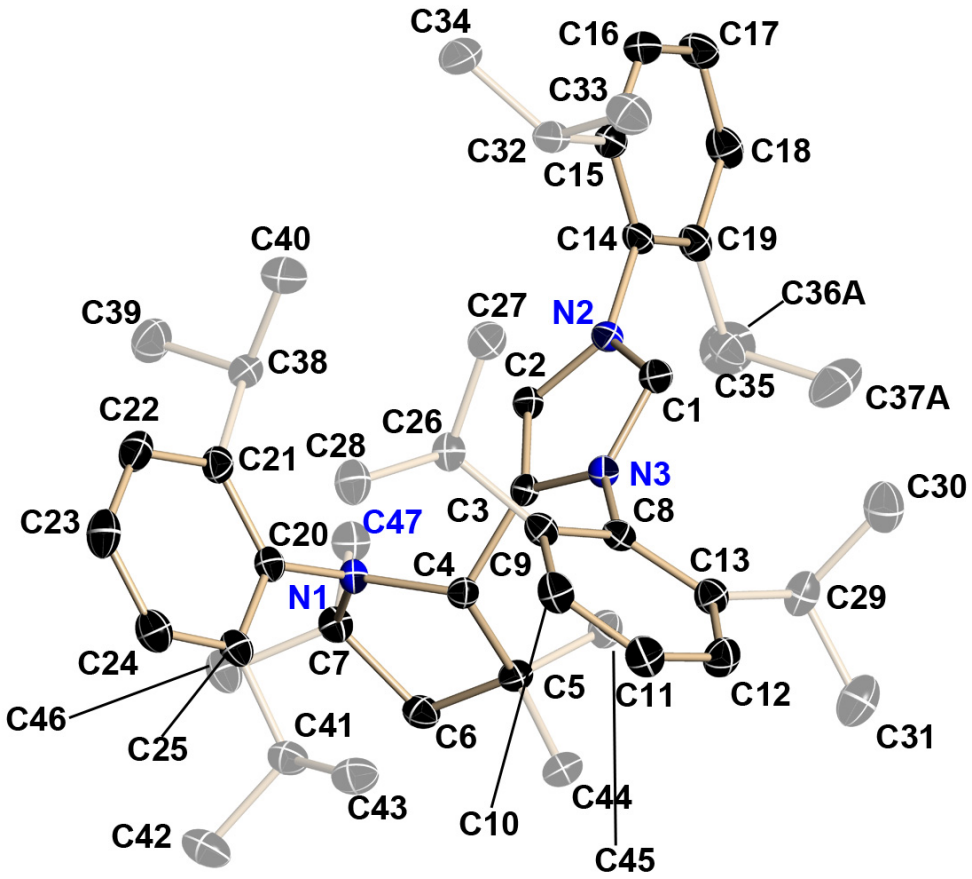

Figure S9. Molecular structure of L^2: (**3**) in the crystal. Anisotropic displacement parameters are depicted at the 50 % probability level.

Table S3. Bond lengths [pm] and angles [°] for **3**.

N(1)-C(20)	143.50(17)	C(26)-C(28)	152.51(19)
N(1)-C(4)	146.99(16)	C(26)-C(27)	153.0(2)
N(1)-C(7)	148.91(17)	C(29)-C(31)	152.5(2)
N(2)-C(1)	137.50(17)	C(29)-C(30)	154.7(2)
N(2)-C(3)	141.11(17)	C(32)-C(34)	152.9(2)
N(2)-C(8)	144.79(16)	C(32)-C(33)	153.2(2)
N(3)-C(1)	136.61(17)	C(19)-C(35)	151.9(2)
N(3)-C(2)	139.12(17)	C(35)-C(36B)	151.4(13)
N(3)-C(14)	144.28(17)	C(35)-C(37A)	151.6(2)
C(2)-C(3)	134.78(18)	C(35)-C(36A)	152.3(2)
C(3)-C(4)	151.40(18)	C(35)-C(37B)	155.9(13)
C(4)-C(5)	159.00(18)	C(38)-C(40)	152.6(2)
C(5)-C(44)	152.93(19)	C(38)-C(39)	153.1(2)
C(5)-C(45)	153.47(19)	C(41)-C(43)	153.4(2)
C(5)-C(6)	154.47(19)	C(41)-C(42)	153.6(2)
C(6)-C(7)	153.84(19)		
C(7)-C(46)	152.81(19)	C(20)-N(1)-C(4)	119.18(10)
C(7)-C(47)	153.52(19)	C(20)-N(1)-C(7)	122.35(10)
C(8)-C(13)	139.93(19)	C(4)-N(1)-C(7)	112.08(10)
C(8)-C(9)	140.73(19)	C(1)-N(2)-C(3)	113.54(11)
C(9)-C(10)	139.62(19)	C(1)-N(2)-C(8)	120.60(11)
C(9)-C(26)	152.03(19)	C(3)-N(2)-C(8)	125.16(11)
C(10)-C(11)	138.3(2)	C(1)-N(3)-C(2)	113.09(11)
C(11)-C(12)	137.6(2)	C(1)-N(3)-C(14)	123.43(11)
C(12)-C(13)	139.82(19)	C(2)-N(3)-C(14)	123.43(11)
C(13)-C(29)	152.1(2)	N(3)-C(1)-N(2)	101.34(11)
C(14)-C(15)	139.97(19)	C(3)-C(2)-N(3)	107.42(12)
C(14)-C(19)	140.32(19)	C(2)-C(3)-N(2)	104.60(11)
C(15)-C(16)	139.6(2)	C(2)-C(3)-C(4)	130.87(12)
C(15)-C(32)	151.7(2)	N(2)-C(3)-C(4)	124.21(11)
C(16)-C(17)	138.0(2)	N(1)-C(4)-C(3)	112.91(10)
C(17)-C(18)	138.1(2)	N(1)-C(4)-C(5)	106.13(10)
C(18)-C(19)	139.05(19)	C(3)-C(4)-C(5)	113.69(10)
C(20)-C(21)	141.20(19)	C(44)-C(5)-C(45)	107.39(12)
C(20)-C(25)	141.75(19)	C(44)-C(5)-C(6)	111.09(11)
C(21)-C(22)	139.7(2)	C(45)-C(5)-C(6)	110.75(11)
C(21)-C(38)	151.8(2)	C(44)-C(5)-C(4)	109.92(11)
C(22)-C(23)	137.7(2)	C(45)-C(5)-C(4)	114.32(11)
C(23)-C(24)	138.0(2)	C(6)-C(5)-C(4)	103.42(10)
C(24)-C(25)	139.1(2)	C(7)-C(6)-C(5)	107.67(11)
C(25)-C(41)	152.3(2)	N(1)-C(7)-C(46)	112.50(11)
		N(1)-C(7)-C(47)	111.02(11)

C(46)-C(7)-C(47)	107.68(11)	C(22)-C(23)-C(24)	119.45(14)
N(1)-C(7)-C(6)	102.85(10)	C(23)-C(24)-C(25)	121.47(14)
C(46)-C(7)-C(6)	111.48(12)	C(24)-C(25)-C(20)	119.39(13)
C(47)-C(7)-C(6)	111.34(11)	C(24)-C(25)-C(41)	117.64(13)
C(13)-C(8)-C(9)	122.16(12)	C(20)-C(25)-C(41)	122.97(12)
C(13)-C(8)-N(2)	119.84(12)	C(9)-C(26)-C(28)	114.36(12)
C(9)-C(8)-N(2)	117.95(12)	C(9)-C(26)-C(27)	109.38(11)
C(10)-C(9)-C(8)	117.60(12)	C(28)-C(26)-C(27)	109.21(12)
C(10)-C(9)-C(26)	120.85(12)	C(13)-C(29)-C(31)	112.85(13)
C(8)-C(9)-C(26)	121.40(12)	C(13)-C(29)-C(30)	110.05(12)
C(11)-C(10)-C(9)	121.14(13)	C(31)-C(29)-C(30)	109.75(13)
C(12)-C(11)-C(10)	119.99(13)	C(15)-C(32)-C(34)	112.86(12)
C(11)-C(12)-C(13)	121.63(13)	C(15)-C(32)-C(33)	110.13(12)
C(12)-C(13)-C(8)	117.37(13)	C(34)-C(32)-C(33)	110.77(13)
C(12)-C(13)-C(29)	119.60(13)	C(18)-C(19)-C(14)	117.71(13)
C(8)-C(13)-C(29)	122.93(12)	C(18)-C(19)-C(35)	120.75(13)
C(15)-C(14)-C(19)	122.32(12)	C(14)-C(19)-C(35)	121.49(12)
C(15)-C(14)-N(3)	119.27(12)	C(36B)-C(35)-C(19)	112.0(9)
C(19)-C(14)-N(3)	118.41(12)	C(37A)-C(35)-C(19)	110.18(13)
C(16)-C(15)-C(14)	117.50(13)	C(37A)-C(35)-C(36A)	110.94(17)
C(16)-C(15)-C(32)	120.58(13)	C(19)-C(35)-C(36A)	113.54(15)
C(14)-C(15)-C(32)	121.89(12)	C(36B)-C(35)-C(37B)	109.1(12)
C(17)-C(16)-C(15)	121.08(14)	C(19)-C(35)-C(37B)	109.3(9)
C(16)-C(17)-C(18)	120.33(13)	C(21)-C(38)-C(40)	111.99(13)
C(17)-C(18)-C(19)	121.06(14)	C(21)-C(38)-C(39)	111.06(12)
C(21)-C(20)-C(25)	118.89(12)	C(40)-C(38)-C(39)	110.64(13)
C(21)-C(20)-N(1)	118.71(12)	C(25)-C(41)-C(43)	111.09(12)
C(25)-C(20)-N(1)	122.40(12)	C(25)-C(41)-C(42)	112.64(12)
C(22)-C(21)-C(20)	119.42(13)	C(43)-C(41)-C(42)	109.53(12)
C(22)-C(21)-C(38)	118.06(13)		
C(20)-C(21)-C(38)	122.50(12)		
C(23)-C(22)-C(21)	121.36(14)		

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sad (compound **3**)

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sad (compound 3)

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:            a=13.078(2)     b=14.822(2)         c=21.866(3)
```

	alpha=90	beta=104.81(1)	gamma=90
Temperature:	111 K		

	Calculated	Reported Volume
	4097.7(10)	4097.7(10) Space group
	P 21/c	P2(1)/c Hall group
	-P 2ybc	-P 2ybc Moiety formula
	C47 H67 N3	?
Sum formula	C47 H67 N3	C47 H67 N3
Mr	674.04	674.04
Dx,g cm-3	1.093	1.093
Z	4	4
Mu (mm-1)	0.063	0.063
F000	1480.0	1480.0
F000'	1480.46	
h,k,lmax	16,18,27	16,18,27
Nref	8421	8403
Tmin,Tmax	0.989,0.997	0.988,0.997
Tmin'	0.987	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.410

R(reflections)= 0.0418(6489) wR2(reflections)= 0.1064(8403) S = 1.023

Npar= 485

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4
PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L= 0.600 16

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 5
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ? PLAT301_ALERT_3_G
Note: Main Residue Disorder ..... 4 Perc.
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C1
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 79
C36B -C35 -C36A 1.555 1.555 1.555 23.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 83
C37A -C35 -C37B 1.555 1.555 1.555 28.00 Deg.
PLAT793_ALERT_4_G The Model has Chirality at C4 (Verify) .... S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 55

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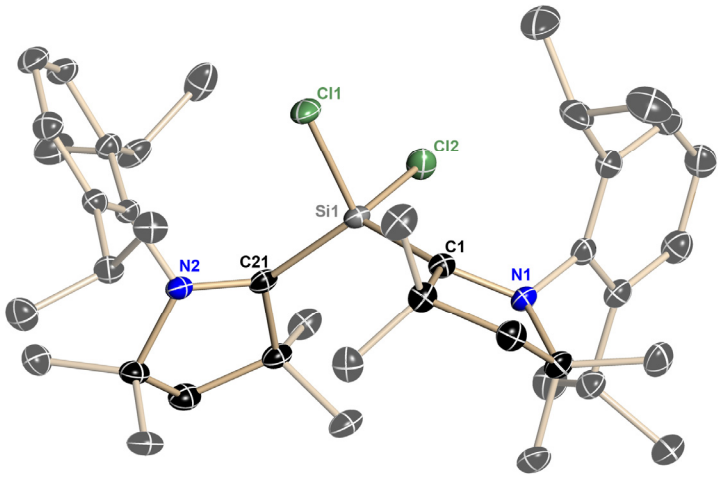
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Center. The crystal data are available from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

(S6) Theoretical calculations on 2

Calculated geometry of the closed-shell singlet and triple state of **2**:



	Exp.[a]	R/U-M05-2X/SVP		
		Singlet	Triplet	Singlet Biradical
d (Si – C1)	1.846	1.860	1.849	1.858
d (Si – C21)	1.848	1.861	1.849	1.858
d (Si – Cl1)	2.066	2.105	2.109	2.101
d (Si – Cl2)	2.069	2.104	2.109	2.101
d (C1 – N1)	1.399	1.378	1.392	1.393
d (C21 – N2)	1.395	1.378	1.392	1.393
d (C1 – C21)	3.246	3.326	3.186	3.262
A (Cl1 – Si – Cl2)	105.5	105.9	102.2	104.9
A (C1 – Si – C21)	123.0	126.8	118.8	122.8
A (C1 – Si – Cl1)	107.0	105.5	107.3	106.3

[a]Bond lengths in Å, angles in degree.

Coordinates of the optimized geometries:

$SiCl_2$

RM052x/def2-SVP Singlet: -1209.562166

Si	-0.086493	0.000000	-0.061479
Cl	0.066661	0.000000	2.027813
Cl	1.933736	0.000000	-0.612993

UM052x/def2-SVP Triplet: -1209.472559

Si	0.059313	0.000000	0.042580
Cl	-0.102288	0.000000	2.111177
Cl	1.956879	0.000000	-0.800417

L:

RM052x/def2-SVP Singlet: -1159.013908

C	0.676369	0.229665	0.580337
N	0.154704	-0.703242	1.424542
N	1.388269	-0.541939	-0.287134
C	0.528387	-2.001304	1.100645
C	1.311074	-1.898843	-0.000017
H	0.204743	-2.861699	1.675759
H	1.815886	-2.650401	-0.596701
C	-0.665690	-0.395863	2.558362
C	2.132025	-0.028241	-1.399092
C	-2.057343	-0.571931	2.451307
C	-2.836557	-0.305114	3.579136
C	-2.250270	0.131707	4.764537
C	-0.874365	0.310829	4.840863
C	-0.051863	0.044708	3.740651
C	-2.693859	-0.947553	1.123301
H	-3.916071	-0.432596	3.531132
H	-2.873832	0.338420	5.633613
H	-0.428504	0.664476	5.769431
C	1.443652	0.294659	3.825968
H	1.913971	-0.173532	2.952966
C	1.713566	1.802642	3.745058
C	2.072423	-0.317344	5.080861
H	-1.986417	-1.588258	0.581619
C	-4.002916	-1.723814	1.271562
C	-2.904721	0.323259	0.287359
H	3.162899	-0.193319	5.048719
H	1.714033	0.174265	5.994844
H	1.847684	-1.388685	5.158447
H	2.792932	2.003341	3.773172
H	1.302453	2.210948	2.813824
H	1.244283	2.321953	4.592467
H	-4.334051	-2.079766	0.287720
H	-3.885619	-2.592236	1.932443
H	-4.804764	-1.090326	1.673268
H	-3.313990	0.070190	-0.700663
H	-3.612783	0.992640	0.795154
H	-1.958795	0.861725	0.151599
C	1.452190	0.277337	-2.587735
C	2.206446	0.755967	-3.664468
C	3.583728	0.910044	-3.559389
C	4.236270	0.597654	-2.369408
C	3.523611	0.125934	-1.264811
C	-0.057758	0.161039	-2.699280
H	1.706500	1.011201	-4.597634
H	4.155191	1.279443	-4.410135
H	5.314203	0.729439	-2.300396
C	4.210365	-0.128354	0.066930
H	3.646885	-0.911624	0.589743
C	5.653963	-0.613208	-0.074619
C	4.142735	1.143696	0.924058
H	-0.410056	-0.451555	-1.860204
C	-0.689104	1.552090	-2.558518
C	-0.501866	-0.522716	-3.995466
H	6.041735	-0.910513	0.908094
H	5.726685	-1.475074	-0.750353
H	6.310523	0.180225	-0.455235
H	4.584682	0.963231	1.913982
H	4.701826	1.954754	0.437151
H	3.103595	1.470237	1.053683
H	-1.587944	-0.682507	-3.978769
H	-0.275746	0.092458	-4.876336
H	-0.010994	-1.495922	-4.122682
H	-1.784367	1.484756	-2.604876
H	-0.401970	2.003443	-1.601102
H	-0.348924	2.209107	-3.371271

UM052x/def2-SVP Triplet: -1158.875159

C	0.310414	0.182513	0.357452
N	0.074298	-0.756646	1.384399
N	0.951136	-0.448927	-0.716187
C	0.329894	-2.000292	0.799416
C	0.859717	-1.824926	-0.431605
H	0.130123	-2.923296	1.332461
H	1.208665	-2.566662	-1.142444
C	-0.602563	-0.510168	2.603456
C	2.018098	0.122333	-1.483960
C	-1.884183	-1.068090	2.828636
C	-2.490703	-0.834620	4.065685
C	-1.884547	-0.035640	5.030825
C	-0.649364	0.546488	4.772042
C	0.017176	0.314204	3.566546
C	-2.643084	-1.789913	1.721748
H	-3.467899	-1.263544	4.274195
H	-2.383111	0.140609	5.982964
H	-0.186368	1.178782	5.527529
C	1.360496	0.964811	3.291551
H	1.869057	0.345307	2.543833
C	1.156473	2.362138	2.689131
C	2.260680	1.039521	4.527016
H	-1.963166	-2.484054	1.216047
C	-3.825972	-2.618314	2.224699
C	-3.114764	-0.771859	0.672268
H	3.263387	1.376650	4.233377
H	1.880219	1.758664	5.264418
H	2.351815	0.061131	5.015415
H	2.122662	2.832248	2.461161
H	0.570376	2.313277	1.760981
H	0.618316	3.004979	3.399743
H	-4.243149	-3.200333	1.393325
H	-3.527028	-3.316843	3.016820
H	-4.630632	-1.978930	2.611354

H	-3.657903	-1.281851	-0.135082
H	-3.789959	-0.040586	1.137491
H	-2.266808	-0.229850	0.233810
C	1.694755	0.687299	-2.733059
C	2.729679	1.226444	-3.500594
C	4.044554	1.203530	-3.041343
C	4.343963	0.647724	-1.803052
C	3.336875	0.103674	-0.998451
C	0.248111	0.740980	-3.193381
H	2.510493	1.665590	-4.471742
H	4.840597	1.623398	-3.655288
H	5.376103	0.635865	-1.453650
C	3.684353	-0.497845	0.352095
H	2.744717	-0.732396	0.863427
C	4.463671	-1.807372	0.183897
C	4.456485	0.491232	1.231424
H	-0.244114	-0.157761	-2.800399
C	-0.452879	1.958984	-2.575173
C	0.093424	0.749265	-4.714484
H	4.677353	-2.254323	1.163953
H	3.891647	-2.531610	-0.409052
H	5.419874	-1.628985	-0.326891
H	4.605479	0.066496	2.233261
H	5.447157	0.713159	0.813035
H	3.908753	1.436469	1.332593
H	-0.965611	0.634928	-4.978578
H	0.435734	1.697581	-5.150191
H	0.656137	-0.068752	-5.182068
H	-1.503568	1.998324	-2.892946
H	-0.428678	1.914302	-1.478863
H	0.042477	2.885494	-2.896989

L^1:

RM052x/def2-SVP Singlet: -834.752590

C	3.071967	4.135420	2.409631
C	3.628813	2.864850	2.499019
C	3.125892	1.917154	3.396449
C	2.058032	2.296490	4.230775
C	1.425895	3.546769	4.093850
C	1.962983	4.461083	3.183149
N	1.570761	1.376121	5.226176
C	0.650127	0.490196	4.945238
C	0.414340	-0.298464	6.221041
C	1.169665	0.457767	7.343968
C	2.147160	1.405189	6.629426
C	0.969900	-1.712137	5.989135
C	-1.088445	-0.384577	6.498884
C	3.587087	0.885320	6.636383
C	2.146008	2.813678	7.222473
C	3.629262	0.484707	3.336137
C	5.152343	0.373748	3.241957
C	0.110168	3.860296	4.787031
C	0.043895	5.279269	5.355645
C	2.944346	-0.229026	2.161655
C	-1.039104	3.595769	3.803892
H	4.456975	2.594701	1.845502
H	3.481768	4.862770	1.709908
H	1.493232	5.436115	3.063674
H	0.796306	-2.333455	6.878818
H	2.048581	-1.694370	5.785496
H	0.472265	-2.175800	5.128803
H	-1.596552	-0.896400	5.672781
H	-1.525428	0.618610	6.596533
H	-1.275629	-0.936649	7.431050
H	3.983734	0.953819	7.657277
H	4.223791	1.493390	5.980890
H	3.646005	-0.161652	6.319357
H	2.571736	2.767189	8.233197
H	1.133798	3.223038	7.303017
H	2.760953	3.498042	6.623588
H	3.306669	-0.025126	4.246594
H	5.650273	0.933531	4.044183
H	5.526593	0.750480	2.281202
H	5.454385	-0.679108	3.316819
H	3.268126	-1.277691	2.109729
H	3.201018	0.260224	1.211914
H	1.855302	-0.199983	2.289519
H	-0.015498	3.154966	5.613366
H	-0.880545	5.407704	5.933805
H	0.035362	6.033509	4.557966
H	0.897075	5.489013	6.013618
H	-1.010498	2.552803	3.464595
H	-0.953768	4.251840	2.926707
H	-2.007851	3.786106	4.285884
H	0.458274	1.043787	7.941278
H	1.696577	-0.220314	8.027706

UM052x/def2-SVP Triplet: -834.676760

C	2.665563	4.166861	2.192573
C	3.445411	3.020260	2.268258
C	3.157829	2.011858	3.194641
C	2.075004	2.187073	4.080873
C	1.262375	3.340927	3.994481
C	1.574773	4.315116	3.044019
N	1.795717	1.175148	5.046690
C	0.690201	0.356559	4.994696
C	0.116605	-0.060791	6.321323
C	1.075041	0.738152	7.258740
C	2.332844	1.136846	6.436274
C	0.215392	-1.579268	6.544519
C	-1.346660	0.359802	6.526551
C	3.434206	0.078764	6.574814
C	2.881662	2.494452	6.861249
C	3.984682	0.739031	3.181029
C	5.462352	1.016336	3.477892
C	0.037519	3.523554	4.872156
C	-0.065803	4.929369	5.472064
C	3.822769	-0.000942	1.847868
C	-1.230192	3.173519	4.082062
H	4.285937	2.894497	1.585863
H	2.899171	4.942178	1.463811
H	0.955159	5.207946	2.969428
H	-0.158069	-1.843949	7.544211
H	1.248137	-1.932716	6.451857
H	-0.391503	-2.107494	5.798131
H	-1.994815	-0.160506	5.809320
H	-1.475669	1.438888	6.383560
H	-1.680170	0.098328	7.540972
H	3.689944	-0.061156	7.633716
H	4.340797	0.390131	6.043053
H	3.103414	-0.881974	6.163470
H	3.218050	2.434832	7.904776
H	2.119530	3.278364	6.783732

H	3.737498	2.782356	6.237064
H	3.585598	0.090301	3.965875
H	5.584208	1.573736	4.415810
H	5.921236	1.610378	2.675786
H	6.021199	0.074176	3.558571
H	4.376658	-0.949241	1.869137
H	4.208637	0.597317	1.011205
H	2.766135	-0.220589	1.651683
H	0.121010	2.810700	5.698331
H	-0.883332	4.964324	6.204374
H	-0.285068	5.681971	4.703598
H	0.864706	5.221409	5.975914
H	-1.182670	2.140163	3.714972
H	-1.336769	3.843186	3.217435
H	-2.123630	3.280701	4.712792
H	0.566137	1.651997	7.594735
H	1.345361	0.157831	8.150739

L:$SiCl_2$

RM052x/def2-SVP Singlet: -2368.651933

C	3.484268	0.222216	-1.134772
C	2.115486	0.130889	-1.427178
C	1.570339	0.427615	-2.682243
C	2.460289	0.822306	-3.683847
C	3.823692	0.927728	-3.428952
C	4.330441	0.634438	-2.166589
N	1.238837	-0.314390	-0.372402
C	0.577349	0.448402	0.520476
N	0.007449	-0.426637	1.379065
C	0.298265	-1.726976	1.023679
C	1.073632	-1.656055	-0.088282
C	-0.739561	-0.064393	2.557925
C	-2.139575	-0.157742	2.530002
C	-2.823330	0.154301	3.709702
C	-2.137967	0.547417	4.852677
C	-0.749033	0.642053	4.844524
C	-0.016545	0.339052	3.695983
C	-2.903720	-0.615302	1.299320
C	-4.150393	0.235988	1.040872
C	1.502422	0.405644	3.706041
C	2.089754	-0.906277	4.243681
C	0.080426	0.334861	-2.956393
C	-0.239839	-0.945521	-3.737701
C	4.033648	-0.033265	0.260003
C	4.327382	1.297968	0.965003
C	-3.288811	-2.095480	1.429845
C	2.033619	1.608764	4.488099
C	-0.446950	1.577333	-3.679286
C	5.272314	-0.933455	0.244683
H	-0.061324	-2.572951	1.596651
H	1.536995	-2.424812	-0.695780
H	-3.909972	0.093909	3.727590
H	-2.690706	0.789658	5.759360
H	-0.228187	0.960750	5.745128
H	1.842614	0.528882	2.671210
H	-2.244016	-0.492432	0.431687
H	3.187446	-0.872118	4.217485
H	1.774336	-1.067301	5.283549
H	1.757519	-1.768632	3.651433
H	3.117678	1.695033	4.338965
H	1.561475	2.535268	4.139133
H	1.858712	1.503317	5.566826
H	-3.821755	-2.430653	0.530494
H	-2.411190	-2.738616	1.568373
H	-3.949956	-2.240961	2.295115
H	-4.582531	-0.033036	0.068544
H	-4.921499	0.062471	1.803240
H	-3.895100	1.300758	1.019807
H	2.076623	1.067189	-4.672784
H	4.498556	1.250092	-4.220820
H	5.397934	0.737063	-1.977647
H	3.263179	-0.554515	0.842823
H	-0.440113	0.293764	-1.992631
H	5.579451	-1.163834	1.273179
H	5.074611	-1.877459	-0.278845
H	6.120017	-0.440739	-0.248539
H	4.654242	1.119262	1.998694
H	5.126647	1.838337	0.439356
H	3.444327	1.948443	0.972058
H	-1.320171	-1.022607	-3.917616
H	0.270475	-0.940247	-4.710821
H	0.084574	-1.841515	-3.191801
H	-1.542719	1.537482	-3.724210
H	-0.160262	2.484941	-3.136142
H	-0.069524	1.638090	-4.709150
Si	0.256215	2.436724	0.825338
Cl	-1.627019	2.260614	-0.315357
Cl	1.544320	3.167672	-0.772780

UM052x/def2-SVP Triplet: -2368.579704

C	3.433079	0.289760	-1.118395
C	2.073196	0.154081	-1.442618
C	1.550567	0.559427	-2.682317
C	2.436787	1.095124	-3.619394
C	3.790501	1.230028	-3.324646
C	4.282853	0.833300	-2.085892
N	1.181160	-0.381128	-0.463968
C	0.546003	0.385228	0.524327
N	0.024736	-0.557026	1.420884
C	0.359991	-1.832804	1.006277
C	1.067149	-1.726292	-0.145130
C	-0.691103	-0.195232	2.598193
C	-2.099348	-0.205787	2.563881
C	-2.781716	0.141242	3.732850
C	-2.088486	0.504725	4.883720
C	-0.697723	0.536028	4.885974
C	0.029417	0.191676	3.743014
C	-2.855178	-0.613743	1.310755
C	-4.090454	0.255235	1.060675
C	1.547479	0.238387	3.762640
C	2.117825	-0.757314	4.779004
C	0.074145	0.399623	-2.998560
C	-0.169966	-0.931949	-3.720264
C	3.975544	-0.096738	0.246786
C	4.414717	1.148180	1.026241
C	-3.249056	-2.095319	1.384776
C	2.047216	1.661211	4.035792
C	-0.486337	1.574867	-3.801708
C	5.111681	-1.118540	0.134968
H	0.071792	-2.709729	1.574102
H	1.515538	-2.492419	-0.767727
H	-3.870308	0.135180	3.740273
H	-2.638129	0.773971	5.784848

H	-0.166727	0.832003	5.790305
H	1.904906	-0.051013	2.767746
H	-2.175857	-0.477993	0.458580
H	3.215501	-0.744390	4.747701
H	1.806245	-0.502348	5.800934
H	1.777061	-1.778267	4.564875
H	3.143927	1.692930	4.001682
H	1.659227	2.361540	3.284137
H	1.728112	2.011018	5.026806
H	-3.771395	-2.398672	0.467945
H	-2.371570	-2.740746	1.510385
H	-3.920585	-2.266169	2.237571
H	-4.512172	0.020488	0.074977
H	-4.873729	0.066435	1.806901
H	-3.832837	1.320217	1.075186
H	2.063449	1.420251	-4.588653
H	4.466140	1.655848	-4.065578
H	5.342194	0.956652	-1.862397
H	3.162191	-0.567671	0.811024
H	-0.467476	0.368292	-2.045117
H	5.444177	-1.426921	1.134938
H	4.786470	-2.012454	-0.412520
H	5.978992	-0.696565	-0.389906
H	4.751629	0.866054	2.033380
H	5.247354	1.654681	0.519063
H	3.585570	1.860661	1.115677
H	-1.239304	-1.064264	-3.931783
H	0.376986	-0.955409	-4.672956
H	0.169710	-1.779747	-3.111660
H	-1.579064	1.493740	-3.860926
H	-0.242248	2.528838	-3.318587
H	-0.097456	1.586948	-4.828831
Si	-0.047493	2.114792	0.495048
Cl	-1.825919	2.615624	-0.606466
Cl	1.416199	3.291135	-0.423812

L^1:$SiCl_2$

RM052x/def2-SVP Singlet: -2044.392183

C	2.853439	3.960050	2.463949
H	3.575183	3.139577	2.362594
H	2.039764	3.617291	3.116425
H	3.373244	4.790018	2.959887
C	2.329483	4.418352	1.098595
C	3.491794	4.789138	0.167816
C	1.424037	3.383773	0.446067
C	0.218884	3.724283	-0.203073
C	-0.556568	2.769073	-0.881879
C	-0.119397	1.440408	-0.856176
C	1.054432	1.078507	-0.210652
C	1.823106	2.047223	0.425626
N	-0.152292	5.121084	-0.170406
C	-1.072611	5.682739	0.885020
C	-0.604384	7.141257	0.924294
C	0.106304	7.418150	-0.425010
C	0.367203	6.018691	-0.981337
C	1.454265	8.112351	-0.152711
C	-0.722463	8.293481	-1.377300
C	-0.922212	4.956077	2.216120
C	-2.527243	5.596310	0.417299
Si	0.691734	5.703414	-2.877282
C	-1.792191	3.104655	-1.700078
C	-3.040992	2.410931	-1.138059
Cl	1.907972	3.931897	-2.945707
Cl	2.189627	7.185423	-3.334353
C	-1.606609	2.717091	-3.174490
H	2.104556	7.480561	0.466014
H	1.257677	9.044372	0.395500
H	1.979982	8.345728	-1.082226
H	0.107459	7.275958	1.749481
H	-1.444219	7.826007	1.091843
H	2.757209	1.760739	0.905536
H	1.382871	0.040046	-0.217078
H	-0.700389	0.681390	-1.378039
H	-1.694404	7.843071	-1.610305
H	-0.179393	8.453569	-2.316540
H	-0.891186	9.271060	-0.905930
H	-1.594168	5.425259	2.945775
H	0.100489	5.018462	2.602814
H	-1.198737	3.898586	2.121026
H	-2.870730	4.560039	0.363448
H	-2.656372	6.065669	-0.565471
H	-3.158314	6.127317	1.141186
H	1.741743	5.327551	1.263724
H	4.088172	3.898306	-0.071038
H	4.146484	5.523841	0.656438
H	3.132959	5.208629	-0.779394
H	-1.935661	4.190514	-1.665859
H	-2.977432	1.326224	-1.296430
H	-3.942393	2.770466	-1.651762
H	-3.162017	2.575693	-0.060324
H	-1.561467	1.625803	-3.288991
H	-0.683537	3.140143	-3.584360
H	-2.456629	3.083024	-3.765108

UM052x/def2-SVP Triplet: -2044.351009

C	2.726873	3.661702	2.619930
H	3.068122	2.622842	2.721845
H	1.799176	3.766462	3.190597
H	3.489594	4.306503	3.076582
C	2.553001	4.025238	1.139073
C	3.897494	3.825108	0.421139
C	1.459691	3.211803	0.459995
C	0.323363	3.782725	-0.156673
C	-0.553858	2.981551	-0.926624
C	-0.317473	1.607246	-0.999903
C	0.760905	1.026040	-0.343582
C	1.643314	1.827896	0.366504
N	0.064617	5.190483	-0.038562
C	-0.775613	5.762492	1.056829
C	-0.743739	7.265428	0.722814
C	-0.393257	7.403092	-0.773756
C	0.357051	6.100659	-1.030413
C	0.456744	8.656063	-1.016121
C	-1.644113	7.492833	-1.665565
C	-0.164012	5.495261	2.430154
C	-2.196042	5.186498	1.066852
Si	1.760014	6.067855	-2.219470
C	-1.707219	3.556578	-1.734018
C	-3.040533	2.859039	-1.439752
Cl	2.216890	4.157258	-2.933754
Cl	3.584345	6.778968	-1.395015
C	-1.406286	3.496307	-3.237411
H	1.396395	8.615449	-0.451682

H	-0.101568	9.552012	-0.711152
H	0.702045	8.766526	-2.082995
H	0.049494	7.743043	1.313251
H	-1.693731	7.754620	0.975040
H	2.511825	1.375351	0.843117
H	0.926737	-0.048744	-0.406418
H	-0.987375	0.983410	-1.590434
H	-2.327426	6.652518	-1.503615
H	-1.349689	7.488556	-2.723870
H	-2.190190	8.424826	-1.460798
H	-0.762258	6.009770	3.193628
H	0.864442	5.867106	2.487102
H	-0.173626	4.421883	2.655802
H	-2.159139	4.094685	1.166608
H	-2.764705	5.439924	0.167248
H	-2.734269	5.590197	1.933844
H	2.284151	5.085059	1.054130
H	4.269834	2.803486	0.575261
H	4.643513	4.521661	0.825527
H	3.813745	4.000407	-0.655556
H	-1.800094	4.610700	-1.467880
H	-3.034130	1.823812	-1.805353
H	-3.858205	3.382186	-1.953691
H	-3.265479	2.836148	-0.367057
H	-1.292742	2.455530	-3.570742
H	-0.479212	4.027067	-3.476916
H	-2.231327	3.948150	-3.804989

$(L^1:)_2SiCl_2$

RM052x/def2-SVP Singlet: -2879.180062
RM052x/def2-TZVPP//def2-SVP: -2881.52173095
CASSCF[2,2]//RM052x/def2-SVP: -2866.0778038504

Cl	2.719007	4.276820	2.291414
Si	3.925345	2.564079	2.487322
N	3.144431	0.293427	4.118353
C	2.815135	1.237418	3.169541
Cl	5.295915	2.997103	4.024987
N	4.573270	2.935094	-0.321125
C	1.525956	0.791765	2.441234
C	2.363285	-0.977461	3.948023
C	3.732684	0.600337	5.398677
C	4.933037	-0.019475	5.807373
C	5.437097	0.245194	7.084307
H	6.366845	-0.230983	7.394107
C	4.791855	1.115568	7.951106
H	5.204865	1.318852	8.938240
C	3.612615	1.724944	7.542176
H	3.098404	2.407371	8.218227
C	3.057358	1.474031	6.285672
C	1.755610	0.458186	0.961231
H	0.809505	0.145381	0.495619
H	2.491010	-0.343095	0.832409
H	2.122608	1.346341	0.436384
C	0.389510	1.830751	2.503702
H	0.630234	2.723825	1.925859
H	0.173732	2.142056	3.531765
H	-0.522096	1.378679	2.086032
C	3.103814	-1.992425	3.065103
H	2.395643	-2.750398	2.705845
H	3.891384	-2.508527	3.622847
H	3.557788	-1.500330	2.199314
C	2.010612	-1.626794	5.281994
H	1.367677	-2.495120	5.086304
H	1.470925	-0.929025	5.931065
H	2.903547	-1.966557	5.816922
C	5.757568	-0.915220	4.901075
H	5.252429	-0.943746	3.932796
C	5.874656	-2.348126	5.434943
H	4.895301	-2.811019	5.604340
H	6.416239	-2.360284	6.390244
H	6.433404	-2.973806	4.725327
C	7.158470	-0.325718	4.688788
H	7.674194	-0.842021	3.867520
H	7.771284	-0.437265	5.593257
H	7.095371	0.741669	4.455340
C	1.747912	2.161535	5.947999
H	1.435159	1.800717	4.968144
C	0.635508	1.823324	6.948053
H	-0.311338	2.272824	6.618630
H	0.860170	2.221151	7.946402
H	0.486699	0.740435	7.044870
C	1.932626	3.680491	5.847883
H	2.757540	3.937645	5.175814
H	2.149726	4.106834	6.837370
H	1.016882	4.152940	5.466824
C	4.935119	2.477285	0.926875
C	6.120165	1.495955	0.779389
C	6.457978	1.604248	-0.720709
H	7.273109	2.328642	-0.857827
H	6.791515	0.644653	-1.136003
C	5.203796	2.136698	-1.424259
C	4.093479	4.269539	-0.582334
C	4.916095	5.376627	-0.260280
C	4.449334	6.665887	-0.523353
H	5.075331	7.517494	-0.259160
C	3.217296	6.882983	-1.126554
H	2.872702	7.896324	-1.328280
C	2.433976	5.792016	-1.474977
H	1.467554	5.955657	-1.950444
C	2.846555	4.483026	-1.208397
C	5.765500	0.057312	1.177785
H	4.954088	-0.347849	0.563808
H	5.447872	0.032409	2.225744
H	6.647339	-0.590766	1.066418
C	7.360824	1.900167	1.600171
H	8.206197	1.268167	1.290506
H	7.195633	1.757003	2.668614
H	7.638327	2.947523	1.439146
C	5.580047	3.000775	-2.623250
H	6.108008	2.372270	-3.352504
H	6.240331	3.822643	-2.326064
H	4.697087	3.431104	-3.107423
C	4.301374	0.982676	-1.886073
H	3.502853	1.336897	-2.545329
H	3.844544	0.476260	-1.029806
H	4.899778	0.253143	-2.447157
C	6.299485	5.239550	0.347151
H	6.538564	4.175581	0.372599
C	6.327642	5.766234	1.786726
H	6.171937	6.854212	1.798696
H	7.300420	5.557531	2.253207
H	5.546757	5.302425	2.397513
C	7.374883	5.935870	-0.496731
H	7.362590	5.592283	-1.538897

H	8.368886	5.730307	-0.076628
H	7.238357	7.025076	-0.501366
C	1.888999	3.359960	-1.559917
H	2.335648	2.433351	-1.192067
C	1.669139	3.230239	-3.072213
H	1.190346	4.135170	-3.469737
H	1.009537	2.378624	-3.288851
H	2.608427	3.085925	-3.618867
C	0.538453	3.551862	-0.856961
H	-0.040234	4.354500	-1.333410
H	0.684411	3.821449	0.193542
H	-0.058809	2.631453	-0.910530
C	1.104491	-0.452798	3.247417
H	0.375066	-0.155793	4.014078
H	0.632850	-1.214469	2.613241

UM052x/def2-SVP Triplet: -2879.194378
UM052x/TZVPP//SVP: -2881.53373845
CASSCF[2,2]//UM052x/def2-SVP: -2866.0801926959

Cl	2.634063	4.002436	2.293805
Si	3.908093	2.322793	2.337366
N	3.233862	0.175274	4.201768
C	3.001913	0.858397	3.011560
Cl	5.341473	2.888953	3.777656
N	4.477397	2.975897	-0.454343
C	1.757871	0.269810	2.314008
C	2.472116	-1.112551	4.219919
C	3.783286	0.696346	5.421216
C	5.009082	0.193627	5.911662
C	5.448988	0.592209	7.177131
H	6.390075	0.199620	7.560905
C	4.718482	1.488289	7.945754
H	5.072393	1.784822	8.932250
C	3.543473	2.021471	7.432402
H	2.982131	2.746239	8.020841
C	3.059469	1.649838	6.174951
C	2.047772	-0.397320	0.959513
H	1.102825	-0.731984	0.509132
H	2.710927	-1.262200	1.042605
H	2.511805	0.329661	0.280922
C	0.659623	1.314196	2.046089
H	0.944431	1.988602	1.231534
H	0.440857	1.922368	2.931698
H	-0.260917	0.792539	1.746214
C	3.277782	-2.246311	3.566402
H	2.609787	-3.085528	3.331494
H	4.058699	-2.615102	4.236945
H	3.755362	-1.910147	2.641316
C	2.065421	-1.541749	5.625061
H	1.449186	-2.447086	5.547936
H	1.485523	-0.763169	6.129095
H	2.940041	-1.767721	6.245913
C	5.914736	-0.721270	5.104249
H	5.449648	-0.861505	4.121403
C	6.095195	-2.089346	5.776736
H	5.136867	-2.560233	6.025203
H	6.659370	-1.982697	6.712949
H	6.658226	-2.768861	5.122343
C	7.292037	-0.076051	4.889123
H	7.883384	-0.671600	4.180177
H	7.852799	-0.026941	5.831910
H	7.193348	0.942789	4.500663
C	1.795857	2.334576	5.677688
H	1.624437	2.010997	4.647652
C	0.558752	1.978449	6.511209
H	-0.320406	2.508954	6.121160
H	0.694996	2.279258	7.558827
H	0.340538	0.904381	6.496326
C	1.987058	3.858023	5.659306
H	2.915383	4.130717	5.146225
H	2.021108	4.260867	6.680657
H	1.150840	4.337616	5.133962
C	4.699973	2.189250	0.671834
C	5.828530	1.178269	0.378011
C	6.292581	1.624626	-1.022905
H	7.118556	2.342548	-0.916010
H	6.647089	0.782989	-1.632174
C	5.102298	2.349076	-1.660557
C	4.061045	4.349097	-0.496747
C	4.926985	5.366149	-0.030806
C	4.560971	6.701427	-0.221914
H	5.230077	7.487310	0.126668
C	3.368070	7.045900	-0.844312
H	3.106454	8.092850	-0.992138
C	2.502362	6.041171	-1.254656
H	1.549868	6.307121	-1.711971
C	2.821297	4.691421	-1.079936
C	5.381731	-0.292754	0.397532
H	4.636147	-0.522330	-0.368257
H	4.955351	-0.538917	1.378286
H	6.254760	-0.939263	0.231426
C	7.006293	1.278734	1.362725
H	7.846696	0.685093	0.974399
H	6.735702	0.877321	2.345000
H	7.344537	2.312578	1.499419
C	5.553357	3.374791	-2.694077
H	6.072982	2.848122	-3.505276
H	6.235555	4.109698	-2.257295
H	4.701606	3.916858	-3.120718
C	4.143717	1.354302	-2.334286
H	3.387895	1.875262	-2.928371
H	3.626877	0.735810	-1.594348
H	4.708809	0.696567	-3.007863
C	6.224684	5.091118	0.713053
H	6.297535	4.010986	0.867306
C	6.198258	5.758974	2.095726
H	6.285626	6.850256	2.003964
H	7.039744	5.402620	2.704184
H	5.269169	5.528106	2.627435
C	7.465700	5.556112	-0.058606
H	7.573713	5.047399	-1.023330
H	8.369328	5.356391	0.533092
H	7.423026	6.636667	-0.251510
C	1.778599	3.660851	-1.478644
H	2.166037	2.674882	-1.195832
C	1.501744	3.681748	-2.988251
H	1.015158	4.624477	-3.272275
H	0.829137	2.859598	-3.268396
H	2.420329	3.596998	-3.580513
C	0.463187	3.890296	-0.719081
H	-0.032150	4.807684	-1.063435
H	0.641140	3.984958	0.357167
H	-0.227051	3.053670	-0.893714
C	1.255805	-0.739466	3.365790
H	0.516417	-0.244841	4.011756

H	0.779291	-1.616498	2.908860

UM052x/def2-SVP Biradical: -2879.198528
UM052x/TZVPP//SVP: -2881.53874807

Cl	2.701556	4.200698	2.283987
Si	3.922341	2.498791	2.443741
N	3.192847	0.246307	4.142581
C	2.868999	1.120118	3.107315
Cl	5.304623	2.964552	3.955843
N	4.519736	2.937584	-0.376539
C	1.606509	0.620220	2.380688
C	2.417071	-1.031609	4.031573
C	3.737710	0.635609	5.418400
C	4.973553	0.111400	5.856812
C	5.437368	0.437210	7.134846
H	6.390645	0.031124	7.471293
C	4.721061	1.281736	7.971366
H	5.102257	1.532309	8.960450
C	3.515496	1.809012	7.528193
H	2.951238	2.478313	8.176783
C	2.999904	1.493516	6.268769
C	1.875761	0.197076	0.928139
H	0.937722	-0.120864	0.451069
H	2.593584	-0.625972	0.860084
H	2.275972	1.047473	0.362314
C	0.468089	1.655321	2.330679
H	0.697746	2.462151	1.631561
H	0.270804	2.103072	3.311212
H	-0.449574	1.155928	1.986798
C	3.192833	-2.090119	3.235853
H	2.524747	-2.926184	2.990090
H	4.030469	-2.487510	3.816377
H	3.587591	-1.674535	2.304023
C	2.037891	-1.607546	5.391985
H	1.410405	-2.494218	5.232442
H	1.475034	-0.881407	5.987051
H	2.922264	-1.903963	5.966859
C	5.867948	-0.753683	4.986458
H	5.408361	-0.799345	3.993880
C	6.004387	-2.179038	5.538667
H	5.032621	-2.662486	5.691598
H	6.519811	-2.162761	6.508464
H	6.596920	-2.800792	4.853442
C	7.264200	-0.130552	4.841415
H	7.824705	-0.630345	4.039687
H	7.841133	-0.242426	5.769029
H	7.194729	0.938419	4.614921
C	1.671230	2.115678	5.879428
H	1.395494	1.713528	4.903688
C	0.545703	1.775958	6.864199
H	-0.404040	2.192760	6.502130
H	0.738877	2.207333	7.855145
H	0.419516	0.693410	6.989540
C	1.811075	3.637146	5.741685
H	2.658438	3.902718	5.101441
H	1.969840	4.096907	6.727114
H	0.900137	4.070652	5.306678
C	4.862874	2.367802	0.847187
C	6.011894	1.361594	0.647657
C	6.377822	1.574531	-0.835186
H	7.213249	2.285575	-0.904191
H	6.692739	0.640632	-1.318706
C	5.147977	2.190440	-1.514448
C	4.100527	4.302638	-0.564915
C	4.977714	5.361621	-0.230055
C	4.571699	6.677909	-0.462859
H	5.242093	7.493210	-0.192955
C	3.341916	6.966416	-1.039292
H	3.046665	7.998925	-1.221324
C	2.491277	5.922712	-1.376661
H	1.521043	6.143719	-1.820068
C	2.843104	4.590679	-1.139316
C	5.602829	-0.091713	0.935287
H	4.807783	-0.440776	0.268855
H	5.246143	-0.182686	1.968462
H	6.471547	-0.754626	0.813887
C	7.245170	1.654619	1.521660
H	8.085868	1.040717	1.166616
H	7.058707	1.401772	2.567510
H	7.541864	2.708765	1.476866
C	5.555721	3.106280	-2.663862
H	6.074926	2.504688	-3.421398
H	6.230801	3.896499	-2.320551
H	4.686410	3.581806	-3.131745
C	4.212034	1.097621	-2.048057
H	3.380942	1.528917	-2.613689
H	3.797803	0.500126	-1.230692
H	4.770492	0.432484	-2.719909
C	6.347149	5.147969	0.388658
H	6.524172	4.071782	0.426517
C	6.380137	5.685246	1.825134
H	6.316365	6.782459	1.824274
H	7.317466	5.399891	2.322242
H	5.545233	5.296012	2.416372
C	7.473116	5.782188	-0.437487
H	7.476930	5.422512	-1.473818
H	8.445898	5.542876	0.013185
H	7.381644	6.875919	-0.463382
C	1.814586	3.522989	-1.466165
H	2.208492	2.571367	-1.095181
C	1.566957	3.405661	-2.976015
H	1.115100	4.330388	-3.359568
H	0.874330	2.579478	-3.187999
H	2.491921	3.234645	-3.538676
C	0.483159	3.802064	-0.753752
H	-0.051518	4.632218	-1.234123
H	0.648688	4.070303	0.294868
H	-0.167772	2.918274	-0.798251
C	1.173416	-0.569993	3.261005
H	0.417179	-0.230545	3.982988
H	0.730435	-1.380570	2.667734

RI-RB3LYP/def2-SVP Singlet: -2878.148858569
RI-RB3LYP/def2-TZVPP//def2-SVP: -2880.379748532

Cl	2.6880814	4.2284955	2.3149170
Si	3.9245101	2.5179804	2.4575773
N	3.1506290	0.2630468	4.1609464
C	2.8158528	1.1817899	3.1720587
Cl	5.3247947	3.0141280	3.9636188
N	4.5620247	2.9555312	-0.3682656
C	1.5275659	0.6932317	2.4429140
C	2.3818069	-1.0389773	4.0095645
C	3.7388547	0.6020940	5.4443942
C	4.9468266	-0.0157419	5.8717547

C	5.4161623	0.2292341	7.1712510
H	6.3418306	-0.2490601	7.5007002
C	4.7453572	1.0800303	8.0421182
H	5.1294017	1.2583776	9.0501229
C	3.5852126	1.7123551	7.6062261
H	3.0621746	2.3919966	8.2834514
C	3.0584392	1.4944836	6.3254166
C	1.7510566	0.3081398	0.9649948
H	0.8107257	-0.0638933	0.5230803
H	2.5133965	-0.4733766	0.8475366
H	2.0730578	1.1802969	0.3801747
C	0.3679862	1.7188673	2.4738681
H	0.5824577	2.6018505	1.8625142
H	0.1492049	2.0623813	3.4948130
H	-0.5459130	1.2429888	2.0782410
C	3.1419945	-2.0650863	3.1431597
H	2.4532038	-2.8668776	2.8322050
H	3.9657947	-2.5367138	3.6923836
H	3.5565547	-1.6041993	2.2378662
C	2.0221784	-1.6844128	5.3520968
H	1.3846190	-2.5625679	5.1613292
H	1.4656109	-0.9954087	6.0014318
H	2.9086288	-2.0245836	5.9042804
C	5.8203709	-0.8900976	4.9746282
H	5.3495952	-0.9138874	3.9834364
C	5.9436447	-2.3387530	5.4839754
H	4.9646170	-2.8193945	5.6299353
H	6.4720614	-2.3766012	6.4507126
H	6.5188445	-2.9532228	4.7711414
C	7.2257730	-0.2820713	4.7998021
H	7.7910612	-0.8295922	4.0274413
H	7.8077272	-0.3369903	5.7342622
H	7.1683502	0.7747536	4.5058298
C	1.7729681	2.2401359	5.9735647
H	1.5237972	2.0005673	4.9352150
C	0.5842441	1.8082884	6.8526780
H	-0.3367222	2.3247957	6.5339048
H	0.7498434	2.0569767	7.9140131
H	0.3981297	0.7241686	6.7939410
C	1.9651741	3.7674062	6.0356722
H	2.8155287	4.0898506	5.4189911
H	2.1409370	4.1127538	7.0682246
H	1.0636088	4.2813324	5.6634096
C	4.9287778	2.4460778	0.8730532
C	6.1079861	1.4448190	0.6805938
C	6.4349734	1.6073745	-0.8244395
H	7.2522415	2.3364584	-0.9427465
H	6.7748848	0.6641252	-1.2791749
C	5.1756997	2.1631323	-1.5104461
C	4.0989799	4.3113427	-0.6054448
C	4.9276460	5.4182511	-0.2536345
C	4.5125853	6.7111661	-0.6023377
H	5.1488745	7.5591432	-0.3374511
C	3.3224642	6.9431641	-1.2846345
H	3.0270486	7.9605152	-1.5550146
C	2.5082823	5.8628354	-1.6043488
H	1.5601924	6.0431505	-2.1169659
C	2.8619884	4.5474265	-1.2672390
C	5.7511048	-0.0181060	1.0198623
H	4.9031838	-0.3893180	0.4291427
H	5.4886714	-0.1179798	2.0816214
H	6.6161730	-0.6750696	0.8247962
C	7.3704270	1.8051181	1.5018327
H	8.2014799	1.1469920	1.1944298
H	7.2136239	1.6732244	2.5777522
H	7.6886701	2.8437739	1.3339125
C	5.5500099	3.0349876	-2.7137808
H	6.0779316	2.4097057	-3.4516309
H	6.2163083	3.8604397	-2.4294483
H	4.6695536	3.4686171	-3.2070534
C	4.2557211	1.0179251	-1.9829976
H	3.4186141	1.3863260	-2.5882189
H	3.8417176	0.4540703	-1.1376025
H	4.8310128	0.3178990	-2.6101066
C	6.2597246	5.2983787	0.4836106
H	6.4147706	4.2410111	0.7193016
C	6.2348562	6.0473016	1.8297053
H	6.1597359	7.1381423	1.6857655
H	7.1616387	5.8505722	2.3936137
H	5.3876258	5.7264472	2.4514905
C	7.4501594	5.7669012	-0.3741992
H	7.5132164	5.2204936	-1.3286465
H	8.3984429	5.6091029	0.1664700
H	7.3832376	6.8411119	-0.6136686
C	1.8414556	3.4554499	-1.5811650
H	2.2401638	2.5124728	-1.1854957
C	1.5958031	3.2787892	-3.0916799
H	1.1336635	4.1799133	-3.5271549
H	0.9096943	2.4353630	-3.2772643
H	2.5241099	3.0875908	-3.6507957
C	0.5016315	3.7218136	-0.8672352
H	-0.0210126	4.5897824	-1.3013649
H	0.6539249	3.9263807	0.2012679
H	-0.1687104	2.8517191	-0.9645560
C	1.1194700	-0.5392623	3.2871060
H	0.3783456	-0.2337761	4.0425215
H	0.6516465	-1.3254052	2.6744867

RI-UB3LYP/def2-SVP Triplet: -2878.153077444
RI-UB3LYP/def2-TZVPP//def2-SVP: -2880.382960713

Cl	2.6381122	4.0494979	2.3187962
Si	3.9114564	2.3581356	2.3606783
N	3.2033508	0.1758465	4.2313093
C	2.9494066	0.9082102	3.0560659
Cl	5.3486695	2.9271829	3.8077408
N	4.5073374	2.9980499	-0.4674808
C	1.6917673	0.3264073	2.3492520
C	2.4521540	-1.1391424	4.2038159
C	3.7523697	0.6682621	5.4759416
C	4.9850528	0.1517699	5.9660041
C	5.4214464	0.5275270	7.2452916
H	6.3633702	0.1250607	7.6261091
C	4.6940368	1.4128975	8.0330981
H	5.0503528	1.6910180	9.0286740
C	3.5163225	1.9553029	7.5290154
H	2.9549189	2.6674442	8.1385538
C	3.0232963	1.6077421	6.2626001
C	1.9741218	-0.2774927	0.9553626
H	1.0365209	-0.6537056	0.5129474
H	2.6866798	-1.1109994	0.9887424
H	2.3793237	0.4859837	0.2744376
C	0.5496338	1.3526404	2.1605915
H	0.7903818	2.1022277	1.3965461
H	0.3142023	1.8873577	3.0919700
H	-0.3624005	0.8245644	1.8324504

C	3.2703059	-2.2510022	3.5101231
H	2.6104247	-3.0991982	3.2661195
H	4.0693864	-2.6333692	4.1561777
H	3.7282661	-1.8989123	2.5770499
C	2.0390855	-1.6305730	5.5944584
H	1.4376511	-2.5468795	5.4820957
H	1.4319776	-0.8896303	6.1299869
H	2.9073746	-1.8720921	6.2234532
C	5.9077841	-0.7561625	5.1541457
H	5.4536294	-0.8841972	4.1618938
C	6.0805407	-2.1471121	5.7947390
H	5.1183357	-2.6439092	5.9904845
H	6.6103100	-2.0757964	6.7589024
H	6.6757655	-2.8061722	5.1406400
C	7.2932720	-0.1123999	4.9453480
H	7.8959379	-0.7158857	4.2463080
H	7.8554688	-0.0483959	5.8913760
H	7.2060063	0.9050100	4.5405664
C	1.7264823	2.2827291	5.8145932
H	1.5361366	1.9860701	4.7767442
C	0.5101348	1.8510553	6.6562225
H	-0.4065295	2.3369879	6.2822337
H	0.6285630	2.1392946	7.7139277
H	0.3462408	0.7630349	6.6279566
C	1.8556840	3.8185364	5.8286843
H	2.7361847	4.1548169	5.2644777
H	1.9381724	4.2080438	6.8569216
H	0.9657311	4.2807727	5.3712072
C	4.7607425	2.2443153	0.6943735
C	5.9036279	1.2281227	0.4091574
C	6.3150029	1.6037820	-1.0365805
H	7.1656538	2.3028993	-1.0028750
H	6.6375338	0.7265702	-1.6189219
C	5.1144649	2.3190263	-1.6775076
C	4.0927394	4.3818940	-0.5478821
C	4.9659520	5.4212426	-0.1117698
C	4.5913353	6.7551629	-0.3309791
H	5.2625832	7.5538157	-0.0061730
C	3.3945647	7.0885860	-0.9568872
H	3.1311890	8.1361131	-1.1266034
C	2.5296917	6.0717635	-1.3462420
H	1.5749695	6.3323008	-1.8098247
C	2.8444238	4.7198241	-1.1427132
C	5.4726898	-0.2521913	0.5118331
H	4.6817910	-0.5161792	-0.2011463
H	5.1057332	-0.4824569	1.5232842
H	6.3367851	-0.9084351	0.3141651
C	7.1323767	1.3930324	1.3346684
H	7.9626597	0.7762852	0.9491165
H	6.9241082	1.0628013	2.3599772
H	7.4792043	2.4352598	1.3824697
C	5.5623457	3.3021854	-2.7633646
H	6.0580497	2.7380708	-3.5695356
H	6.2751049	4.0430307	-2.3796075
H	4.7155209	3.8466410	-3.2043716
C	4.1425326	1.2969255	-2.3075922
H	3.3446251	1.7889643	-2.8761084
H	3.6730550	0.6584124	-1.5484738
H	4.6919138	0.6461221	-3.0068960
C	6.2994689	5.1839331	0.5977019
H	6.3975980	4.1066053	0.7740936
C	6.3351197	5.8731796	1.9757391
H	6.3488530	6.9712950	1.8775313
H	7.2437005	5.5795878	2.5265272
H	5.4667440	5.5959852	2.5885311
C	7.5091350	5.6333569	-0.2443531
H	7.5503666	5.1281179	-1.2213434
H	8.4495479	5.4112459	0.2871670
H	7.4868598	6.7190536	-0.4356678
C	1.7828288	3.6917242	-1.5311060
H	2.1576190	2.7029250	-1.2323117
C	1.5081351	3.6715306	-3.0474304
H	1.0518442	4.6185835	-3.3795338
H	0.8068946	2.8603260	-3.3056520
H	2.4241335	3.5287191	-3.6402722
C	0.4607293	3.9298185	-0.7741315
H	-0.0322296	4.8588272	-1.1044599
H	0.6268746	4.0079907	0.3088725
H	-0.2431317	3.1016162	-0.9604064
C	1.2280489	-0.7552989	3.3566862
H	0.4593950	-0.3286085	4.0203980
H	0.7783464	-1.6261525	2.8549944

RI-UB3LYP/def2-SVP Biradical: -2878.158226430
RI-UB3LYP/def2-TZVPP//def2-SVP: -2880.388584964

Cl	2.6756437	4.1867610	2.3213607
Si	3.9206801	2.4837217	2.4374903
N	3.1741221	0.2284922	4.1764870
C	2.8549950	1.0999593	3.1226384
Cl	5.3267493	2.9978786	3.9282280
N	4.5384229	2.9686164	-0.3995724
C	1.5773525	0.5876116	2.3984197
C	2.4007103	-1.0711207	4.0601562
C	3.7373776	0.6165754	5.4551597
C	4.9631268	0.0474361	5.9009091
C	5.4213944	0.3392146	7.1945969
H	6.3596709	-0.1027168	7.5387575
C	4.7223490	1.1914044	8.0419737
H	5.0983152	1.4072013	9.0457432
C	3.5443834	1.7761286	7.5886998
H	2.9996284	2.4567115	8.2476218
C	3.0275549	1.5079872	6.3128679
C	1.8269179	0.1398384	0.9411414
H	0.8919982	-0.2393830	0.4948516
H	2.5815612	-0.6542375	0.8673829
H	2.1686769	0.9852289	0.3265400
C	0.4206951	1.6148532	2.3594427
H	0.6344963	2.4517216	1.6853353
H	0.2044426	2.0320048	3.3532443
H	-0.4947987	1.1160774	1.9970139
C	3.1764217	-2.1299501	3.2477853
H	2.5002138	-2.9573774	2.9786802
H	4.0068099	-2.5588790	3.8215355
H	3.5859378	-1.7116133	2.3199048
C	2.0192809	-1.6706043	5.4179388
H	1.3914889	-2.5599641	5.2480623
H	1.4467681	-0.9635965	6.0325319
H	2.8986763	-1.9841226	5.9972654
C	5.8595846	-0.8305569	5.0298430
H	5.4024434	-0.8759776	4.0321165
C	5.9882757	-2.2680352	5.5696695
H	5.0113026	-2.7518386	5.7181723
H	6.5081622	-2.2806483	6.5417582
H	6.5738479	-2.8937164	4.8752057
C	7.2634451	-0.2151272	4.8667508

H	7.8406111	-0.7655829	4.1053810
H	7.8358158	-0.2605443	5.8076430
H	7.2050666	0.8393819	4.5643789
C	1.7211157	2.2056087	5.9380319
H	1.4738660	1.9190952	4.9108512
C	0.5449108	1.7785583	6.8367705
H	-0.3891010	2.2582908	6.4992763
H	0.7056114	2.0748729	7.8864784
H	0.3857370	0.6889114	6.8232874
C	1.8734280	3.7388790	5.9504844
H	2.7175093	4.0657610	5.3279850
H	2.0359396	4.1197433	6.9726242
H	0.9604973	4.2180450	5.5598880
C	4.8779707	2.3766720	0.8276267
C	6.0458582	1.3725315	0.6104024
C	6.4013743	1.6052954	-0.8790301
H	7.2319269	2.3258873	-0.9459752
H	6.7350166	0.6806312	-1.3750730
C	5.1630060	2.2146390	-1.5580694
C	4.1029241	4.3389962	-0.5877933
C	4.9555923	5.4216959	-0.2206608
C	4.5549781	6.7316272	-0.5214408
H	5.2091399	7.5616572	-0.2434869
C	3.3561607	7.0020865	-1.1731150
H	3.0722532	8.0315846	-1.4076018
C	2.5180391	5.9448320	-1.5087840
H	1.5639930	6.1556438	-1.9981568
C	2.8567829	4.6147940	-1.2172414
C	5.6578560	-0.0987714	0.8772854
H	4.8211491	-0.4345291	0.2506527
H	5.3676493	-0.2409816	1.9283137
H	6.5175344	-0.7605858	0.6771345
C	7.2983509	1.6682867	1.4697294
H	8.1313014	1.0295606	1.1283975
H	7.1291228	1.4576850	2.5315429
H	7.6216648	2.7154598	1.3830523
C	5.5670242	3.1244466	-2.7231866
H	6.0876307	2.5180247	-3.4816103
H	6.2475678	3.9239109	-2.4022921
H	4.6991894	3.5952997	-3.2054015
C	4.2300321	1.1063838	-2.0909973
H	3.3973104	1.5179745	-2.6739200
H	3.8083632	0.5025561	-1.2777071
H	4.7964710	0.4341422	-2.7556104
C	6.2979297	5.2576909	0.4904039
H	6.4449868	4.1898465	0.6815475
C	6.3023420	5.9617847	1.8610058
H	6.2485020	7.0577858	1.7515226
H	7.2303812	5.7287608	2.4087351
H	5.4552864	5.6404268	2.4823764
C	7.4829206	5.7455814	-0.3646305
H	7.5304408	5.2346446	-1.3390515
H	8.4355090	5.5592027	0.1589815
H	7.4236268	6.8284485	-0.5632638
C	1.8174410	3.5461453	-1.5504904
H	2.2011721	2.5883815	-1.1737951
C	1.5713976	3.4077727	-3.0652827
H	1.1173704	4.3237305	-3.4779494
H	0.8785570	2.5749234	-3.2725110
H	2.4986731	3.2238004	-3.6283030
C	0.4795473	3.8204180	-0.8354364
H	-0.0316528	4.7003236	-1.2590405
H	0.6303160	4.0084264	0.2364102
H	-0.2016723	2.9605671	-0.9468000
C	1.1521681	-0.6026625	3.2936401
H	0.3992523	-0.2595604	4.0207678
H	0.6921975	-1.4161537	2.7113041

RI-RPBE0/def2-SVP Singlet: -2877.069133549

RI-RPBE0/def2-TZVPP//def2-SVP: -2879.223533552

Cl	2.6966370	4.2272416	2.3091389
Si	3.9247690	2.5330591	2.4677797
N	3.1716413	0.2741409	4.1344947
C	2.8297906	1.1941775	3.1621702
Cl	5.3130967	3.0093110	3.9676835
N	4.5403578	2.9415497	-0.3430075
C	1.5479226	0.7147788	2.4415692
C	2.4102416	-1.0138015	3.9836157
C	3.7564864	0.6090731	5.4061036
C	4.9519367	-0.0169134	5.8354871
C	5.4190943	0.2234632	7.1317654
H	6.3398412	-0.2640050	7.4623298
C	4.7549530	1.0798830	7.9967769
H	5.1365257	1.2557414	9.0054930
C	3.6062263	1.7224720	7.5560772
H	3.0856791	2.4096405	8.2279316
C	3.0850934	1.5076821	6.2774537
C	1.7726984	0.3429809	0.9706694
H	0.8327852	-0.0180889	0.5207913
H	2.5318293	-0.4407420	0.8503614
H	2.1049835	1.2203792	0.3991258
C	0.3985343	1.7368121	2.4810839
H	0.6190768	2.6263078	1.8813979
H	0.1775810	2.0684977	3.5051949
H	-0.5142897	1.2686546	2.0767166
C	3.1583972	-2.0270490	3.1082268
H	2.4682847	-2.8255771	2.7953909
H	3.9867253	-2.5023283	3.6476411
H	3.5656600	-1.5559409	2.2049555
C	2.0681479	-1.6590626	5.3208263
H	1.4297761	-2.5365718	5.1365970
H	1.5213412	-0.9690199	5.9770949
H	2.9623785	-1.9967957	5.8614447
C	5.8120011	-0.8879451	4.9379830
H	5.3302108	-0.9078441	3.9509404
C	5.9367072	-2.3268838	5.4439053
H	4.9590584	-2.8096757	5.5884022
H	6.4625632	-2.3620226	6.4112958
H	6.5149136	-2.9399146	4.7340039
C	7.2046367	-0.2774462	4.7578015
H	7.7703053	-0.8196944	3.9834394
H	7.7886360	-0.3291569	5.6903046
H	7.1388796	0.7793883	4.4665582
C	1.8174762	2.2579913	5.9119532
H	1.5916138	2.0262928	4.8643199
C	0.6216243	1.8259577	6.7631035
H	-0.2909729	2.3521905	6.4397972
H	0.7764439	2.0608972	7.8284986
H	0.4294770	0.7446711	6.6898541
C	2.0195042	3.7730524	5.9882957
H	2.8823721	4.0913838	5.3875109
H	2.1827779	4.1082470	7.0253817
H	1.1296193	4.2977727	5.6064921
C	4.9147694	2.4458316	0.8912132
C	6.0902539	1.4581747	0.7035042

C	6.4115849	1.6213784	-0.7933045
H	7.2160652	2.3648542	-0.9110476
H	6.7654616	0.6837918	-1.2480795
C	5.1495134	2.1580667	-1.4726326
C	4.0791129	4.2844959	-0.5787865
C	4.8997023	5.3864518	-0.2183624
C	4.4913776	6.6751163	-0.5723211
H	5.1266446	7.5218275	-0.3001086
C	3.3121786	6.9052347	-1.2674755
H	3.0202894	7.9214743	-1.5433541
C	2.5029082	5.8270889	-1.5922722
H	1.5589309	6.0036987	-2.1141847
C	2.8538261	4.5171688	-1.2496028
C	5.7352535	0.0070468	1.0507586
H	4.8905619	-0.3684780	0.4587546
H	5.4639324	-0.0785183	2.1118049
H	6.6012173	-0.6511949	0.8688505
C	7.3421968	1.8262919	1.5188976
H	8.1732666	1.1652634	1.2216332
H	7.1809026	1.7069006	2.5956082
H	7.6602437	2.8628956	1.3401327
C	5.5064869	3.0281709	-2.6713996
H	6.0370298	2.4097744	-3.4114510
H	6.1626375	3.8616711	-2.3875103
H	4.6179370	3.4528166	-3.1574478
C	4.2431552	1.0092801	-1.9319190
H	3.3988407	1.3681989	-2.5330267
H	3.8402751	0.4480933	-1.0795674
H	4.8199940	0.3115661	-2.5583441
C	6.2128907	5.2583687	0.5315570
H	6.3452221	4.1984743	0.7790607
C	6.1755720	6.0143413	1.8617084
H	6.1096398	7.1034691	1.7065944
H	7.0915170	5.8166181	2.4405745
H	5.3168958	5.7047730	2.4729324
C	7.4094735	5.7026781	-0.3122041
H	7.4778464	5.1470170	-1.2598924
H	8.3497242	5.5430912	0.2397441
H	7.3534449	6.7742734	-0.5627957
C	1.8464690	3.4249422	-1.5596302
H	2.2562225	2.4867284	-1.1611519
C	1.6009388	3.2468292	-3.0596275
H	1.1420192	4.1486185	-3.4952625
H	0.9122116	2.4066807	-3.2436687
H	2.5277937	3.0522862	-3.6189701
C	0.5190268	3.6884210	-0.8430964
H	-0.0050525	4.5552048	-1.2760109
H	0.6793352	3.8972761	0.2231390
H	-0.1513678	2.8188283	-0.9328095
C	1.1464886	-0.5114006	3.2814940
H	0.4194338	-0.2011611	4.0487676
H	0.6657130	-1.2933016	2.6742797

RI-UPBE0/def2-SVP Triplet: -2877.076274247
RI-UPBE0/def2-TZVPP//def2-SVP: -2879.229996956

Cl	2.6507264	4.0324617	2.3040433
Si	3.9115100	2.3529499	2.3570808
N	3.2191312	0.1826626	4.2132306
C	2.9626375	0.9053882	3.0462045
Cl	5.3351156	2.9075012	3.7987783
N	4.4914057	2.9867045	-0.4531013
C	1.7137690	0.3263525	2.3470720
C	2.4756191	-1.1187420	4.1948717
C	3.7637911	0.6801538	5.4434178
C	4.9894770	0.1678040	5.9361536
C	5.4220274	0.5475918	7.2106930
H	6.3634558	0.1459773	7.5942476
C	4.6935124	1.4346294	7.9896498
H	5.0456632	1.7166650	8.9849584
C	3.5221953	1.9761398	7.4788471
H	2.9581064	2.6936755	8.0798968
C	3.0372746	1.6234767	6.2157238
C	1.9976601	-0.2804893	0.9656632
H	1.0602068	-0.6486850	0.5184362
H	2.7034015	-1.1189182	1.0044331
H	2.4138355	0.4808038	0.2884102
C	0.5875789	1.3537711	2.1513846
H	0.8395796	2.0980092	1.3854054
H	0.3534906	1.8948405	3.0792294
H	-0.3264727	0.8324177	1.8214350
C	3.2856722	-2.2229941	3.5007673
H	2.6278350	-3.0728275	3.2616249
H	4.0912203	-2.6005914	4.1416898
H	3.7356492	-1.8676810	2.5650682
C	2.0791936	-1.5995584	5.5844314
H	1.4778100	-2.5160539	5.4853488
H	1.4803552	-0.8529543	6.1212131
H	2.9557425	-1.8338713	6.2043520
C	5.9030382	-0.7361317	5.1269600
H	5.4414991	-0.8606070	4.1362144
C	6.0744734	-2.1167217	5.7663331
H	5.1128972	-2.6130543	5.9632889
H	6.6019353	-2.0406490	6.7305785
H	6.6711996	-2.7770563	5.1167739
C	7.2773596	-0.0918636	4.9189882
H	7.8834152	-0.6917389	4.2214809
H	7.8368149	-0.0251806	5.8655580
H	7.1854541	0.9254033	4.5153274
C	1.7561276	2.2941738	5.7487114
H	1.5877577	1.9941172	4.7062775
C	0.5354826	1.8671747	6.5677378
H	-0.3741596	2.3561847	6.1839497
H	0.6428923	2.1539726	7.6262676
H	0.3684587	0.7805118	6.5368969
C	1.8920862	3.8192961	5.7639982
H	2.7832566	4.1492736	5.2135572
H	1.9616614	4.2073158	6.7929354
H	1.0131373	4.2869231	5.2935183
C	4.7470655	2.2358704	0.6962677
C	5.8819679	1.2287101	0.4106101
C	6.2944064	1.6181628	-1.0214085
H	7.1339240	2.3301227	-0.9749918
H	6.6313153	0.7512523	-1.6101685
C	5.0928011	2.3224593	-1.6546873
C	4.0808924	4.3593566	-0.5228114
C	4.9504957	5.3877507	-0.0753146
C	4.5859772	6.7200954	-0.2920256
H	5.2598013	7.5131521	0.0416841
C	3.3979689	7.0593008	-0.9241917
H	3.1406706	8.1078289	-1.0932474
C	2.5320619	6.0499333	-1.3186760
H	1.5791989	6.3132961	-1.7849818
C	2.8411763	4.7009319	-1.1176540
C	5.4499891	-0.2415755	0.5055223
H	4.6655964	-0.5038131	-0.2145253

H	5.0722243	-0.4680315	1.5142005
H	6.3144202	-0.8986572	0.3173327
C	7.0948674	1.3895728	1.3409644
H	7.9275916	0.7738642	0.9618909
H	6.8751253	1.0565639	2.3632044
H	7.4407939	2.4315721	1.3957996
C	5.5253225	3.3109822	-2.7294630
H	6.0221272	2.7585497	-3.5414377
H	6.2303404	4.0563740	-2.3404282
H	4.6705934	3.8513015	-3.1598112
C	4.1296600	1.3024443	-2.2782892
H	3.3258196	1.7925669	-2.8402018
H	3.6679655	0.6625175	-1.5156295
H	4.6770242	0.6551292	-2.9808418
C	6.2641060	5.1329061	0.6447649
H	6.3368538	4.0525431	0.8253621
C	6.2890276	5.8231847	2.0113342
H	6.3185590	6.9197490	1.9076738
H	7.1839000	5.5206383	2.5773255
H	5.4073800	5.5605395	2.6110074
C	7.4808717	5.5583249	-0.1808208
H	7.5274748	5.0476744	-1.1538495
H	8.4117859	5.3293171	0.3621424
H	7.4722010	6.6424089	-0.3781647
C	1.7881343	3.6764535	-1.5023650
H	2.1700642	2.6897913	-1.2008310
C	1.5141105	3.6583088	-3.0086430
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H	0.8109292	2.8508223	-3.2684623
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C	1.2511561	-0.7368856	3.3608415
H	0.4955753	-0.2943870	4.0294552
H	0.7879253	-1.6074434	2.8720753

RI-UPBE0/def2-SVP Biradical: -2877.081234260

RI-UPBE0/def2-TZVPP//def2-SVP: -2879.235212952

Cl	2.6932165	4.1831012	2.3058590
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C	4.7182713	1.2094570	7.9993569
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C	0.4503189	1.6320380	2.3567953
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C	2.0485156	-1.6422600	5.3916774
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C	5.8486968	-0.8096934	4.9991478
H	5.3842036	-0.8490555	4.0033393
C	5.9745339	-2.2381858	5.5349927
H	4.9976988	-2.7226718	5.6783242
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H	2.7253931	4.0336492	5.2530258
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C	4.9507106	5.3896193	-0.1969595
C	4.5535936	6.6981748	-0.4869678
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H	4.7861729	0.4308037	-2.7123811
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H	6.4240311	4.1359821	0.6737831
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Cl	2.695308	4.215351	2.350965
Si	3.923084	2.531621	2.468434
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C	2.849389	1.137679	3.140189
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C	1.811148	0.231509	0.952647
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H	-0.181664	2.974576	-0.942826	H	0.697459	-1.356867	2.674782

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