Electronic Supplementary Information

Reactions of a tetrasilabicyclo[1.1.0]but-1(3)-ene with carbon tetrachloride and methanol

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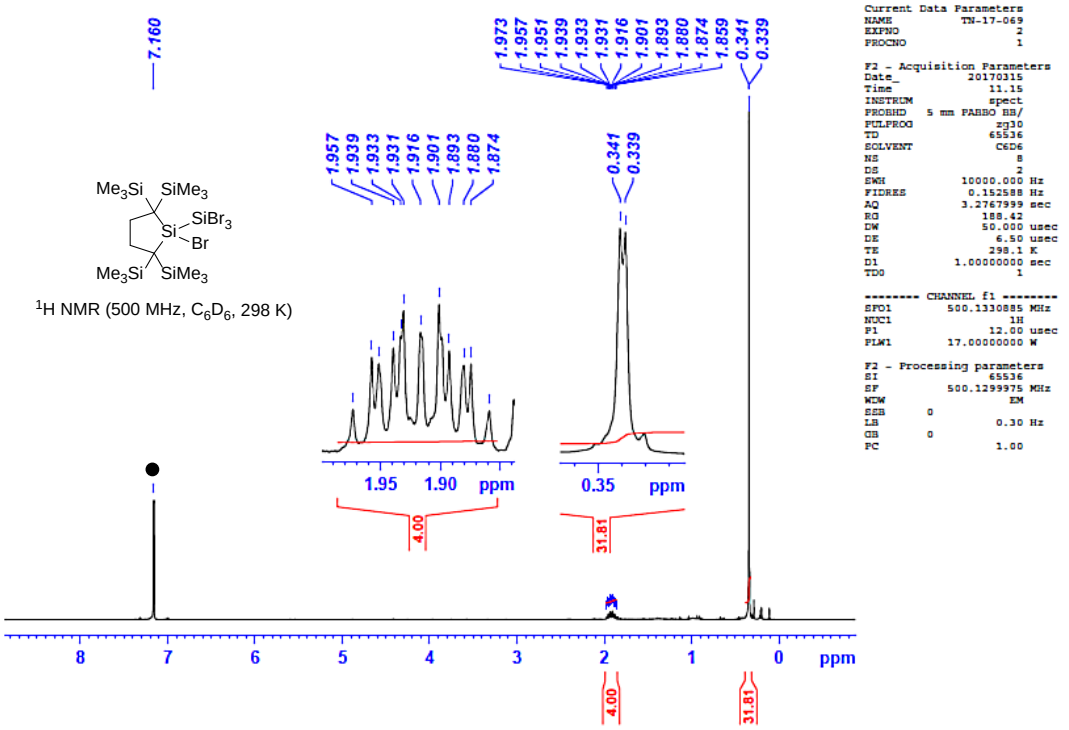


Figure S1. ^{1}H NMR spectrum of **3** in C_6D_6 at 298 K (● = C_6HD_5).

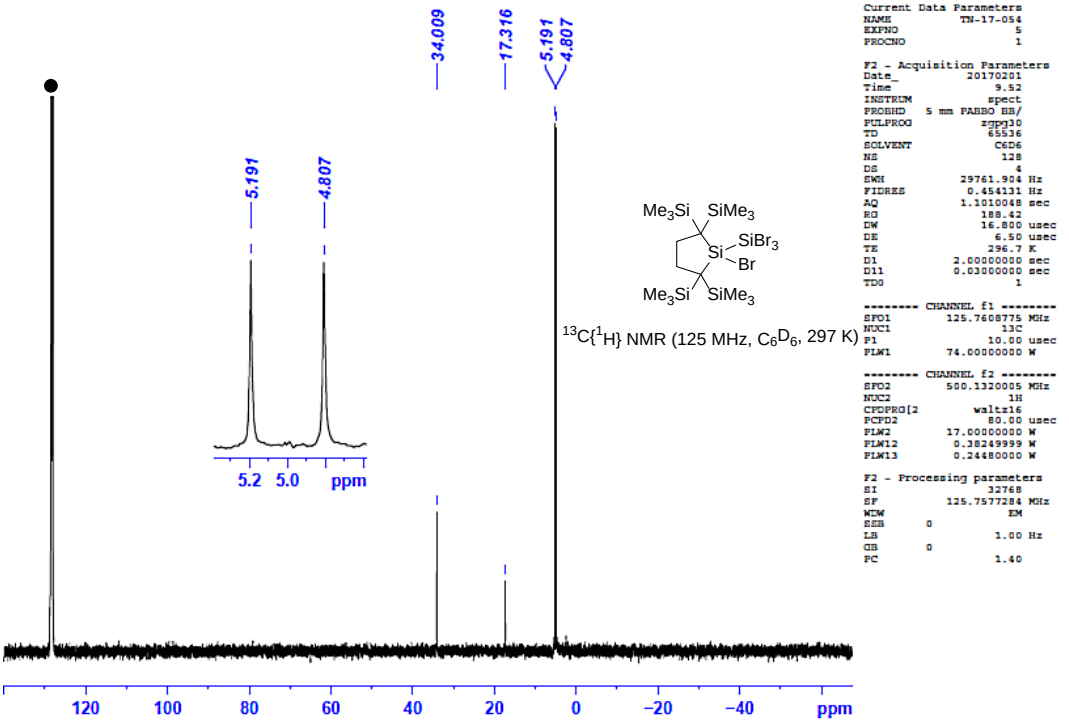
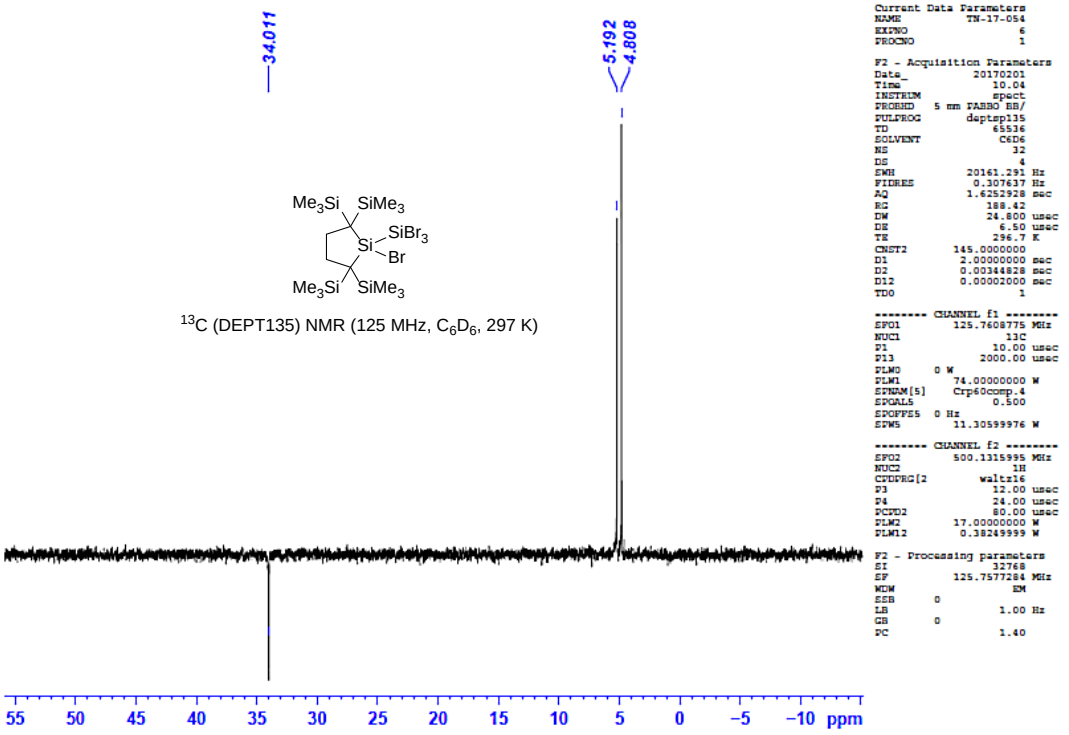


Figure S2. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6 in 297 K (● = C_6D_6).



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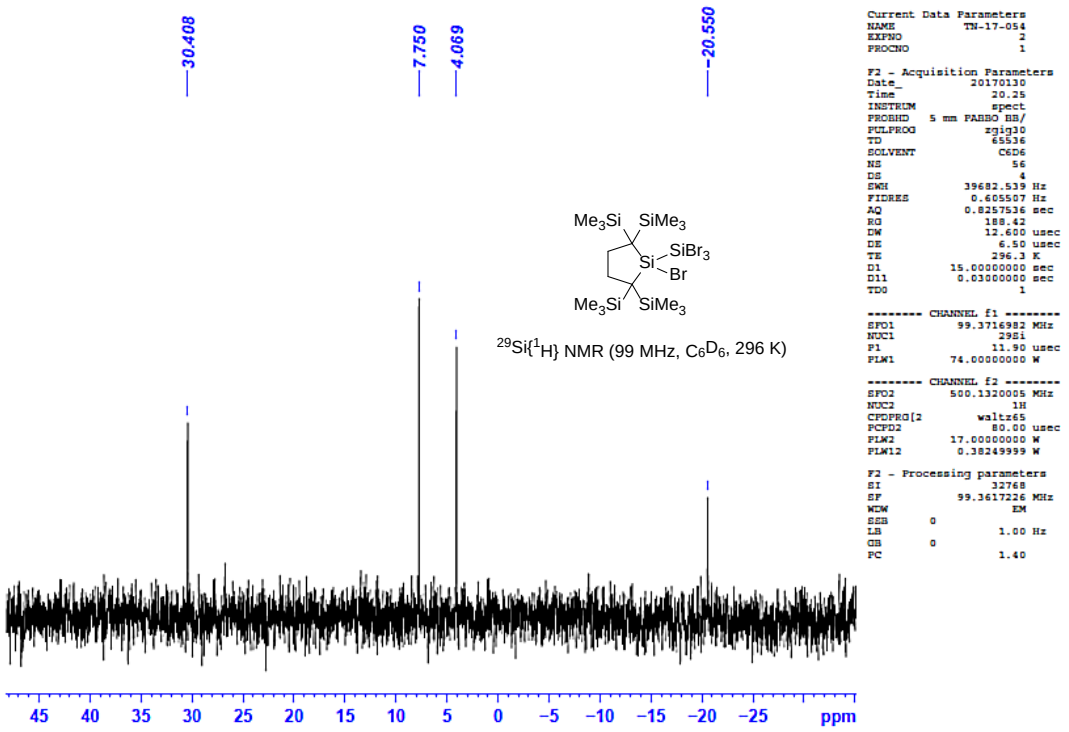

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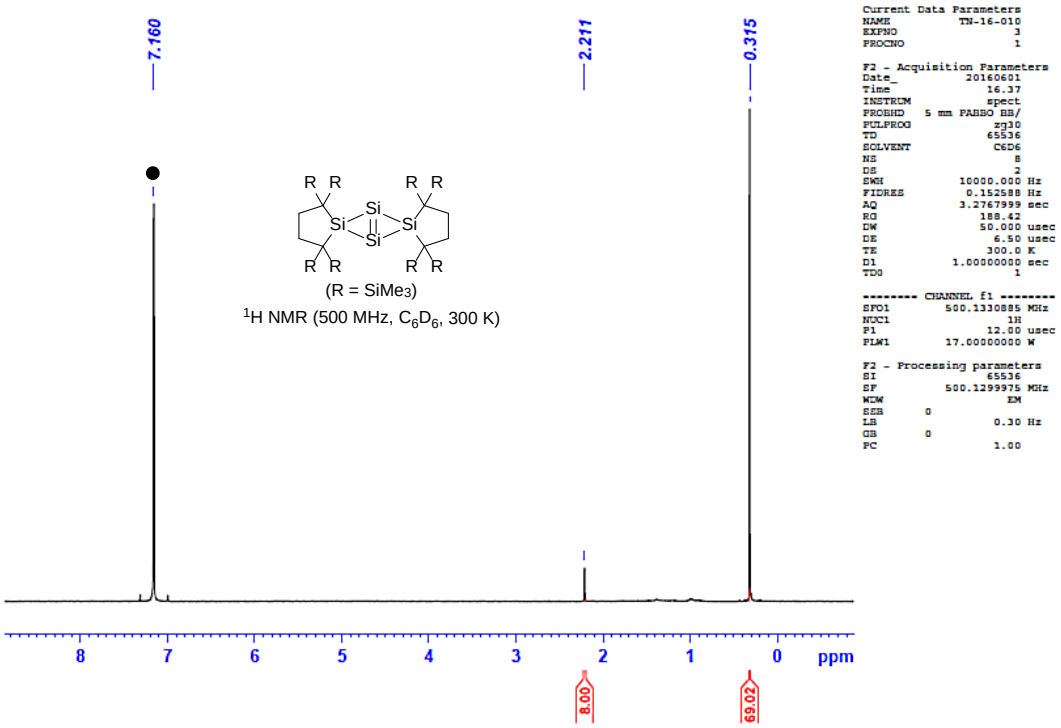

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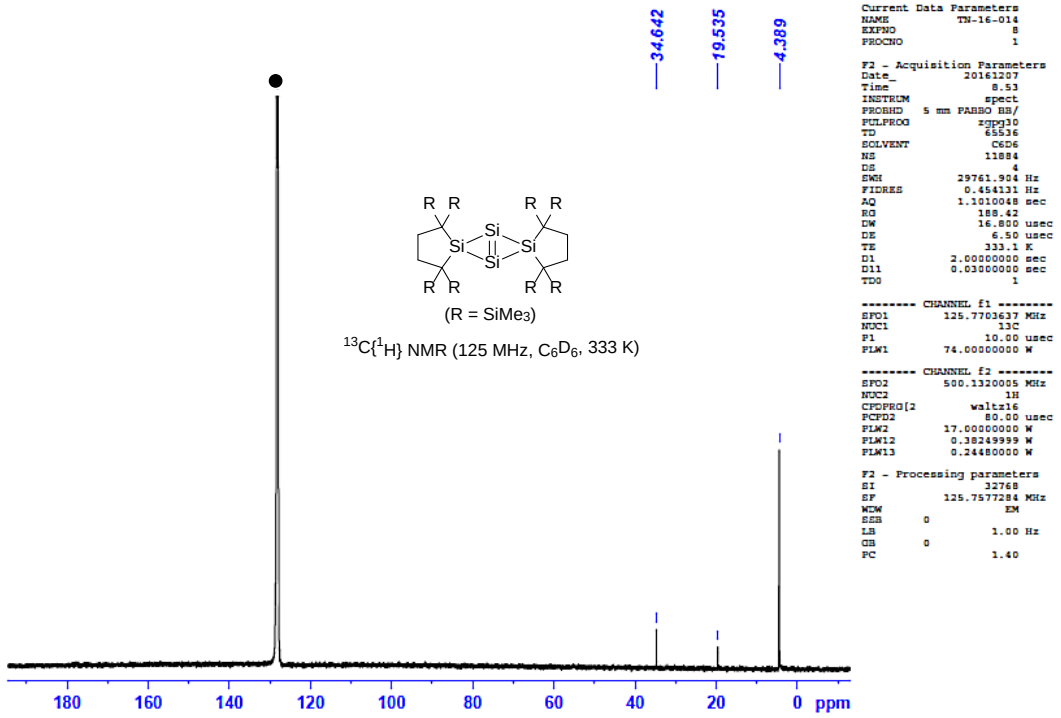

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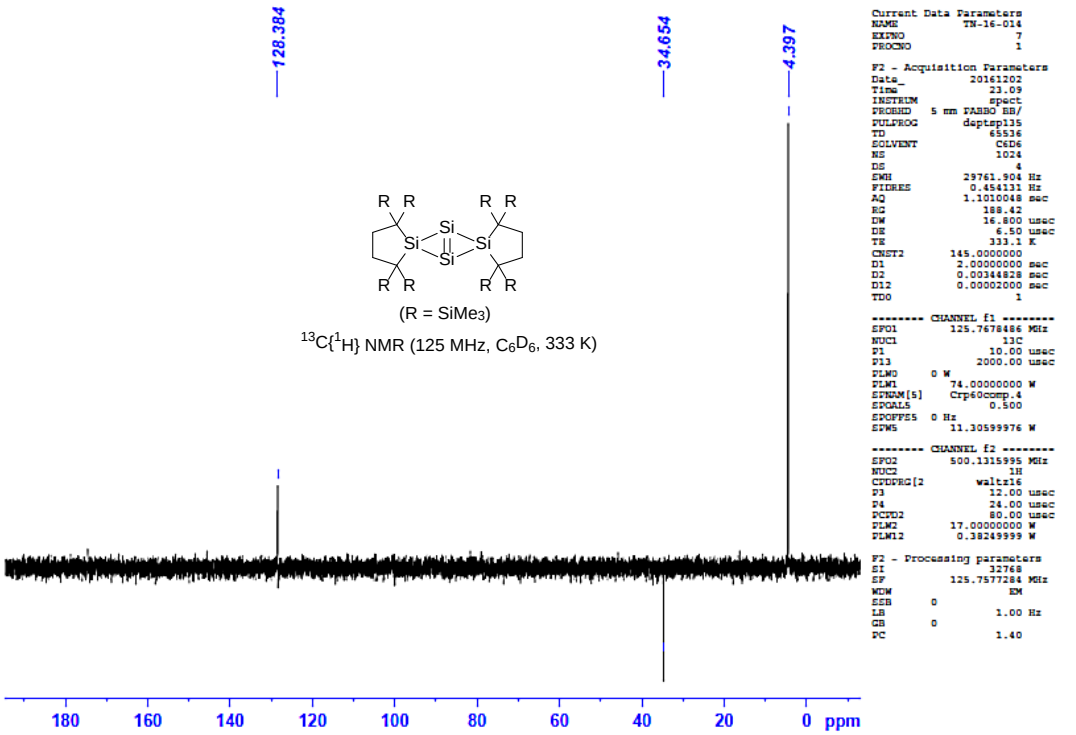

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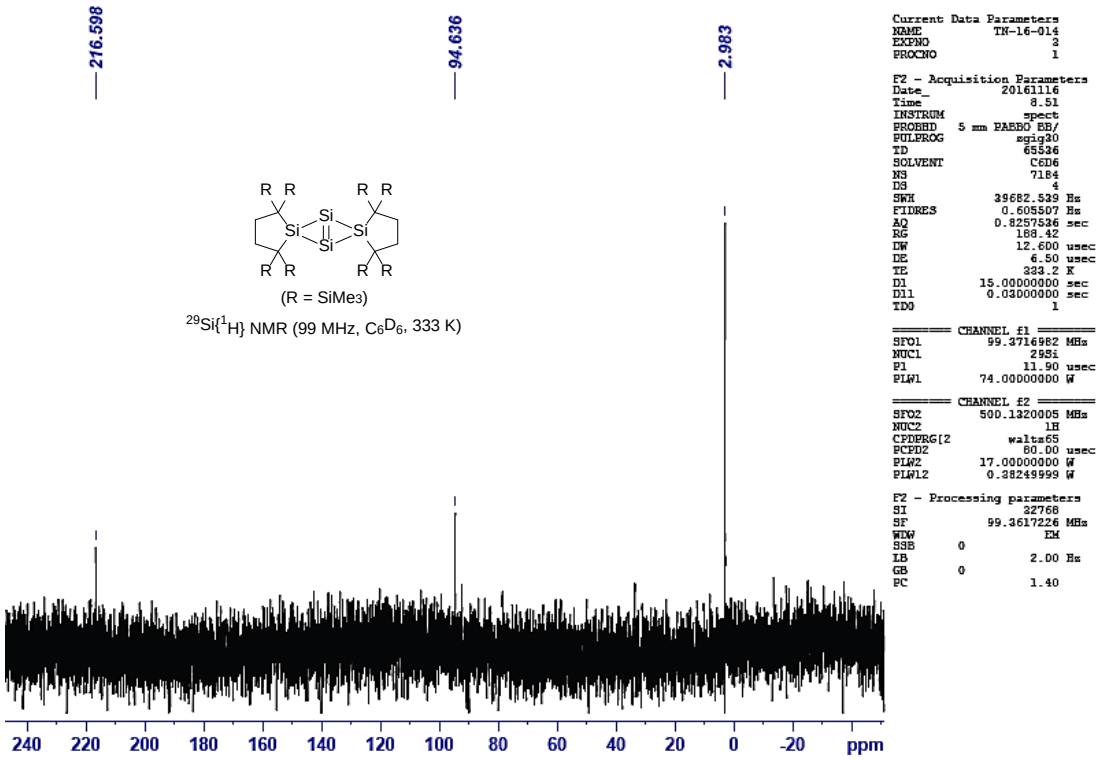
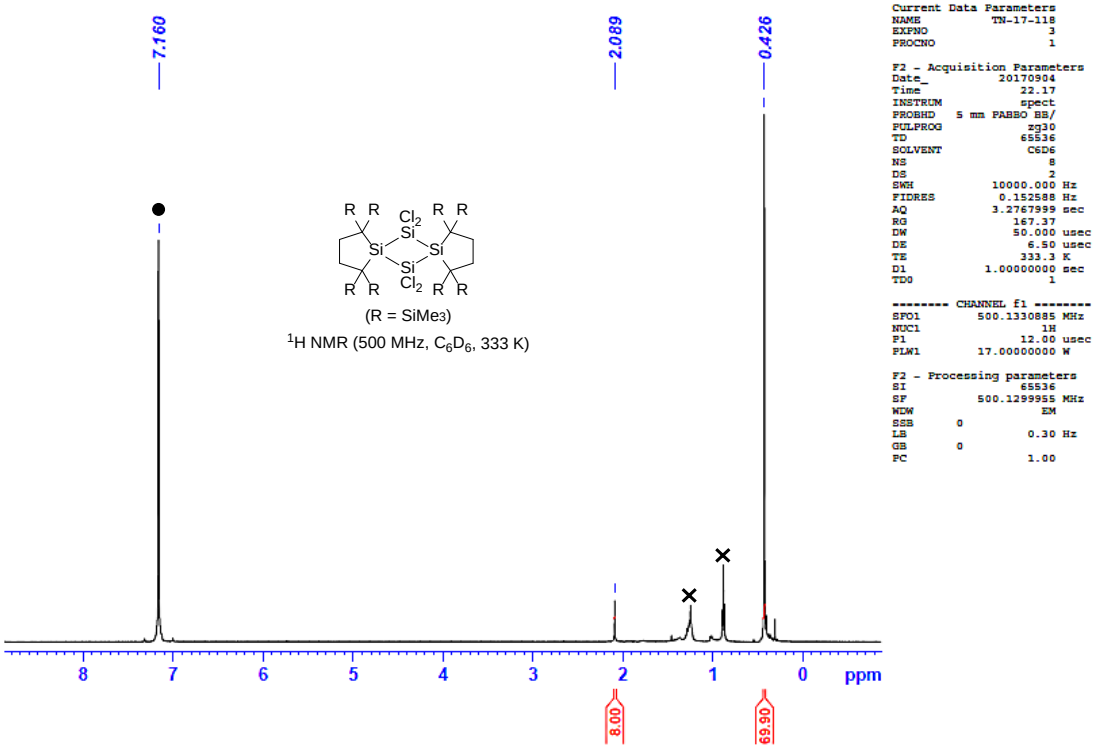


Figure S8. $^{29}Si\{^1H\}$ NMR spectrum of **1b** in C_6D_6 at 333 K.



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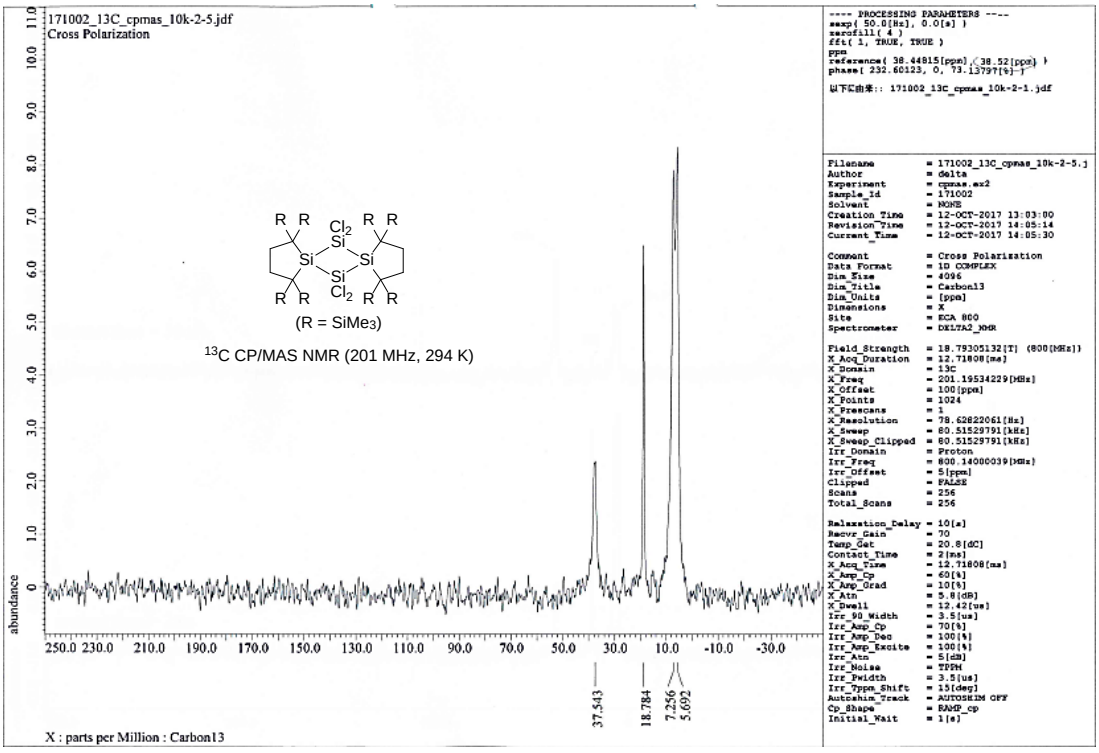

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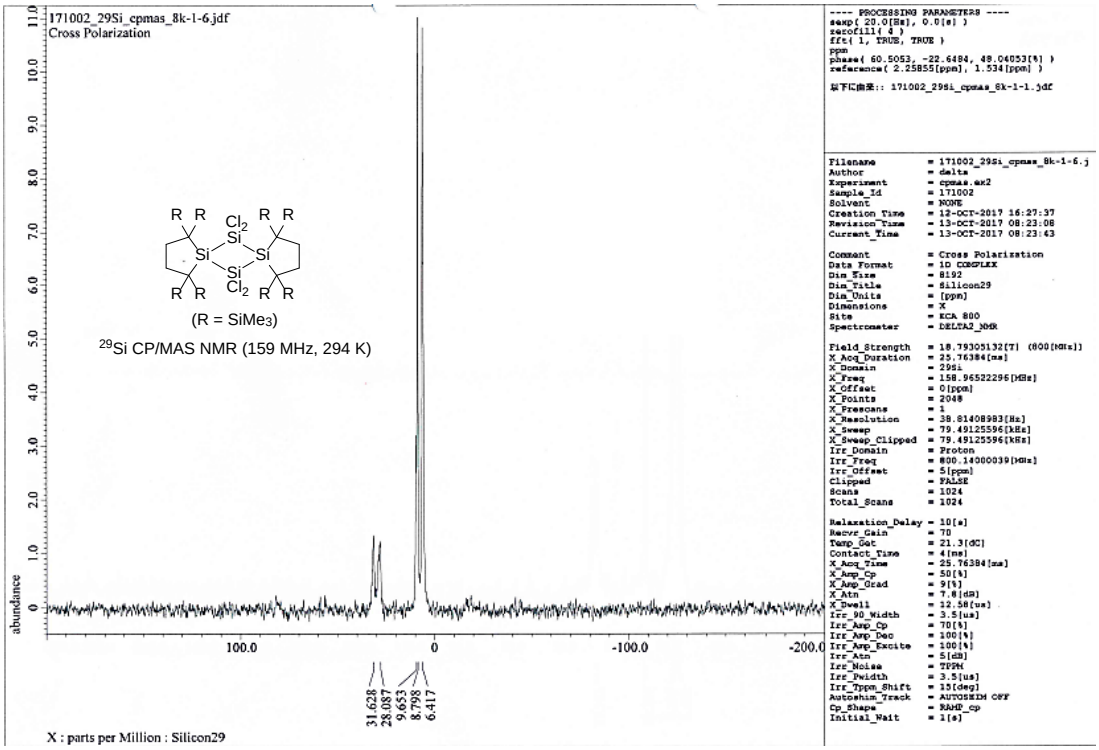

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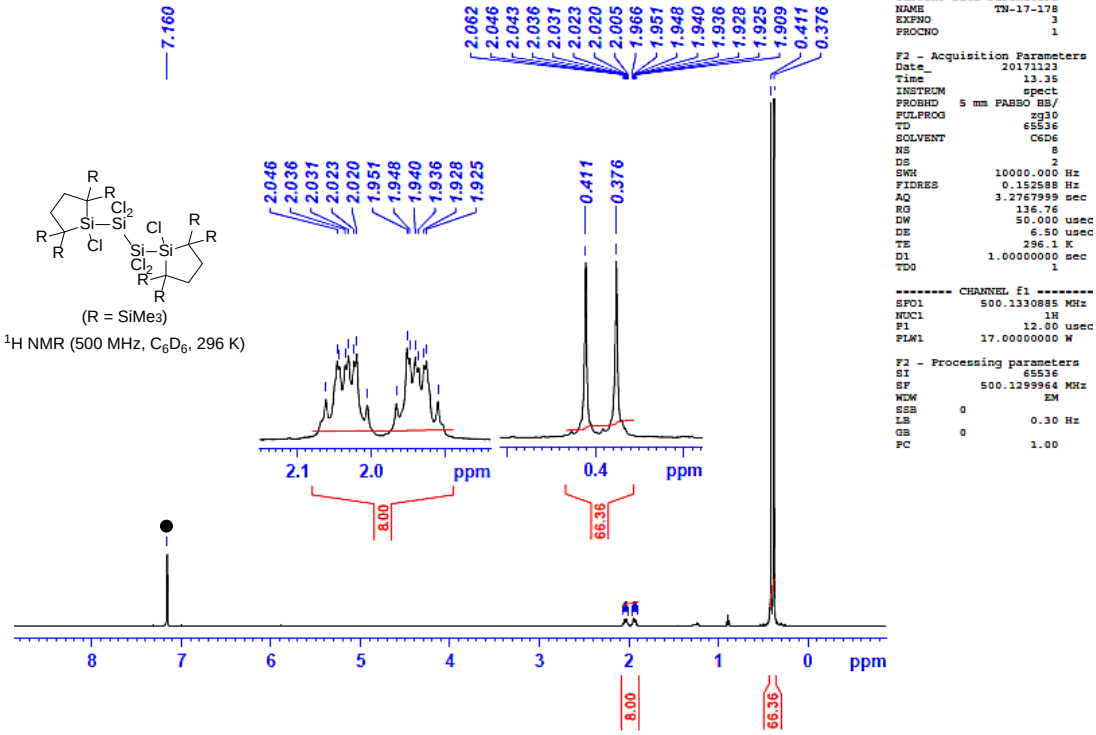

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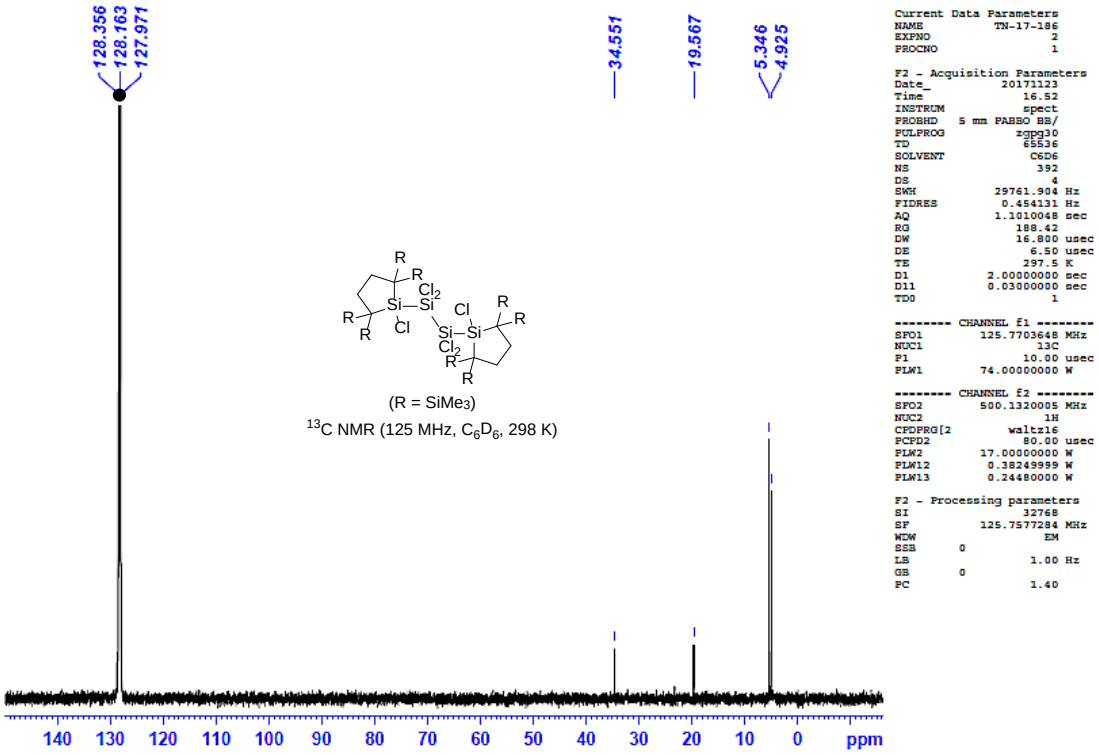
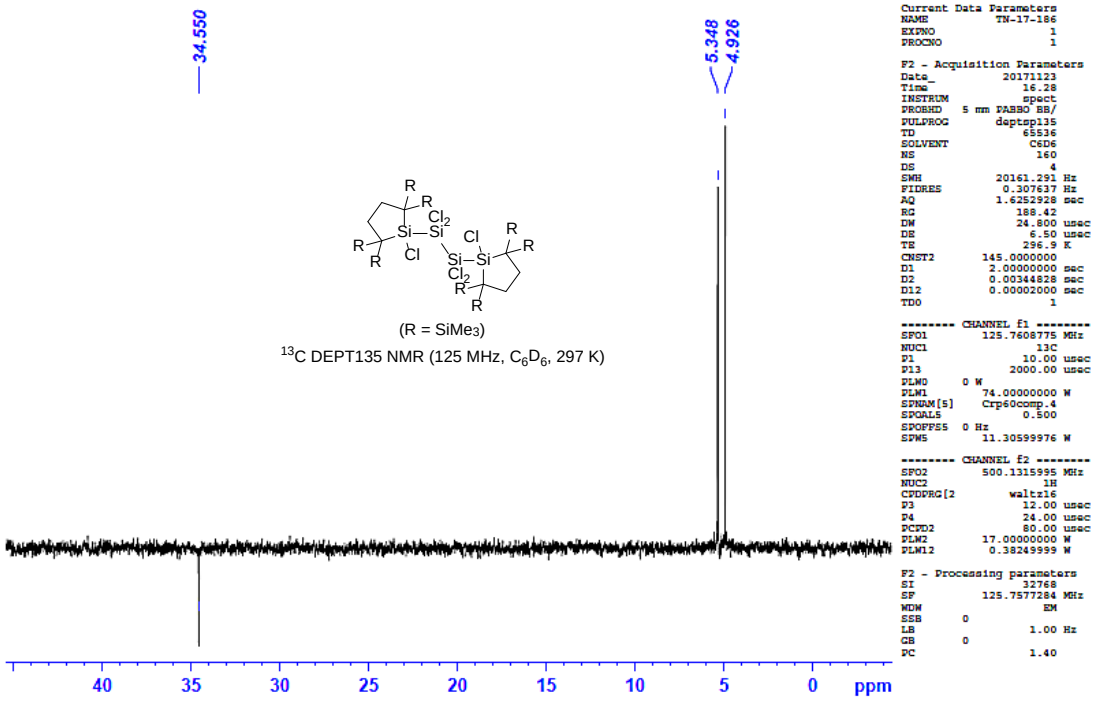


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 298 K (● = C_6D_6).



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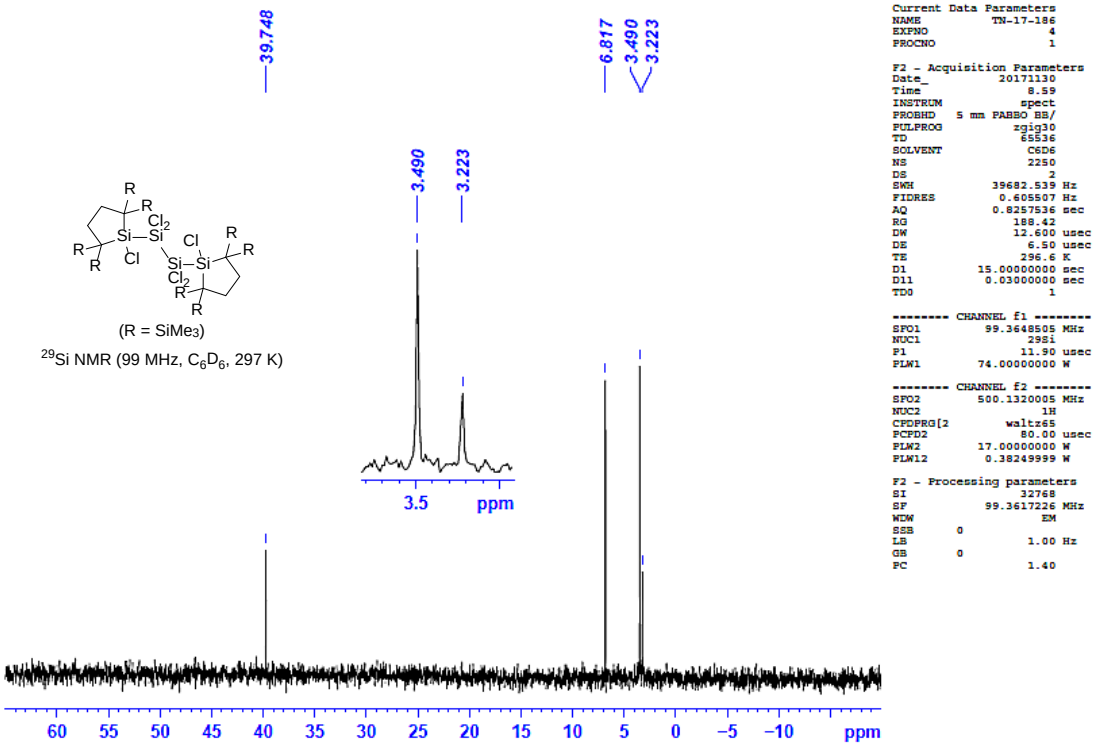

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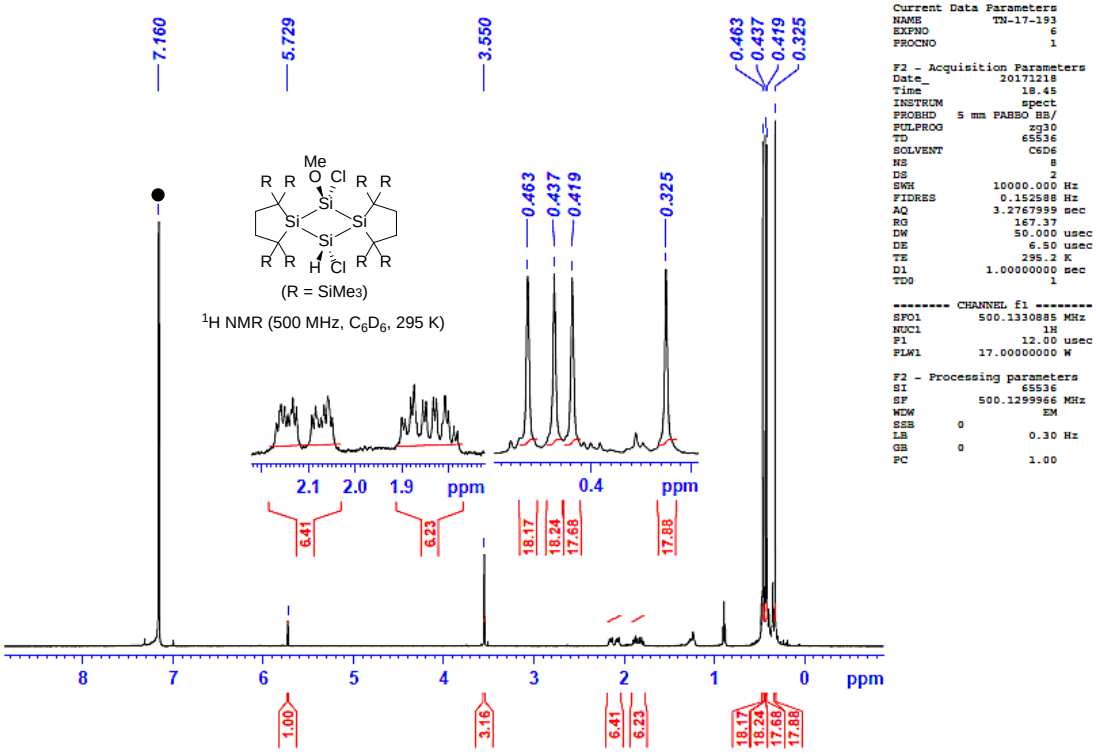

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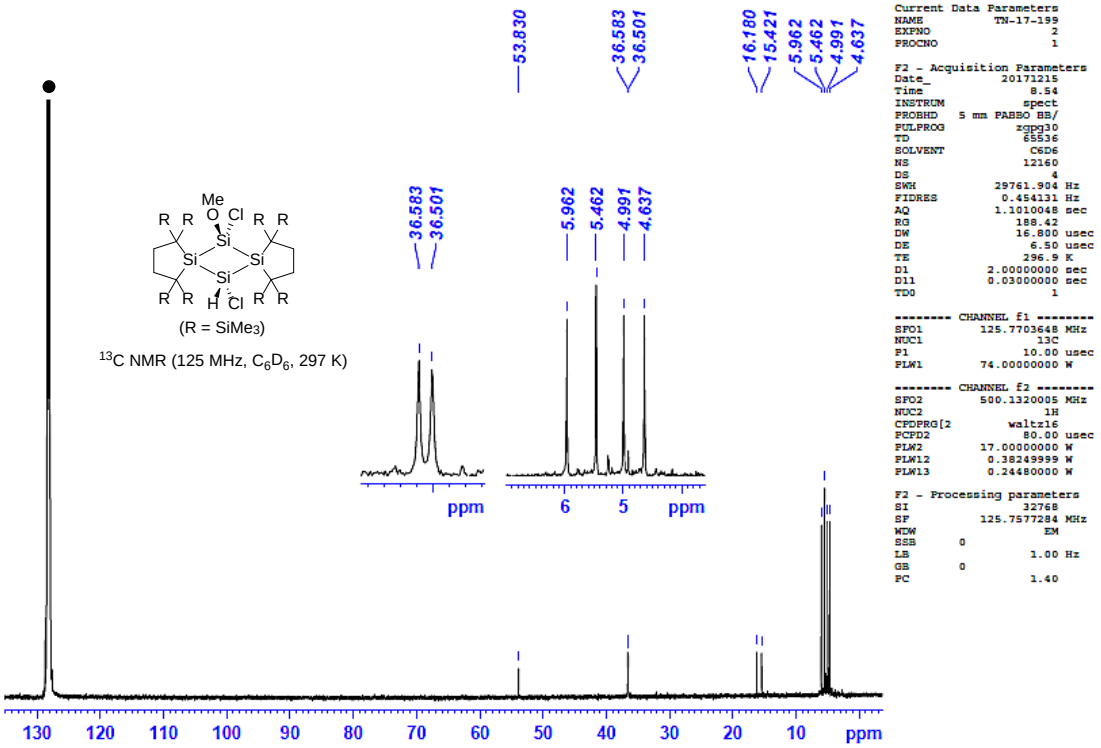

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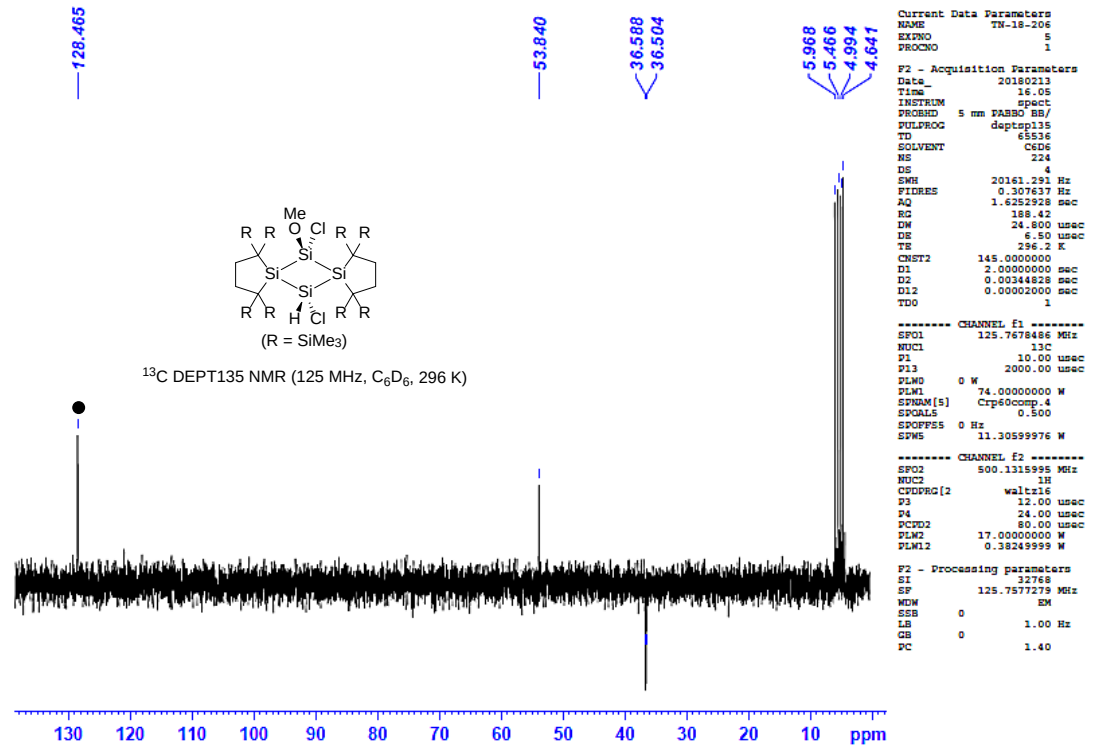

Figure S18. ^{13}C (DEPT135) NMR spectrum of **6** in C_6D_6 at 296 K (● = C_6D_6).

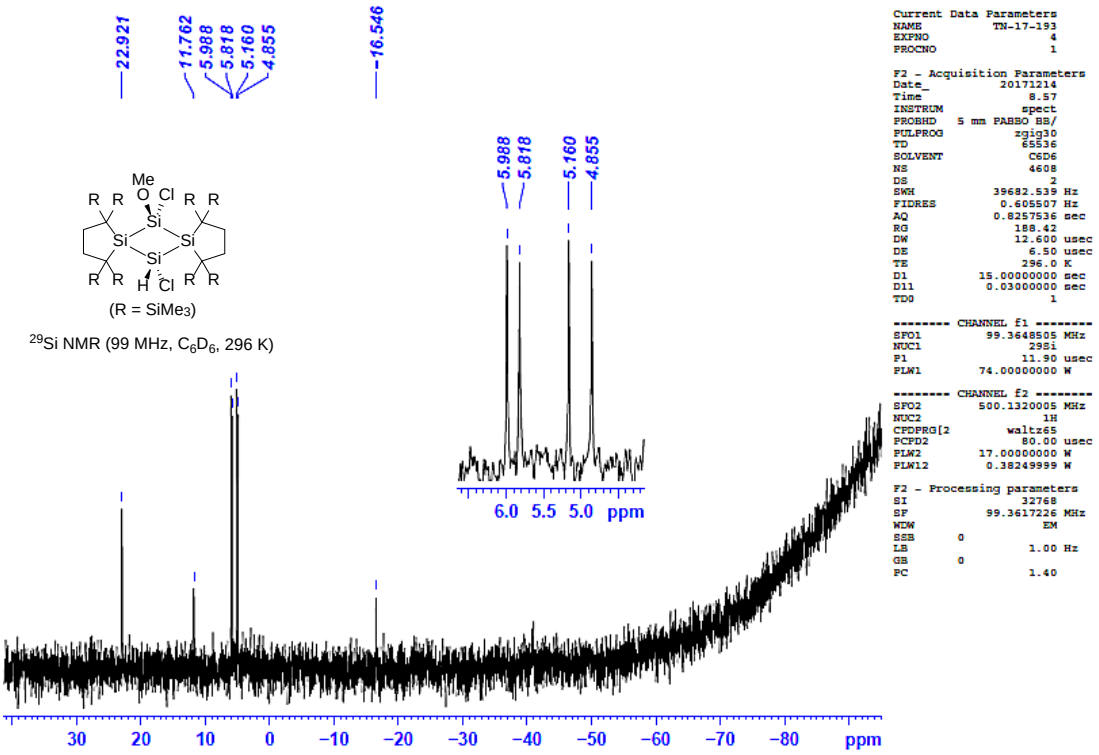

Figure S19. $^{29}Si\{^{1}H\}$ NMR spectrum of **6** in C_6D_6 at 296 K.

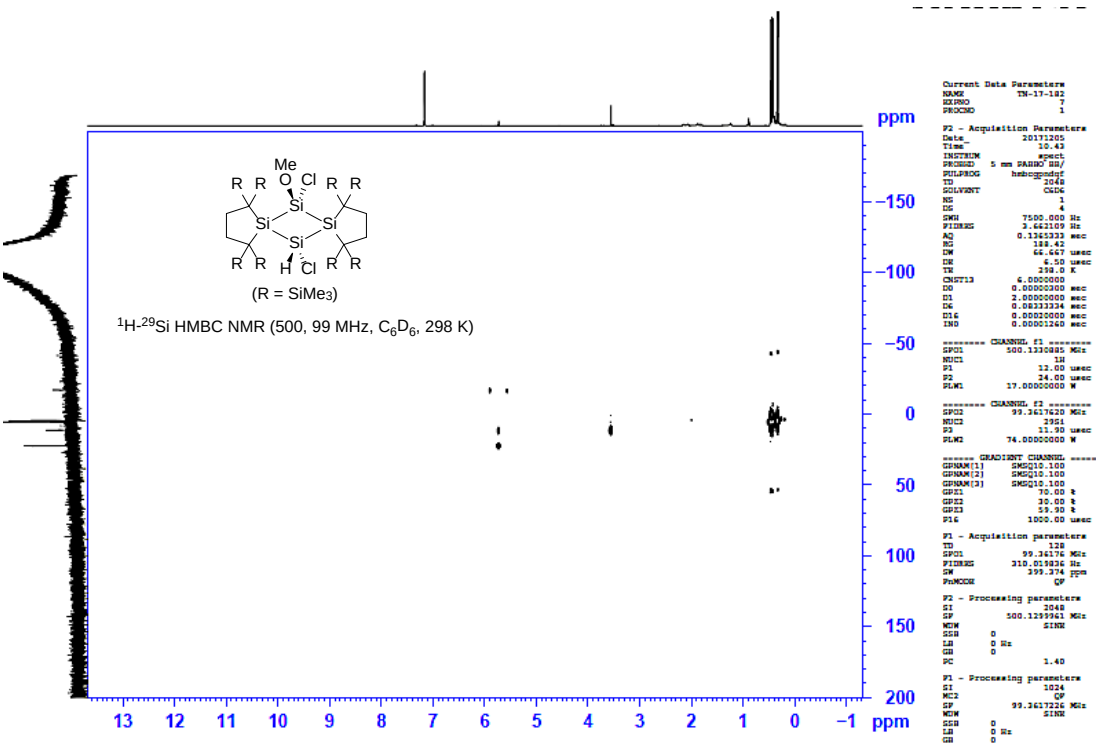

Figure S20. ^{1}H-^{29}Si HMBC NMR spectrum of **6** in C_6D_6 at 298 K.

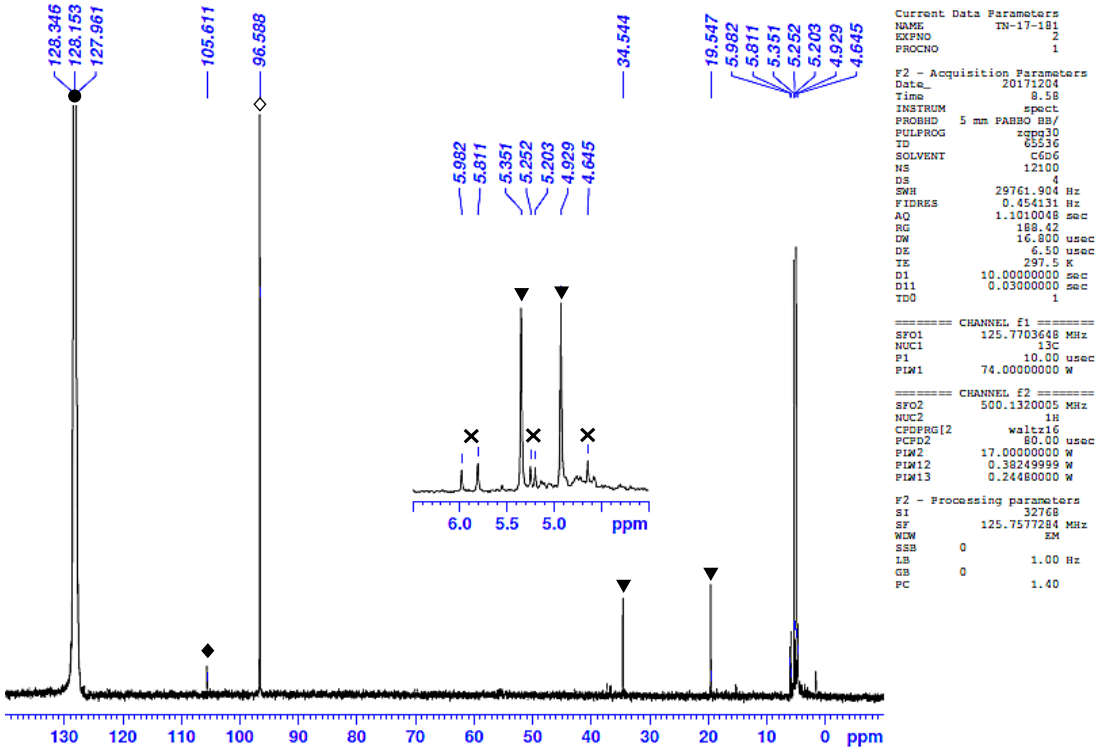

Figure S21. ^{1}H NMR spectrum of a mixture obtained from the reaction of **1b** with CCl_4 in C_6D_6 at 298 K (● = C_6D_6, ▼ = **5**, ◊ = carbon tetrachloride, ♦ = hexachloroethane, × = by products).

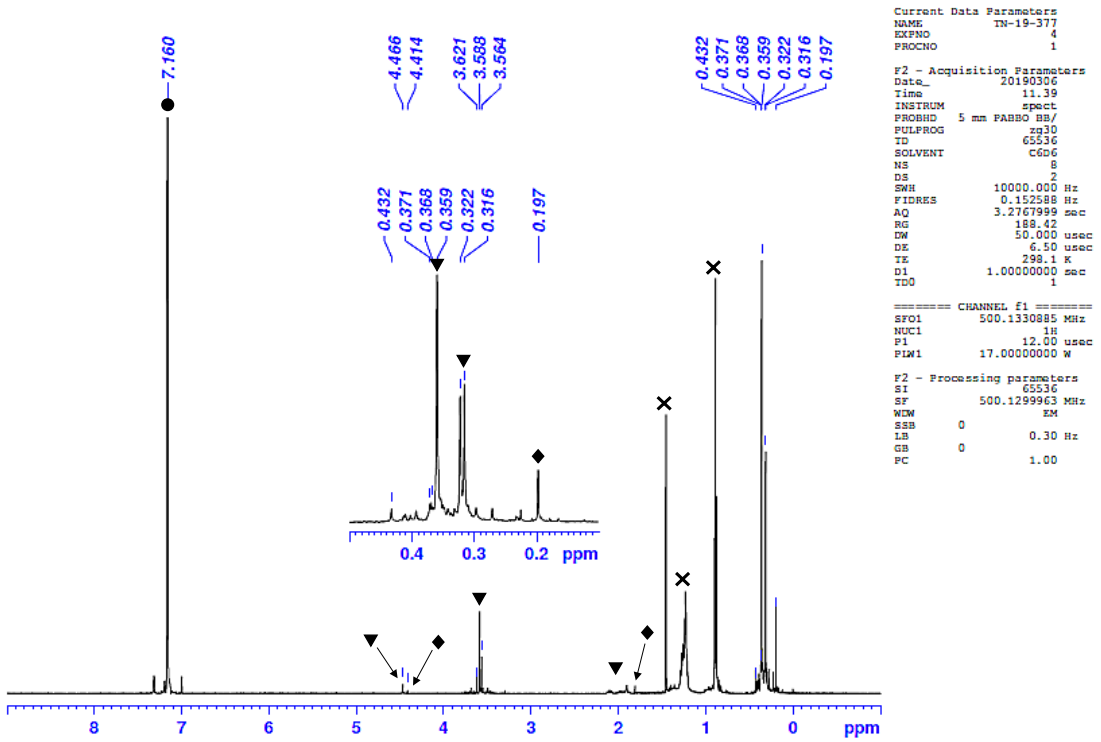

Figure S22. ^{1}H NMR spectrum of a mixture obtained from the reaction of **1b** with MeOH in C_6D_6 at 298 K (● = C_6HD_5, ▼ = **9**, ♦ = dihydrosilane[1], × = impurity).

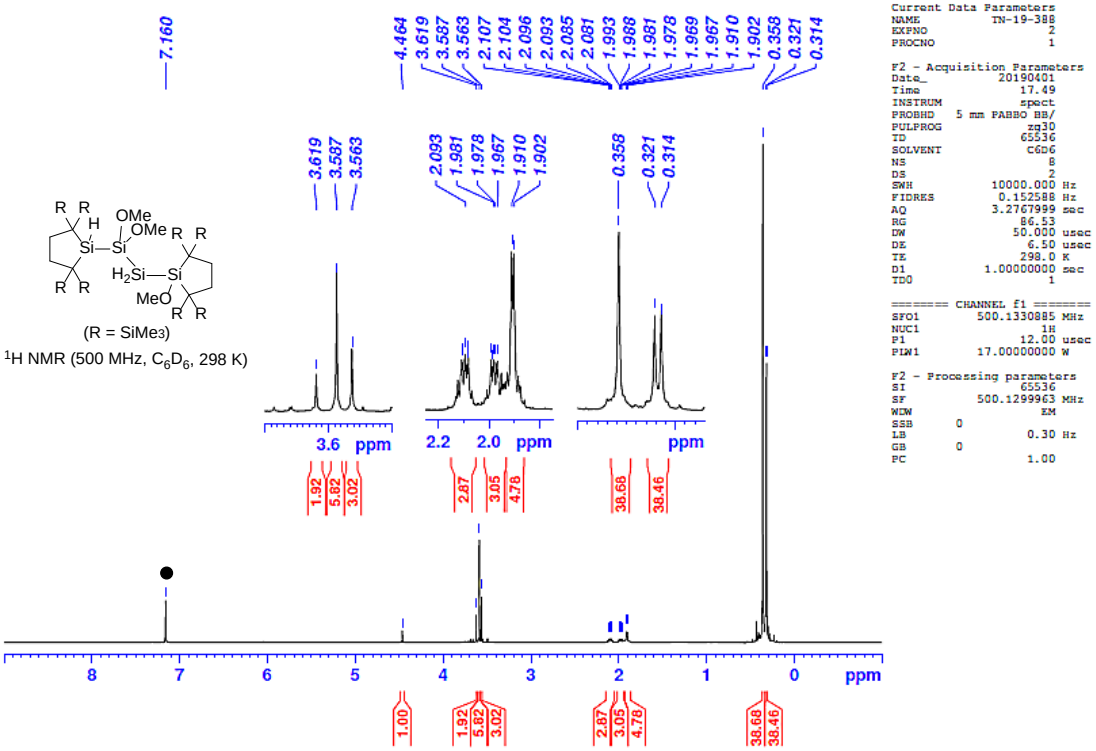

Figure S23. ^{1}H NMR spectrum of **9** in C_6D_6 at 298 K (● = C_6HD_5).

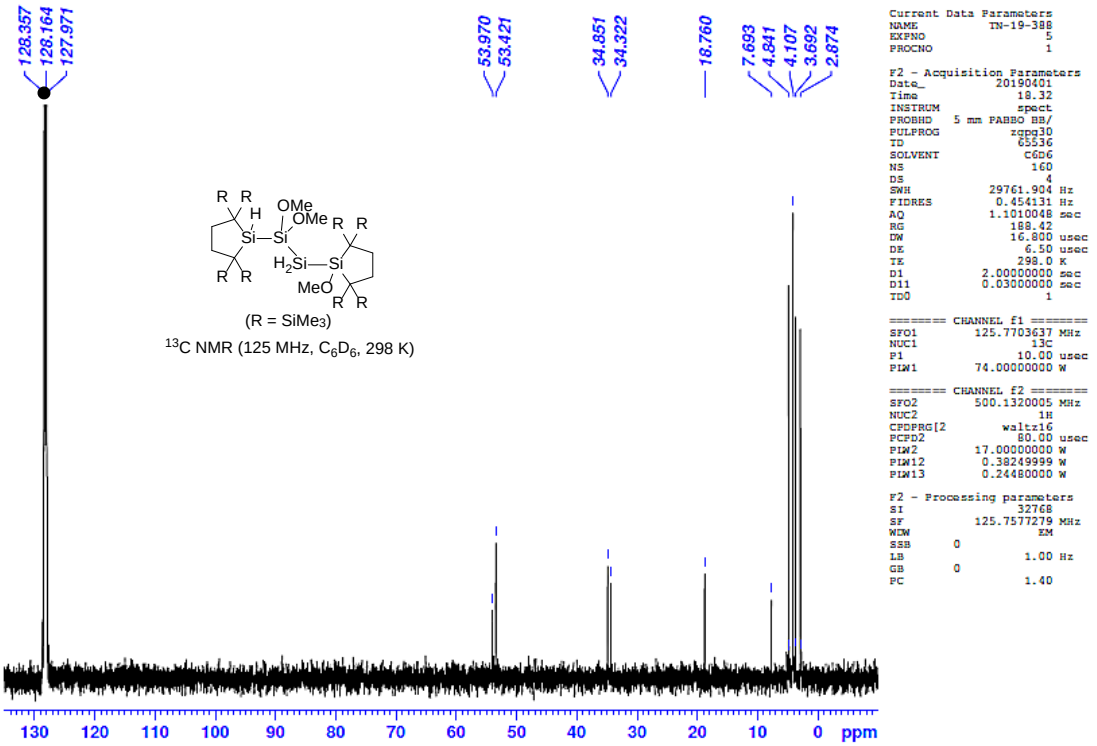

Figure S24. ^{13}C{^{1}H} spectrum of **9** in C_6D_6 at 298 K (● = C_6D_6).

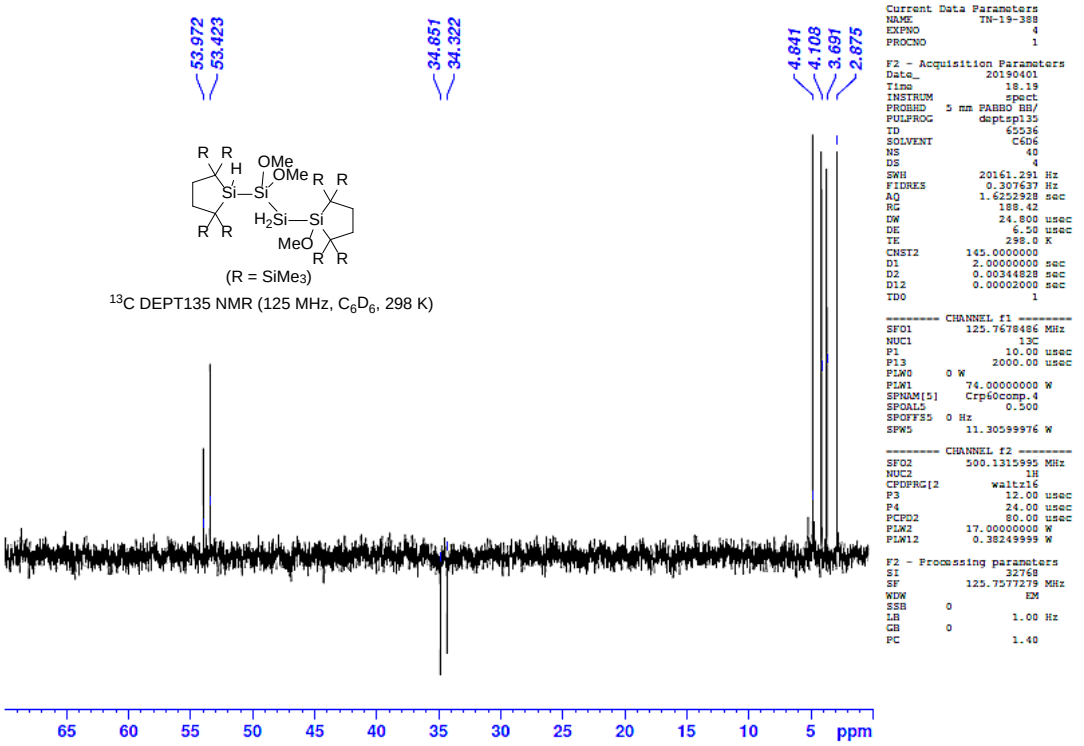

Figure S25. ^{13}C (DEPT135) NMR spectrum of **9** in C_6D_6 at 298 K.

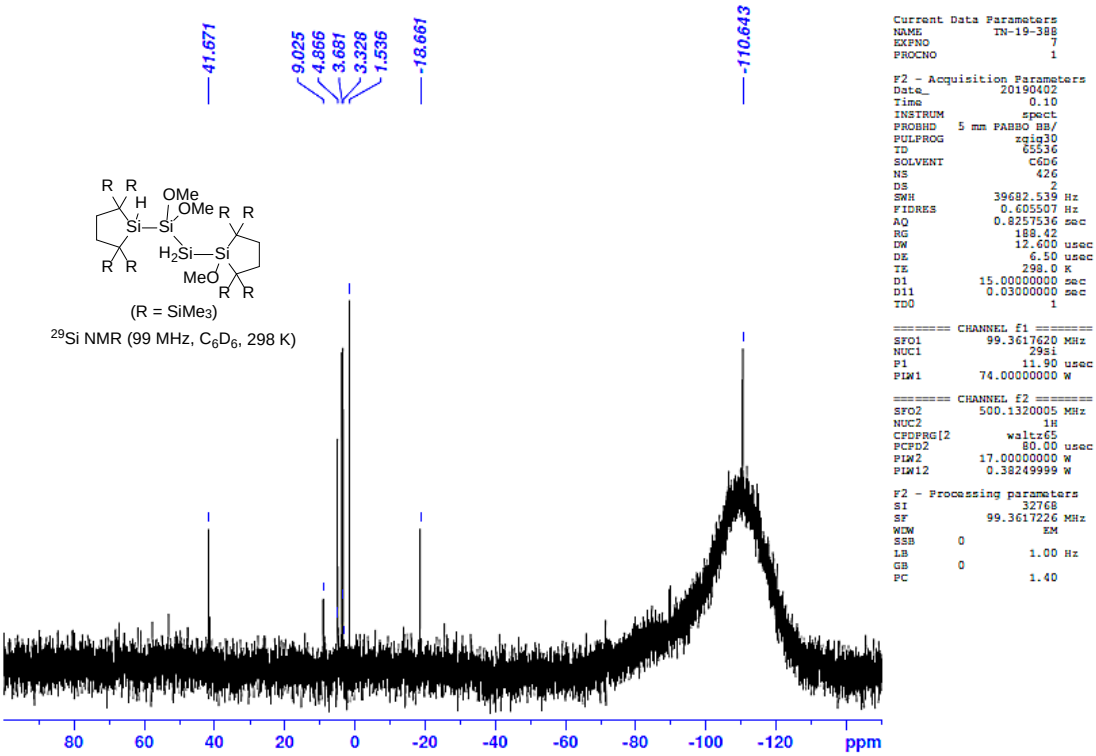

Figure S26. $^{29}Si\{^1H\}$ spectrum of **9** in C_6D_6 at 298 K.

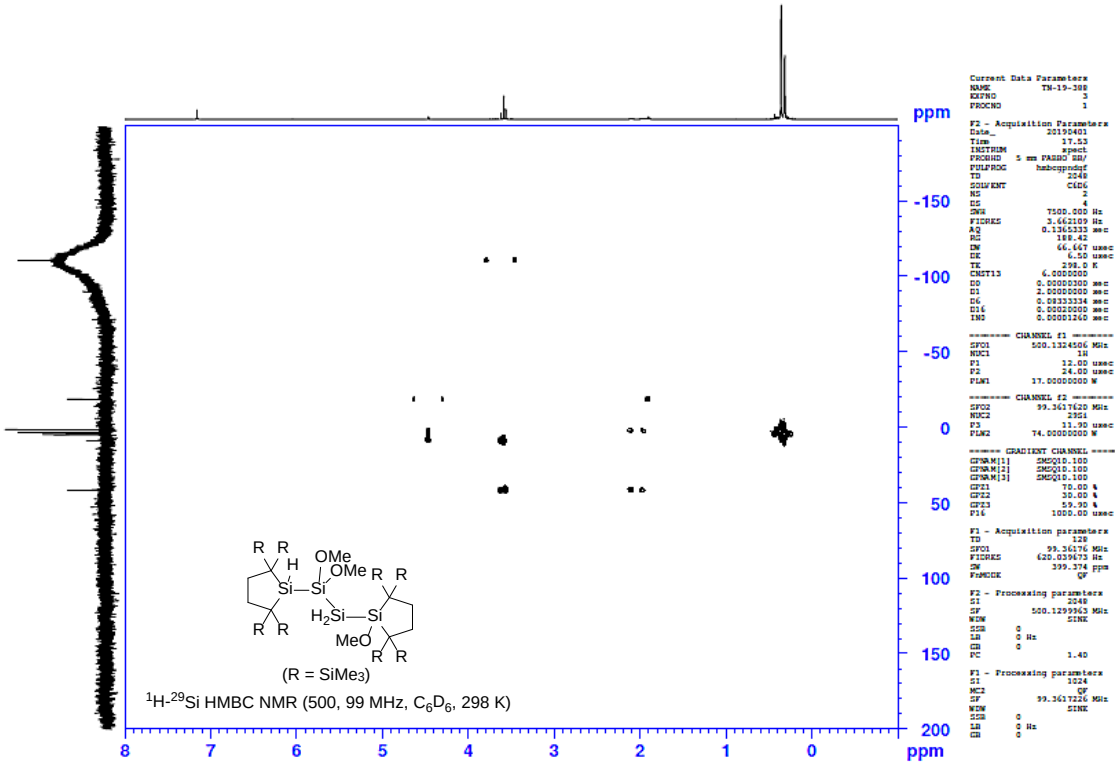

Figure S27. ^{1}H-^{29}Si HMBC NMR spectrum of **9** in C_6D_6 at 298 K.

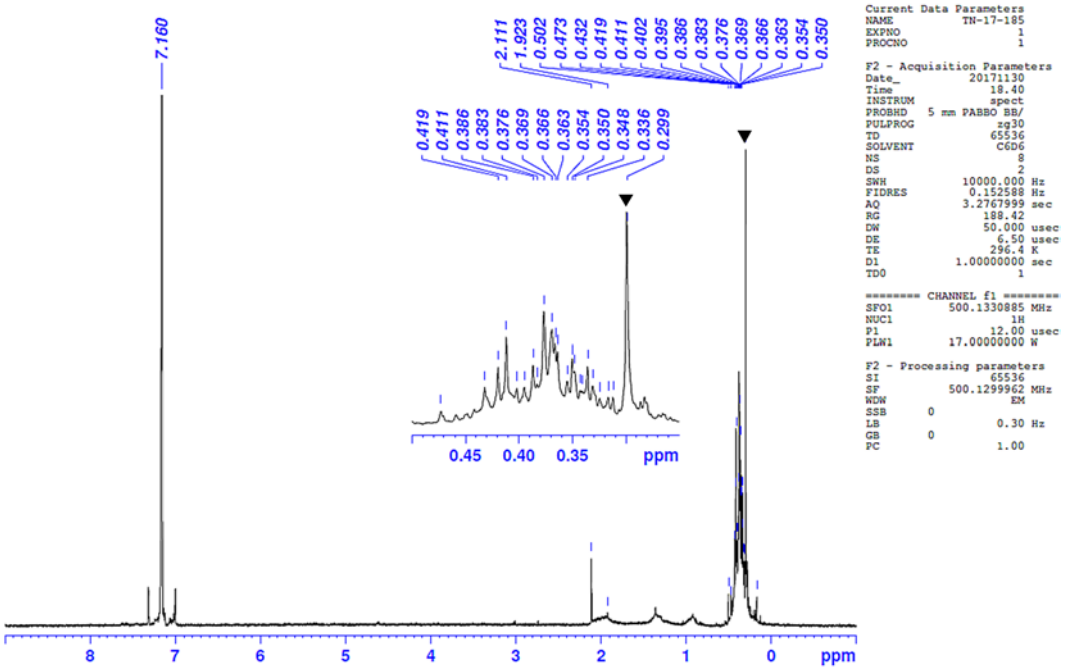

Figure S28. ^{1}H NMR spectrum for the reaction mixture of **1b** with 2 equivalents of CCl_4 recorded in C_6D_6 at 296 K (▼ = silicon grease).

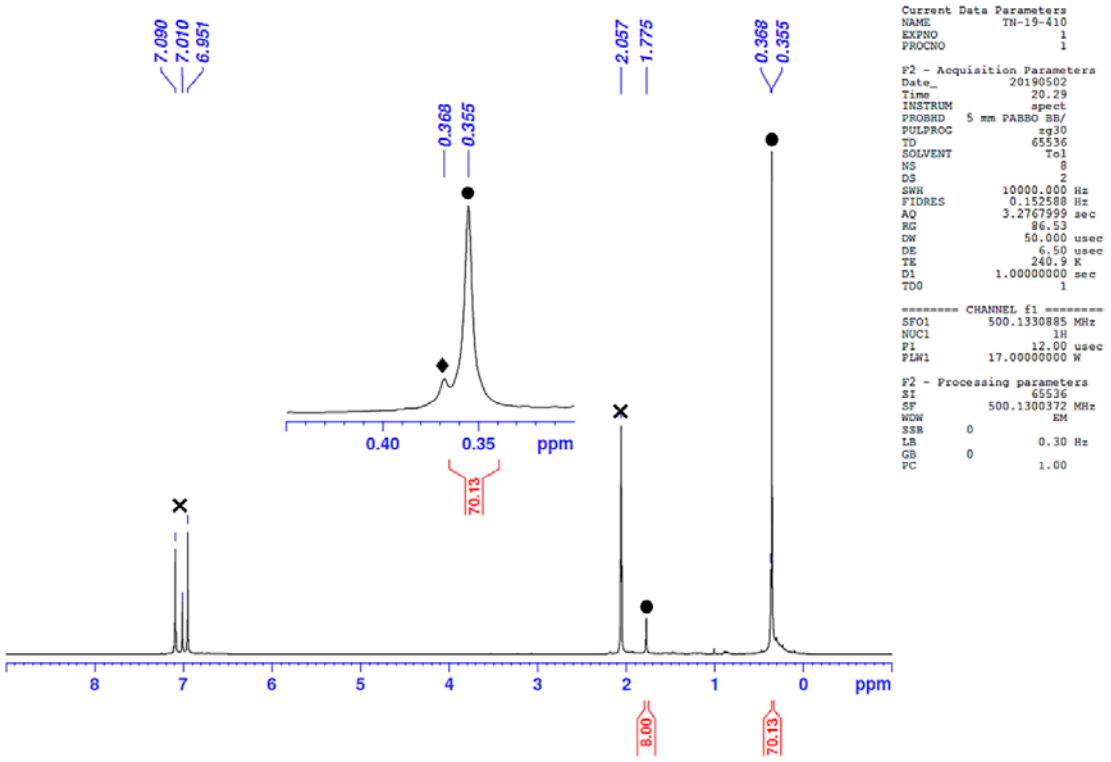

Figure S29. ^{1}H NMR spectrum of the mixture after addition of excess carbon tetrachloride to a toluene-d_8 solution of **1b** at 241 K (● = intermediate, ♦ = **4**, × = C_7D_7H).

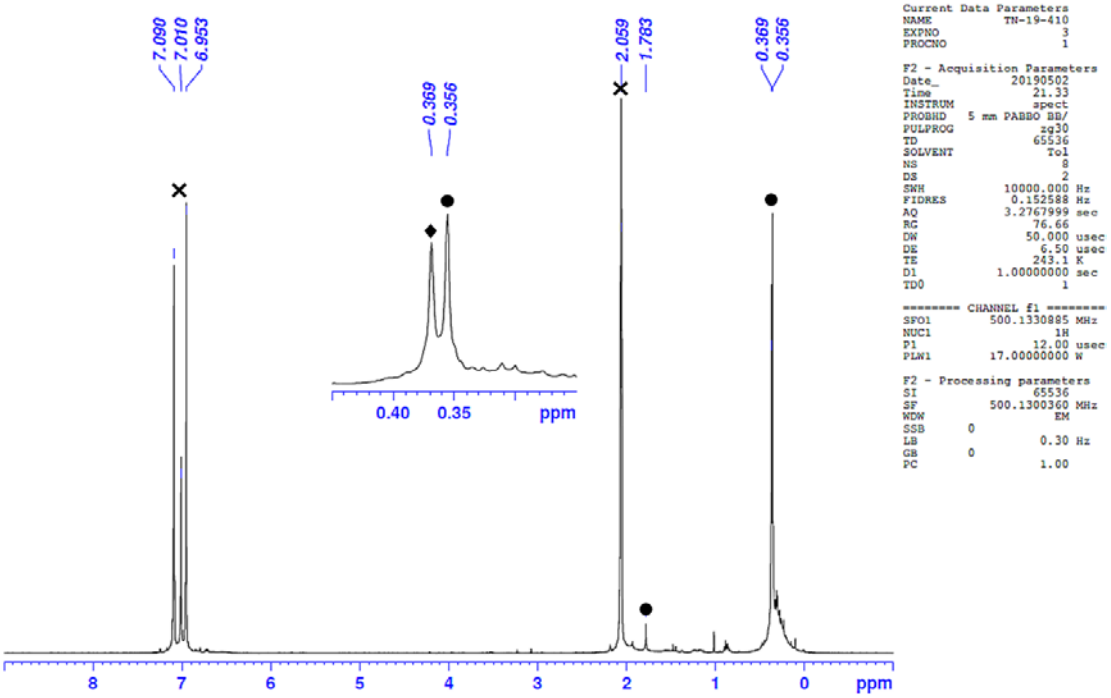

Figure S30. ^{1}H NMR spectrum of the reaction mixture after the reaction of **1b** with excess carbon tetrachloride for 1 hour in toluene-d_8 at 243 K (● = intermediate, ♦ = **4**, × = C_7D_7H).

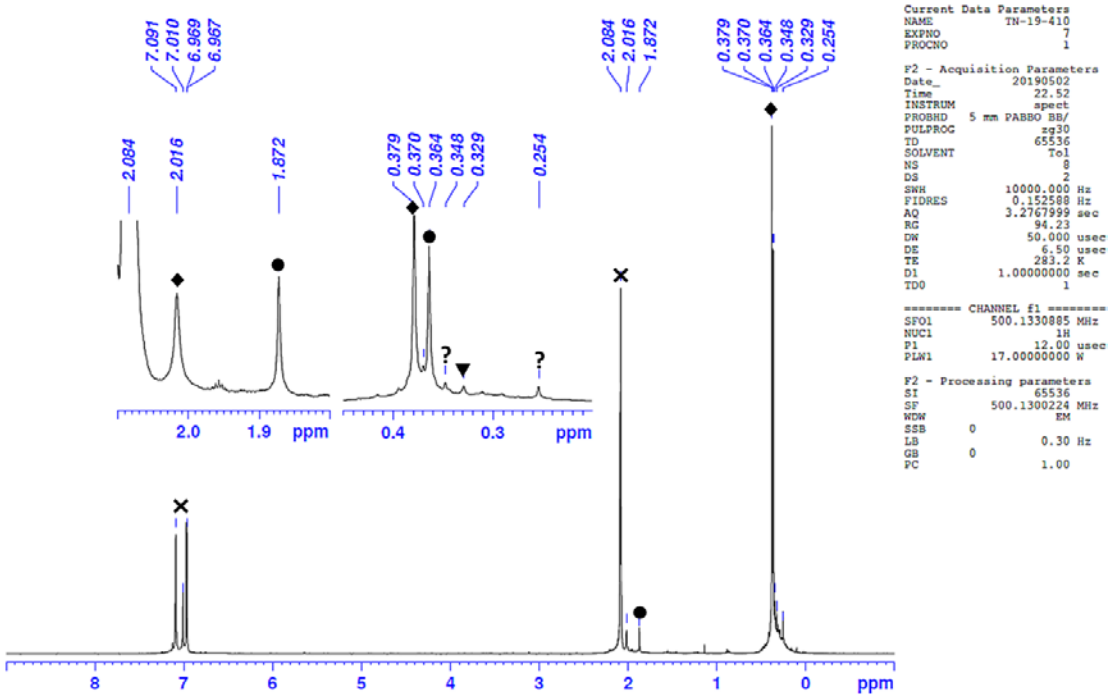

Figure S31. ^{1}H NMR spectrum of the reaction mixture of the reaction of **1b** with excess carbon tetrachloride in toluene-d_8 at 283 K (● = intermediate, ♦ = **4**, ▼ = **5**, × = C_7D_7H).

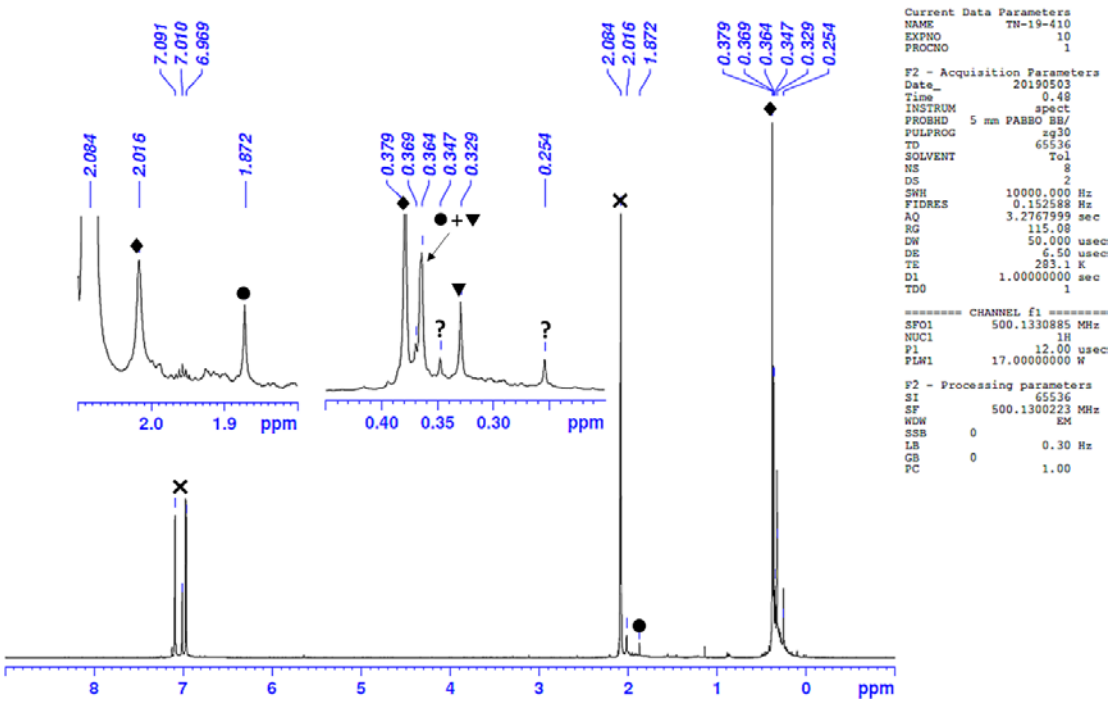

Figure S32. ^{1}H NMR spectrum of the reaction mixture of the reaction of **1b** with excess carbon tetrachloride in toluene-d_8 for additional two hours at 283 K (● = intermediate, ♦ = **4**, ▼ = **5**, × = C_7D_7H).

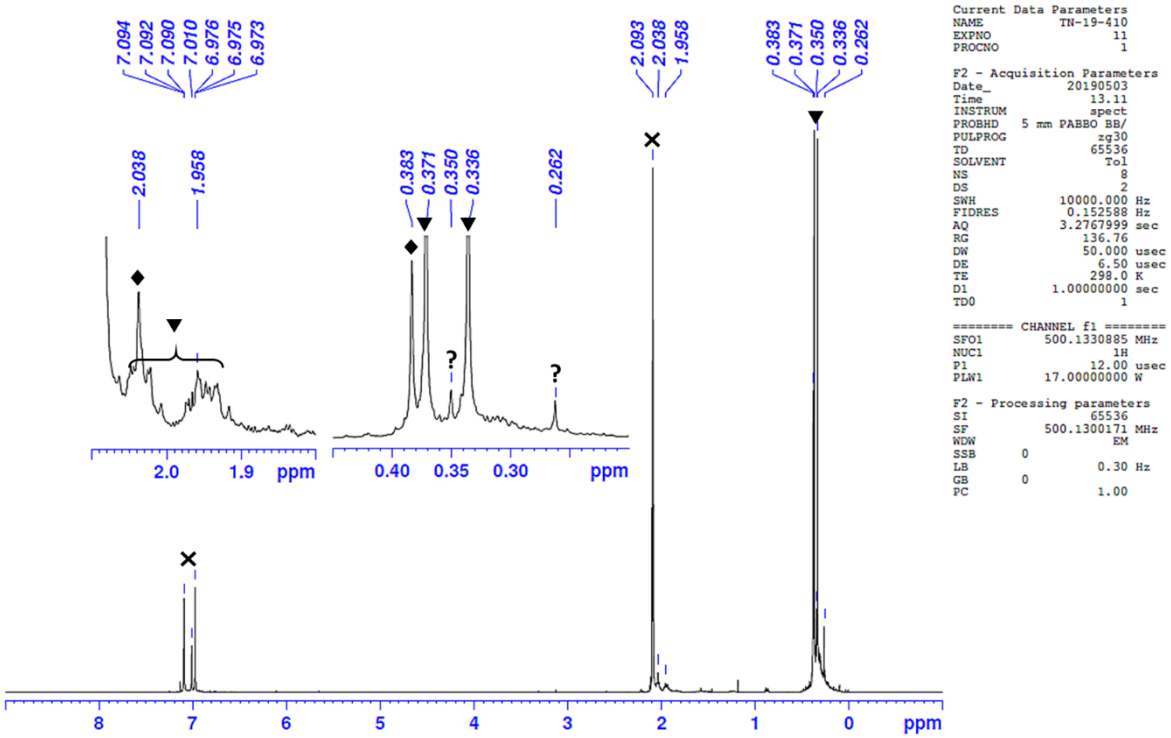

Figure S33. ^{1}H NMR spectrum of the reaction mixture of the reaction of **1b** with excess carbon tetrachloride in toluene-d_8 for additional several hours at 298 K (♦ = **4**, ▼ = **5**, × = C_7D_7H).

2. XRD Analysis

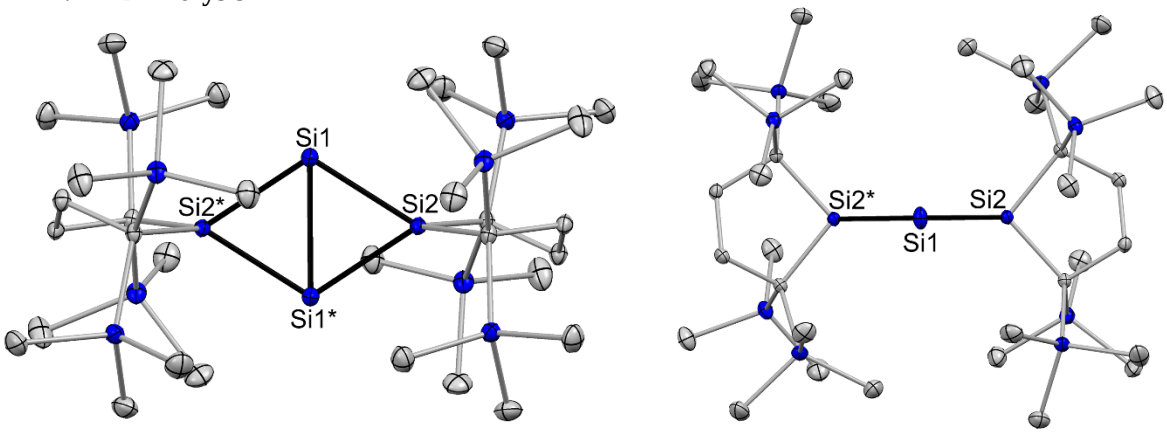

Figure S34. ORTEP drawings of **1b**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

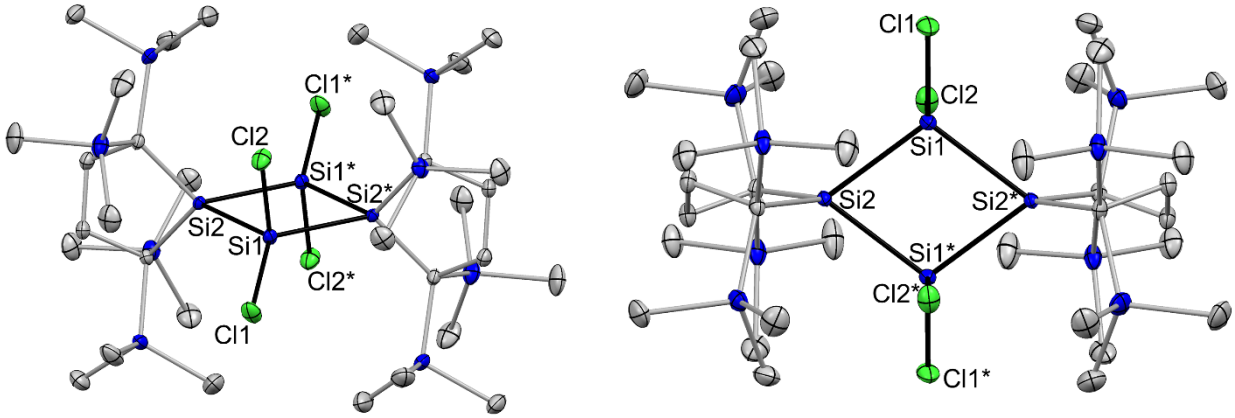

Figure S35. ORTEP drawings of **4**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

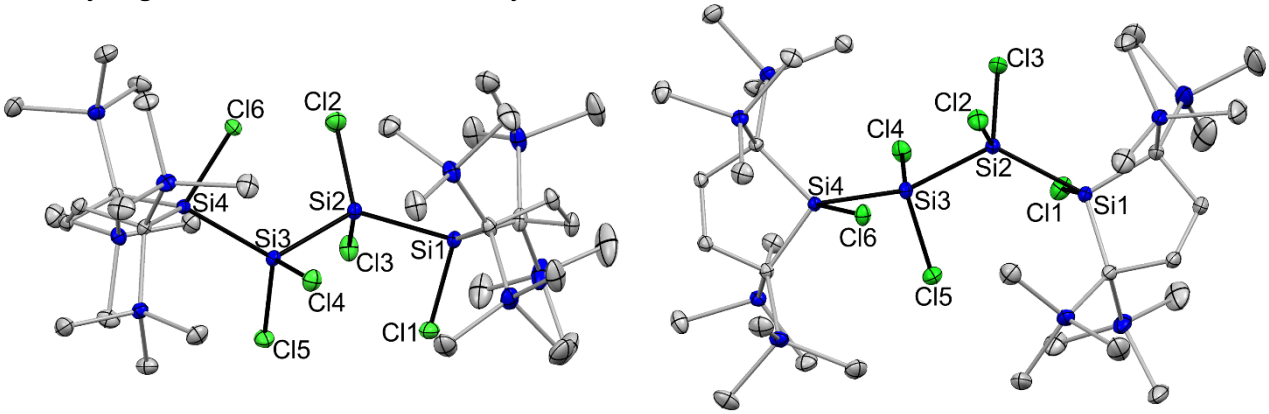

Figure S36. ORTEP drawings of **5**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

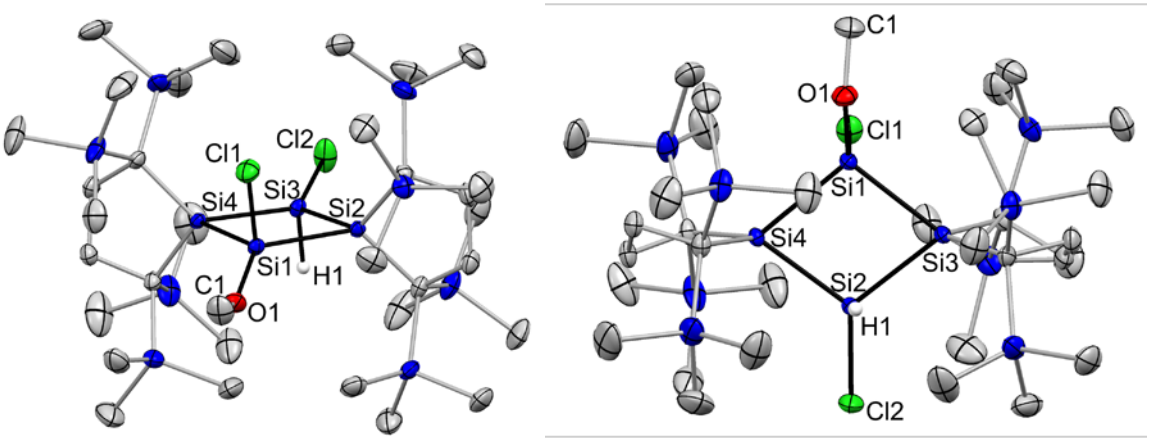

Figure S37. ORTEP drawings of **6**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

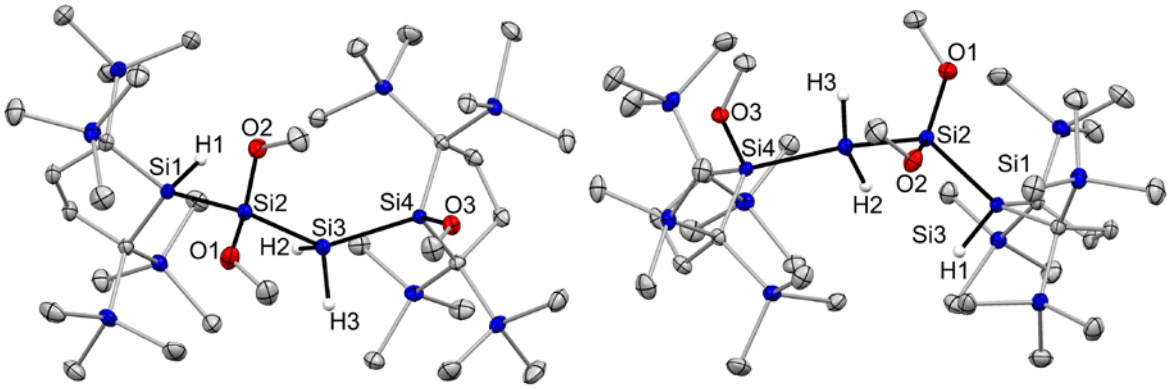

Figure S38. ORTEP drawings of **9**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

3. UV-vis Absorption Spectrum of 1b

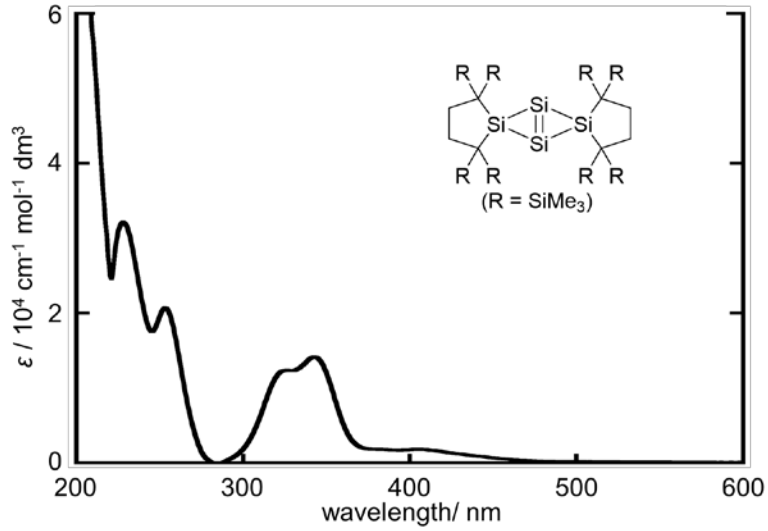

Figure S39. UV/Vis absorption spectrum of **1b** in hexane at room temperature.

Table S1. UV-vis Absorption Bands of **1b**

Absorption maximum / nm	ε / 10^4 cm^{-1} mol^{-1} dm^3
405 sh [a)]	1,800
342	14,000
326 sh [a)]	12,000
253	20,000
228	32,000

a) sh = shoulder

4. Theoretical Studies

All theoretical calculations were performed using a Gaussian 09[S2] (Rev. D.01) program. Geometry optimization was carried out at the B3LYP-D3/6-31G(d) level of theory. For bicyclo[1.1.0]tetrasilanes **7** and **10**, two conformers, which differ primarily in the geometry around the bridgehead silicon atoms, were located. Although the free energy differences between the two conformers are rather small (13.2 and 27.7 kJ mol^{-1} for **7** and **10**, respectively), the energies of more stable conformers were used to estimate the free energy differences for the isomerization of bicyclo[1.1.0]tetrasilanes to the corresponding tetrasila-1,3-dienes.

Table S2. Atomic Coordinates of **7**

Atom	X	Y	Z
Si	0.0442091195	1.2271276015	0.0491167086
Si	0.0508583763	-1.2270579803	0.04370215
Si	-1.6088816335	-0.0195568032	1.1266099575
Si	1.0537451361	0.0192361516	-1.6559799213
C	3.0093720023	-0.0158627755	-1.7611526686
C	3.1770519156	-0.3140229673	-3.2935595434
C	2.087705982	0.3947752555	-4.1174459936
C	0.6514623208	0.069634806	-3.549474391
C	-3.5182222973	-0.0713226813	0.8081068778
C	-4.0222051534	-0.3959518137	2.2681514496
C	-3.151618612	0.3139990045	3.3197662425
C	-1.6278830788	0.0166945932	3.0849561954
Cl	0.5859271666	3.196743634	0.5682382301
Cl	0.5945458605	-3.1960146584	0.5632946537
Si	3.913697695	1.6375149344	-1.3180368718
C	5.6318197073	1.7172909625	-2.131898094
C	4.1215500069	1.8338629123	0.5536553805
C	3.1245867017	3.2262954218	-1.9701145259
Si	3.837136969	-1.4566534962	-0.7749530485
C	3.3307561733	-3.1261063119	-1.5199045281
C	3.4961076467	-1.4091405361	1.093925997
C	5.7301260718	-1.4763714189	-0.9397243442
Si	-0.4655442576	1.5318362141	-4.1157644513
C	-2.2895675619	1.3623803617	-3.654478951
C	-0.2458196289	1.7455934495	-5.9922644197
C	0.0044825313	3.224505106	-3.4091609333
Si	0.0031076582	-1.6215907633	-4.2848194192
C	-0.3519067827	-3.0039920529	-3.0374347967
C	1.2562201728	-2.3177261125	-5.532483813
C	-1.6255578594	-1.5387609508	-5.2666321513
Si	-0.6071560408	1.4586256454	3.8676622191
C	1.2449071753	1.412111703	3.4446490288
C	-0.6884193697	1.4793630945	5.7660592438
C	-1.3748158531	3.1272907861	3.3936462611
Si	-1.1443396806	-1.6358589414	3.9698568519
C	-1.8295286353	-3.2255094324	3.2111367797
C	-1.8817863124	-1.715125383	5.7221645944
C	0.7348089215	-1.8309250552	4.0952683006
Si	-4.2824350551	1.6190828856	0.1918124121
C	-3.0527024433	3.0019739706	-0.218571302
C	-5.4741464587	2.315209176	1.4982554859
C	-5.3349752068	1.534753834	-1.3919876782
Si	-4.1322795306	-1.534530369	-0.2820258399
C	-3.4046068979	-3.2265010577	0.1573864653
C	-3.7519441911	-1.3659077118	-2.124707884
C	-5.9971479935	-1.7492476577	0.0202819213
H	3.0969616603	-1.390515042	-3.4817257276
H	4.1694332849	-0.0201626401	-3.6560250481
H	2.2745330968	1.4752166064	-4.0728125841
H	2.1776531875	0.1202579274	-5.1732723692
H	-3.9687063579	-1.4762537696	2.4534471016
H	-5.0732221425	-0.1220227773	2.4043347943
H	-3.3438278735	1.3903257083	3.2474326862

H	-3.469852015	0.0204961738	4.3273084674
H	5.5477295988	1.7893571388	-3.2229153668
H	6.1094214982	2.6453280433	-1.7910481785
H	6.3081726902	0.8934959435	-1.9004617372
H	3.1901026694	1.6712718957	1.1034789819
H	4.4492044612	2.8589718723	0.7654074375
H	4.8765182549	1.1541337603	0.9616536852
H	3.7286398783	4.0624702497	-1.5939715083
H	3.1567880028	3.272950239	-3.0639967481
H	2.1009242663	3.394082486	-1.6424313249
H	3.9012873912	-3.3324859854	-2.4331072942
H	3.5576705022	-3.9226311652	-0.8015738623
H	2.2699240266	-3.2024286782	-1.7586557954
H	4.3652639562	-1.0116752897	1.6283327209
H	3.3020064742	-2.4190240925	1.4682561914
H	2.6381377733	-0.7883919925	1.3638669908
H	6.0837478568	-2.429056647	-0.5235951044
H	6.0668695127	-1.4299666059	-1.9813289887
H	6.2222947619	-0.6741740106	-0.3809464201
H	-2.3893202935	1.1051918561	-2.5965719543
H	-2.7701831719	2.3380696185	-3.7970121412
H	-2.8472757687	0.625535457	-4.2336666313
H	0.7509131873	2.1497586935	-6.2063899858
H	-0.9789689602	2.4677320939	-6.3724515857
H	-0.3560328337	0.822924739	-6.569321723
H	-0.0641704265	3.2888877833	-2.3194829577
H	0.9986077065	3.5630976793	-3.7077830261
H	-0.7184198211	3.9417034099	-3.8202728288
H	0.5131097085	-3.3303414946	-2.4574708819
H	-1.1485309513	-2.7458744738	-2.3331819499
H	-0.7034124214	-3.8706252652	-3.6129330201
H	1.376097292	-1.6633280912	-6.4038649119
H	0.8690189771	-3.2771736939	-5.8973753988
H	2.2491888745	-2.5032356636	-5.1118058867
H	-2.5009204167	-1.4773289492	-4.6147957853
H	-1.6912640901	-0.7366910992	-6.0054575696
H	-1.6977709034	-2.4897232095	-5.8107606168
H	1.4771299346	0.7913329618	2.575733312
H	1.6097267779	2.422167258	3.2340324112
H	1.8173388159	1.0151464398	4.2894795437
H	-1.7141657816	1.4325174413	6.1483428505
H	-0.2577322826	2.4325024478	6.1005021568
H	-0.1080213408	0.6777832059	6.2335984938
H	-1.6600192766	3.2028765765	2.3442986024
H	-2.2621929918	3.3333734688	4.0036699093
H	-0.6477525417	3.9244180484	3.5883561887
H	-1.5471538972	-3.3937250424	2.1741327155
H	-1.4266239496	-4.0610918555	3.7985236035
H	-2.9209011326	-3.2727931602	3.291523935
H	-1.6216393339	-0.8906470894	6.3871528251
H	-1.519410518	-2.6425173846	6.1849435594
H	-2.9753766385	-1.7882485447	5.6861272985
H	0.9614467122	-2.8557394135	4.4137579498
H	1.2430362	-1.6684204829	3.1404735713
H	1.17515348	-1.1505714647	4.8312634037
H	-3.6436137147	3.8680600464	-0.5449520368
H	-2.4354447921	3.3291910153	0.6199029374
H	-2.3840168661	2.743745272	-1.0452418024
H	-5.8563026704	3.2742294015	1.1269770832
H	-5.0103103374	2.5015087597	2.4716606851
H	-6.3390129146	1.6603657986	1.6566855755
H	-4.722306303	1.4730396734	-2.2951762199
H	-6.0756049494	0.7323177075	-1.4245758469
H	-5.8821970317	2.4854320533	-1.4407513249
H	-3.6589750275	-3.5647012688	1.1638780671
H	-3.8466758966	-3.9443650971	-0.5463322623
H	-2.3189666851	-3.2902572533	0.0408796902
H	-4.3556303038	-0.629766147	-2.6567751158
H	-3.9148853767	-2.3419796718	-2.5980057266
H	-2.6996313925	-1.1081160086	-2.2711462997
H	-6.4088338363	-2.4720437584	-0.6949902656
H	-6.1669239333	-2.1529267431	1.0257142282
H	-6.5790466741	-0.8269725819	-0.0649440569

Sum of electronic and zero-point Energies= -5661.395411
Sum of electronic and thermal Energies= -5661.319348
Sum of electronic and thermal Enthalpies= -5661.318404
Sum of electronic and thermal Free Energies= -5661.498712
No imaginary frequency

Table S3. Atomic Coordinates of **7** (metastable conformer)

Atom	X	Y	Z
Si	-0.2696530305	1.436001817	-0.2998776909
Si	-0.3118095275	-1.4364240065	-0.2546581865
Si	-1.6661382226	0.020925348	1.1273509816
Si	1.0523636588	-0.0213711319	-1.7127968379
C	3.0119650913	0.0515416019	-1.7246882445
C	3.2584043375	-0.4414279673	-3.2005197384
C	2.2292322687	0.1999309108	-4.1333075305
C	0.7742780035	-0.1517572841	-3.6388709089
C	-3.6025908195	0.1504190872	0.9337929516
C	-4.0327283962	-0.2008061503	2.4091430797
C	-3.056042593	0.441343547	3.3962517739
C	-1.5922121652	-0.051145208	3.0856280976
Cl	1.2147563899	2.2957038412	0.9834526293
Cl	1.0355803306	-2.2950278315	1.1725105129
Si	3.8138769433	1.8429616466	-1.5704103194
C	5.2242688882	1.9990666595	-2.8405009556
C	4.6123003242	2.224876789	0.1073013367
C	2.7183172572	3.3302095156	-1.9948129128
Si	4.0408951365	-1.1290547532	-0.5856001695
C	3.6547181404	-2.9554009398	-0.9141580874
C	3.9191853604	-0.7317530078	1.2614619251
C	5.879698078	-1.0205233196	-1.0723170712
Si	-0.396787599	1.1236710012	-4.4835674847
C	-2.1772914433	1.067216313	-3.8796716183
C	-0.3799529979	0.8702891171	-6.3659891976
C	0.135534324	2.9210078242	-4.230913437
Si	0.359083994	-1.9513215678	-4.2802096319
C	0.9327900734	-3.4053521762	-3.2093427855
C	1.2342266356	-2.2563691158	-5.9409553615
C	-1.4850938874	-2.2631382375	-4.5719614875
Si	-0.4096456674	1.1303265389	4.0632394831
C	1.4304718131	0.7337343949	3.8608378556
C	-0.8152926982	1.022286449	5.9216383661
C	-0.7555951025	2.9563977322	3.6912107167
Si	-1.4022126235	-1.842101587	3.8808382968
C	-1.8736434099	-3.3300980187	2.8057198141
C	-2.6091403112	-1.9979184164	5.3456771384
C	0.309041922	-2.2229531395	4.6051702501
Si	-4.2622819192	1.9495051883	0.546204674
C	-3.1680618051	3.404304406	1.0718779244
C	-5.8833284635	2.2542126974	1.4929623421
C	-4.6345172441	2.2603021885	-1.2835959054
Si	-4.4971810897	-1.1258960208	-0.1986108775
C	-4.2208052042	-2.9228775237	0.3230201876
C	-3.9716980224	-1.0701020089	-2.0038341652
C	-6.3771645281	-0.873213001	-0.0996273938
H	3.1595649046	-1.5322601196	-3.2651054191
H	4.274062589	-0.2152202852	-3.5370833393
H	2.3877232205	1.2858667329	-4.1255694057
H	2.3901490869	-0.1185281168	-5.1682127072
H	-4.017642255	-1.2866709338	2.567595064
H	-5.0597293706	0.1173263293	2.6150646692
H	-3.1253434358	1.5321060013	3.2999126965
H	-3.3477140733	0.2154067354	4.4257609048
H	4.8557424305	2.0043819865	-3.8727656697
H	5.7116002737	2.9672202874	-2.6669858343
H	5.991907466	1.2247248837	-2.7566115558
H	3.9377681069	2.103022051	0.955445807
H	4.9185058311	3.2782924798	0.075079542
H	5.5106538084	1.6306968905	0.2959777021
H	3.2301241962	4.2243348937	-1.6166059432
H	2.6139979995	3.4501865018	-3.0759573436
H	1.7221723955	3.3228135263	-1.5523402987
H	4.0621998243	-3.2752122606	-1.8803291202
H	4.1584858256	-3.5478666053	-0.1397331275
H	2.5965487408	-3.212916602	-0.8800119429
H	4.8170387065	-0.2111508507	1.6088213308
H	3.8141754874	-1.6541953586	1.8409634986
H	3.0587976819	-0.1011729491	1.4912123719
H	6.4158300955	-1.7977389796	-0.5119325767
H	6.0366017858	-1.2252953199	-2.1375504633
H	6.3555064347	-0.0644343499	-0.8380283198
H	-2.208651959	1.0888597423	-2.7870160318
H	-2.7000144274	1.9624841481	-4.2380692389
H	-2.7367334124	0.1935840375	-4.2156973069
H	0.6373696712	0.9212921221	-6.7709641548

H	-0.9575757799	1.6779388235	-6.8331270567
H	-0.8226303887	-0.0778839477	-6.685718046
H	0.1407152753	3.2166165514	-3.1787649251
H	1.1137981142	3.1563636672	-4.6601118109
H	-0.6033592341	3.5487056821	-4.7456770153
H	2.018150155	-3.4487927771	-3.0954689452
H	0.4854289434	-3.4283778097	-2.2115938303
H	0.62277994	-4.3221652456	-3.7280585571
H	1.0431060943	-1.490121621	-6.6971201124
H	0.8708086356	-3.2124597025	-6.3387938966
H	2.3195988491	-2.3499949489	-5.820048721
H	-2.0786549825	-2.1795409891	-3.6590291905
H	-1.9269850404	-1.6062946288	-5.3265870674
H	-1.5856598405	-3.2942774599	-4.933807314
H	1.6225591775	0.1028804472	2.99146164
H	2.0044206026	1.6563664901	3.7301510076
H	1.817069264	0.2136430614	4.7428131336
H	-1.8727264526	1.2266081714	6.1249987524
H	-0.2323383188	1.7999873087	6.4324010671
H	-0.5599056916	0.0664975491	6.3870783415
H	-0.7679103757	3.2135556024	2.6324772005
H	-1.7031449585	3.2759354913	4.1404889324
H	0.0398624328	3.5493857105	4.1604061658
H	-1.4752052503	-3.3231253768	1.7911554271
H	-1.4730650865	-4.2238000896	3.3009785361
H	-2.958273026	-3.4505081227	2.7488951164
H	-2.4919391241	-1.2231218113	6.1084815845
H	-2.4140291538	-2.9657390713	5.8254404153
H	-3.6565782968	-2.0038023799	5.0228021534
H	0.2906693484	-3.2762024218	4.913090725
H	1.1267696147	-2.1011776657	3.8940608655
H	0.5366769604	-1.6281992006	5.4940658612
H	-3.7003141337	4.3207215576	0.7844629799
H	-3.0068451314	3.4482914275	2.1511910824
H	-2.1908499351	3.4276169689	0.5812877905
H	-6.2971355394	3.2099537258	1.1468696269
H	-5.7151323649	2.3483960445	2.5719697523
H	-6.646755204	1.4875262731	1.3354264682
H	-3.7483830863	2.1768188884	-1.9164786672
H	-5.4074621335	1.60293162	-1.6917538095
H	-5.0008676784	3.2912436379	-1.3687044859
H	-4.6067126692	-3.1579087228	1.3192345755
H	-4.7671509336	-3.5511287641	-0.3923522346
H	-3.169324379	-3.218099943	0.2823109513
H	-4.3321903443	-0.1968891891	-2.5485013678
H	-4.352230053	-1.9657709323	-2.5099650758
H	-2.8814430159	-1.0913634476	-2.0828974122
H	-6.8687751016	-1.6813131988	-0.6559151116
H	-6.7372565206	-0.9238953238	0.9344501686
H	-6.716322011	0.074631272	-0.5283317937

Sum of electronic and zero-point Energies=	-5661.393862
Sum of electronic and thermal Energies=	-5661.319038
Sum of electronic and thermal Enthalpies=	-5661.318094
Sum of electronic and thermal Free Energies=	-5661.493676

No imaginary frequency

Table S4. Atomic Coordinates of **8**

Atom	X	Y	Z
C	-4.5405149746	4.2420452629	-0.7250266577
C	-5.4190596154	2.9881276411	-0.5718044227
C	-4.6365349241	1.7005246138	-1.0432922495
Si	-2.8846065482	2.1315357174	-0.3731812343
C	-3.1250436523	4.0208083616	-0.0628848244
Si	-0.9784469566	1.1449926683	-1.1893607301
Si	0.7168056381	0.4108976025	0.3585049018
Si	2.6395572585	0.239168781	-0.9751795393
C	4.1905622382	1.3109155028	-1.0384180744
C	5.225412727	0.3678178468	-1.7713936628
C	4.5242326664	-0.7398534314	-2.5890150293
C	3.294669479	-1.33061399	-1.8071844816
Cl	-1.634818327	-0.7003452661	-2.0871381643
Cl	1.1009563361	2.2903390121	1.3958212645
Si	-1.8588270303	5.2230910443	-0.9137573944
Si	-3.2065177323	4.4674012904	1.8283563886
C	-0.2936904698	5.5052746248	0.1091422479
C	-2.7226525474	6.8846413042	-1.2397563117

Si	2.0346260951	-2.0617971281	-3.0789106389
C	-1.2615160991	4.7028780654	-2.6336861645
C	-3.2155898988	6.3459983977	2.1283584372
C	-1.7961716262	3.6937883329	2.8125354202
C	-4.8228239815	3.9385504584	2.6692389837
Si	3.873664221	-2.701393048	-0.5596621927
Si	-5.37744649	0.1785637587	-0.1131458015
Si	-4.8532979363	1.4784838502	-2.9658143796
C	-7.1980106812	-0.0221421339	-0.6178501613
Si	4.8875960235	1.8496373309	0.7005194745
C	-5.4051777925	0.4450612779	1.7664975838
C	-4.4526804404	-1.4510761414	-0.3355508519
Si	3.8813266971	2.8654638409	-2.1518344717
C	-4.9074015891	-0.3097387365	-3.5884870385
C	-3.5451510465	2.3578913812	-4.0085116248
C	-6.5154743036	2.2447532644	-3.4834925344
C	1.2406306376	-0.666986015	-4.0883628513
C	0.725544797	-3.1247723105	-2.226901879
C	2.9477396401	-3.098935474	-4.3802538295
C	4.1219347519	-4.3747834803	-1.4214438344
C	2.6659226364	-2.9395315681	0.8719783747
C	5.605507529	-2.3615705596	0.144513137
C	6.7826156576	1.7906943599	0.5935027431
C	4.3330778322	0.6967852747	2.0995964888
C	4.4425942237	3.5960647589	1.2780995758
C	5.480004326	3.8823549614	-2.2534056506
C	2.4322312992	3.92464763	-1.5786014142
C	3.4950485899	2.3580947306	-3.9365572711
H	-5.05067675	5.116716856	-0.2983553052
H	-4.4299007767	4.4537397706	-1.7984595566
H	-6.3591714631	3.1178420977	-1.11638148
H	-5.69857719	2.8900765896	0.4808786842
H	5.8926650657	0.9398637905	-2.428936124
H	5.8787271355	-0.1099023082	-1.0411210237
H	5.2492791572	-1.5231432721	-2.8480213565
H	4.1880808593	-0.3196210646	-3.5447705404
H	0.2214898042	4.5639226808	0.3155085729
H	0.390603016	6.12980915	-0.4779858144
H	-0.4678018305	6.0088680536	1.0635747543
H	-3.5611299973	6.759825355	-1.9346630752
H	-2.0033718966	7.5599222546	-1.7206280379
H	-3.1004187116	7.3854207879	-0.3460070686
H	-0.8083871836	3.7086058785	-2.6633963331
H	-2.0617950426	4.7325817361	-3.3779293479
H	-0.4997640845	5.4310098767	-2.942417672
H	-4.0806283622	6.8203938255	1.6501948608
H	-3.319095501	6.502153425	3.2098327591
H	-2.3170110267	6.8755612132	1.8034325179
H	-1.7538724032	2.6068880001	2.6811567036
H	-1.9519567611	3.895183949	3.8800619225
H	-0.8162317189	4.0874667179	2.5347077402
H	-5.713487736	4.32591494	2.1622093151
H	-4.9283071018	2.8583311324	2.777750367
H	-4.8146068353	4.3677482437	3.6797290366
H	-7.329720556	-0.3167519657	-1.663613137
H	-7.6714251618	-0.7902413427	0.0062856728
H	-7.7494396117	0.9132601	-0.4635418114
H	-4.4160379957	0.6871753579	2.1725763634
H	-5.7254668156	-0.4948175614	2.2339508233
H	-6.1094142214	1.2203429905	2.0828020973
H	-4.3649960124	-1.7891807114	-1.3683899384
H	-3.4395715406	-1.3802362253	0.0731796231
H	-4.9891695928	-2.2228114591	0.2322589341
H	-5.7099655147	-0.9083506307	-3.147674909
H	-5.0928322595	-0.259923645	-4.6694480608
H	-3.9612646556	-0.8325601107	-3.4375908111
H	-3.6207519358	3.4448192879	-3.9078086846
H	-3.7159489186	2.1123281955	-5.0644705278
H	-2.5209480595	2.0665934455	-3.7575376854
H	-7.3632041463	1.8416852743	-2.9188369806
H	-6.5275623643	3.3359612819	-3.3815372932
H	-6.6847061854	2.0148457336	-4.5430496673
H	1.9681949306	-0.2400184346	-4.7880525987
H	0.414074348	-1.0769340603	-4.6806782187
H	0.8223357456	0.1475211326	-3.4893089076
H	1.1349394226	-4.0798186603	-1.8813269273
H	-0.0856348023	-3.3434608251	-2.9306272235
H	0.2710612677	-2.6186834266	-1.3711869712
H	2.2680088568	-3.2781435225	-5.2231290294
H	3.8193458342	-2.5645871382	-4.776384551
H	3.2856714585	-4.0720106457	-4.0159378468
H	4.817865445	-4.2953448882	-2.2639591596

H	4.5699730166	-5.0602950729	-0.6908689904
H	3.2008849797	-4.8374298133	-1.7846851798
H	2.6182162393	-2.0670121004	1.5315245671
H	2.9889247367	-3.7989420453	1.4732653865
H	1.6471354508	-3.1388283408	0.5246515245
H	6.3589585465	-2.3394293207	-0.6516491481
H	5.7039848358	-1.4441967347	0.7281122169
H	5.8627345429	-3.198586331	0.8064993719
H	7.1578153689	2.3247228511	-0.2863666449
H	7.2015712819	2.2770242264	1.483090678
H	7.1787990158	0.7700191825	0.5613804443
H	3.3023590409	0.9130731804	2.3962106786
H	4.9715291301	0.8730887193	2.9749949779
H	4.3998443384	-0.3674206571	1.8586221181
H	4.8239736762	4.3924556257	0.6326857882
H	3.3665359364	3.7326247196	1.4000503092
H	4.9036971946	3.7279379124	2.2659069431
H	6.3044348769	3.2826884888	-2.6570079245
H	5.3266333108	4.7264052893	-2.9374287274
H	5.8043046705	4.2889091287	-1.2917784049
H	1.5166818335	3.3291747905	-1.4945117192
H	2.2456113495	4.7059605111	-2.3261588922
H	2.5967369397	4.4111158652	-0.6160944951
H	3.4144685282	3.2680197205	-4.5448595891
H	4.2780850639	1.7359674764	-4.3833096152
H	2.5427762939	1.8260756274	-4.0218610105

Sum of electronic and zero-point Energies= -5661.372998
Sum of electronic and thermal Energies= -5661.295663
Sum of electronic and thermal Enthalpies= -5661.294719
Sum of electronic and thermal Free Energies= -5661.479784
No imaginary frequency

Table S5. Atomic Coordinates of **10**

Atom	X	Y	Z
C	-4.730330135	-0.6014987919	1.261088912
C	-4.215784983	-2.0375297153	1.1017698487
C	-3.0840653513	-2.1036857255	0.0132183441
Si	-2.1487140396	-0.4435989267	0.4040253045
C	-3.5446193171	0.4240094289	1.4582380245
Si	-0.8944798007	0.5702467525	-1.3220699699
Si	0.1684797111	-0.3865898366	1.187255311
Si	1.2425087744	1.0621021745	-0.3985198822
C	1.8251180488	2.8816400258	-0.0148465111
C	3.3221555769	2.8072178742	-0.5128470077
C	3.4707271851	1.8414802495	-1.6966218444
C	2.8206279684	0.4529730132	-1.3558448639
Si	-3.0785792888	0.5131433908	3.331462481
Si	-4.2530830413	2.1626694002	0.9468832406
C	-4.5587345073	1.0993526704	4.374340956
C	-1.609904814	1.676195639	3.643840785
C	-2.6242290282	-1.1505417695	4.1178719967
C	-3.5468537196	3.6405764633	1.9071138991
C	-6.1186546591	2.1836616961	1.3218641818
C	-4.1170907165	2.6390576681	-0.8822497922
C	-0.5888879929	-4.0609301918	-0.7015998933
C	-3.3377851686	-5.2362073709	-0.1253857465
C	-1.7428052898	-4.0420524845	2.1048424934
C	-4.4187937125	-0.4129649802	-2.4357596186
C	-5.5386338801	-3.0596080161	-1.7232205683
Si	-2.1751294624	-3.7850701282	0.2760154329
Si	4.0684526812	-0.5833378119	-0.2896009876
C	-2.7829672447	-2.854398552	-3.0896520555
O	0.9623249042	-1.8812585332	1.005151954
Si	-3.8964921186	-2.1009422533	-1.75422204
Si	2.5128674962	-0.4675554868	-3.0208490645
C	1.4351995475	-2.679623937	2.0843722328
C	1.6245351181	-2.1294473555	-2.8246331538
C	4.1752487717	-0.7788463911	-3.8926654951
C	1.5335749067	0.5683909023	-4.273276655
Si	0.8722870599	4.1888957253	-1.075025199
C	4.0343419745	-0.2125816605	1.5681021731
C	5.8512528562	-0.1506303931	-0.7906766946
Si	1.8810561292	3.5301805268	1.8174575661
C	3.8805866354	-2.4566567025	-0.4895569926
C	0.9413141134	3.8977134288	-2.9454190468
C	1.6402097209	5.9171563412	-0.8664095262

C	-0.96357067	4.2759684514	-0.6103405241
C	2.0936592966	2.2303976201	3.1806318025
C	0.3801317914	4.558146644	2.3512102979
C	3.3865049423	4.6765980596	2.0049893065
H	-5.3083200551	-0.349777407	0.3633900372
H	-5.4442633817	-0.5492298093	2.0929204192
H	-5.0510264228	-2.7064337794	0.8617314465
H	-3.8284751447	-2.3760167499	2.0667642884
H	-0.5932102165	-0.6733404699	-2.1100342108
H	3.9766311078	2.4556634078	0.2952975758
H	3.7017187344	3.8004056286	-0.78471077
H	2.9829792046	2.2802591921	-2.5718884498
H	4.5286035794	1.7408838154	-1.9641404561
H	-5.4292292378	0.4435017434	4.2554991561
H	-4.2674956327	1.0594277511	5.4318529227
H	-4.8797675438	2.1221042698	4.159718343
H	-1.0885670161	1.9385133136	2.720484711
H	-0.8747912356	1.1912316147	4.2951891011
H	-1.9208603819	2.6099346064	4.1234132303
H	-3.4422889781	-1.8780470364	4.1005272604
H	-1.7487922194	-1.6098437351	3.6542318301
H	-2.3778429085	-0.9608050617	5.1708008437
H	-2.4714106651	3.7738468505	1.7874293582
H	-4.027453425	4.5389843952	1.4993294965
H	-3.76453898	3.6129947679	2.9781949227
H	-6.6832441898	1.5139208006	0.6640895771
H	-6.4916037279	3.201035873	1.1478082336
H	-6.3563242286	1.9160818115	2.3555352054
H	-3.157382828	2.3847667142	-1.3366926
H	-4.9075148137	2.182801531	-1.4831710714
H	-4.2385670403	3.7274177478	-0.9482678162
H	0.1812810907	-3.3593965278	-0.3782885166
H	-0.2341111185	-5.0778851561	-0.4875300193
H	-0.7045292837	-3.9716758558	-1.782647474
H	-4.2937932776	-5.166244336	0.4058457403
H	-2.8474315664	-6.1612443428	0.2041244102
H	-3.5495378383	-5.3427522522	-1.1939779744
H	-1.1741754791	-3.2116171609	2.5253381675
H	-2.6291037301	-4.19230982	2.7298985498
H	-1.1242082376	-4.9441370714	2.191128175
H	-3.5995933601	0.3011210639	-2.5507876082
H	-4.8542040548	-0.5826443825	-3.4293588874
H	-5.1912403108	0.0561481861	-1.819282867
H	-5.4712253488	-4.0743766891	-1.3248079542
H	-5.9079132456	-3.1299218169	-2.7544010997
H	-6.299271572	-2.5194860254	-1.1468186292
H	-3.2611335757	-2.6888934255	-4.0632126572
H	-1.7985592788	-2.3763452101	-3.1180000992
H	-2.6354710387	-3.9324367497	-2.9733853904
H	1.165581975	-3.7231760014	1.8934773842
H	2.5256269739	-2.6015438334	2.1534037669
H	1.0031459497	-2.3805849749	3.0497064976
H	1.1796309258	-2.2353276984	-1.8355629027
H	0.8159326974	-2.2158612123	-3.5596654512
H	2.3077754275	-2.9713307471	-2.9760116483
H	4.7621797981	0.1407304523	-4.0009436114
H	3.9737058022	-1.1594375676	-4.902068223
H	4.7990232304	-1.5197409172	-3.3824784169
H	0.5093974843	0.781740625	-3.9535933212
H	2.0185357444	1.5172110392	-4.522997047
H	1.4694364557	-0.0185815779	-5.1990233631
H	3.0407091469	-0.2713972047	2.0160447429
H	4.6791089435	-0.9368180992	2.0823204142
H	4.4376765389	0.7842901388	1.7735193389
H	6.0418968795	-0.2431789317	-1.8634663251
H	6.5311135322	-0.8381529946	-0.2714282827
H	6.1240467838	0.8665161324	-0.4855598276
H	4.5324451385	-2.9462703189	0.2452368031
H	2.8564999598	-2.7886515575	-0.3111213153
H	4.185946999	-2.8063046153	-1.4806485142
H	0.5296680951	2.930453849	-3.2406834271
H	0.3265362506	4.6748999287	-3.4184762134
H	1.9511483081	3.9871032944	-3.3596369483
H	1.536443752	6.3366251997	0.1383134349
H	1.1340570253	6.5996906924	-1.5612492579
H	2.7055503517	5.9272826588	-1.125145799
H	-1.5770635527	4.3271391152	-1.5159324143
H	-1.2904841042	3.3922304723	-0.0582854477
H	-1.1922983822	5.153616991	0.0012846279
H	3.0909141175	1.7851952151	3.1854103834
H	1.9577218875	2.7450436926	4.1407395946
H	1.3599758639	1.4217672749	3.130597481

H	0.5144865884	4.8010060267	3.412699454
H	-0.5650192535	4.0219444163	2.2624172195
H	0.2843882132	5.5017969129	1.8079801832
H	4.3328049617	4.1294258271	1.9334281352
H	3.4103392394	5.4838364631	1.2674517573
H	3.350616805	5.1365644882	3.0006374069

Sum of electronic and zero-point Energies= -4856.623293
Sum of electronic and thermal Energies= -4856.547613
Sum of electronic and thermal Enthalpies= -4856.546669
Sum of electronic and thermal Free Energies= -4856.722926
No imaginary frequency

Table S6. Atomic Coordinates of **10** (metastable conformer)

Atom	X	Y	Z
C	-4.4974264645	0.956148829	-0.0021058323
C	-4.5185020754	-0.4938352232	0.5130263562
C	-3.3129963058	-1.3110665428	-0.0702062652
Si	-1.9194650357	0.0598929971	-0.0440889026
C	-3.0743295986	1.6142995364	0.1688101012
Si	-0.0822693689	-0.2958755307	-1.3779633249
Si	-0.0002847047	-0.3528456311	1.1956032341
Si	1.8671246108	-0.0214263062	-0.1585846
C	3.0529309113	1.5288179923	-0.1926414457
C	4.4675995955	0.8390669208	-0.147107913
C	4.4457698755	-0.5261692228	-0.8544703268
C	3.2464802356	-1.40155589	-0.3427555495
Si	-2.9000644256	2.3490461234	1.9459138642
Si	-2.9535853393	3.0638790412	-1.1093452192
C	-4.220764755	3.685461767	2.2414815712
C	-1.1806245986	3.0913972335	2.250569107
C	-3.139570597	1.1060712533	3.3554492462
C	-1.9271969	4.5627329231	-0.5568422656
C	-4.6996885281	3.7560135196	-1.4074510124
C	-2.2788222634	2.6123396916	-2.8241475099
C	-1.4350887331	-3.7942332736	0.7833604623
C	-4.4507103498	-4.1411084065	0.7796509891
C	-3.1781883831	-2.4504745513	2.8880675744
C	-3.5279306213	-0.5762126009	-3.2269214358
C	-5.5652645118	-2.3605872483	-2.0087500364
Si	-3.0647992313	-2.8649751739	1.0430757332
Si	3.7445708558	-2.2060060258	1.3367358863
C	-2.6706258177	-3.3448792324	-2.4512072282
O	-0.1800913455	-0.9715107606	2.7312220142
Si	-3.7303988549	-1.8829746708	-1.8708640685
Si	2.9376864237	-2.7746119594	-1.6617509079
C	0.2512315707	-2.0472539647	3.5476916437
C	1.371947109	-3.8123282882	-1.4367929568
C	4.4055771907	-3.9834580884	-1.7260798711
C	2.824777247	-2.0868199567	-3.4263237379
Si	2.8825605471	2.506388118	-1.8496261756
C	3.6148183921	-1.0552301898	2.838851526
C	5.5762883204	-2.7092921803	1.3437983288
Si	2.9750555918	2.8058994297	1.2648900119
C	2.7221130392	-3.7583304036	1.7200073733
C	3.1478511257	1.4684020269	-3.4131158306
C	4.2220353277	3.8519518196	-1.9722729612
C	1.1745002467	3.3048441279	-2.051314147
C	2.3288929383	2.1704327468	2.935103953
C	1.9669153035	4.3742680765	0.9132717481
C	4.7416211031	3.4124864166	1.6206042081
H	-4.7880434023	0.9420447988	-1.0596427748
H	-5.2748849232	1.5413900069	0.5057107868
H	-5.4830015751	-0.957090675	0.2698794986
H	-4.465009328	-0.4712613351	1.6046837654
H	-0.1397049436	-0.878668617	-2.7528095647
H	4.785424366	0.6815861983	0.890385401
H	5.2430602316	1.4759415779	-0.5918915378
H	4.3565548051	-0.356658094	-1.9305252067
H	5.4083276348	-1.0323025481	-0.7116013376
H	-5.2362611856	3.2908442335	2.1182731766
H	-4.1348413366	4.0411910028	3.2761164865
H	-4.118733787	4.5542371032	1.5845580539
H	-0.435266603	2.6774527686	1.5667246174
H	-0.8506050979	2.8541627448	3.2684095315
H	-1.1652696175	4.1790307853	2.1399943851
H	-4.108286935	0.5979501438	3.3547607504

H	-2.3496207654	0.3504021793	3.3653933414
H	-3.0648292056	1.6680808286	4.2961106727
H	-0.8869194768	4.3246871062	-0.3321303946
H	-1.9215580046	5.269321083	-1.3966812115
H	-2.3484836884	5.0867227922	0.3059651589
H	-5.3549462193	3.0406667206	-1.9160740971
H	-4.6204262489	4.6418691125	-2.0502967849
H	-5.1952557568	4.0625994618	-0.4804934303
H	-1.4031386365	1.9591303021	-2.7895492814
H	-3.0326580113	2.1354014871	-3.4546445845
H	-1.9737910502	3.5428187538	-3.3189040464
H	-0.5586669199	-3.1498287083	0.8899560932
H	-1.3640350023	-4.5857191648	1.5409425824
H	-1.3664126221	-4.2694920186	-0.197240212
H	-5.4419359493	-3.7037779983	0.9457314461
H	-4.3216385981	-4.9432009445	1.5178991455
H	-4.4472341005	-4.6046323587	-0.2116540335
H	-2.4472054181	-1.7031390803	3.1966305205
H	-4.1733389987	-2.0975529296	3.1784406439
H	-2.9819519851	-3.3702206912	3.4541698179
H	-2.5023295686	-0.2213771487	-3.3500209352
H	-3.8327068326	-1.0390067613	-4.1748435089
H	-4.1732673973	0.292947955	-3.0688867696
H	-5.9048110005	-3.083424991	-1.2635799757
H	-5.7363964872	-2.7974841805	-3.0008462521
H	-6.2059993227	-1.4738167305	-1.9335756329
H	-2.8806592786	-3.5169248257	-3.5144148378
H	-1.5995700088	-3.1382927821	-2.3599222449
H	-2.8811968796	-4.2782350851	-1.9203362083
H	-0.2052821286	-2.9855926341	3.2157325751
H	1.3369725132	-2.157100441	3.5414715142
H	-0.0806074446	-1.8390701613	4.5696414502
H	0.4836375211	-3.1844641959	-1.3395633776
H	1.24446304	-4.4290067111	-2.3358705008
H	1.3998684483	-4.4833089054	-0.5757195831
H	5.3622318354	-3.4640893782	-1.8549944127
H	4.271579124	-4.6420901899	-2.593456598
H	4.4848495845	-4.6223618756	-0.8404347103
H	1.9401380584	-1.4641848262	-3.583369785
H	3.7041656047	-1.5143618146	-3.7359157221
H	2.7400955509	-2.9467764632	-4.1033574483
H	2.6469221087	-0.564926787	2.9511273943
H	3.8007050553	-1.6415711543	3.748276276
H	4.3788098747	-0.2716852309	2.800751324
H	5.8708079791	-3.3383328298	0.5005841759
H	5.7797111744	-3.2690499569	2.2657531084
H	6.2287476166	-1.8282348849	1.3511367753
H	2.888760246	-4.0550393158	2.7629301029
H	1.6473750298	-3.610964355	1.582801401
H	3.0223684336	-4.6006946124	1.0882396843
H	2.4382907384	0.6427433488	-3.5020146116
H	2.9879193395	2.1313209474	-4.2737355348
H	4.1601595224	1.0610061208	-3.5020373032
H	4.1351108009	4.6396699808	-1.2184801984
H	4.1429932183	4.3288614908	-2.9577066891
H	5.2314454006	3.430116523	-1.8990619393
H	0.8223475584	3.1765156515	-3.0809398897
H	0.4297656408	2.8439097373	-1.398843226
H	1.1913815377	4.3770995567	-1.8369227597
H	3.081639987	1.5839610187	3.467694884
H	2.1042103031	3.0504358612	3.5510753266
H	1.4132554194	1.5758731087	2.8782889154
H	1.9678447199	4.9711336879	1.8340761687
H	0.9253544609	4.1742521867	0.661039713
H	2.3931526635	4.9950722165	0.1207147089
H	5.3718518074	2.6273903612	2.0526478935
H	5.2458776451	3.7891936646	0.7251605853
H	4.6958240503	4.2330307155	2.347662172

Sum of electronic and zero-point Energies= -4856.612432
Sum of electronic and thermal Energies= -4856.536719
Sum of electronic and thermal Enthalpies= -4856.535775
Sum of electronic and thermal Free Energies= -4856.712362
No imaginary frequency

Table S7. Atomic Coordinates of **11**

Atom	X	Y	Z

C	-3.4227080783	1.6427884371	3.0712952186
C	-4.1144936155	0.3057517859	2.7193195517
C	-3.9469225979	-0.0414318128	1.1942619971
Si	-2.1644229123	0.5934871686	0.9165041642
C	-1.9952939047	1.7868495182	2.4007163984
Si	-1.0898307922	0.7453948305	-1.0287500043
Si	1.2216707637	0.9643954697	-0.9089158184
Si	2.613854173	-0.6042995492	-1.6112271278
C	4.4008306542	-0.2828197032	-2.1846182941
C	5.0736793333	-1.6736629704	-1.8849576
C	4.0608524817	-2.8366282095	-2.0156538491
C	2.6749973714	-2.4851559319	-1.3503796442
O	-1.6480580504	-0.4837312146	-2.0688321441
Si	-1.7257600586	3.6294808939	1.8800507603
Si	-0.6568286446	1.2377296724	3.6759082026
C	-1.7400238733	-0.2508025178	-3.4690722386
C	0.0983455575	4.1191107961	1.7438833195
C	-2.5524593454	4.7585341688	3.1655514717
C	-2.4786552878	4.0987579254	0.2028834253
C	-0.6894327791	2.3893167131	5.1873087991
C	1.1205141323	1.2250423376	3.0275271461
C	-1.0134505045	-0.5089227633	4.318335801
C	-5.5110878764	-2.6740291044	1.9030619152
Si	-4.0209381244	-1.9565051846	0.9665905343
C	-2.5271414396	-2.8196625342	1.7525446898
C	-4.0722981536	-2.4612533159	-0.8538483311
C	-4.7476007721	1.1296406205	-1.6473000793
C	-5.9066014106	2.4569508895	0.899853595
C	-6.9160762664	-0.1846514221	0.046561431
Si	-5.3063179053	0.8245707026	0.1319518195
C	0.8675093534	-2.6200355325	-3.9728920422
C	-0.3615539392	-3.4404709634	-1.3079455984
Si	1.2531302072	-3.4022276828	-2.2849795039
Si	5.2998210324	1.0916361147	-1.1650028558
C	1.7926253269	-5.1755872754	-2.697116757
C	2.4387335673	-4.8902300369	0.6917891313
Si	2.6547819976	-3.0118523124	0.5040560092
C	1.2910216673	-2.1313170811	1.4765059022
C	4.3042445708	-2.6584354496	1.3632028458
C	7.1793828009	0.8706642099	-1.3242451725
C	4.9748745393	0.9846637776	0.700949083
C	4.8204376044	2.8424861539	-1.7015467968
Si	4.4472473593	0.1480123251	-4.0680677483
C	6.1216542246	0.8617484092	-4.6113270688
C	3.084981084	1.369832559	-4.5492717912
C	4.251125705	-1.3957153144	-5.1498409813
H	-3.3605155636	1.7439756236	4.1624934751
H	-4.0725185966	2.4573487284	2.7435543192
H	-5.1731674069	0.3550643743	3.0080942978
H	-3.677228643	-0.4899606096	3.3355708009
H	1.6498570138	2.2010754768	-1.6385613358
H	5.9322315755	-1.8580030537	-2.5450241287
H	5.4755780935	-1.6774938694	-0.8651968063
H	4.4899648653	-3.750092375	-1.5821695678
H	3.9202043415	-3.0541827402	-3.079924778
H	-1.9490251462	-1.2091459012	-3.9541988588
H	-2.5517489455	0.4512308382	-3.7046858027
H	-0.8015858978	0.1485359283	-3.878817028
H	0.667395637	3.4223674655	1.1177955292
H	0.1511193513	5.107610764	1.2704519601
H	0.5997337627	4.1903647915	2.7142942687
H	-3.6456119138	4.7204898361	3.0948796768
H	-2.2504579791	5.7962892341	2.9762692259
H	-2.2762271009	4.511873444	4.1948237165
H	-1.8133811855	3.8168191937	-0.6186830942
H	-3.4489325526	3.6398109456	0.0001853125
H	-2.6113885266	5.1886533247	0.1777118265
H	-1.6870109069	2.4872539765	5.6303091044
H	-0.0267995995	1.9781648333	5.9594443196
H	-0.3274139156	3.3952951571	4.9483950218
H	1.1903223184	0.9180220647	1.9793255965
H	1.7034970927	0.5126536045	3.6247362516
H	1.6042354154	2.2013783027	3.1177881459
H	-0.2863442796	-0.7548846339	5.1026113279
H	-2.0136784014	-0.6083235178	4.7533459704
H	-0.9066430268	-1.2552977262	3.5254848918
H	-6.4697048488	-2.5112346714	1.4044694549
H	-5.3722303097	-3.7573586276	2.0098688505
H	-5.5820718688	-2.25577788	2.9143348895
H	-1.5735016672	-2.5063954328	1.3212261864
H	-2.6275049644	-3.8995568577	1.5825809906
H	-2.4838402801	-2.6626447484	2.8352404042

H	-4.9892429314	-2.1433226432	-1.3606532981
H	-3.2206962949	-2.0366507977	-1.3941875114
H	-4.0130656629	-3.5543705735	-0.9272369071
H	-4.3132325674	0.2248094515	-2.0831720634
H	-5.6082500361	1.4268998165	-2.2591541076
H	-3.9937741449	1.9207101053	-1.7108341307
H	-6.3187904392	2.2907041017	1.9022316358
H	-6.7235118746	2.8413855269	0.2755982746
H	-5.1532317332	3.2440699255	0.9718850657
H	-7.6585113387	0.4174820427	-0.4927928617
H	-6.8176224091	-1.1363182829	-0.4831355647
H	-7.3240462799	-0.3916017062	1.0421191197
H	1.5665308135	-2.9598234475	-4.7441078552
H	-0.1351311391	-2.9395239688	-4.2829838635
H	0.8722132982	-1.5257647554	-3.9608274983
H	-0.2694847645	-3.8829380991	-0.3123878727
H	-1.0935326583	-4.0367169753	-1.8678381948
H	-0.7812020268	-2.4359090685	-1.2079231604
H	1.0531282567	-5.6151109819	-3.378875386
H	2.7597408885	-5.1927961553	-3.2129703565
H	1.8661568443	-5.8283037715	-1.8238724123
H	3.1862933222	-5.4504718061	0.1187263194
H	2.5837322752	-5.14104302	1.7505066031
H	1.4480139579	-5.2518520997	0.4015668635
H	1.7235472565	-1.3377353258	2.0913414336
H	0.7758086695	-2.8308042421	2.145213117
H	0.5370761208	-1.6645213618	0.8364056365
H	5.1495151992	-3.1596511934	0.878220243
H	4.5223416198	-1.5902842637	1.4227841599
H	4.2442999881	-3.0399795206	2.3906637145
H	7.5738213874	1.1324412714	-2.3087430191
H	7.6738547382	1.5134928274	-0.5849072661
H	7.476304425	-0.162051322	-1.1064145651
H	3.9175961676	0.8806573547	0.9635793214
H	5.3398605607	1.9123843339	1.1605996175
H	5.533184849	0.1614442503	1.158671911
H	5.0290692808	3.0500696174	-2.7551989507
H	3.7582803185	3.0378086411	-1.5227284105
H	5.3943502617	3.5610470949	-1.1030006071
H	6.9467896221	0.1816063371	-4.3713334084
H	6.1020892852	0.9779403529	-5.7026253832
H	6.3534539718	1.8401638014	-4.1809068474
H	2.0993079058	0.8924278872	-4.5351835855
H	3.267226315	1.7381140161	-5.5668033893
H	3.0338200116	2.2332689229	-3.8794715665
H	4.3498674021	-1.0967433031	-6.201161383
H	5.0275911625	-2.1428018035	-4.9493716762
H	3.2765950101	-1.8743800498	-5.0354561133

Sum of electronic and zero-point Energies= -4856.598911
Sum of electronic and thermal Energies= -4856.521244
Sum of electronic and thermal Enthalpies= -4856.520300
Sum of electronic and thermal Free Energies= -4856.705569
No imaginary frequency

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