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Supplementary Information for

Zinc-Silylene Complexes

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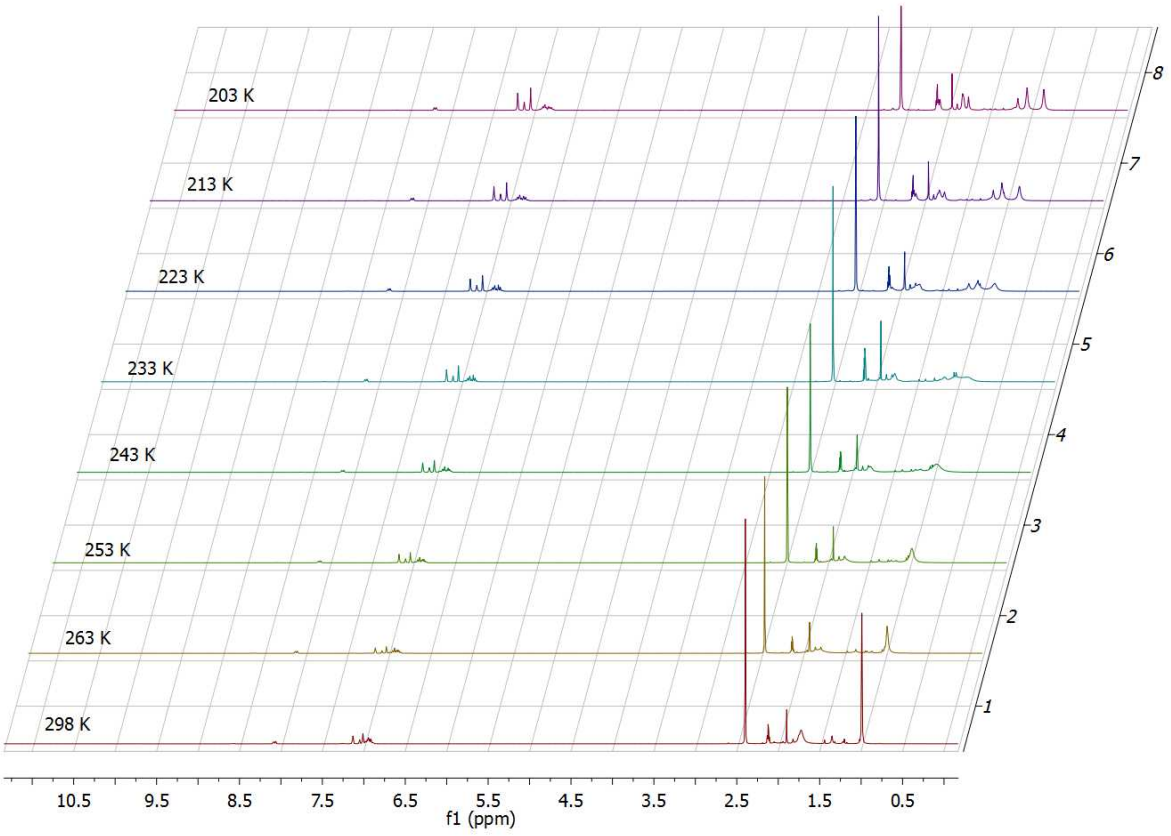
Experimental section

General Procedures. All manipulations were performed with the rigorous exclusion of oxygen and moisture in flame-dried Schlenk-type glassware either on a dual-manifold Schlenk line, interfaced to a high vacuum (10^{-3} Torr) line, or in an argon-filled MBraun glovebox. Hydrocarbon solvents (toluene and *n*-pentane) were dried using an *MBraun* solvent purification system (SPS-800). Deuterated solvents were obtained from *Carl Roth GmbH* and *Euroiso-Top GmbH* (99.5 atom % D). NMR spectra were recorded on a *Bruker* Avance II 300 MHz or Avance 400 MHz. Chemical shifts are referenced to the residue ^{1}H, ^{13}C and ^{29}Si resonances of the deuterated solvents and are reported relative to tetramethylsilane. FT-Raman spectra were taken using a *Bruker MultiRam* spectrometer; the excitation wavelength of the Nd-YAG laser was 1064 nm. The FT-IR spectra were recorded using a *Bruker Tensor 37* spectrometer equipped with a room temperature DLaTGS detector and a diamond ATR (attenuated total reflection) unit; for the mid infrared region a KBr beamsplitter and for the far infrared region a silicon beamsplitter was used. The spectrometer software *Bruker OPUS* was used to obtain Figure S3. Elemental analyses were carried out with an Elementar vario micro cube. Mass spectra were recorded at 70 eV on a Finnigan MAT 8200. [PhC(N^tBu)$_2$]SiCl (**SiCl**) was prepared according to a literature methods[1]. Diethylzinc-hexane solution (1 M) was obtained by Sigma-Aldrich and used as received. Decamethylzincocene[2] and diphenylzinc[3] were prepared according to literature methods.

Synthesis of [PhC(N^tBu)$_2$(η^1-C_5Me_5)Si-Zn(η^2-C_5Me_5)Cl] (**1**).

10 mL toluene were condensed onto a mixture of decamethylzincocene (100.0 mg, 0.30 mmol) and **SiCl** (87.8 mg, 0.30 mmol) at -78 °C. The solution slowly warmed to room temperature and subsequently was stirred for 18 h. The volume was reduced by half and the colorless solution was cooled to -30 C°. After 3d colorless crystals of **1** formed, which were separated by filtration and dried *in vacuo* (61.2 mg, 33%). Elemental analysis (%) calcd for $C_{35}H_{53}ClN_2SiZn$: C: 66.65; H: 8.47: N: 4.44; found: C, 66.80; H, 8.86; N, 4.28; ^{1}H NMR (300.13 MHz, C_6D_6, 25 °C): δ 0.97 (s, 18 H, tBu), 1.35 (s, isomer), 1.70 (b, 15 H, C_5Me_5-Si), 1.88 (s, isomer), 2.43 (s, 15 H, C_5Me_5-Zn), 6.81-6.98 (m, 4H, Ph), 8.08 (m, 1H, Ph) ppm; ^{13}C{^{1}H} NMR (75.47 MHz, C_6D_6, 25 °C): δ 12.7 (C_5***Me***$_5$-Zn), 31.0 (tBu-CH_3), 54.8 (tBu-C), 114.8 (***C***$_5Me_5$-Zn), 127.6, 130.2, 130.7, 131.3 (Ph), 171.0 (NCN); ^{29}Si{^{1}H} NMR (59.6 MHz, C_6D_6, 25 °C): δ 60.5 ppm; EI-MS, m/z (%): 592 ([M - HCl]$^+$, 8), 457 ([M-HCl- C_5Me_5]$^+$, 24), 394([PhC(N^tbu)$_2$]Si C_5Me_5]$^+$, 45) 334 ([Zn C_5Me_5-]$^+$, 100), 323 ([PhC(N^tBu)$_2$]SiZn$^+$, 48).

Figure S1. VT 1H NMR of compound **1** (300 MHz NMR).



Synthesis of $[PhC(N^tBu)_2PhSi\text{-}ZnPh(\mu\text{-}Cl)]_2$ (**2**).

To a mixture of solid diphenylzinc (64.0 mg, 0.29 mmol) and **SiCl** (85.9, 0.29 mmol) 10 mL of toluene was added at -78 °C. The resulting colorless solution was warmed to room temperature and subsequently was stirred for 18 h. The solution was concentrated to about two thirds of its volume and 10 mL of pentane were layered on top. After one day, a white microcrystalline precipitate of **2** was formed, which was separated by filtration and dried *in vacuo* (97.7 mg, 65%). Elemental analysis (%) calcd for $C_{54}H_{66}Cl_2N_4Si_2Zn_2$: C, 63.03; H, 6.46; N, 5.44; found: C, 62.59; H, 6.38; N, 5.27; ^{1}H NMR (300.13 MHz, C_6D_6, 25 °C): δ 1.02 (s, 18 H, tBu), 6.89 - 6.98 (m, 4 H, Ph), 7.20-7.29 (m, 4H, Ph), 7.38 (m, 1 H, Ph), 7.54 (t, $J_{H,H}$=7.3 Hz, 2H, Ph), 8.17 (m,

2H, Ph), 8.49 (d, $J_{H,H}$=6.4 Hz, 2H, Ph) ppm; $^{13}C\{^1H\}$ NMR (75.47 MHz, C_6D_6, 25 °C): δ 31.1 (tBu-CH_3), 54.4 (tBu-C), 125.4, 127.1, 128.6, 128.8, 129.9, 130.3, 131.1, 131.8, 135.7, 137.6, 139.5 (Ph) (two resonances not located); ^{29} Si/^{1}H (HMBC) NMR (59.63/ 300.13 MHz, C_6D_6, 25 °C): δ 34.4 ppm.

Synthesis of $[PhC(N^tBu)_2SiEt]_2ZnCl_2$ (**3**)

The synthesis was carried out under exclusion of light. To 10 mL of a toluene solution of **SiCl** (80 mg, 0.27 mmol) a hexane solution of diethylzinc (1 M, 0.15 mL, 0.15 mmol) was added via syringe at room temperature. During the addition the solution turned to slightly yellowish color. The mixture was stirred for 18 h. Then, the volume was reduced to about 3 mL and 10 mL of pentane were layered on top. After several days in the dark, colorless crystals were formed. These were filtered off and dried *in vacuo* (33.12 mg, 34%). Due to the unstable nature of **3** in solution impurities could not be avoided in the recorded NMR-spectra. Elemental analysis (%) calcd for $C_{34}H_{56}Cl_2N_4Si_2Zn$: C, 57.25; H, 7.91; N, 7.85; found: C, 56.36; H, 7.58; N, 7.23; ^{1}H NMR (400.3 MHz, C_6D_6, 25 °C): δ 1.13, 1.19, (b, Si-Et); 1.30 (s, 18 H, tBu), 6.85 - 6.99 ppm (m, 4 H, Ph), 8.21 (m, 1H, Ph) ppm; $^{13}C\{^1H\}$ NMR (100.66 MHz, C_6D_6, 25 °C): δ 7.1 (Et-CH_3), 13.9 (Et-CH_2), 31.23 (tBu-CH_3), 54.10 (tBu-C), 127.3, 128.5, 128.9, 130.2, 131.0, 132.2 (Ph, one extra signal due to decomposition), 168.4 ppm (NCN); $^{29}Si\{^1H\}$ NMR (59.63 MHz, C_6D_6, 25 °C): δ 55.4 ppm.

X-ray Crystallographic Studies of 1-3. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber. The crystal was transferred directly to the cold stream of a STOE IPDS 2 or STOE StadiVari diffractometer.

All structures were solved by the Patterson method (SHELXS-2013[4]). The remaining non-hydrogen atoms were located from difference in Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F, minimizing the function $(F_o\text{-}F_c)^2$, where the weight is defined as $4F_0^2/2(F_o^2)$ and F_o and F_c are the observed and calculated structure factor amplitudes using the program SHELXL-2013[4]. Carbon-bound hydrogen atom positions were calculated. The locations of the largest peaks in the final difference Fourier map calculation as well as the magnitude of the residual electron densities in each case were of no chemical significance. Positional parameters, hydrogen atom parameters, thermal parameters, bond lengths and angles have been deposited as supporting information.

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{35}H_{53}ClN_2SiZn$
Formula weight	630.70
Temperature	150.15 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 11.089(2) Å
	b = 17.537(4) Å beta = 98.91(3)°
	c = 17.947(4) Å
Volume	3448.0(12) $Å^3$
Z, Calculated density	4, 1.215 mg/m^3
Absorption coefficient	0.850 mm^{-1}
F(000)	1352
Crystal size	0.185 x 0.161 x 0.114 mm
Theta range for data collection	1.633 to 25.500°
Limiting indices	-13<=h<=10, -19<=k<=21, -21<=l<=21
Reflections collected / unique	15445 / 6404 [R(int) = 0.0620]
Completeness to theta =	25.242 99.5 %
Absorption correction	Integration
Max. and min. transmission	0.9426 and 0.8475
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6404 / 0 / 377
Goodness-of-fit on F^2	0.924
Final R indices [I>2sigma(I)]	$R1$ = 0.0428, w$R2$ = 0.0955
R indices (all data)	$R1$ = 0.0636, w$R2$ = 0.1019

Table S2. Crystal data and structure refinement for **2**.

Empirical formula	$C_{54}H_{66}Cl_2N_4Si_2Zn_2$
Formula weight	1028.92
Temperature	200.15 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 12.479(3) Å
	b = 14.937(3) Å beta = 104.21(3)°
	c = 14.850(3) Å
Volume	2683.5(10) $Å^3$
Z, Calculated density	2, 1.273 mg/m^3
Absorption coefficient	1.076 mm^{-1}
F(000)	1080
Crystal size	0.701 x 0.525 x 0.319 mm
Theta range for data collection	1.915 to 25.511°
Limiting indices	-11<=h<=15, -17<=k<=18, -17<=l<=17
Reflections collected / unique	20474 / 4991 [R(int) = 0.0388]
Completeness to theta =	25.242 99.8 %
Absorption correction	Integration
Max. and min. transmission	0.7779 and 0.5936
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4991 / 0 / 295
Goodness-of-fit on F^2	0.920
Final R indices [I>2sigma(I)]	$R1$ = 0.0265, w$R2$ = 0.0608
R indices (all data)	$R1$ = 0.0377, w$R2$ = 0.0628

Table S3. Crystal data and structure refinement for **3**.

Empirical formula	$C_{34}H_{56}Cl_2N_4Si_2Zn$
Formula weight	713.27
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 11.432(2) Å
	b = 23.618(5) Å beta = 105.97(3)°
	c = 16.420(3) Å
Volume	4262.1(16) $Å^3$
Z, Calculated density	4, 1.112 mg/m^3
Absorption coefficient	0.79 mm^{-1}
F(000)	1520
Crystal size	0.260 x 0.165 x 0.103 mm
Theta range for data collection	1.552 to 25.260°.
Limiting indices	-13<=h<=13, -26<=k<=28, -19<=l<=19
Reflections collected / unique	36794 / 7732 [R(int) = 0.1577]
Completeness to theta =	26.000 92.3 %
Absorption correction	Integration
Max. and min. transmission	0.9369 and 0.8350
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7732 / 0 / 402
Goodness-of-fit on F^2	0.669
Final R indices [I>2sigma(I)]	$R1$ = 0.0485, w$R2$ = 0.0652
R indices (all data)	$R1$ = 0.1638, w$R2$ = 0.0850

DFT calculation

All calculations were performed using the program package TURBOMOLE.[5] The geometries of the molecules were obtained without the constraint of symmetry at the RI-BP86 level using a def-SV(P) basis set[6] for each atom. Vibrational frequency calculations related to the optimized structure of each molecule at this level of theory were performed by diagonalization of the analytically computed Hessian using the module AOFORCE.[7] Atomic charges were calculated according to Mulliken's procedure.

Table S4 Results of the quantum-chemical DFT-calculations (distances r (Å), partial charges Q, experimental distances in parentheses).

	r(Zn-Cl)	r(Si-N)	r(Si-Cl)	r(Zn-Si)	Q(Cl)	Q(Zn)	Q(Si)
1	2.330	1.881		2.414	-0.39	0.40	0.51
	(2.315)	(1.826)		(2.375)			
Zn(Cl)(C_5Me_5)	2.138				-0.33	0.43	
Si(C_5Me_5)		1.934					0.36
(C_5Me_5)$_2$Zn-**SiCl**		1.908	2.147	2.613	-0.25	0.46	0.45
Zn(C_5Me_5)$_2$						0.44	
SiCl		1.929	2.180		-0.33		0.39
$ZnCl_2$	2.104				-0.28	0.55	
$SiCl_2$			2.115		-0.22		0.43
$SiCl_4$			2.055		-0.16		0.64
Zn(Si(CH_3)$_3$)$_2$				2.421		0.14	0.31

Figure S2. Energy diagram of **1** resulting from DFT calculations.

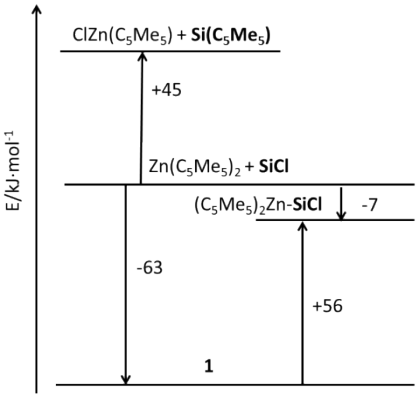
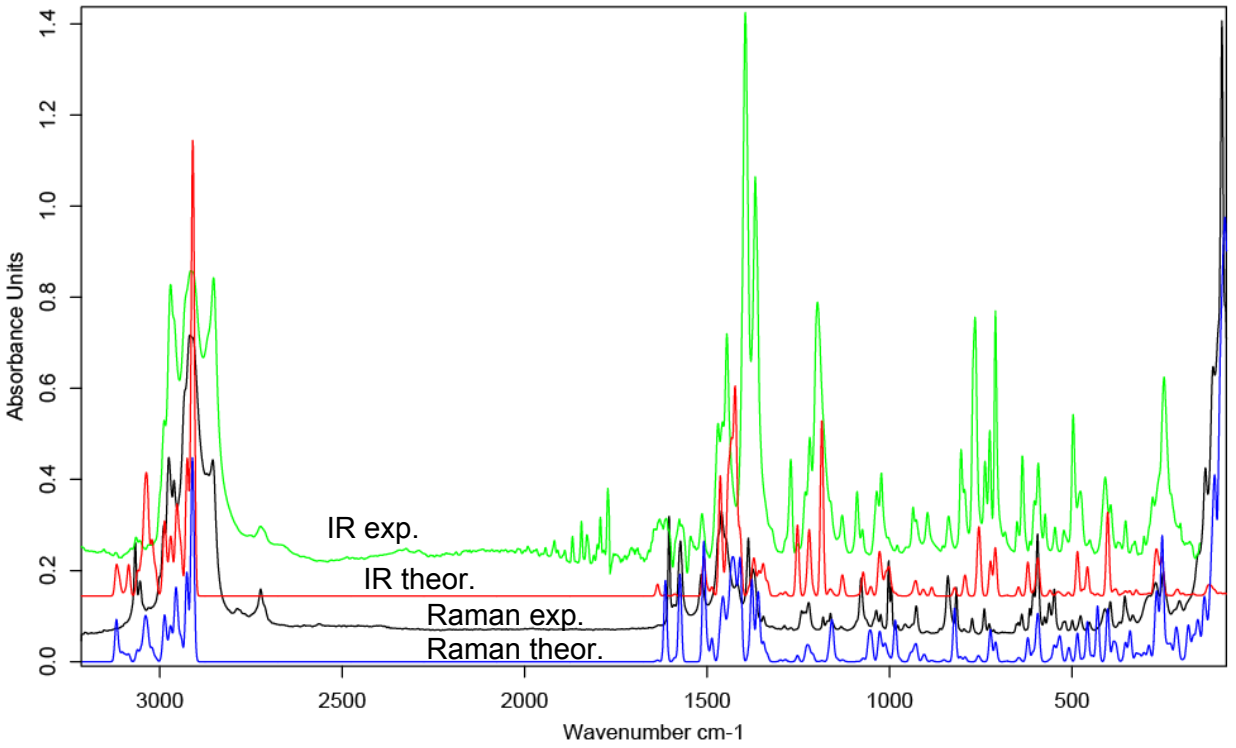


Figure S3 Experimental and theoretical IR and Raman spectra of **1**.



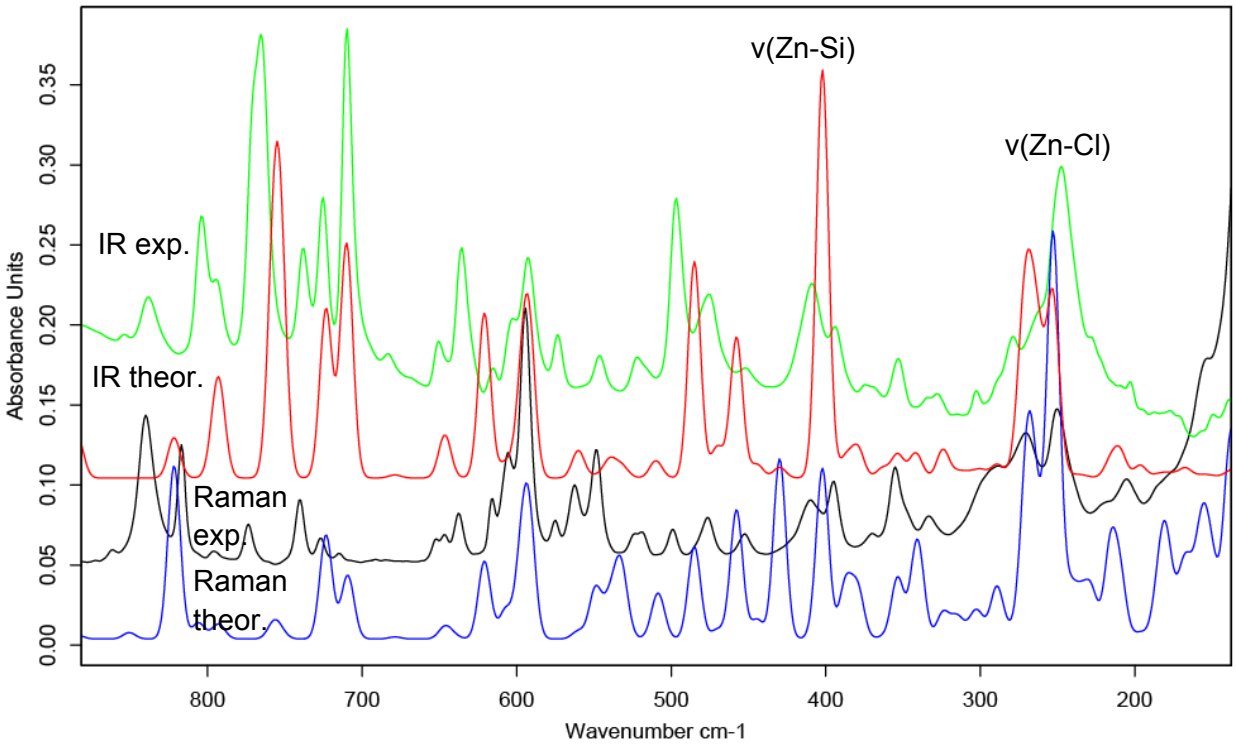


Table S5: Signals of the experimental Raman and IR spectra of **1**. The highlighted signals refer to the Zn-Si and Zn-Cl stretching vibrations (see text).

Raman spectrum		IR spectrum	
v/cm-1	Int./a.u.	v/cm-1	Int./a.u.
3067.2459	0.045	2970.5857	0.059
3053.9657	0.027	2915.5427	0.059
2975.4376	0.083	2852.774	0.057
2960.9987	0.073	2090.0155	0.021
2917.3199	0.138	2054.5476	0.014
2854.7369	0.082	1995.493	0.016
2723.5377	0.024	1810.2558	0.014
1604.2631	0.057	1611.69	0.025
1573.0124	0.045	1576.0601	0.019
1515.9696	0.03	1513.7345	0.022
1460.4721	0.059	1445.8388	0.043
1386.9926	0.047	1395.3693	0.08
1374.5797	0.033	1368.0407	0.061
1221.582	0.018	1270.7412	0.027
1161.9266	0.013	1218.5115	0.03
1078.1295	0.029	1197.5145	0.046
1036.3707	0.014	1129.8844	0.021
1002.4249	0.037	1088.9301	0.025
995.0216	0.025	1022.5313	0.027
926.8574	0.016	935.5099	0.021
840.0648	0.03	896.0376	0.019
816.9226	0.025	838.3701	0.018
773.6412	0.011	803.8732	0.023

740.2943	0.015	803.8477	0.025
637.5016	0.012	765.6124	0.04
594.442	0.049	765.4302	0.038
562.4717	0.017	738.3253	0.023
548.4312	0.024	725.3649	0.024
499.0229	0.01	709.859	0.038
476.3511	0.012	635.8069	0.022
394.9627	0.018	592.3593	0.021
355.0665	0.021	573.457	0.013
270.469	0.027	546.3571	0.012
250.3476	0.031	521.9038	0.011
205.343	0.018	496.8035	0.026
134.2916	0.078	475.5887	0.017
89.1232	0.28	408.9447	0.017
		393.969	0.014
		353.1188	0.011
		247.546	0.027

Energies (given in Hartree), geometries (cartesian coordinates given in a.u.) and vibrational frequencies obtained from DFT-calculations

a) 1

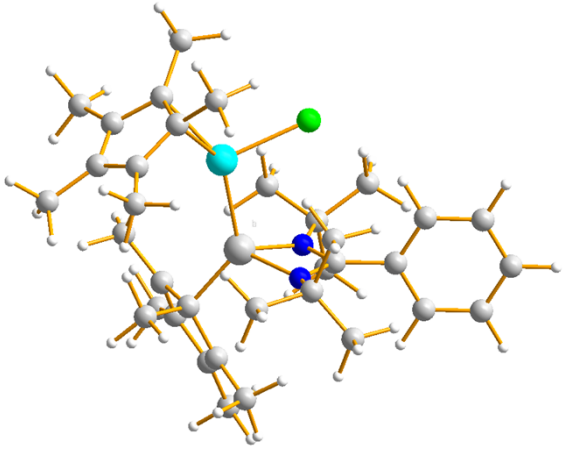
Total energy = -4003.0663310030 |dE/dxyz| = 0.000169

Cartesian Coordinates (given in a.u.):

0.08923361560705	-1.05132802759343	0.50479164165167	si
2.48209772940427	0.89370335700669	2.30028553379970	n
2.99922188764318	-0.66415525227345	-1.47420061693456	n
3.99964958361808	0.94464666475002	0.23256782086488	c
2.20114620002145	-5.69704999034272	2.61936223393971	c
2.76434011775198	-7.63893299896843	0.97768849174189	c
0.73406451275573	-7.87125131179924	-0.91082241313750	c
-1.09421277415525	-6.07839594130565	-0.44091453980320	c
-0.27690888957083	-4.51098967021982	1.82756634885066	c
-3.07207627087522	1.90018955721263	-0.94805663318487	zn
-0.53219746839502	4.86086427304203	-2.98998915263166	cl
-8.03087795843492	0.03999659333428	-1.43669033052387	c
-6.98886065792860	2.50293093203308	-1.96795899823156	c
-6.51925328495512	3.73033644274379	0.48825556598850	c
-7.26898742506807	1.96625155102947	2.41534698310925	c
-8.20927341295503	-0.26433794729359	1.22869044699233	c
2.38982080345598	2.59832044570541	4.54343680367821	c
3.77212058744345	-1.31571593486217	-4.10311424844539	c
1.68076144603157	5.32648923516070	3.77599044108580	c
3.23671261949292	6.25312739577320	2.71965888976871	h
1.30089911819180	6.47438474282132	5.49576458650980	h
-0.02109125182179	5.35417945074013	2.54931345234609	h
4.86962474889400	0.95512083480147	-5.57088057638972	c
6.76438223518451	1.52202028803170	-4.87973549846018	h
5.07315173755989	0.40616804268243	-7.58976672104074	h
3.56789228359151	2.59847677796322	-5.45575332298149	h
0.31584001879234	1.53884427763624	6.29234249967135	c
0.09292043158469	2.77604125582371	7.97338935782461	h
0.80395354669898	-0.38814972756153	6.96435683747869	h
-1.54088818196811	1.46538701730156	5.30647496662817	h
1.35923924782456	-2.19540169029882	-5.48295571137698	c
1.83712353629338	-2.81800103383072	-7.43082817449677	h
0.47047934066491	-3.81439071121763	-4.48175821195890	h
-0.02060871586226	-0.61589883227492	-5.61869074133916	h
4.93082930896830	2.59935652736669	5.98163293681406	c
5.48545872219279	0.65612224294479	6.55559191174584	h
4.74219002895912	3.75855993719318	7.72442679143013	h
6.48092187213883	3.42361792212391	4.83587730335480	h
5.71772535761299	-3.48793865549968	-3.99177823288511	c
4.92734579814030	-5.13334174384638	-2.95439329156216	h
6.23883586686934	-4.09925746045465	-5.93462850921436	h
7.47380043554575	-2.86681363650493	-3.01756759461640	h
-7.24131406248024	3.88978882674609	-4.45631958179136	c

-9.12040260876645	4.84248672709607	-4.60665304546347	h
-7.08317112216070	2.58109228027323	-6.09387831214058	h
-5.75997266654797	5.35653980787563	-4.70027139679107	h
-6.12648442745267	6.54111431694258	0.83300390819881	c
-7.94569082846311	7.59476845330236	0.63801588027018	h
-5.36029898506503	6.99732938801973	2.73708721516265	h
-4.78422431821151	7.32818417440116	-0.57797068849655	h
-8.99413615519357	-1.77899760729433	-3.40194857568694	c
-10.97578380103948	-1.32655115084583	-3.97620595403158	h
-9.01465461707695	-3.76240046323635	-2.70610561213004	h
-7.84044688313391	-1.74033131502514	-5.15863342121726	h
-7.21444705862428	2.44706895623320	5.22131344187460	c
-9.13157303752733	2.90197920641610	5.97865979034844	h
-6.53006393879808	0.78093767310292	6.31340444918929	h
-5.97266613254371	4.06709670840858	5.71660077035887	h
5.01654463752864	-9.37349112917619	1.02294015184414	c
6.28996585247385	-8.98265273878993	2.64233887609144	h
6.16842289932888	-9.20624439703734	-0.73360415193193	h
4.43002670875972	-11.39242291365906	1.15184681506549	h
0.73491371212189	-9.86038645991184	-2.93988685106942	c
-0.91544261782407	-9.68484205161084	-4.22228810444138	h
2.47434407202501	-9.76220712894712	-4.12403379932215	h
0.68752054283236	-11.80069564531498	-2.12006010353782	h
3.67072910330452	-4.91726492454099	4.91482639460879	c
4.43971292158784	-2.96584656982774	4.74266073866987	h
5.28690190133257	-6.20719614796321	5.27186437333197	h
2.47409229921372	-4.93421473297234	6.65117038294345	h
-3.62043717760626	-5.79372861827649	-1.70031599910016	c
-5.16460189731598	-6.60445631810204	-0.51202071833597	h
-4.14080950246473	-3.77753880578813	-2.01781079586815	h
-3.69030199957356	-6.77868529150313	-3.55205875393282	h
-2.32415500901878	-4.46998730468820	3.91876855467373	c
-2.81310859260225	-6.44453858502591	4.45833508877670	h
-4.08026398231455	-3.51790684208699	3.26380539314863	h
-1.66863544128468	-3.47784491326142	5.64784799035316	h
-9.27786459965114	-2.53474983241273	2.57969842349135	c
-11.38393716830488	-2.46133164292782	2.70305039552385	h
-8.57638812548599	-2.68404791203063	4.55583990784931	h
-8.80846436408149	-4.34422052158285	1.61246877123786	h
6.33597463673856	2.49988995529942	-0.08346553747687	c
6.19896588964005	4.99400223792986	-1.02315268368455	c
8.42045310432099	6.41766973151535	-1.30276071776117	c
10.77827976067266	5.37320920027376	-0.65942815507130	c
10.91809208068991	2.88605474433492	0.26309501210585	c
8.70440140220491	1.44907355305336	0.55145610787851	c
4.34497032334265	5.76762379087500	-1.58111936798763	h
8.30596725304664	8.36051613876861	-2.04558270004179	h
12.51640882078365	6.49973281618634	-0.88528782324348	h
12.76184529789267	2.05556083811923	0.76387236763117	h
8.80831298888947	-0.49685914196617	1.28700165374362	h

Figure S4: Representation of the calculated molecular structure of **1**.



Vibrational frequencies, IR and Raman intensities

(Raman Intensities: The scattered wave has its electric field unpolarized to the scattering plane and the incident radiation is polarized orthogonal to the scattering plane. All cross sections are given in % relative to the most active single mode.)

			v/cm^{-1}	IR Int./km mol^{-1}	rel. Raman Int./%
7	a	18.99	0.04627	23.35	
8	a	23.05	0.04427	35.14	
9	a	26.34	0.21135	62.75	
10	a	31.52	0.29144	50.97	
11	a	34.26	0.13941	26.71	
12	a	44.15	0.61887	44.04	
13	a	54.88	0.16165	100	
14	a	57.54	0.30438	4.62	
15	a	62.18	0.12935	59.89	
16	a	63.82	0.41584	25.1	
17	a	69.73	0.38493	26.02	
18	a	72.67	0.57050	24.08	
19	a	79.23	0.96228	42.9	
20	a	81.97	0.88304	8.77	
21	a	86.48	0.61780	37.77	
22	a	92.38	1.31999	24.18	
23	a	94.77	0.44834	4.24	
24	a	97.29	0.99058	16.46	
25	a	106.06	1.98593	15.14	
26	a	109.87	2.47813	9.87	
27	a	113.17	0.77271	9.36	
28	a	116.77	1.90581	3.93	
29	a	118.70	3.50289	3.78	
30	a	122.45	3.11402	5.25	
31	a	128.07	6.15138	1.03	
32	a	132.14	0.59124	4.27	
33	a	137.27	0.42560	3.98	
34	a	139.75	0.53905	4.52	
35	a	149.78	0.29333	2.89	

36	a	155.83	0.43640	4.66
37	a	161.52	0.13061	1.61
38	a	167.04	1.29430	2.11
39	a	169.67	0.34838	1.35
40	a	177.04	0.58986	1.02
41	a	180.46	0.26250	3.81
42	a	185.06	0.51661	1.68
43	a	196.47	2.02543	0.3
44	a	209.55	4.12840	2.73
45	a	215.81	2.60403	4.06
46	a	228.12	0.09176	2.1
47	a	234.74	0.43437	1.63
48	a	241.43	0.36544	1.95
49	a	249.43	1.43436	2.64
50	a	253.02	27.35417	16.28
51	a	256.61	0.49435	0.59
52	a	261.32	9.28127	1.26
53	a	263.55	9.96365	2.67
54	a	267.08	7.20484	2.13
55	a	268.87	4.31613	3.11
56	a	269.79	14.00774	3.43
57	a	273.54	12.25088	1.25
58	a	281.29	0.36242	0.17
59	a	285.64	0.06114	0.22
60	a	289.22	2.04365	1.88
61	a	290.39	0.04436	0.38
62	a	299.53	1.17074	0.44
63	a	303.16	0.19081	0.94
64	a	307.51	0.71832	0.18
65	a	314.08	0.81167	0.58
66	a	316.19	0.12441	0.46
67	a	324.08	4.52994	1.2
68	a	339.63	0.78550	2.74
69	a	342.17	3.31179	2.06
70	a	353.48	3.75852	2.81
71	a	363.18	1.57600	0.09
72	a	379.25	4.72788	2.27
73	a	386.72	2.29667	1.17
74	a	387.45	0.96266	1.41
75	a	402.10	64.76694	7.77
76	a	407.44	0.18861	0.15
77	a	429.83	1.69205	8.26
78	a	444.47	2.14089	0.89
79	a	457.73	22.37735	5.93
80	a	470.16	4.92981	0.43
81	a	485.01	34.38426	4.24
82	a	507.37	0.30054	1.3
83	a	510.15	2.50052	0.93
84	a	530.03	0.79775	0.94
85	a	533.49	1.37086	2.79
86	a	540.02	2.78947	1.54

87	a	545.03	0.05130	0.08
88	a	549.10	0.32498	2.26
89	a	560.13	4.35811	0.36
90	a	591.45	14.06347	3.53
91	a	593.31	9.76879	1.88
92	a	596.97	10.59055	3.17
93	a	607.20	2.43790	1.33
94	a	620.85	26.19629	3.56
95	a	641.15	0.05641	0.17
96	a	646.53	6.83071	0.54
97	a	678.78	0.49626	0.09
98	a	708.44	6.78524	1.64
99	a	710.44	31.14265	1.37
100	a	723.41	26.84033	4.77
101	a	752.75	31.73190	0.31
102	a	757.34	31.33320	0.7
103	a	791.30	5.48663	0.17
104	a	793.21	7.47870	0.47
105	a	795.24	3.17086	0.03
106	a	796.20	1.24251	0.05
107	a	805.96	0.03255	0.74
108	a	821.71	6.40017	7.94
109	a	850.73	0.01657	0.29
110	a	884.36	6.67415	0.18
111	a	902.89	0.32266	0.47
112	a	904.49	1.13586	0.32
113	a	907.83	1.86245	0.3
114	a	909.09	2.41895	0.2
115	a	926.36	3.21272	1.69
116	a	927.15	2.56067	0.55
117	a	928.28	4.54507	0.05
118	a	933.46	4.33071	1.2
119	a	934.59	0.19183	0.18
120	a	935.37	0.18862	0.14
121	a	942.61	1.08265	1.19
122	a	972.95	0.14585	0.48
123	a	984.51	2.25323	6.15
124	a	994.49	4.15172	0.23
125	a	1000.65	2.00544	0.13
126	a	1001.35	17.30839	0.32
127	a	1004.88	1.61210	0.45
128	a	1009.81	12.25801	0.66
129	a	1011.98	3.96386	1.48
130	a	1014.78	0.67552	0.58
131	a	1019.73	4.51447	0.58
132	a	1019.94	1.64302	0.25
133	a	1022.33	3.30640	0.09
134	a	1024.81	9.08281	1.73
135	a	1026.60	2.58513	0.22
136	a	1028.35	2.23394	1.4
137	a	1028.41	9.91798	0.68

138	a	1029.13	10.78603	0.68
139	a	1033.07	1.09217	0.09
140	a	1049.21	0.49162	2.68
141	a	1050.48	2.23800	0.56
142	a	1052.14	4.60127	0.38
143	a	1056.73	0.44372	3.34
144	a	1071.66	11.10462	0.35
145	a	1072.68	6.99750	0.16
146	a	1078.17	1.42979	0.05
147	a	1086.43	0.54354	0.02
148	a	1126.36	5.64864	0.13
149	a	1130.31	12.36290	0.18
150	a	1143.52	0.12807	0.43
151	a	1152.59	0.63459	0.46
152	a	1155.90	0.46501	3.09
153	a	1159.67	2.91933	3.35
154	a	1165.14	3.56050	1.46
155	a	1185.56	136.24572	0.16
156	a	1209.99	4.44972	1.06
157	a	1217.79	17.69156	0.52
158	a	1220.91	35.47115	1.41
159	a	1227.01	7.09579	1.41
160	a	1229.41	0.17286	0.62
161	a	1252.32	54.90384	0.91
162	a	1285.52	3.11898	0.31
163	a	1298.89	2.13346	0.25
164	a	1333.91	8.84638	0.3
165	a	1336.29	1.74733	0.83
166	a	1342.71	6.76529	0.26
167	a	1345.15	2.92707	1.01
168	a	1345.84	4.79200	0.91
169	a	1346.14	6.81710	0.56
170	a	1350.18	9.26234	0.38
171	a	1357.65	7.51099	2.41
172	a	1357.92	3.05561	2.08
173	a	1358.63	0.47170	0.73
174	a	1358.78	3.57844	0.7
175	a	1359.92	2.57612	1.41
176	a	1361.92	1.10054	2.47
177	a	1364.60	1.26264	2.91
178	a	1368.66	4.03262	0.41
179	a	1370.84	20.68569	0.58
180	a	1376.59	5.33142	2.71
181	a	1376.94	5.09257	4.79
182	a	1377.80	3.22560	4.41
183	a	1385.52	5.79643	1.43
184	a	1408.00	21.01263	9.62
185	a	1409.61	5.08596	0.86
186	a	1410.17	12.23563	0.72
187	a	1411.15	7.97287	2.33
188	a	1412.30	1.72301	0.6

189	a	1413.88	0.43335	1.67
190	a	1415.17	4.07826	2.44
191	a	1416.52	5.82291	1.14
192	a	1418.03	14.14037	0.93
193	a	1419.49	5.19660	0.93
194	a	1420.51	10.51322	0.82
195	a	1421.76	29.01470	1.78
196	a	1422.37	21.31993	1.55
197	a	1423.92	72.72746	1.75
198	a	1425.18	7.95367	2.09
199	a	1426.20	7.37568	2.42
200	a	1426.37	2.59889	0.65
201	a	1428.19	0.64581	1.82
202	a	1428.86	7.60743	2.08
203	a	1430.93	5.96005	2.36
204	a	1432.04	26.59585	1.5
205	a	1433.38	49.70832	2.06
206	a	1434.93	4.85363	4.72
207	a	1435.94	14.46232	0.89
208	a	1438.62	12.99942	1.45
209	a	1439.16	0.98428	0.82
210	a	1440.89	20.90670	1.45
211	a	1441.99	26.81020	1.03
212	a	1442.40	11.61403	0.68
213	a	1445.24	17.33958	0.72
214	a	1446.69	7.21029	2.14
215	a	1451.61	6.51486	2.84
216	a	1456.26	3.19364	6.1
217	a	1460.11	10.24811	2.39
218	a	1463.75	67.28597	2.15
219	a	1465.83	20.81609	1.74
220	a	1486.89	6.90056	3.47
221	a	1499.49	6.11911	2.27
222	a	1508.99	29.48005	17.7
223	a	1574.35	0.42748	13.01
224	a	1588.72	1.45464	0.58
225	a	1614.40	0.88913	12.1
226	a	1635.87	9.00111	0.22
227	a	2907.45	19.57372	1.64
228	a	2907.80	104.29346	5.3
229	a	2908.63	27.16061	1.93
230	a	2909.34	91.08209	3.09
231	a	2911.50	100.90080	13.62
232	a	2911.74	40.42550	7.37
233	a	2922.06	40.65266	1.8
234	a	2923.95	10.72832	0.43
235	a	2926.32	68.18674	11.77
236	a	2940.65	20.93523	2.84
237	a	2944.38	14.63223	0.14
238	a	2946.93	6.55636	1.46
239	a	2948.41	12.11966	0.71

240	a	2952.63	12.45829	0.25
241	a	2953.17	38.15644	4.9
242	a	2957.43	19.63486	7.18
243	a	2967.45	27.81923	2.9
244	a	2972.00	7.70439	0.38
245	a	2972.65	20.38971	3.16
246	a	2981.21	14.03636	1.61
247	a	2985.16	6.12601	0.52
248	a	2986.66	2.86423	2.6
249	a	2986.87	27.55406	1.6
250	a	2987.66	12.23677	1
251	a	2991.59	9.63278	1.36
252	a	3011.04	18.33450	0.53
253	a	3018.72	13.44431	0.59
254	a	3020.86	17.46513	0.4
255	a	3022.14	6.33071	0.96
256	a	3025.16	11.41629	0.28
257	a	3030.20	5.82414	0.61
258	a	3031.56	11.80800	0.67
259	a	3033.43	5.82800	0.51
260	a	3033.72	11.98550	0.61
261	a	3034.12	14.06370	0.37
262	a	3034.14	5.29212	0.69
263	a	3034.98	15.65478	0.94
264	a	3038.23	4.89384	0.82
265	a	3038.54	16.69102	0.81
266	a	3040.07	22.88109	1.78
267	a	3042.83	9.49691	0.72
268	a	3042.99	5.95311	1.3
269	a	3043.59	21.57668	1.07
270	a	3050.67	7.55699	0.77
271	a	3051.61	15.00744	0.95
272	a	3059.23	5.65640	0.44
273	a	3061.84	4.17134	0.52
274	a	3062.19	9.83747	0.82
275	a	3085.25	23.95129	1.07
276	a	3094.32	3.39313	0.9
277	a	3102.61	1.38484	1.22
278	a	3111.20	12.17991	1.08
279	a	3119.00	22.22716	6.1

b) Second isomer

This isomer is calculated to be 13.1 kJ·mol^{-1} higher in energy compared to the most stable one of **1**.

Its structure is best described to be formed from **1** after rotation of the Cp*-Zn-Cl around the Zn-Si axis by about 120 °.

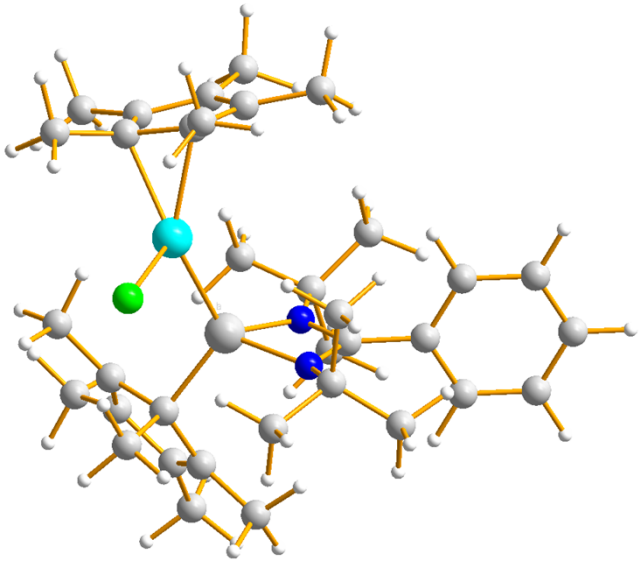
Total energy = -4003.0613259100 |dE/dxyz| = 0.000181

Cartesian Coordinates (given in a.u.):

0.56287439167932	-0.51881167818965	0.40903547045609	si
2.66153583904512	1.02168991965852	2.88070344231224	n
3.82642584271028	-0.06642985210566	-0.91529556154875	n
4.56849200832750	1.19076263873382	1.17870055438407	c
2.24611143700764	-5.64337323011463	1.65731248467038	c
2.51255039499510	-7.40799265532106	-0.23683200078828	c
0.40910910636044	-7.14684137109217	-2.04628611052957	c
-1.16481003165757	-5.22334510247585	-1.27555962580729	c
-0.11341044852111	-4.10289569042171	1.16188647215133	c
-2.95570634466250	2.15847454635662	-0.73732130364095	zn
-5.44936251063543	1.79210148970780	2.82284869557099	cl
-1.46741142114073	6.20210727384558	-4.10373546828538	c
-3.71465802948519	5.78584620660953	-2.64093157962921	c
-5.10781761921575	3.70189089581261	-3.86525422654576	c
-3.64925465223359	2.94732578546301	-6.04287104232794	c
-1.46250836186406	4.50056316923728	-6.19390407802867	c
2.22458899174991	2.44833268802907	5.27785095044079	c
5.13638160451938	-0.58006050906369	-3.34870972089267	c
1.14163229369629	5.09245075649940	4.66216805497204	c
2.47514615889957	6.21139950116082	3.48755434099573	h
0.79142146791384	6.15904683856180	6.43952160680388	h
-0.69113906245816	4.91976318874727	3.64905333857292	h
6.43715655980643	1.79992224803300	-4.42654168484506	c
8.13096380103411	2.35650741824187	-3.32522520198160	h
7.05879277892257	1.40954928638621	-6.39484969490290	h
5.10538731801393	3.42185393458576	-4.47969102756009	h
0.25857155053117	0.95968802769483	6.82647948055163	c
-0.17539429345270	2.00640834111295	8.59534238720756	h
0.99823214321050	-0.93243418395085	7.35848629402536	h
-1.54710207417309	0.75148827725496	5.76943494667083	h
3.06548227058512	-1.45112713276276	-5.20183035691054	c
3.90647877715691	-1.87888084528882	-7.07729491200148	h
2.11682992160951	-3.18803130134148	-4.49383605854393	h
1.61521356210220	0.04991406284220	-5.45294986653258	h
4.66063845186647	2.69088223744763	6.86647519043039	c
5.56871202910066	0.81824258528022	7.15604473799480	h
4.15366744890442	3.45704858537480	8.75592927989202	h
6.06776301521524	3.98993691755317	6.01723416557639	h
7.10155269747815	-2.70765802485710	-2.98042778394280	c
6.18826601404195	-4.41645780761069	-2.17436257692192	h
7.96911573947527	-3.21427614503595	-4.82733521005796	h
8.64502594999692	-2.09694061260063	-1.69311619451811	h
-4.86999643716147	7.62675066490865	-0.78381656655342	c
-6.13822465925643	9.00101692652247	-1.76546905857010	h
-3.40136949794836	8.75598393045765	0.21079488688048	h
-6.00429657295399	6.65541857110267	0.69278015436273	h
-7.90174282375483	3.20279097388628	-3.49976799564007	c
-9.06726377175317	4.61338477365981	-4.55411062908992	h
-8.45397482846550	1.30137637368568	-4.20486327893643	h

-8.46548672948984	3.29416613257351	-1.47927697035834	h
0.50261209898810	8.19350123527932	-3.59502446786321	c
0.25181253568856	9.89671955914434	-4.81739261018211	h
2.45734649152883	7.49607573406889	-3.96577921462502	h
0.44244956681864	8.86515316661418	-1.60462978323990	h
-4.42605663069019	0.96541568480412	-7.93379957917354	c
-5.40193777285039	1.80843400814765	-9.60531348226912	h
-2.78148354796391	-0.11123114730315	-8.68635164059772	h
-5.75671487449278	-0.43458335403539	-7.10603761313241	h
4.52316678825952	-9.40073829078045	-0.50567123159431	c
5.99845966720518	-9.25262992806239	0.97977646348828	h
5.49279453636732	-9.29105834866622	-2.37254737070763	h
3.70529999369128	-11.33865872380766	-0.38151084577807	h
0.12303673224489	-8.83237855958190	-4.31770469454882	c
-1.61233783897429	-8.40224970796796	-5.41417862382716	h
1.75927636378631	-8.64492433964603	-5.63260376025380	h
0.03686611802173	-10.86301628518034	-3.76595516702741	h
3.84922765513940	-5.34548191131248	3.97993605045101	c
4.50634531959008	-3.36431314675606	4.24532141527301	h
5.54132403195102	-6.58659419636050	3.92439915708457	h
2.78019032133872	-5.84394724791369	5.72944685660687	h
-3.62570768977949	-4.41460768329602	-2.43132458578659	c
-5.21665601935233	-4.56574377682001	-1.05879689414015	h
-3.60092410539008	-2.39800614710976	-3.06258804853485	h
-4.11911845488817	-5.57884080110827	-4.10593912952648	h
-2.07364396103614	-4.31837716600259	3.33858837232969	c
-2.74501078502220	-6.31019314475790	3.44227526519736	h
-3.72938935854352	-3.05604690760484	3.05693177611778	h
-1.22547394291069	-3.82584107397564	5.19055993704554	h
0.48334232874220	4.45112075253147	-8.27314730864579	c
0.10449626654152	5.93116392213306	-9.73067095542024	h
0.51559875802000	2.61301239556265	-9.29202460310142	h
2.43455910937524	4.81126472248558	-7.57160428948190	h
7.01543802049500	2.56411581857497	1.50896945002510	c
7.20971231428871	5.15909180343216	0.92087713860653	c
9.51625590416571	6.42872195865624	1.24547863296545	c
11.64481514231171	5.12325110340172	2.15436756267895	c
11.46174374860254	2.53825954339863	2.73475845366376	c
9.15836585682718	1.25988260066377	2.41309876339579	c
5.55355420293459	6.18001922649164	0.17938497738405	h
9.65144787009366	8.45413924451192	0.77814685655675	h
13.45361082802232	6.12532053462263	2.40821976644480	h
13.12395705200624	1.50563790120866	3.44870095058718	h
9.00958063315613	-0.76139285390053	2.88908726952186	h

Figure S5: Representation of the calculated molecular structure of the less stable isomer of **1**.



c) Zn(Cl)(C_5Me_5)

Total energy = -2629.3740308480 |dE/dxyz| = 0.000460

Cartesian coordinates:

0.00000000000000	0.00000000000000	3.28172389979369	zn
0.00000000000000	0.00000000000000	7.32177162985373	cl
1.88412214613512	-1.36889486712391	-0.25880499273521	c
1.88412214613512	1.36889486712391	-0.25880499273521	c
-0.71967062086723	2.21491842203173	-0.25880499273521	c
-2.32890305053579	0.00000000000000	-0.25880499273521	c
-0.71967062086723	-2.21491842203173	-0.25880499273521	c
4.18273633071167	3.03893582769514	-0.43996413100513	c
4.70121241351401	3.41563075160466	-2.44901018358619	h
5.86412375584686	2.17052011426073	0.47131603128245	h
3.87640119609190	4.90638550842015	0.47131603128245	h
-1.59766311235283	4.91710145884051	-0.43996413100513	c
-1.79570335362943	5.52660664911568	-2.44901018358619	h
-3.46837606263132	5.20283312037431	0.47131603128245	h
-0.25217340074286	6.24784071229858	0.47131603128245	h
4.18273633071167	-3.03893582769514	-0.43996413100513	c
4.70121241351401	-3.41563075160466	-2.44901018358619	h
3.87640119609190	-4.90638550842015	0.47131603128245	h
5.86412375584686	-2.17052011426073	0.47131603128245	h
-5.17014643671768	0.00000000000000	-0.43996413100513	c
-5.81101811976918	0.00000000000000	-2.44901018358619	h
-6.01997548856458	-1.69085780223513	0.47131603128245	h
-6.01997548856458	1.69085780223513	0.47131603128245	h

-1.59766311235283	-4.91710145884051	-0.43996413100513	c
-1.79570335362943	-5.52660664911568	-2.44901018358619	h
-3.46837606263132	-5.20283312037431	0.47131603128245	h
-0.25217340074286	-6.24784071229858	0.47131603128245	h

d) $Si(C_5Me_5)$

Total energy = -1373.6509298540 |dE/dxyz| = 0.000502

Cartesian coordinates:

-3.24456909301077	0.67492988452094	-0.01242723130361	si
-0.68477958870460	2.44503551477917	1.93717779163591	n
-0.12838856729773	0.98752900510812	-1.86577127383399	n
0.88755988028827	2.50231461744004	-0.08947722323774	c
-0.81918546058919	-4.15608353285316	1.90500521743827	c
-0.46383837091460	-6.13454426863580	0.23826155976526	c
-2.69693084372886	-6.35551912444887	-1.40132528698223	c
-4.42509504367468	-4.51521528527801	-0.74917960676083	c
-3.33223371728639	-2.93876158213361	1.37276518281723	c
-0.90752555337845	4.28379929898294	4.04635398274306	c
0.78336586425067	0.26750489640829	-4.41334136898344	c
-1.91758967876370	6.85020728792582	3.06851970877613	c
-0.54150825441872	7.76886438220851	1.77728725902542	h
-2.26503035086951	8.16772443522452	4.67109706645046	h
-3.72474225461108	6.57580440323826	2.03123294605049	h
1.57032551332731	2.57854397553189	-6.02138339694600	c
3.31751224250341	3.49329641043033	-5.31240715830308	h
1.93674865557480	1.95943258157094	-7.99708517396141	h
0.03316499815089	4.01260099096021	-6.07068348919858	h
-2.84087742572341	3.18126434937356	5.92648102676991	c
-3.18783295981217	4.54032260374535	7.48974637864135	h
-2.13747928116118	1.38752378893698	6.75868044686918	h
-4.67891471172504	2.80196497628176	4.97772548663872	h
-1.44245856791905	-1.05174889811934	-5.75550313494623	c
-0.84622947059264	-1.71110830204052	-7.65862561822136	h
-2.10365291849836	-2.70976055655003	-4.64847333446130	h
-3.05673886776819	0.27339660599213	-5.99444555038079	h
1.62329402464370	4.66850020908667	5.45162690262473	c
2.42890438908999	2.82625935621881	6.06122655967552	h
1.29690424782799	5.83297783493211	7.17184080918883	h
3.04879980593553	5.65896443409048	4.27822709015635	h
3.02169537513511	-1.59136588832838	-4.16370797153999	c
2.46097638567783	-3.23958585296046	-2.99073589995062	h
3.62095290787858	-2.27830649016098	-6.05900799560115	h
4.67699498692665	-0.66264881961542	-3.26284904967665	h
1.75809627533647	-7.90191860236958	0.05221788795651	c
3.22453279494864	-7.48810081167853	1.49525636888169	h
2.69744982639707	-7.80899612406554	-1.83390241375403	h

1.17294709423306	-9.91036047955524	0.31244096786687	h
-2.94155804103734	-8.34770492832058	-3.41561804179767	c
-4.73276057378306	-8.16936245740617	-4.49393787016349	h
-1.35762867892674	-8.25635941802924	-4.80423460180421	h
-2.89479589399900	-10.29028259555955	-2.59877912819852	h
0.90415711620657	-3.36742972873265	4.01644524641507	c
1.60983929823134	-1.39857207207745	3.76931371941121	h
2.56747099305576	-4.63812553239731	4.17877452494877	h
-0.08066098066596	-3.40236381820960	5.88247185293066	h
-7.03910125790516	-4.12482466971873	-1.78639687380132	c
-8.52758305125331	-4.65996303011995	-0.38880230518689	h
-7.39745196570198	-2.10162896247323	-2.26975125261343	h
-7.37923006968006	-5.26778563069570	-3.51535639367492	h
-5.12624875914165	-2.84711668351360	3.68259995656075	c
-5.63663074192413	-4.80482968301385	4.27063400048607	h
-6.91460102684490	-1.82326108024656	3.24954937019688	h
-4.24486144219191	-1.89782336245064	5.33256062324934	h
3.26817113785380	4.02466084704986	-0.32427977712216	c
3.27557265294949	6.48386628621861	-1.36204051255855	c
5.53287793865506	7.86999034837687	-1.52579325585502	c
7.81430805645892	6.81423743486270	-0.66617317301015	c
7.82878689918042	4.36213008690098	0.35413119125331	c
5.57093338212268	2.97642209691871	0.52624480520352	c
1.50081594517482	7.30794733253830	-2.07271662686703	h
5.50884908643294	9.78826971936242	-2.33854069169649	h
9.58540148696692	7.90372709513735	-0.79622464006396	h
9.61153753067518	3.51924500042949	1.02659446715065	h
5.57976667141374	1.06220018097518	1.34648692467880	h

e) $(C_5Me_5)_2$Zn-**SiCl**

Total energy = -4003.0448367060 |dE/dxyz| = 0.000420

Cartesian coordinates:

-0.11769812449498	-0.17408114303307	-2.90180995234002	zn
-1.25392611839177	4.38991160981176	-4.54205810894457	c
-0.31488510179990	4.55495159538814	-7.01408993412633	c
2.37732218886320	4.05700674662548	-6.97883553621337	c
3.11941583575910	3.55593740976627	-4.49348896669414	c
0.86447435393422	3.68951923190108	-2.85321233278698	c
-2.91507291464026	-3.24871501734736	-5.43725331438246	c
-0.14668961695509	-2.99454695995213	-5.64140203761098	c
0.92018624245747	-5.11922021410592	-4.20413719748084	c
-1.08714461274984	-6.54461063702323	-3.19729292996540	c
-3.44499096395290	-5.38173863578184	-3.93964911324496	c
-3.71506630877924	-4.75132229253148	2.94362988452629	cl
-1.37360961748109	-1.71445394279409	1.61808893022576	si
1.17533406751583	-1.74519875569489	4.16772922035359	n
-2.14961834957375	0.65901906172164	4.21997671216007	n
0.03723360948297	0.15574849365781	5.42961014039663	c

3.73079630613884	-2.88392556611268	4.30302164936639	c
-4.46573103402284	2.01440036509677	5.04668981539924	c
-5.70306952200453	0.58353104423581	7.27730707257375	c
-7.54181544919625	1.47190922083947	7.77696850604237	h
-4.48267295517565	0.64204314071949	8.98523106221658	h
-6.04782175936083	-1.42245135825735	6.76515851687290	h
-3.90863701458170	4.77473802069968	5.81268709783707	c
-5.71704949103676	5.75715529865462	6.24015090806063	h
-2.95568118750603	5.81537688297976	4.25775551985414	h
-2.70280416219939	4.88979056660972	7.52433672515797	h
5.60442209950595	-1.28151963466667	2.74150024107606	c
7.51084214882977	-2.16644957301461	2.73652220943002	h
5.78693526298628	0.65649730544358	3.53441153879277	h
4.95530367070110	-1.12517927911941	0.74934771754510	h
4.69051471850654	-3.16049844315352	7.04219933081271	c
5.12646010725542	-1.31440562887375	7.93388090862005	h
6.45895840693076	-4.29469556363129	7.02672496595729	h
3.28825813376988	-4.16910417263625	8.23726310600971	h
-6.01479868681631	-6.41967539932407	-3.29658859518315	c
-7.55741954364687	-5.13664582133144	-3.91703339684903	h
-6.24827846279598	-6.73581072793548	-1.23001379163919	h
-6.35110622779975	-8.27981069578406	-4.23505870205678	h
-0.91032774284834	-8.96789276604023	-1.71384166094502	c
-1.87697637090432	-10.54784508481638	-2.72199829776170	h
-1.82750319632329	-8.81737659047339	0.17515591665674	h
1.07967806558284	-9.56621626997585	-1.41003826828450	h
3.68023959170031	-5.82015556850677	-4.26922710387458	c
4.19729321894062	-7.18388712892308	-2.75749998293069	h
4.93746776816686	-4.14619884686807	-4.06399249856514	h
4.20172339262435	-6.72876467058153	-6.10440248815894	h
1.09810549127247	-2.14065579864201	-8.09299773965088	c
0.16999704823234	-0.44090097643040	-8.89558527050280	h
0.98006085871743	-3.67738545315071	-9.54004919496452	h
3.12599564187791	-1.66378823824257	-7.84140089046976	h
-4.78567888636994	-1.72144802310775	-6.95269188016421	c
-4.12673336731985	0.25001771946041	-7.26128135894662	h
-6.66552121054528	-1.61598818988392	-6.01809538869619	h
-5.10595787173153	-2.56432958739744	-8.86319630582276	h
1.09020000005467	4.80564239457930	-0.21371445715387	c
-0.65215526942438	4.53240892080816	0.92460191919285	h
1.47174243724533	6.88342275309819	-0.29474535549861	h
2.67281469828552	3.93306780605320	0.86533209580469	h
5.78783913681466	3.24083608120710	-3.54981367412779	c
7.04546117779782	2.38523213183968	-5.00120618253388	h
5.89492532541199	2.01670900425469	-1.84627948840617	h
6.66011042709727	5.08859290431660	-3.01105477709837	h
4.01784107343516	4.07825076259239	-9.30305786553335	c
3.30280409680934	2.77333407151223	-10.79725193519998	h
5.99568718019780	3.51301024991026	-8.87991567166962	h
4.10100810390976	5.99284663136046	-10.18357002746825	h
-1.77099030305346	5.10821454350288	-9.39430519491001	c

-1.81605036772017	3.45595178762343	-10.70761694823607 h
-0.90644371697413	6.69333384350550	-10.48139704692838 h
-3.76789076824915	5.63094368533910	-9.00758348525816 h
-3.89391691634507	5.03777524693823	-3.67865376971666 c
-4.94937386319922	6.06648249947633	-5.17518599620121 h
-3.87578408088618	6.28415590120523	-1.97956161827668 h
-5.06852059754481	3.35744427919984	-3.18196559353473 h
1.04676880006682	1.51264214159946	7.69628454012444 c
2.47020137703898	3.74652221985683	7.38067135208728 c
3.43952268292418	5.01885315252778	9.49827699257914 c
2.98863651762060	4.07985664821468	11.94222994356279 c
1.56776213099001	1.85845967652398	12.26449986007635 c
0.60262505579482	0.57364926371930	10.15271034338104 c
2.80462194692360	4.49220459450957	5.46581092303463 h
4.55113681351838	6.76050155385864	9.23421714356058 h
3.74731863663197	5.08355946733331	13.60260582430373 h
1.21113293659639	1.11292216966152	14.17652192954953 h
-0.48610585210080	-1.18230836088687	10.40757095266030 h
-6.28266721254713	1.99524362178350	2.76909032518865 c
-5.45020612998235	3.00230385195065	1.12659377612983 h
-8.08210068558626	2.95195462144499	3.27613276240094 h
-6.74158268385782	0.02923785865299	2.18705903609571 h
3.46690860658859	-5.53624809911346	3.11951825293558 c
2.69068698150249	-5.41242006037149	1.16796337257800 h
2.17276554532835	-6.73603457346652	4.25625854315701 h
5.34053440013857	-6.47921630458846	3.01580374266125 h

f) $Zn(C_5Me_5)_2$

Total energy = -2559.0073082420 |dE/dxyz| = 0.000195

Cartesian coordinates:

2.52927530463639	2.54822850177576	-0.00172796198996 c
1.17890122338316	3.59758202108347	2.23662021078384 c
-0.84788719418470	5.03961607463747	1.37457644218325 c
-0.84821063057645	5.03769912369829	-1.38071800011268 c
1.17841665558879	3.59452287153249	-2.24122923948200 c
5.41010399447353	2.36592885072287	-0.00189525365597 c
6.14406040295317	1.35966714160305	-1.69425706139537 h
6.14438511041590	1.36162586655144	1.69148940143159 h
6.26523595551446	4.29632538789955	-0.00308574902874 h
2.07893433791063	3.26567785682844	4.91631498779821 c
-2.81935951926705	6.36946262626035	2.93539877188809 c
-2.82011550880752	6.36524647466860	-2.94294430042075 c
2.07781934242480	3.25894225055790	-4.92067607530018 c
2.70315422711806	1.29434697270260	5.31237762925632 h
-2.51760543683546	6.09586672632114	4.99512504843288 h
-4.76862686688645	5.69320485918962	-2.49710849919656 h
0.58018056784132	3.72299761948813	-6.31799232485114 h
2.70233785664789	1.28716513355716	-5.31404529648864 h

-2.51905485169746	6.08845401652028	-5.00234653388094	h
-4.76799315609405	5.69665338420471	2.49124761260173	h
0.58175155520533	3.73205168823109	6.31334754950700	h
3.72748044331860	4.51270093203804	5.34937019514084	h
-2.82181382453465	8.44738547514877	2.58142071301798	h
-2.82236382223603	8.44371725826644	-2.59218131006448	h
3.72599798688533	4.50567296700256	-5.35596705330831	h
0.73633477104927	-0.80236938788515	0.00054895583920	zn
-2.81005490304870	-3.08752011399613	0.00270001344532	c
-1.36784620300099	-3.80657347965886	2.21605225176684	c
0.95876298220192	-4.95418657483874	1.36747581955715	c
0.95801729436024	-4.95552128154463	-1.36231715308595	c
-1.36905674112617	-3.80873960424410	-2.21074324367122	c
-5.45534777406457	-2.03373620702292	0.00291347991801	c
-2.25155759006342	-3.58491370054969	4.91309862727744	c
2.95823712674467	-6.11000009883577	3.03278019697483	c
2.95656062776316	-6.11297254230093	-3.02760088608773	c
-2.25421513293903	-3.58973326651856	-4.90753001992619	c
-5.82939820921749	-0.84620968421378	-1.68793515522721	h
-3.41123203244673	-1.86176609754022	5.22570004640286	h
3.06905590569223	-5.16647360684396	4.90665515449876	h
4.86834320917302	-6.00312339565761	-2.16216612204121	h
-0.64774795560620	-3.51222914819317	-6.25874818880799	h
-5.82849544777688	-0.84463856222691	1.69285161786410	h
-3.41448924687174	-1.86716208710746	-5.22106672979978	h
3.06658259131794	-5.17106241767788	-4.90233764632091	h
4.86959671551283	-6.00068212654332	2.16633806323260	h
-0.64437244097561	-3.50661559059311	6.26341345896390	h
-6.89689120954968	-3.57457348576142	0.00401919222434	h
-3.44160541479123	-5.23385724855092	5.47293862131800	h
2.57601414662083	-8.15167838649139	3.40170751512709	h
2.57393338988191	-8.15492218734056	-3.39459856579013	h
-3.44413261203741	-5.23948179835293	-5.46526320651821	h

g) SiCl

Total energy = -1444.0349408510 |dE/dxyz| = 0.000406

Cartesian coordinates:

0.33397045918920	-1.42520989844695	0.68807135357932	si
2.40631496445693	1.18507359480490	2.13047886665035	n
2.73892040822746	-0.11633182453758	-1.73843258657149	n
3.87746093564719	1.29477836631830	0.05573614919268	c
-2.95347059399380	0.83324993698413	-0.34171896506494	cl
2.34304199481638	2.67224043069587	4.49091503219158	c
3.62468042527570	-1.07815335452416	-4.20809141680968	c
1.63302133932001	5.43979868648576	3.86789245840947	c
3.13533926738854	6.36568784703744	2.72732904403907	h
1.38863843103992	6.55351358158047	5.63452093016880	h
-0.16182584311704	5.49809709850080	2.77992943286800	h

4.34166198227629	1.12484136896865	-5.98624363438087	c
6.03734107084279	2.15934073326141	-5.31014363459598	h
4.77046700328795	0.38074959653537	-7.90493694907514	h
2.75020708733627	2.48687237201759	-6.15206024062182	h
0.25160944684209	1.49290026995201	6.15033768254910	c
0.05685558866738	2.57062204855470	7.94251985099434	h
0.70744172568976	-0.50254951833658	6.63024087069868	h
-1.60005933961198	1.52716037538063	5.15774827905517	h
1.36334307718331	-2.51969179271284	-5.36005931804972	c
1.86530489254855	-3.27451416355357	-7.25477112355250	h
0.80863933732067	-4.14260731441358	-4.14081290033587	h
-0.30297997214004	-1.25750355532252	-5.55590758827928	h
4.87562739702916	2.56913873697292	5.94187661595089	c
5.44252966985585	0.57769635567348	6.30348664781793	h
4.67235597368207	3.53554383795622	7.79822909810879	h
6.42398581429809	3.52119737775626	4.89508895495851	h
5.88088705378319	-2.90823650090498	-3.89036447770547	c
5.37905864505665	-4.47156572786092	-2.57816680279356	h
6.40977100574927	-3.75288201359768	-5.74272690515965	h
7.57055904374142	-1.91793169007817	-3.13206026244339	h
6.38631796403996	2.59757532217625	-0.14732593550594	c
6.55658881939065	5.04854128287502	-1.18709706817010	c
8.90505310290436	6.27676875538251	-1.35023403970894	c
11.10665276370364	5.06720924191441	-0.48837905036454	c
10.95196438118794	2.62403737672051	0.54451994050971	c
8.60578522193341	1.39684648451122	0.72156713023317	c
4.83384542407954	5.99229020973710	-1.87807309513647	h
9.01244938580593	8.19289075287394	-2.16058446092143	h
12.94908192160173	6.03078666897650	-0.62038561988104	h
12.67241773672905	1.66548589711712	1.22460535032190	h
8.48590139243515	-0.50882871735918	1.55308650259789	h

h) $ZnCl_2$

Total energy = -2699.7206369050 |dE/dxyz| = 0.000012

Cartesian coordinates:

0.00000000000000	0.00000000000000	0.00000000005772	zn
3.97560557627799	0.00000000000000	-0.00000000002886	cl
-3.97560557627799	0.00000000000000	-0.00000000002886	cl

Vibrational frequencies (cm^{-1}) and IR intensities (km/mol)

6	a1	94.81	13.09692
7	b2	94.81	13.09692
8	a1	345.40	0.00000
9	b1	496.12	65.48643

i)$SiCl_2$

Total energy = -1209.7106622350 |dE/dxyz| = 0.000093

Cartesian coordinates:

0.00000000000000	0.00000000000000	-1.00544289252805	si
3.11135786658331	0.00000000000000	1.50272144626404	cl
-3.11135786658331	0.00000000000000	1.50272144626404	cl

j) $SiCl_4$

Total energy = -2130.0570022760 |dE/dxyz| = 0.000002

Cartesian coordinates:

0.00000000000000	0.00000000000000	0.00000000000000	si
2.24183532062485	2.24183532062485	2.24183532062485	cl
-2.24183532062485	2.24183532062485	-2.24183532062485	cl
-2.24183532062485	-2.24183532062485	2.24183532062485	cl
2.24183532062485	-2.24183532062485	-2.24183532062485	cl

k) $Zn(Si(CH_3)_3)_2$

Total energy = -2597.6021720090 |dE/dxyz| = 0.000163

Cartesian coordinates:

0.00000000000000	0.00000000000000	0.00000000000000	zn
0.00000000000000	0.00000000000000	4.57416853690879	si
2.92106319918001	-1.68647662436649	5.89671193179722	c
-2.92106319918001	-1.68647662436649	5.89671193179722	c
0.00000000000000	3.37295324873296	5.89671193179722	c
2.89684990743105	-1.67249707385725	8.00394207665005	h
-4.70210082206676	-0.75430825935805	5.27639048742075	h
1.69780029614489	4.44929289274452	5.27639048742075	h
-2.89684990743105	-1.67249707385725	8.00394207665005	h
3.00430052592188	-3.69498463338649	5.27639048742075	h
4.70210082206676	-0.75430825935805	5.27639048742075	h
-1.69780029614488	4.44929289274452	5.27639048742075	h
-3.00430052592188	-3.69498463338649	5.27639048742075	h
0.00000000000000	3.34499414771454	8.00394207665005	h
0.00000000000000	0.00000000000000	-4.57416853690879	si
-2.92106319918001	1.68647662436649	-5.89671193179722	c
2.92106319918001	1.68647662436649	-5.89671193179722	c
0.00000000000000	-3.37295324873296	-5.89671193179722	c
-2.89684990743105	1.67249707385725	-8.00394207665005	h
4.70210082206676	0.75430825935805	-5.27639048742075	h
-1.69780029614488	-4.44929289274452	-5.27639048742075	h
2.89684990743105	1.67249707385725	-8.00394207665005	h
-3.00430052592188	3.69498463338649	-5.27639048742075	h
-4.70210082206676	0.75430825935805	-5.27639048742075	h

1.69780029614489	-4.44929289274452	-5.27639048742075	h
3.00430052592188	3.69498463338649	-5.27639048742075	h
0.00000000000000	-3.34499414771454	-8.00394207665005	h

Vibrational frequencies (cm^{-1}) and IR intensities (km/mol)

7	a1u	29.93	0.00000
8	eu	39.59	0.27062
9	eu	39.59	0.27062
10	eg	105.81	0.00000
11	eg	105.81	0.00000
12	a1g	131.61	0.00000
13	eu	159.62	0.34976
14	eu	159.62	0.34976
15	a2g	169.60	0.00000
16	a1u	169.81	0.00000
17	eg	179.03	0.00000
18	eg	179.03	0.00000
19	eu	179.26	0.00010
20	eu	179.26	0.00010
21	a2u	189.31	26.20969
22	eg	198.30	0.00000
23	eg	198.30	0.00000
24	eu	207.37	0.60489
25	eu	207.37	0.60489
26	a1g	283.31	0.00000
27	a2u	336.25	3.24337
28	a2u	590.34	22.29928
29	a1g	590.93	0.00000
30	eg	662.83	0.00000
31	eg	662.83	0.00000
32	eu	663.36	26.85885
33	eu	663.36	26.85885
34	a2g	671.73	0.00000
35	a1u	671.76	0.00000
36	eg	721.61	0.00000
37	eg	721.61	0.00000
38	eu	731.29	16.92527
39	eu	731.29	16.92527
40	eg	837.23	0.00000
41	eg	837.23	0.00000
42	eu	838.51	94.48389
43	eu	838.51	94.48389
44	a2u	839.64	476.25782
45	a1g	860.18	0.00000
46	eg	1231.41	0.00000
47	eg	1231.41	0.00000
48	eu	1231.86	33.05096
49	eu	1231.86	33.05096
50	a2u	1243.14	0.10285
51	a1g	1244.11	0.00000

52	a2g	1397.63	0.00000
53	a1u	1397.83	0.00000
54	eg	1400.38	0.00000
55	eg	1400.38	0.00000
56	eu	1400.67	1.99685
57	eu	1400.67	1.99685
58	eu	1410.36	18.32091
59	eu	1410.36	18.32091
60	eg	1410.51	0.00000
61	eg	1410.51	0.00000
62	a2u	1416.36	4.55225
63	a1g	1416.72	0.00000
64	a2u	2926.69	58.10859
65	eg	2926.88	0.00000
66	eg	2926.88	0.00000
67	eu	2926.92	27.76565
68	eu	2926.92	27.76565
69	a1g	2927.20	0.00000
70	eg	3013.19	0.00000
71	eg	3013.19	0.00000
72	eu	3013.24	3.97761
73	eu	3013.24	3.97761
74	a2u	3013.76	56.57819
75	a1g	3013.86	0.00000
76	a2g	3028.01	0.00000
77	a1u	3028.03	0.00000
78	eg	3028.10	0.00000
79	eg	3028.10	0.00000
80	eu	3028.14	27.61614
81	eu	3028.14	27.61614

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