

Electronic Supplementary Information for:

A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory

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General considerations. All starting materials were purchased from the Aldrich Chemical Company and were used as received. *E,E*-1,5-Bis(trimethylsilyl)-1,3-pentadiene was prepared according to a literature procedure.¹ Hexane solvent was pre-dried over sodium wire and was dried by refluxing under an atmosphere of N₂ over potassium metal. Also under N₂, toluene-*d*₈ was dried by stirring over sodium-potassium alloy before being distilled from the alloy, and was then stored over activated 4 Å molecular sieves. X-ray diffraction data for complex **2** was collected on an Oxford XCalibur 2 instrument. NMR spectra were recorded on a Bruker Avance 400 MHz instrument.

Synthesis of pro-ligand 1. A solution of *E,E*-1,5-bis(trimethylsilyl)-1,3-pentadiene (12.0 mmol, 2.54 g) in thf (30 ml) was cooled to -78°C and n-butyllithium (12.0 mmol, 7.50 ml, 1.6 M solution in hexane) was added dropwise over 10 minutes to give a yellow solution. The reaction was stirred for 15 minutes at -78°C and then warmed to room temperature, giving an orange solution that was stirred 2.5 hours. A solution of 2-(methoxy)ethyltosylate (2.99 g, 13.0 mmol) in thf (15ml) was added dropwise to the reaction mixture at -10°C, and the solution developed a dark orange/brown colour, which became dark grey/blue on warming to room temperature. Stirring for 18 hours resulted in the formation of a grey solution and a colourless precipitate. The reaction mixture was cooled to -10°C and the solvent removed *in vacuo* to give a colourless oil and a white precipitate. Pentane (120 ml) was added to the residue and the resulting suspension was filtered (porosity 3, Celite) to give a colourless solution. The pentane was removed under vacuum and the residue was subsequently distilled (10⁻² mm Hg, 45-50°C) to yield **1** as a colourless oil (1.93 g, 60%). Elemental analysis calculated for C₁₄H₃₀OSi₂, C 62.15, H 11.18; found C 62.02, H 11.07 %. ¹H NMR spectrum, recorded at 400.13 MHz at 300 K, using CDCl₃ as the solvent. Data are stated as: chemical shift δ /ppm, number of protons, signal multiplicity, coupling constant *J* (where relevant), structure assignment. 0.06 ppm, 18H, s, 2 × SiMe₃; 1.68 ppm, 2H, quartet, 8.0 Hz, CHCH₂CH₂OMe; 2.87 ppm, 1H, quintet, 8.0 Hz, CHCH₂CH₂OMe; 3.32 ppm, 3H, s, OCH₃; 3.35 ppm, 2H, t, 8.0 Hz, CH₂OMe; 5.68 ppm, 2H, d, 20.0 Hz, Me₃SiCH; 5.94 ppm, 2H, dd, 20.0 Hz, 8.0 Hz, Me₃SiCHCH. ¹³C NMR spectrum (100.61 MHz, CDCl₃, 300.0 K): -1.16 ppm, SiMe₃; 33.66 ppm, CHCH₂CH₂OMe; 49.46 ppm, CHCH₂CH₂OMe; 58.51 ppm, OCH₃; 70.52 ppm, CH₂OMe; 129.96 ppm, Me₃SiCH; 148.19 ppm, Me₃SiCHCH. Mass spectrometry, APCI (*m/z*); 269, molecular mass minus H⁺.

Synthesis of complex 2. A solution of **1** (2.0 mmol, 0.54 g) in hexane (20 ml) was cooled to -78°C and *n*-butyllithium (2.0 mmol, 1.25 ml) was added. The reaction was stirred for 15 minutes before being warmed to room temperature, and was then stirred vigorously for an additional one hour, resulting in the formation of a yellow precipitate. Addition of tmeda (2.0 mmol, 0.23 g) produced an orange solution, which was stirred for two hours. The solution was filtered (porosity 3, Celite) and the solvent volume was reduced until precipitation occurred. Gently heating the precipitate back into solution produced an orange solution, which, on storage at room-temperature overnight, produced orange crystals of **2** (0.30 g, 38% isolated yield). Anal. calc. for $\text{C}_{20}\text{H}_{45}\text{N}_2\text{OSi}_2\text{Li}$, C 63.10, H 11.31, N 6.69; found C 62.95, H 11.19, N 6.51 %. ^1H NMR spectrum (400.13 MHz, toluene- D_8 , 300.0 K): 0.29 ppm, 18H, s, $2 \times \text{SiMe}_3$; 1.70 ppm, 4H, s, tmeda CH_2 ; 1.90, 12H, s, tmeda CH_3 ; 2.65 ppm, 2H, t, 5.6 Hz $\text{CH}_2\text{CH}_2\text{OMe}$; 2.89 ppm, 3H, s, OCH_3 ; 3.48 ppm, 2H, t, 5.6 Hz, $\text{CH}_2\text{CH}_2\text{OMe}$; 3.64, 2H, d, 17.5 Hz, Me_3SiCHCH ; 6.80, 2H, d, 17.5 Hz, Me_3SiCHCH . ^{13}C NMR spectrum (100.61 MHz, toluene- D_8 , 300.0 K): 1.86 ppm, SiMe_3 ; 45.89 tmeda CH_3 ; 56.94 tmeda CH_2 ; 58.48 OCH_3 ; 74.99, CH_2OMe ; 76.91 Me_3SiCH ; 99.97, Me_3SiCHCH ; 151.07, Me_3SiCHCH . ^7Li NMR spectrum (155.51 MHz, toluene- D_8 , 300.0 K): -0.77 ppm.

Crystal data for complex **2**. Formula $\text{C}_{20}\text{H}_{45}\text{LiN}_2\text{OSi}_2$, formula weight 392.70, $T = 100(2)$, $\lambda = 0.71073 \text{ \AA}$, monoclinic, $P2_1/c$, $a = 17.4496(6) \text{ \AA}$, $b = 17.7496(11) \text{ \AA}$, $c = 17.2174(7) \text{ \AA}$, $\beta = 101.374(4)^{\circ}$, $V = 5227.9(4) \text{ \AA}^3$, $Z = 8$, density (calculated) = 0.998 Mg/m^3 , absorption coefficient = 0.146 mm^{-1} , $F(000) = 1744$, crystal size $0.50 \times 0.15 \times 0.15 \text{ mm}$, θ range for data collection $3.04\text{--}28.42^{\circ}$, 22053 reflections collected, 11675 independent reflections [$R(\text{int}) = 0.0535$], 99.8% completeness to $\theta = 28.42^{\circ}$, data / restraints / parameters 11675 / 30 / 513, goodness-of-fit on F^2 1.026, final R indices [$I > 2\sigma(I)$] $R1 = 0.0634$, $wR2 = 0.1611$, R indices (all data) $R1 = 0.0820$, $wR2 = 0.1786$, largest diff. peak and hole 1.410 and -0.585 e\AA^{-3} . CCDC 805551.

1. H. Yasuda T. Nishi K. Lee and A. Nakamura, *Organometallics* 1983, **2**, 21.

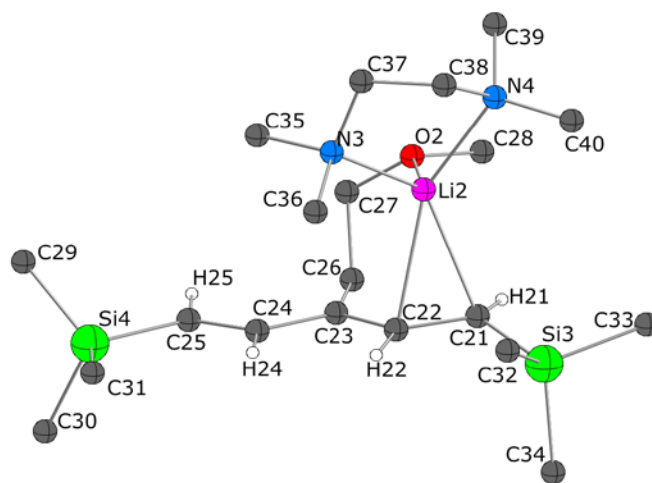


Figure S1. Molecular structure of **2b**, the second unique molecule in the unit cell of complex **2**. Selected bond lengths [Å] and angles [°]: C(21)–C(22) 1.393(3), C(22)–C(23) 1.403(3), C(23)–C(24) 1.423(3), C(24)–C(25) 1.365(3), Li(2)–C(21) 2.399(4), Li(2)–C(22) 2.427(4), Li(2)···C(23) 2.839, Li(2)–O(2) 1.990(4), Li(2)–N(3) 2.159(4), Li(2)–N(4) 2.161(4), Si(3)–C(21)–C(22) 121.41(15), C(21)–C(22)–C(23) 132.04(19), C(22)–C(23)–C(24) 119.48(18), C(23)–C(24)–C(25) 131.15(19), C(24)–C(25)–Si(4) 122.94(16).

Table S1. Selected bond lengths and angles for the experimental structures of **2a**, **2b**, and for the calculated structures of **2**.

	2a	2b ^a	BP86/TZ2P ^b	BP86/TZ2P ^c	BP86/QZAP ^b
C(1)–C(2)	1.400(3)	1.393(3)	1.408	1.406	1.410
C(2)–C(3)	1.400(3)	1.403(3)	1.406	1.408	1.405
C(3)–C(4)	1.430(3)	1.423(3)	1.433	1.432	1.435
C(4)–C(5)	1.360(3)	1.365(2)	1.375	1.378	1.374
C(1)–Li(1)	2.368(4)	2.399(4)	2.346	2.396	2.309
C(2)–Li(1)	2.446(4)	2.427(4)	2.400	2.471	2.409
C(3)···Li(1)	2.798	2.839	2.769	2.857	2.821
O(1)–Li(1)	1.986(4)	1.990(4)	2.061	2.048	2.033
N(1)–Li(1)	2.132(4)	2.159(4)	2.241	2.220	2.203
N(2)–Li(1)	2.192(4)	2.161(4)	2.315	2.269	2.299
C(2)–C(1)–Si(1)	120.89(15)	121.41(15)	123.0	123.3	122.0
C(1)–C(2)–C(3)	132.43(19)	132.04(19)	131.0	131.0	131.6
C(2)–C(3)–C(4)	119.38(19)	119.48(18)	119.6	119.5	119.4
C(3)–C(4)–C(5)	130.5(2)	131.15(19)	129.5	129.6	129.6
C(4)–C(5)–Si(2)	123.0(3)	122.94(16)	125.9	125.9	125.9

^a The bond lengths and angles listed for **2b** are the equivalents of those in **2a**, although the actual atom labels used in the structure of **2b** are different (see Figure S1). ^b Gas-phase. ^c COSMO simulation in toluene.

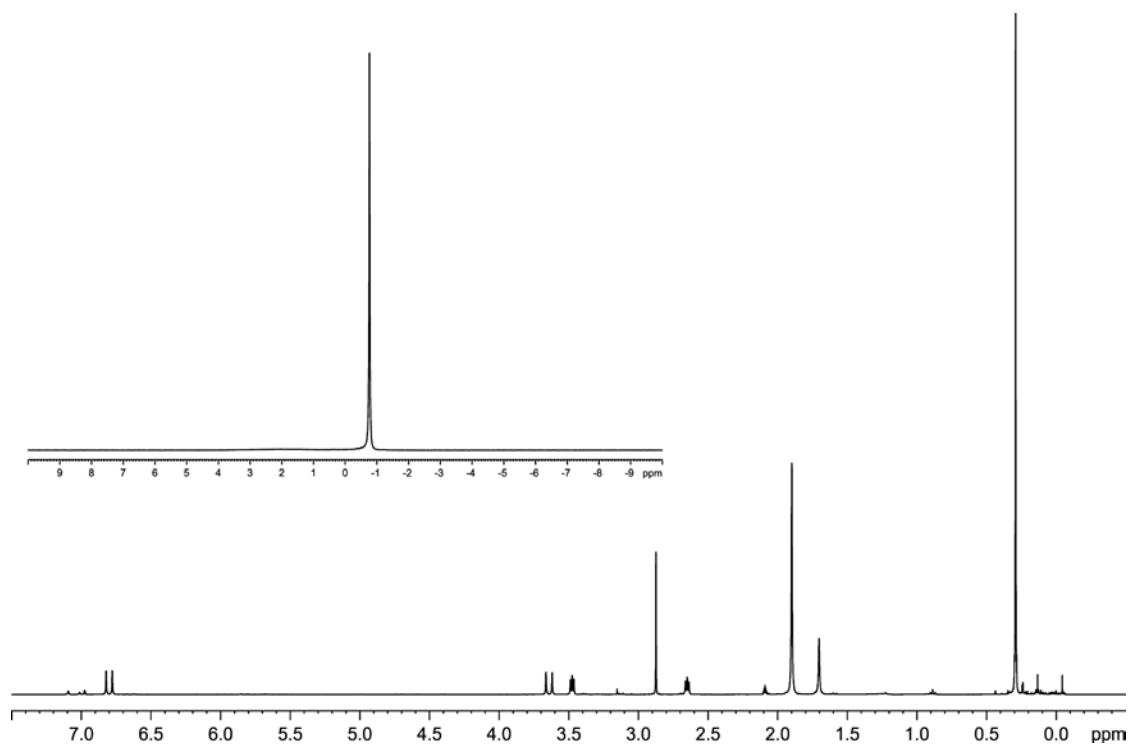


Figure S2. ^1H NMR and ^7Li NMR (inset) spectra of **2** recorded in toluene- d_8 at 300 K.

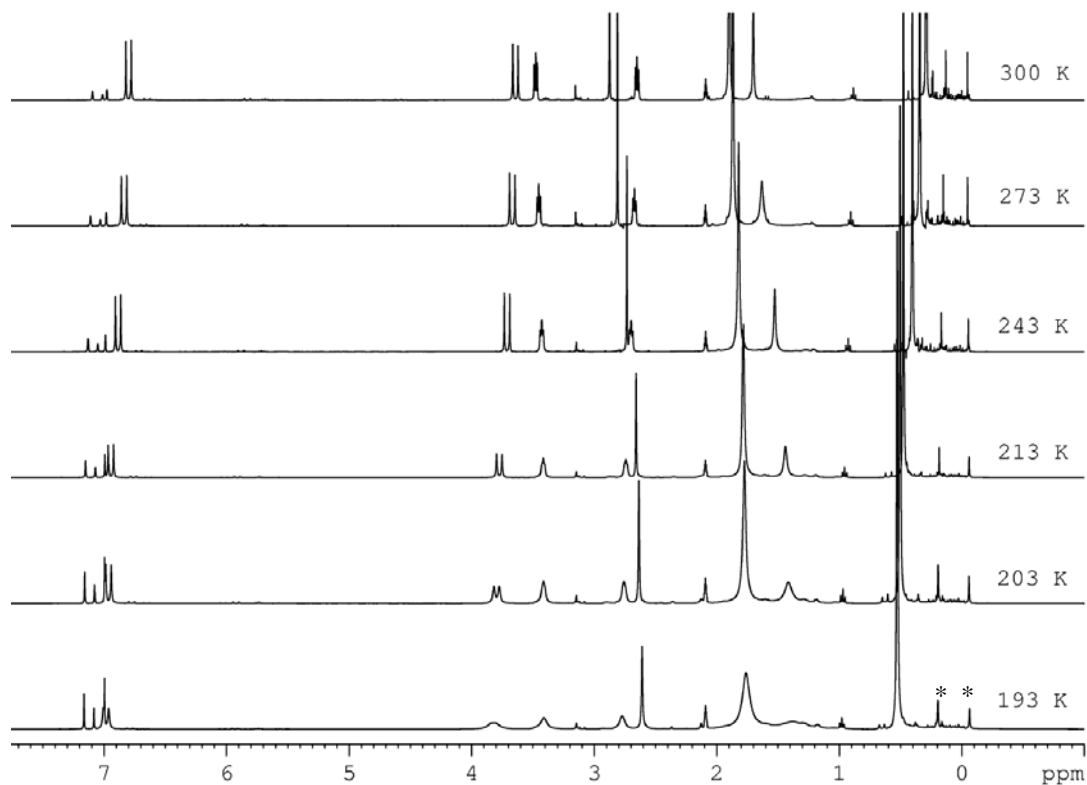


Figure S3. ^1H NMR spectrum of **2** in the temperature range 193-300 K in toluene- d_8 . The weak resonances labeled with an asterisk arise from a hydrolysis product, and contributes approximately 1% of the spectrum. This was found to be unavoidable even with rigorous drying of the solvent.

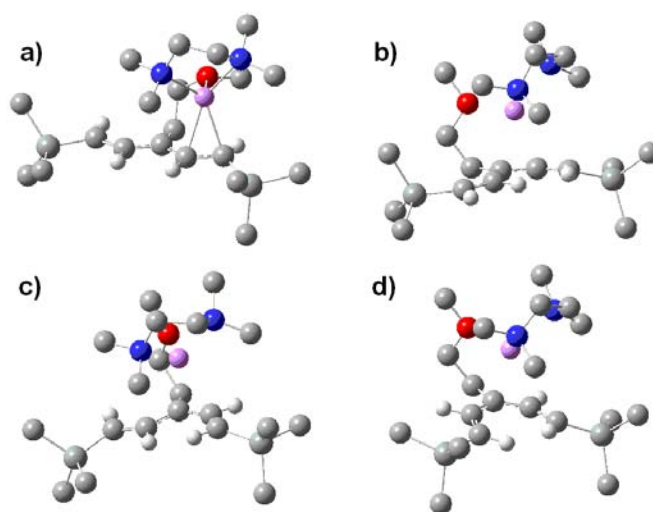


Figure S4. Structures of complex **2** calculated at the BP86/TZ2P level of theory: a) (*exo,exo*)-**W-2**, 0.0 kcal mol⁻¹; b) (*exo,exo*)-**S-2**, +10.4 kcal mol⁻¹; c) (*exo,exo*)-**S-2**, +3.1 kcal mol⁻¹; d) (*exo,exo*)-**U-2**, +5.3 kcal mol⁻¹.

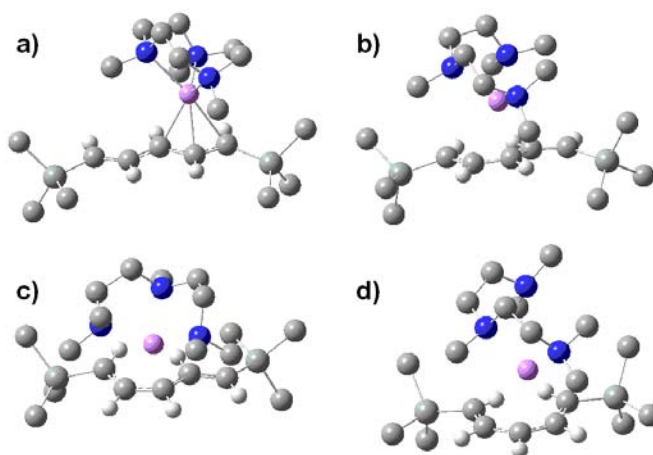


Figure S5. Structures of [(pmdeta)Li{1,5-(Me₃Si)₂C₅H₅}] (**4**) calculated at the BP86/TZ2P level of theory: a) (*exo,exo*)-**W-4**, 0.0 kcal mol⁻¹; b) (*exo,endo*)-**S-4** +5.9 kcal mol⁻¹; c) (*exo,exo*)-**S-4**, +1.5 kcal mol⁻¹; d) (*exo,exo*)-**U-4**, +4.7 kcal mol⁻¹. Pertinent bond lengths for (*exo,exo*)-**W-4** [Å]: C(1)–C(2) 1.398, C(2)–C(3) 1.408, C(3)–C(4) 1.426, C(4)–C(5) 1.374.

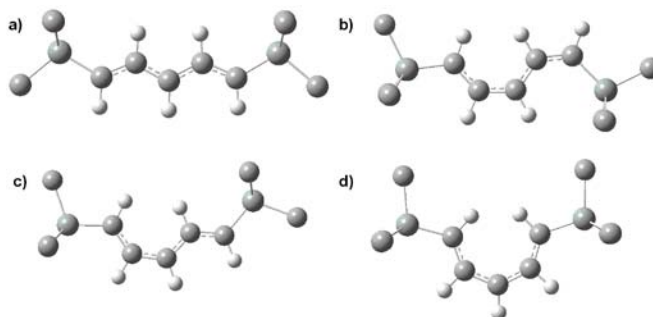


Figure S6. Structures of the 1,5-bis(trimethylsilyl)pentadienyl anion (**5**), [(Me₃Si)₂C₅H₅]⁻, calculated at the BP86/TZ2P level of theory: a) (*exo,exo*)-**W-5**, 0.0 kcal mol⁻¹; b) (*exo,endo*)-**S-5**, +3.9 kcal mol⁻¹; c) (*exo,exo*)-**S'-6**, +2.9 kcal mol⁻¹; d) (*exo,exo*)-**U-5**, +4.6 kcal mol⁻¹. Pertinent bond lengths for (*exo,exo*)-**W-5** [Å]: C(1)–C(2) 1.393, C(2)–C(3) 1.406.

Cartesian coordinates in Å for complexes 2-5 as calculated by Density Functional Theory

All calculations were carried out at the BP86/TZP level of theory in the gas-phase, unless otherwise stated.

Coordinates for complex 2.

(*exo,exo*)-W-2

C	-1.553611621	-1.577973363	0.455974977
C	-0.206439110	-1.404503259	0.083619592
C	0.898623042	-0.927506289	0.810847669
C	2.167432578	-0.789907483	0.159253162
C	3.364737014	-0.339971878	0.664118004
C	0.809076421	-0.668168226	2.297315513
H	0.051532493	-1.327308230	2.753926068
H	1.770836035	-0.932487122	2.770639198
C	0.505858051	0.782030020	2.672088760
H	0.617520979	0.963121134	3.755639862
H	1.179681547	1.463097976	2.136260678
C	-1.807448902	0.825836467	3.276634878
H	-1.772400887	-0.247914570	3.518890593
H	-2.798881843	1.059350608	2.874339961
H	-1.641969026	1.408969376	4.197963005
C	5.731699186	1.439753108	-0.251909817
H	6.726706783	1.449670313	-0.724387470
H	5.848493165	1.820201083	0.774915569
H	5.090929122	2.149387714	-0.797132619
C	6.259201956	-1.429299642	0.625307322
H	5.923553163	-2.477163285	0.641221143
H	6.406611068	-1.114089079	1.670136965
H	7.239475731	-1.390942261	0.123935200
C	4.771064601	-0.900745834	-2.033703253
H	4.078550949	-0.255767902	-2.595593584
H	4.383767850	-1.929768499	-2.077020629
H	5.737450580	-0.887135294	-2.560863762
C	-2.848920320	-2.182733133	-2.315741423
H	-3.251408140	-1.166573590	-2.450727156
H	-3.502319422	-2.876822536	-2.867231731
H	-1.859531897	-2.214110674	-2.798347518
C	-4.451611050	-2.582695703	0.321163083
H	-4.398465143	-2.870897952	1.382738307
H	-5.150651041	-3.275573452	-0.171641354
H	-4.890034666	-1.575439998	0.272438934
C	-2.212600423	-4.506585342	-0.456395973
H	-1.216718955	-4.642155072	-0.906283346
H	-2.923948464	-5.137424548	-1.013993060
H	-2.158114871	-4.887934341	0.575161244
C	1.004021530	2.648342555	-0.761149088
H	1.713263708	1.850862234	-0.503332886
H	0.822922074	3.259379178	0.132932982
H	1.461203749	3.294330768	-1.537682132
C	-0.004688251	1.211609391	-2.402824028
H	-0.926833466	0.723693553	-2.742362801
H	0.715029364	0.429420900	-2.137118676

H	0.408515535	1.807672046	-3.242271763
C	-1.249063961	3.104548087	-1.529261981
H	-1.136504331	3.902703693	-0.782877803
H	-1.047454929	3.568776590	-2.516558508
C	-2.682178081	2.582584334	-1.510757197
H	-2.785446926	1.759014855	-2.231505489
H	-3.366463560	3.389822104	-1.847799091
C	-3.260767386	3.167937106	0.774663561
H	-3.993948913	3.918586110	0.413502689
H	-2.307598302	3.672206953	0.969552292
H	-3.625487398	2.767716971	1.728129956
C	-4.345474228	1.318487357	-0.309302379
H	-4.633690132	0.917538288	0.670060532
H	-4.208697703	0.474294385	-0.994606965
H	-5.174524079	1.952076833	-0.684875210
H	-1.792118884	-1.424245543	1.519261909
H	0.038105679	-1.654159483	-0.959387496
H	2.157715322	-1.104180142	-0.893871513
H	3.384376706	-0.018406497	1.715107392
Li	-1.251660793	0.743640711	0.309236202
N	-0.263584586	2.051542832	-1.219493386
N	-3.085607068	2.066960084	-0.186089607
O	-0.842436429	1.178561721	2.281891516
Si	-2.724719254	-2.670817715	-0.475513870
Si	4.984087471	-0.313093525	-0.239506917

(exo,exo)-S-2

C	1.847947335	-1.513169873	0.535623174
C	0.935831510	-1.384853765	-0.506301239
H	1.453642288	-1.431249915	1.559169111
H	1.354754676	-1.499688919	-1.517064356
C	-0.476870839	-1.133679082	-0.512056830
C	-1.222342250	-1.193751457	0.703590152
C	-2.564530464	-1.141457080	1.051840870
H	-0.560013559	-1.360325737	1.561778659
H	-2.701995172	-1.282333967	2.135396780
Li	0.426144366	1.016954948	-0.365779257
Si	3.527098921	-2.284516353	0.411149501
Si	-4.278474082	-1.052498638	0.319523669
C	4.775021709	-1.392446694	1.544863517
H	4.399698733	-1.368105629	2.580178854
H	5.744157416	-1.915396532	1.559883811
H	4.962170989	-0.352560497	1.236492700
C	4.189307402	-2.281647866	-1.373467848
H	3.519939370	-2.835435322	-2.049140967
H	4.312235213	-1.267341264	-1.780886898
H	5.173069280	-2.774849121	-1.411188228
C	3.510622687	-4.094646923	1.006599053
H	4.517361392	-4.542145847	0.974357539
H	3.146524067	-4.163065613	2.043600811
H	2.842878979	-4.709093102	0.383711364
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H	-6.451592944	-1.916907521	1.262046732

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C	-1.157707137	-1.042939854	-1.862147966
H	-1.956020099	-1.797889992	-1.957170990
H	-0.426563023	-1.262365653	-2.656056882
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H	-2.178792176	0.339066280	-3.204309491
H	-2.642399588	0.508217546	-1.486971002
O	-0.822797616	1.363538974	-1.999289442
C	-1.355288909	2.617726888	-2.422656124
H	-0.591297780	3.382117409	-2.249363008
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C	3.396579613	1.529753032	-1.042838538
H	3.274491924	1.209313458	-2.085217120
H	3.432698122	0.634722124	-0.409966160
H	4.352891077	2.083641007	-0.959003335
C	2.133386863	3.499069014	-1.567310805
H	1.299226048	4.151484632	-1.281452028
H	1.952210866	3.135607543	-2.586607784
H	3.058409209	4.111781624	-1.573256426
C	2.396543926	2.814462245	0.749714810
H	2.784986911	1.967735261	1.332307261
H	3.147045530	3.628332519	0.824841059
C	1.073143757	3.282717090	1.351047001
H	0.631711378	4.062627392	0.714520373
H	1.263972083	3.752774085	2.337258355
C	0.378858930	1.351149934	2.650395543
H	0.332414148	1.952218858	3.581278957
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H	-0.362953101	0.547060030	2.708256456
C	-1.280986972	2.694682268	1.551994895
H	-1.978692953	1.847002345	1.570260913
H	-1.505274913	3.315331233	0.674579407
H	-1.439571588	3.308328875	2.461259780
N	2.242828887	2.356421487	-0.648351678
N	0.096449269	2.180208486	1.462695841

(exo,exo)-S-2

C	-1.304341207	-1.760969424	0.094905138
C	-0.804914828	-1.057706138	1.185866195
H	-0.629705406	-1.893450295	-0.763310346
H	-1.491697881	-0.950831573	2.038733621
C	0.468129240	-0.441828223	1.405393647
C	1.584949684	-0.722240509	0.556889630

C	2.903623572	-0.331038673	0.667189554
H	1.346289194	-1.397699192	-0.273947069
H	3.176768767	0.327875834	1.502976712
Li	-0.633304577	1.238340852	0.259742350
Si	-2.783728692	-2.872522866	0.109484780
Si	4.310068008	-0.950888983	-0.372052075
C	-3.884527839	-2.566939145	1.631777238
H	-4.747892838	-3.250126451	1.618432990
H	-3.332804071	-2.752570478	2.565734414
H	-4.277137873	-1.539982658	1.673567512
C	-2.272833071	-4.708159956	0.122311137
H	-3.150002695	-5.374755687	0.092157339
H	-1.643664332	-4.944440098	-0.750164512
H	-1.688933614	-4.950645107	1.023137668
C	-3.835231121	-2.659780032	-1.468943619
H	-3.213987363	-2.812301440	-2.365767204
H	-4.652357733	-3.397443305	-1.507041013
H	-4.286681133	-1.658706032	-1.545569750
C	5.237730639	0.486656756	-1.214198796
H	5.582168000	1.218825386	-0.466980802
H	6.125176025	0.127584390	-1.759309404
H	4.597133971	1.022179109	-1.931771451
C	5.599693474	-1.842708579	0.705794408
H	6.465967042	-2.174964712	0.111603303
H	5.974761891	-1.174186852	1.496619960
H	5.163703626	-2.724736239	1.198646579
C	3.700794166	-2.146793897	-1.716981025
H	3.189848122	-3.017441787	-1.279832220
H	3.001036265	-1.662594675	-2.415157279
H	4.549452697	-2.520844904	-2.310262399
C	0.697532143	0.270409163	2.724430083
H	1.541209295	-0.190917492	3.273924674
H	-0.193739346	0.157293161	3.361691444
C	1.034398832	1.756669086	2.628462661
H	1.036741680	2.225416338	3.629195102
H	2.024892654	1.911687378	2.170914940
O	0.051150835	2.435221119	1.805612940
C	0.305383867	3.838032115	1.764139213
H	1.312960694	4.049130057	1.366302311
H	-0.445027775	4.296555611	1.112127481
H	0.225138961	4.282908448	2.770426741
C	-3.708412521	1.143582740	0.219992476
H	-3.774842194	1.242655795	1.310900567
H	-3.436071928	0.107886496	-0.016676910
H	-4.703045822	1.373781457	-0.211254129
C	-2.975548718	3.425320556	0.118174904
H	-2.229010183	4.127051629	-0.273525350
H	-2.970017228	3.495102347	1.213138747
H	-3.971625021	3.747320998	-0.249483910
C	-2.559783662	1.935686933	-1.759983348
H	-2.632323921	0.868839839	-2.012803413
H	-3.407917129	2.444937405	-2.262677484
C	-1.242276917	2.497922980	-2.290572945

H	-1.128049856	3.543003791	-1.969564903
H	-1.270191671	2.511399496	-3.399105003
C	0.108110493	0.494934120	-2.561632450
H	0.289495878	0.706705212	-3.634980998
H	-0.774381105	-0.149080455	-2.468114403
H	0.966759525	-0.052098834	-2.156650452
C	1.155835166	2.542898956	-1.872451849
H	1.985691914	1.971664047	-1.436496230
H	1.034218123	3.473417218	-1.302565502
H	1.415458311	2.806402052	-2.917296877
N	-2.662738870	2.047754908	-0.288827439
N	-0.076028336	1.740003509	-1.791693312

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C	-0.991163494	-1.878391485	0.210479318
C	-0.779196764	-0.990543546	1.256067312
H	-0.179929732	-2.024440478	-0.508817635
H	-1.621433472	-0.891130123	1.958052453
C	0.331988891	-0.166447684	1.618354027
C	1.659910813	-0.226640953	1.076848465
C	2.237050156	-0.973577818	0.068187176
H	2.358707951	0.445537207	1.597782644
H	1.613242338	-1.705586408	-0.454002519
Li	-0.574885176	1.350024847	0.205411467
Si	4.052979460	-1.020334548	-0.309862575
Si	-2.395379544	-3.078625511	0.073774065
C	-3.278925165	-2.955442160	-1.614354972
H	-4.043628175	-3.740740978	-1.724967746
H	-3.776336998	-1.983506450	-1.757007887
H	-2.556478872	-3.081407298	-2.436219708
C	-3.683709220	-2.824421550	1.451482557
H	-4.492051270	-3.566087820	1.357490028
H	-3.232482993	-2.950765680	2.447180624
H	-4.147814339	-1.827184333	1.418655028
C	-1.756391720	-4.869040492	0.176195430
H	-1.012191836	-5.060640293	-0.612640443
H	-1.265908783	-5.060018699	1.142558181
H	-2.571019004	-5.600711442	0.052528335
C	4.355803655	-0.954840645	-2.190267797
H	4.016062707	-0.005767427	-2.632642378
H	5.424799856	-1.072713652	-2.427758149
H	3.814593362	-1.769191955	-2.697154305
C	4.970931361	0.432711719	0.507879499
H	4.888366079	0.398852502	1.604834897
H	6.042762759	0.396563782	0.258494645
H	4.583582623	1.406470311	0.170802851
C	4.852118541	-2.640847496	0.289331545
H	4.763557024	-2.745348632	1.381435087
H	4.353316726	-3.511325104	-0.164605540
H	5.920818688	-2.689782533	0.024639856
C	0.176934984	0.648249599	2.904132878
H	0.762443061	0.219839771	3.740995285
H	-0.873627051	0.620963883	3.230634022

C	0.609824376	2.104732444	2.799789442
H	0.380864658	2.657649040	3.728891989
H	1.695494211	2.183576975	2.617032650
O	-0.083021830	2.739842767	1.697602095
C	0.296323224	4.107367928	1.562366788
H	-0.256087974	4.525779539	0.713873434
H	0.043083188	4.680612175	2.470310781
H	1.379247733	4.204642734	1.374215359
C	1.154882152	2.618094823	-2.031849077
H	2.017991921	2.106603942	-1.588965594
H	1.014660361	3.580454318	-1.521811591
H	1.376351849	2.819383600	-3.099204934
C	0.185525684	0.479095932	-2.530098440
H	-0.664773654	-0.193515107	-2.364174979
H	1.070025389	0.003225011	-2.087303745
H	0.339723442	0.609521758	-3.620653163
C	-1.238087991	2.453077657	-2.399802425
H	-1.184847294	3.513088051	-2.111490032
H	-1.250641767	2.428780983	-3.508913703
C	-2.533360307	1.838250492	-1.873155352
H	-2.566469068	0.772395491	-2.136173844
H	-3.397776784	2.319813983	-2.375237105
C	-3.013477215	3.295496904	0.016162153
H	-4.020392557	3.581035168	-0.351819458
H	-2.292416835	4.027699903	-0.367199397
H	-3.008524902	3.356793277	1.111306989
C	-3.648481195	0.980797904	0.097433313
H	-3.719771850	1.065012422	1.189069778
H	-3.334186448	-0.040437961	-0.148001491
H	-4.652591298	1.169867696	-0.332045461
N	-0.040604121	1.777188890	-1.862108667
N	-2.644446367	1.935001009	-0.402008594

Coordinates for complex 2 with toluene solvation.

(*exo,exo*)-W-2

C	1.487354458	1.622850083	0.499190899
C	0.152636764	1.411406934	0.109858627
C	-0.949540204	0.902493720	0.824054077
C	-2.207103756	0.744057829	0.158794480
C	-3.405825833	0.272999791	0.648705648
C	-0.857076822	0.601984776	2.303009568
H	-0.120233136	1.266956017	2.784413331
H	-1.827036172	0.818278079	2.783724096
C	-0.508404612	-0.849584761	2.635879759
H	-0.631088950	-1.065570028	3.710938203
H	-1.152058877	-1.534682730	2.068895813
C	1.796775708	-0.833283199	3.277440997
H	1.727549436	0.232727435	3.543801256
H	2.800270340	-1.032402959	2.887864371
H	1.630176370	-1.441787976	4.180979913
C	-5.693208859	-1.584734046	-0.315382037
H	-6.675934208	-1.626394730	-0.811934454
H	-5.820696756	-1.966883540	0.709766434
H	-5.014136940	-2.271221858	-0.843947507
C	-6.341147056	1.256351142	0.554543850
H	-6.053843699	2.318981918	0.567517589
H	-6.489012093	0.939224130	1.598950342
H	-7.310453449	1.169812386	0.037649221
C	-4.782835381	0.791994267	-2.073901526
H	-4.058672570	0.172629718	-2.624649800
H	-4.429694946	1.833830667	-2.108196567
H	-5.740662677	0.746154966	-2.615196032
C	2.818621876	2.249425773	-2.256858225
H	3.246192665	1.242814163	-2.383698316
H	3.466143564	2.960839557	-2.793785357
H	1.836756893	2.257890312	-2.755680894
C	4.362167827	2.693065088	0.410340268
H	4.281597680	2.997717816	1.465710518
H	5.057555053	3.389707901	-0.082927339
H	4.815786879	1.691651950	0.387312670
C	2.094641498	4.559145430	-0.420735612
H	1.105705834	4.668302398	-0.893556563
H	2.803504335	5.201464137	-0.968670057
H	2.012107668	4.944927789	0.607663752
C	-0.895141935	-2.653864640	-0.835347495
H	-1.627082383	-1.876688859	-0.579719729
H	-0.720096193	-3.277276894	0.051070557
H	-1.320400684	-3.295246276	-1.633174381
C	0.116138861	-1.171430695	-2.433903621
H	1.035766927	-0.664698356	-2.751462311
H	-0.622488700	-0.404719394	-2.174323053
H	-0.269728314	-1.764839946	-3.287483068
C	1.383068094	-3.050564926	-1.560981396
H	1.272647109	-3.860858413	-0.827914442
H	1.209710082	-3.502835135	-2.558134336

C	2.802864139	-2.498014760	-1.506347933
H	2.905564889	-1.665248081	-2.216416733
H	3.511636107	-3.286301260	-1.833802328
C	3.345167047	-3.100343250	0.784416165
H	4.105146141	-3.824398284	0.426840990
H	2.401624332	-3.633132576	0.946770957
H	3.677832006	-2.706593657	1.751916408
C	4.415624060	-1.217894638	-0.253143796
H	4.677398891	-0.824512582	0.736651718
H	4.282632767	-0.371243915	-0.936392598
H	5.260753821	-1.835722107	-0.616731815
H	1.728075364	1.447736710	1.557856074
H	-0.088592588	1.666097643	-0.932813842
H	-2.189867585	1.057923138	-0.894499293
H	-3.430898007	-0.059332741	1.696089653
Li	1.316130120	-0.759551728	0.306877892
N	0.368446531	-2.020877462	-1.255407093
N	3.164254601	-1.987728300	-0.165064772
O	0.856380522	-1.188337071	2.255960705
Si	2.650650267	2.733276879	-0.419965947
Si	-5.003916198	0.191444357	-0.284704282

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C	-1.876185559	-1.675123193	-0.355419822
C	-0.977027575	-1.316971387	0.638438828
H	-1.484581085	-1.781584268	-1.377654608
H	-1.395061275	-1.255926649	1.653845439
C	0.432378366	-1.030553133	0.597029415
C	1.156456443	-1.183083414	-0.622559063
C	2.494942938	-1.223978211	-0.995028001
H	0.472615967	-1.326531770	-1.468277827
H	2.604992315	-1.357391685	-2.083372726
Li	-0.298992642	1.178723847	0.250647097
Si	-3.595350047	-2.309484892	-0.108536259
Si	4.219859384	-1.266483302	-0.287995698
C	-4.842391145	-1.446985026	-1.267142708
H	-4.514510003	-1.541922773	-2.314524790
H	-5.841582415	-1.904682291	-1.188920580
H	-4.944964686	-0.373029581	-1.048636136
C	-4.184251732	-2.114427966	1.690552986
H	-3.526462247	-2.657369712	2.386396641
H	-4.217981123	-1.063227189	2.012767170
H	-5.198587546	-2.528865762	1.801462473
C	-3.710979585	-4.160233984	-0.554317809
H	-4.744573659	-4.533440492	-0.467972466
H	-3.377758811	-4.332212690	-1.589999099
H	-3.071684357	-4.768172770	0.104438169
C	5.215332339	-2.389152818	-1.460608839
H	6.280212128	-2.412509836	-1.180574142
H	4.835644969	-3.422094025	-1.438255239
H	5.148571250	-2.032006099	-2.499930356
C	5.101065787	0.430453881	-0.350303190
H	5.085043027	0.833726831	-1.374781889

H	4.632817463	1.179159697	0.306863087
H	6.154891370	0.329642190	-0.043283869
C	4.474687765	-1.959741636	1.468573767
H	4.115645757	-1.287342305	2.261043280
H	3.975331306	-2.931894211	1.596846093
H	5.553923876	-2.111575944	1.633811406
C	1.128939981	-0.806730019	1.926656383
H	1.855324746	-1.608735995	2.145477274
H	0.384982171	-0.841342949	2.737839259
C	1.895807759	0.504913766	2.041146318
H	2.301436573	0.637537175	3.059139716
H	2.732811977	0.541475373	1.327385318
O	1.010124783	1.614596089	1.748489238
C	1.672223525	2.866509951	1.951773169
H	0.967397699	3.663532791	1.695748751
H	1.976533983	2.980856454	3.004828160
H	2.566675447	2.950813392	1.313056292
C	-3.227839340	1.653433019	1.073021082
H	-3.020610876	1.390224776	2.117852955
H	-3.331623360	0.726328911	0.496704248
H	-4.181778977	2.215804609	1.039500775
C	-1.906167026	3.632390618	1.376372141
H	-1.098127758	4.258574398	0.979973959
H	-1.634837661	3.324147499	2.393533261
H	-2.824027758	4.252212061	1.428909064
C	-2.376033496	2.822341438	-0.868902945
H	-2.820105881	1.950666288	-1.368880199
H	-3.123551360	3.639248903	-0.924287705
C	-1.107833329	3.245766842	-1.605479972
H	-0.630024953	4.079339045	-1.072234897
H	-1.379085666	3.627573731	-2.610124493
C	-0.504198062	1.195860910	-2.764311879
H	-0.574676793	1.701658145	-3.748320127
H	-1.467802474	0.722874284	-2.538874899
H	0.252001242	0.405594788	-2.826466572
C	1.224395017	2.665496778	-1.973645643
H	1.938337039	1.831808691	-1.972062983
H	1.516405762	3.378699321	-1.192237055
H	1.280767088	3.181351330	-2.952630944
N	-2.104244185	2.439931547	0.535227273
N	-0.125864934	2.143924814	-1.698366035

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C	-1.368922708	-1.806944861	0.035916527
C	-0.889432046	-1.070108395	1.110494281
H	-0.669194888	-2.007165071	-0.788293136
H	-1.606510274	-0.897461432	1.926623703
C	0.401112142	-0.498120305	1.366973636
C	1.527281753	-0.820834232	0.546531511
C	2.870197576	-0.555101946	0.730346287
H	1.270644893	-1.412820372	-0.340600259
H	3.165374399	0.016048144	1.620971724
Li	-0.513688157	1.367524761	0.292225972

Si	-2.948495794	-2.763371482	-0.024121523
Si	4.252624484	-1.159111288	-0.346292811
C	-4.019078769	-2.468667595	1.521537375
H	-4.943127346	-3.064814555	1.461859751
H	-3.486423934	-2.770543531	2.436306492
H	-4.312009210	-1.414485127	1.637641412
C	-2.603219784	-4.634260644	-0.152762137
H	-3.536648414	-5.213158391	-0.245170412
H	-1.984597648	-4.852827583	-1.037569562
H	-2.057961441	-5.000529901	0.730542172
C	-3.987519733	-2.355640840	-1.573458099
H	-3.388670832	-2.511423830	-2.484956729
H	-4.873261617	-3.007605205	-1.642387174
H	-4.336593449	-1.311579238	-1.581181053
C	5.245210656	0.287131379	-1.095716705
H	5.624973063	0.948621839	-0.301061170
H	6.112103145	-0.076413019	-1.670843436
H	4.624446658	0.898683848	-1.768692932
C	5.506108227	-2.169720742	0.669944288
H	6.364418985	-2.484897356	0.054961628
H	5.896939848	-1.570955240	1.507853885
H	5.039974173	-3.071827115	1.095020126
C	3.604861479	-2.240629881	-1.768545641
H	3.064863353	-3.121509317	-1.390058769
H	2.920690562	-1.685813276	-2.428479734
H	4.441767433	-2.600068048	-2.387351346
C	0.626780950	0.167741803	2.713874405
H	1.382828944	-0.386559464	3.305346901
H	-0.306768207	0.137172587	3.297582429
C	1.123513779	1.611598161	2.679828027
H	1.133263337	2.044440464	3.695600273
H	2.142812261	1.674021090	2.267019752
O	0.252487314	2.413872871	1.844196483
C	0.673818109	3.780225290	1.826340728
H	1.705036695	3.871587626	1.446623166
H	-0.005200756	4.332291256	1.168929306
H	0.628536896	4.216900461	2.837370232
C	-3.589935104	1.352435472	0.376355554
H	-3.595388677	1.405001772	1.472379860
H	-3.408261285	0.312962305	0.078927657
H	-4.585745899	1.670139666	0.008841882
C	-2.708869912	3.583591590	0.327143348
H	-1.931533197	4.248393476	-0.067691974
H	-2.653667990	3.604821853	1.422502243
H	-3.693980975	3.986412029	0.015872422
C	-2.489363321	2.147918201	-1.627680418
H	-2.632868320	1.097991881	-1.918006654
H	-3.332772383	2.720705049	-2.063775100
C	-1.176038004	2.666851943	-2.208440867
H	-1.011510616	3.704413506	-1.886265342
H	-1.251103387	2.687845117	-3.313938233
C	0.076670960	0.605753430	-2.528311198
H	0.189987806	0.796709438	-3.614357954

H	-0.816054622	-0.010097371	-2.364566280
H	0.943852832	0.035808833	-2.175747384
C	1.237894661	2.622993597	-1.930743755
H	2.073772797	2.027117828	-1.543076132
H	1.186193798	3.562028376	-1.365059856
H	1.440620412	2.867382037	-2.992309960
N	-2.509806358	2.204839270	-0.148956417
N	-0.014344345	1.865544601	-1.765196400

(*exo,exo*)-U-2

C	-0.945246350	-1.978447070	0.184284713
C	-0.779409147	-1.059255977	1.210469537
H	-0.118179523	-2.121088275	-0.517104122
H	-1.642900174	-0.957870582	1.885568556
C	0.309227393	-0.210016309	1.587330315
C	1.645651101	-0.249298077	1.066972910
C	2.251599262	-0.988688331	0.067406385
H	2.324919744	0.436835913	1.594789646
H	1.646981090	-1.720113849	-0.477111001
Li	-0.584807866	1.432793279	0.239391073
Si	4.063726062	-0.969458142	-0.322053421
Si	-2.365886359	-3.146806900	-0.017652218
C	-3.241746711	-2.942134400	-1.702326315
H	-4.024372636	-3.705392636	-1.841566520
H	-3.713273699	-1.952622596	-1.807041318
H	-2.517999934	-3.052763680	-2.525369967
C	-3.661908287	-2.940047387	1.360709663
H	-4.482394367	-3.661392399	1.222110676
H	-3.221088141	-3.121472074	2.352768597
H	-4.105464202	-1.932980669	1.371213341
C	-1.750644831	-4.950143273	0.001309926
H	-0.996001425	-5.106514471	-0.785675031
H	-1.280041505	-5.200976116	0.964243470
H	-2.572871924	-5.662295511	-0.175942206
C	4.358612589	-0.830319477	-2.200205839
H	3.984297523	0.122106814	-2.605965419
H	5.430725371	-0.904906384	-2.442488105
H	3.840313191	-1.644135814	-2.731491429
C	4.952083962	0.473148613	0.544451124
H	4.872576314	0.398407255	1.639769348
H	6.023435111	0.469699684	0.289491635
H	4.538635415	1.447682684	0.242714528
C	4.915514278	-2.590497807	0.206492022
H	4.849913196	-2.736512209	1.295760036
H	4.431819824	-3.456066245	-0.273094305
H	5.980524762	-2.599620984	-0.077722327
C	0.119863264	0.586633107	2.883349997
H	0.660663870	0.128931727	3.734892796
H	-0.943551193	0.574007974	3.166892318
C	0.582877148	2.036670074	2.836225592
H	0.332578195	2.562322208	3.774573934
H	1.674898494	2.104179493	2.692516734
O	-0.064923764	2.713099352	1.733689408

C	0.330372436	4.083823432	1.649076288
H	-0.192565517	4.530068319	0.796783454
H	0.053371042	4.629740409	2.565648008
H	1.418584600	4.173828622	1.496400460
C	1.092290638	2.749702391	-2.016430506
H	1.977654053	2.264096854	-1.588741130
H	0.939599479	3.712257491	-1.511451109
H	1.286383053	2.947481035	-3.089449542
C	0.160132759	0.584905094	-2.480675573
H	-0.675954383	-0.102069343	-2.300361879
H	1.058618677	0.124750616	-2.049280811
H	0.295675344	0.710246673	-3.574127862
C	-1.301760381	2.531041561	-2.336886467
H	-1.267905431	3.591144842	-2.048186008
H	-1.329584511	2.506096149	-3.445108515
C	-2.575072449	1.886464572	-1.794004315
H	-2.600861923	0.825788265	-2.078152359
H	-3.455842687	2.366506821	-2.266657624
C	-3.019299932	3.305375027	0.134895840
H	-4.027517213	3.599809514	-0.220524373
H	-2.299111358	4.044797542	-0.235092297
H	-3.008313341	3.340267734	1.231043236
C	-3.653356385	0.989134013	0.178010520
H	-3.705472524	1.047904149	1.272328408
H	-3.348939703	-0.026876550	-0.099261078
H	-4.664114058	1.190164696	-0.229026839
N	-0.079908032	1.881964578	-1.816759397
N	-2.655954648	1.952275746	-0.317918081

Coordinates for complex 2 calculated at the BP86/QZ4P level of theory.

(exo,exo)-W-2

C	1.535606935	-1.558122362	-0.506124530
C	0.182582044	-1.399508057	-0.143228279
C	-0.924032930	-0.910135610	-0.857304685
C	-2.194273085	-0.800663694	-0.199209545
C	-3.394219330	-0.338070780	-0.682371236
C	-0.829379746	-0.565985101	-2.327032309
H	-0.074724639	-1.197990960	-2.825099824
H	-1.788739858	-0.793273747	-2.822483562
C	-0.516275125	0.902916503	-2.602359374
H	-0.633530101	1.163628818	-3.668028688
H	-1.176432619	1.551993488	-2.014887183
C	1.785292516	0.950282221	-3.228860699
H	1.721325569	-0.103063296	-3.539935223
H	2.786509427	1.135137269	-2.826984326
H	1.618310887	1.595683451	-4.105518258
C	-5.686142998	1.474031871	0.308361272
H	-6.672070249	1.509917553	0.794282422
H	-5.802173561	1.887195329	-0.703852956
H	-5.014300411	2.144511210	0.862082434
C	-6.307150675	-1.367316901	-0.611142273
H	-6.001189136	-2.422167277	-0.633433742
H	-6.457802040	-1.046996830	-1.651935662
H	-7.279903293	-1.306714900	-0.101683106
C	-4.773075425	-0.916087324	2.022820218
H	-4.061855448	-0.295818549	2.586012057
H	-4.408463182	-1.952176423	2.048622911
H	-5.730440365	-0.889898113	2.562321529
C	2.816648493	-2.193137827	2.252495661
H	3.279022799	-1.204556483	2.381773997
H	3.423851871	-2.917508989	2.813749915
H	1.827619518	-2.160493337	2.731056080
C	4.398166700	-2.659741890	-0.364832856
H	4.347175659	-2.958828902	-1.421370894
H	5.072013112	-3.365181398	0.141380779
H	4.866344207	-1.667476663	-0.324481071
C	2.084545691	-4.487584330	0.407879239
H	1.081651265	-4.575616533	0.848590884
H	2.758333807	-5.148482236	0.972715740
H	2.020991578	-4.870120070	-0.620239299
C	-0.947401263	2.568700387	0.801085636
H	-1.656114466	1.773532804	0.537542527
H	-0.772040022	3.192826700	-0.084106521
H	-1.400826750	3.201665844	1.588234768
C	0.069502504	1.123266065	2.424826333
H	0.993536264	0.640077548	2.762689354
H	-0.647165128	0.339695801	2.157958170
H	-0.344767196	1.715017614	3.264031100
C	1.303887645	3.028089534	1.569869470
H	1.186197231	3.835769796	0.834605835
H	1.095489051	3.476497608	2.561760924

C	2.736310477	2.509455789	1.542450375
H	2.843546052	1.669212565	2.244263675
H	3.422007605	3.307631521	1.895595367
C	3.320477050	3.159003972	-0.720778555
H	4.055886642	3.889060484	-0.328268715
H	2.373164424	3.678305695	-0.902388279
H	3.690200664	2.791920196	-1.685227604
C	4.397655287	1.277404578	0.303432324
H	4.683693870	0.897726354	-0.685154666
H	4.267481960	0.420009089	0.973584548
H	5.224543500	1.907396912	0.687328862
H	1.787067516	-1.389173630	-1.563507184
H	-0.067196447	-1.684156370	0.889486142
H	-2.179526766	-1.150832838	0.842027181
H	-3.421397687	0.016333297	-1.721063778
Li	1.301053720	0.728738507	-0.291207689
N	0.324492529	1.969984478	1.244923710
N	3.134570499	2.025762802	0.201527122
O	0.839749508	1.255395508	-2.199455467
Si	2.673263434	-2.683222400	0.421188198
Si	-4.997693227	-0.295476240	0.246752255

Coordinates for the 1,5-bis(trimethylsilyl)pentadienyl anion, 5.

(*exo,exo*)-W-5

C	2.524999087	-0.842466470	-0.000035382
C	1.243590710	-0.294914521	0.000781584
H	2.590763850	-1.939733037	-0.001562112
H	1.169298493	0.804424754	0.002461206
C	0.000231106	-0.952142354	-0.000307009
C	-1.243453364	-0.295519121	-0.000080904
H	0.000495340	-2.048886025	-0.001503608
H	-1.169684822	0.803848071	0.000931037
C	-2.524606676	-0.843667398	-0.000646677
H	-2.589863596	-1.940974165	-0.001034510
Si	4.099341460	0.090275591	0.002481995
Si	-4.099366067	0.088398014	-0.002470110
C	5.562682655	-1.138323014	-0.012759277
H	6.533034640	-0.616922897	-0.012172897
H	5.531684470	-1.795176054	0.870678381
H	5.525037210	-1.781191728	-0.906159826
C	4.343473404	1.230603708	1.523972567
H	3.521195949	1.960585828	1.593844859
H	4.337680331	0.645726583	2.457144249
H	5.290853380	1.794003781	1.473367576
C	4.330848074	1.256463862	-1.501126660
H	5.276826931	1.821814370	-1.446731733
H	4.321066558	0.687211853	-2.443879134
H	3.506061463	1.985057631	-1.553832634
C	-5.562135236	-1.140905219	0.011065858
H	-6.532745968	-0.619984958	0.008563332
H	-5.529263099	-1.798093163	-0.872060331
H	-5.525739192	-1.783407022	0.904784076
C	-4.331734472	1.253024682	1.502173768
H	-4.318590935	0.683398260	2.444632885
H	-3.509190653	1.984243764	1.553810319
H	-5.279536189	1.815483257	1.449628391
C	-4.343655233	1.230205541	-1.522851727
H	-4.340356688	0.645895721	-2.456405154
H	-5.289860041	1.795439561	-1.470567643
H	-3.519988291	1.958554314	-1.593461357

(*exo,exo*)-S-5

C	2.082877673	0.431835960	-0.000303225
C	1.043232630	-0.497943042	-0.003209653
H	1.817600282	1.497444222	0.000806730
H	1.352058678	-1.554301017	-0.005621270
C	-0.363580700	-0.331989123	-0.003751327
C	-1.044440908	0.902470607	-0.001575893
C	-2.410803150	1.174792067	-0.000856831
H	-0.383157104	1.780144354	-0.000240755
H	-2.688032914	2.236364609	0.001163722
H	-0.959111829	-1.249790554	-0.006495677
Si	3.867332650	0.031259701	0.001830798
Si	-3.817623362	-0.011476195	-0.001195017

C	-5.449186806	0.988830733	0.000121870
H	-5.515016928	1.632967831	-0.891001673
H	-6.331875814	0.329642955	0.005891579
H	-5.508764404	1.640086914	0.886489484
C	-3.881027786	-1.170949005	-1.523087348
H	-3.985748294	-0.590062172	-2.453107849
H	-2.949827029	-1.752297768	-1.605902653
H	-4.723557515	-1.880243778	-1.461528893
C	-3.877926717	-1.172515440	1.519789225
H	-3.999537091	-0.593670286	2.449071964
H	-4.708683519	-1.894950385	1.451296303
H	-2.938249738	-1.738933779	1.610171161
C	4.454705409	-0.998234142	-1.506469859
H	5.528028504	-1.247651737	-1.446882156
H	3.892414594	-1.943623873	-1.570430106
H	4.277606411	-0.451531161	-2.446051044
C	4.886126259	1.648204897	-0.001454790
H	4.654119114	2.259470316	0.884767455
H	5.969283292	1.447031331	0.000944336
H	4.656980346	2.254243059	-0.891993046
C	4.454338747	-0.990628023	1.515552762
H	4.274955047	-0.440149961	2.452509786
H	3.893538211	-1.936693769	1.582859158
H	5.528179233	-1.238478323	1.458650798

(exo,endo)-S-5

C	-1.970798052	-0.012687044	0.005114523
C	-1.356872297	1.239587737	0.009320248
H	-1.326526916	-0.901858618	0.004552741
H	-2.041066716	2.101716729	0.013497173
C	0.006815715	1.618731645	0.009626296
C	1.113160282	0.747031143	0.006185230
C	2.470464492	1.055726282	0.005857143
H	0.852113851	-0.321519039	0.003657132
H	2.738032295	2.122549031	0.009904041
H	0.218753612	2.692916857	0.012802325
Si	-3.777508292	-0.296797849	-0.000389498
Si	3.838801812	-0.165253578	-0.000552046
C	5.513644070	0.755418127	-0.000720777
H	5.609907120	1.395774603	0.890145059
H	6.362897844	0.053717164	-0.005243902
H	5.605968746	1.402549458	-0.887080064
C	3.848565012	-1.345219586	1.508718305
H	3.955455134	-0.781784904	2.448887679
H	2.898398328	-1.899340239	1.568931856
H	4.666774703	-2.083337232	1.451441981
C	3.842218402	-1.335820065	-1.517174793
H	3.947030132	-0.766611725	-2.454085991
H	4.659460499	-2.075501289	-1.467113520
H	2.891010072	-1.888078872	-1.577915504
C	-4.133714611	-2.174094681	0.005815640
H	-3.699629887	-2.652371633	0.897810432
H	-5.215136164	-2.384026678	0.002116643

H	-3.692363312	-2.659376050	-0.878802377
C	-4.701423299	0.452729106	1.504402177
H	-5.791465287	0.290732705	1.447121851
H	-4.334821177	0.015415081	2.446392717
H	-4.525384257	1.538988775	1.561326987
C	-4.692229806	0.439336409	-1.517539252
H	-4.318811976	-0.005371361	-2.453379514
H	-5.782527166	0.276754582	-1.466491537
H	-4.516677373	1.525249503	-1.582245457

(exo,exo)-U-5

C	-1.712253706	0.177243509	-0.002138017
C	-1.285385988	1.503220216	-0.008768638
H	-0.955726242	-0.612602133	0.001551712
H	-2.090771144	2.255682244	-0.011576528
C	0.001094002	2.095650639	-0.012818208
C	1.286959140	1.501880951	-0.010751728
H	0.001680691	3.189307643	-0.018271850
C	1.712493137	0.175470878	-0.004688322
H	2.093104327	2.253520096	-0.014775319
H	0.955195553	-0.613643977	-0.001408126
Si	-3.468318311	-0.353981352	0.002268010
Si	3.468055057	-0.357411350	0.000075380
C	4.482168330	0.263641235	-1.504023897
H	4.460014226	1.364018766	-1.556062080
H	5.538673790	-0.050376518	-1.450261820
H	4.055595533	-0.114514366	-2.446332985
C	3.563275867	-2.265054670	-0.011327433
H	4.605754651	-2.621427880	-0.003050580
H	3.054391964	-2.687569735	0.869165395
H	3.071949396	-2.676748066	-0.906766144
C	4.469732661	0.242202191	1.521343019
H	4.036718377	-0.151319402	2.454420695
H	5.527340687	-0.068831835	1.471181403
H	4.444396250	1.341591831	1.590165564
C	-3.565303347	-2.261562443	0.003505489
H	-3.063429786	-2.678631092	0.890576747
H	-4.608154635	-2.616907630	0.006304147
H	-3.067695600	-2.679698928	-0.885461644
C	-4.478862345	0.257190431	-1.508314332
H	-5.536205100	-0.053861792	-1.453713011
H	-4.453812462	1.357040542	-1.569197927
H	-4.051777061	-0.129585899	-2.446908849
C	-4.472457170	0.257473268	1.517127499
H	-5.529814664	-0.054479640	1.467753604
H	-4.040696018	-0.128292352	2.454001490
H	-4.447905900	1.357394565	1.577123581

Coordinates for [(pmdeta)Li{1,5-(Me₃Si)₂C₅H₅}] (4).

(*exo,exo*)-W-4

C	1.813834234	-1.527426906	-0.636141416
C	0.494613655	-1.589825093	-0.176419109
C	-0.659705467	-1.002076852	-0.728812190
C	-1.975375732	-1.174765721	-0.207152671
C	-3.166177819	-0.780028834	-0.767670118
C	-5.865138381	0.509998640	0.035694371
H	-6.898111269	0.316089920	0.365642149
H	-5.919897734	1.011821647	-0.943245939
H	-5.410597746	1.217382680	0.746039814
C	-5.854113602	-2.250728481	-1.240589725
H	-5.368196899	-3.233391358	-1.337516097
H	-5.928718721	-1.819593252	-2.251264108
H	-6.879041511	-2.410044003	-0.868905701
C	-4.763661511	-1.900856115	1.630709119
H	-4.240902127	-1.252556088	2.350516707
H	-4.234457496	-2.865197078	1.600296032
H	-5.773941605	-2.089584331	2.025497873
C	2.686677481	-3.734181175	1.351376866
H	2.333931025	-3.172878605	2.230294468
H	3.532041336	-4.358456346	1.679822264
H	1.873971985	-4.407149152	1.039777404
C	4.745447221	-1.605330528	0.519364578
H	5.066011775	-0.875441795	-0.240687025
H	5.597503605	-2.277644983	0.709357157
H	4.549923346	-1.052512700	1.451312246
C	3.858108316	-3.647317152	-1.520343759
H	3.070660081	-4.310180128	-1.909323838
H	4.717116401	-4.270617360	-1.224738592
H	4.187367810	-3.004317763	-2.352223627
C	1.467525461	0.065581006	2.902521821
H	2.145960180	-0.701432009	2.512072689
H	0.452771060	-0.350231688	2.917621310
H	1.767147712	0.311109571	3.941275571
C	2.883653507	1.768837539	1.980630406
H	2.942635643	2.649120363	1.328156665
H	3.555157121	1.000764820	1.577984145
H	3.243829461	2.063303780	2.988232579
C	0.555605571	2.270059467	2.481637554
H	-0.366372506	1.753897433	2.782005317
H	0.932870204	2.800584628	3.380552731
C	0.230348984	3.289694635	1.390887065
H	1.154949387	3.791377386	1.075550873
H	-0.424460208	4.078962262	1.814279472
C	-1.830758841	2.434518124	0.442976634
H	-2.385073831	3.392387666	0.516800135
H	-1.984711917	1.875008532	1.372885587
H	-2.256512324	1.823090964	-0.361548584
C	-0.177748527	3.425830655	-1.018908436
H	-0.896495900	3.057057259	-1.763123579
H	-0.404144755	4.503371533	-0.877584666

H	1.948869642	-1.049038823	-1.619188999
H	0.321187601	-2.139801862	0.759310444
H	-2.017847213	-1.701647126	0.756886054
H	-3.102073243	-0.285041864	-1.749303539
Li	0.822595283	0.708896150	-0.053777693
N	1.510292008	1.243425189	2.021013954
N	-0.391759013	2.652030854	0.215880273
Si	3.217459603	-2.589933755	-0.071400198
Si	-4.859209957	-1.104291174	-0.092208054
H	-0.578098844	-0.548123257	-1.723681859
C	1.243011016	3.291417413	-1.565110350
H	1.962663406	3.676237548	-0.827907873
H	1.342451901	3.937585036	-2.462614996
N	1.621410312	1.896551796	-1.864674387
C	3.079716975	1.792908575	-2.030687936
H	3.352388764	0.746743668	-2.212325702
H	3.448806902	2.407257308	-2.876886500
H	3.585605543	2.123398552	-1.114880037
C	0.961924841	1.422814790	-3.093887216
H	1.254132939	2.030437118	-3.974928482
H	1.241734715	0.379078311	-3.279913483
H	-0.128097375	1.460859012	-2.988005347

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C	-1.462692743	2.070401572	-0.837323674
C	-0.259320594	1.451263076	-1.144665399
H	-1.597967210	2.409023372	0.200683617
H	-0.124031049	1.165875303	-2.197517935
C	0.861321799	1.120777343	-0.318045976
C	1.018511164	1.563971445	1.026106696
C	2.092214320	1.493684680	1.894551690
H	0.127451520	2.068717829	1.422370459
H	1.913063637	1.946891106	2.878486483
Li	-0.266566084	-0.807343442	0.113094034
Si	-2.677247327	2.740029693	-2.060216788
Si	3.856929090	0.964920114	1.646357305
C	-4.477197217	2.408375634	-1.518172001
H	-4.648771010	2.803753277	-0.504435853
H	-5.193604145	2.906730338	-2.190236945
H	-4.727873566	1.336658758	-1.500748695
C	-2.406994090	2.001271006	-3.794338640
H	-1.397739508	2.225865978	-4.171395740
H	-2.535906442	0.908611432	-3.809400549
H	-3.126942524	2.429505470	-4.508867505
C	-2.550225095	4.635066345	-2.215726943
H	-3.301802599	5.038271153	-2.913846768
H	-2.708010493	5.117839570	-1.238545485
H	-1.553756894	4.936920601	-2.572569784
C	4.926910330	1.990667461	2.837424523
H	5.985689929	1.692024497	2.791580254
H	4.866262070	3.063545120	2.600661089
H	4.588440890	1.861367837	3.877242703
C	4.176190454	-0.868223696	2.086285275

H	3.886756579	-1.084748747	3.126190868
H	3.600357448	-1.544021352	1.435016208
H	5.241427963	-1.126399324	1.972789362
C	4.506484932	1.222049186	-0.124069024
H	4.054594750	0.522076668	-0.842574684
H	4.293285343	2.240651773	-0.480654762
H	5.596952965	1.069013487	-0.156819113
C	-2.884993752	-2.108251981	0.652864995
H	-3.478122794	-1.187569274	0.731992031
H	-3.610465352	-2.943899694	0.577177723
C	-2.824951016	-1.362524079	-1.649214894
H	-2.216625198	-1.315384279	-2.560280998
H	-3.072628318	-0.331086581	-1.370703903
H	-3.752409307	-1.923673154	-1.880356033
C	-1.503513627	-3.290314381	-0.992720456
H	-1.331890209	-3.913904892	-0.105533636
H	-2.225722802	-3.842796666	-1.626754249
C	-0.191531040	-3.121196018	-1.755949810
H	-0.356776398	-2.459263549	-2.617559807
H	0.127728973	-4.103026582	-2.163624253
C	1.426138224	-3.494798347	0.021157799
H	1.892848579	-4.356125334	-0.499801325
H	0.643354155	-3.880748714	0.685476912
H	2.189512332	-3.011032954	0.642741196
C	1.953619594	-2.009482451	-1.786612376
H	2.730589028	-1.550281649	-1.164987311
H	1.562338684	-1.243772046	-2.466816763
H	2.417958865	-2.816789845	-2.387813972
N	-2.056029775	-1.990637549	-0.562957251
N	0.870372651	-2.515480483	-0.926904651
H	1.738809066	0.722654727	-0.831207015
C	-2.047159371	-2.287658708	1.918408380
H	-1.469644819	-3.221741817	1.856397408
H	-2.731228215	-2.401049207	2.785580777
N	-1.090673664	-1.185442767	2.127464803
C	-0.077002125	-1.555467434	3.130646442
H	0.667493496	-0.750984788	3.198568065
H	-0.522834663	-1.723484950	4.131503008
H	0.434003710	-2.476765857	2.822615666
C	-1.785748440	0.038787136	2.570396774
H	-2.380918927	-0.143474023	3.488528065
H	-1.040334351	0.813136955	2.780034273
H	-2.448958626	0.417692187	1.783037923

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C	-1.596986377	1.882523446	-0.113400955
C	-1.093024963	1.209741343	-1.216113724
H	-0.894967862	2.081586969	0.710136987
H	-1.798641055	1.039234546	-2.040786741
C	0.220786697	0.705973166	-1.480262715
C	1.373901742	1.098927160	-0.733274876
C	2.710194270	0.919741282	-1.016229859
H	1.143326474	1.663320350	0.179573350

H	2.952998107	0.403343091	-1.957074019
Li	-0.443770017	-1.273890016	-0.509620408
Si	-3.191009187	2.818870935	-0.031173599
Si	4.124369429	1.649532294	-0.065253697
C	-4.210190572	2.607625185	-1.624366148
H	-5.141270594	3.191963753	-1.561406854
H	-3.651643484	2.964805602	-2.502538231
H	-4.493145098	1.560713149	-1.811505322
C	-2.860795999	4.675644510	0.230742439
H	-3.798616379	5.246501891	0.324664591
H	-2.277735447	4.839952575	1.150617824
H	-2.282989971	5.099043808	-0.604545386
C	-4.276298122	2.293226453	1.450089437
H	-3.715318316	2.389739134	2.393263908
H	-5.171840066	2.929513138	1.533879046
H	-4.616023603	1.248984357	1.371861911
C	5.337804761	0.305575413	0.536227268
H	5.707986906	-0.294781314	-0.309660282
H	6.214163408	0.750582374	1.033955864
H	4.861545783	-0.384561161	1.249942967
C	5.147550604	2.819949297	-1.162089069
H	6.017437287	3.225354667	-0.620846126
H	5.524918633	2.291599796	-2.051600484
H	4.538618736	3.666042224	-1.514694017
C	3.508935548	2.616652622	1.451119012
H	2.838926387	3.438903538	1.159185919
H	2.963548177	1.975087013	2.160062099
H	4.359631637	3.056365903	1.994443443
C	-3.588538012	-1.205294447	-0.631568535
H	-3.619915768	-1.374958686	-1.715618507
H	-3.353265072	-0.151427118	-0.445789943
H	-4.588580496	-1.438234578	-0.214580012
C	-2.851103804	-3.457301163	-0.302433586
H	-2.085485050	-4.121468443	0.115796753
H	-2.889710797	-3.622018311	-1.386876231
H	-3.831786995	-3.749331349	0.126821661
C	-2.458956485	-1.782732822	1.422833776
H	-2.468399468	-0.690327560	1.552177249
H	-3.350232298	-2.185329506	1.948454508
C	-1.193031138	-2.358740486	2.056653966
H	-1.137119508	-3.437105273	1.858879312
H	-1.256383681	-2.248983363	3.156445996
C	0.362665090	-0.516009941	2.332603296
H	0.602704343	-0.777868857	3.382375419
H	-0.483661608	0.182119933	2.327644306
H	1.221171631	-0.003682001	1.883599667
C	1.186005918	-2.622843836	1.454396572
H	2.076076435	-2.002162479	1.284871591
H	1.352063193	-3.162885974	2.408960702
N	-2.536327038	-2.046658758	-0.031932387
N	0.029551541	-1.707670219	1.532634448
H	0.392300141	0.310386561	-2.486890901
C	1.056880906	-3.650711513	0.329083903

H	0.192863301	-4.304297715	0.518226556
H	1.952951260	-4.306012846	0.348805550
N	0.870156971	-3.042501656	-1.004225862
C	2.129310326	-2.450081031	-1.495278873
H	2.935296815	-3.209630101	-1.560217898
H	1.962491890	-2.030951180	-2.495046124
H	2.457134357	-1.623728832	-0.852899980
C	0.418044693	-4.061768372	-1.963699582
H	0.246882280	-3.593141949	-2.941236519
H	1.165396410	-4.870100623	-2.096274037
H	-0.522151894	-4.513323425	-1.625396845

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C	-0.189624517	2.178613158	-1.198360936
C	0.275406837	1.316217207	-2.176717056
H	0.290079611	2.147453495	-0.214334103
H	-0.189448404	1.429352323	-3.165318182
C	1.269196226	0.288995059	-2.160590190
C	2.126327473	-0.114745906	-1.102483601
C	2.120037870	0.194883202	0.256510938
H	2.882213805	-0.845470063	-1.418226978
H	1.428800296	0.972385453	0.599554529
Li	0.021577075	-0.842389173	-0.606194545
Si	3.445823799	-0.295136722	1.460790902
Si	-1.306268475	3.630268721	-1.515103385
C	-2.811817433	3.662257672	-0.345518298
H	-3.389629969	4.590990578	-0.476364041
H	-3.496684104	2.818985102	-0.523865951
H	-2.494403753	3.619494924	0.708014967
C	-1.944066899	3.622346388	-3.305403024
H	-2.593967679	4.493050029	-3.483307523
H	-1.116342086	3.673355665	-4.028414685
H	-2.532676714	2.720243985	-3.532512506
C	-0.377730564	5.259193410	-1.193383380
H	-0.007061317	5.295256332	-0.156903112
H	0.493864517	5.359664236	-1.857430793
H	-1.029428201	6.134520902	-1.345430283
C	2.720081694	-0.915463768	3.110157498
H	2.076488463	-1.797914373	2.978258110
H	3.520578782	-1.181400968	3.818469990
H	2.113446852	-0.128724027	3.585538341
C	4.555720778	-1.658298165	0.734065616
H	5.050510932	-1.325303912	-0.190532010
H	5.345895464	-1.930453754	1.450732209
H	3.992945431	-2.575417595	0.501689986
C	4.541314204	1.192518691	1.916260153
H	5.050156664	1.599627124	1.029577615
H	3.933152721	2.003778825	2.346264706
H	5.308890134	0.920751041	2.658717402
C	1.153063458	-3.548784051	-1.692063783
H	2.147251929	-3.213543132	-1.374698887
H	0.970548165	-3.166898822	-2.704230985
H	1.147929138	-4.657096109	-1.723715796

C	0.422943890	-3.470485712	0.603541959
H	-0.255835527	-2.981868989	1.313847315
H	1.445316576	-3.177652425	0.870170079
H	0.330482339	-4.571860222	0.703907256
C	-1.207793608	-3.423138475	-1.211647627
H	-1.267560118	-3.243829257	-2.294153833
H	-1.368588516	-4.511878692	-1.061532927
C	-2.322693929	-2.668145631	-0.489854414
H	-2.281433719	-2.915518006	0.576643514
H	-3.300326831	-3.032736846	-0.870382250
C	-2.548383840	-0.771538516	-1.991959354
H	-3.593148623	-1.037371668	-2.253562886
H	-1.875760654	-1.228913297	-2.727329404
H	-2.425565305	0.315407426	-2.062480946
C	-3.098337247	-0.480662109	0.309535461
H	-2.890928651	0.589433250	0.171212555
H	-4.159286761	-0.636208956	0.018056908
N	0.139414966	-3.016730449	-0.769595716
N	-2.202954585	-1.204463601	-0.624794790
H	1.478148678	-0.166223582	-3.129693666
C	-2.995352135	-0.849827521	1.790473296
H	-3.359805803	-1.875451221	1.947875584
H	-3.716029420	-0.190144826	2.327693834
N	-1.652930186	-0.761796736	2.364581986
C	-1.190224159	0.624094526	2.464307485
H	-1.833086932	1.232935103	3.138694524
H	-0.165177418	0.638223515	2.855583254
H	-1.178283211	1.100064436	1.475565025
C	-1.607534180	-1.407146183	3.675996020
H	-0.581667897	-1.377853598	4.065246647
H	-2.272470215	-0.916969136	4.420940910
H	-1.913546988	-2.459071288	3.590110656