Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

LiHMDS reacts with water at ultracold conditions

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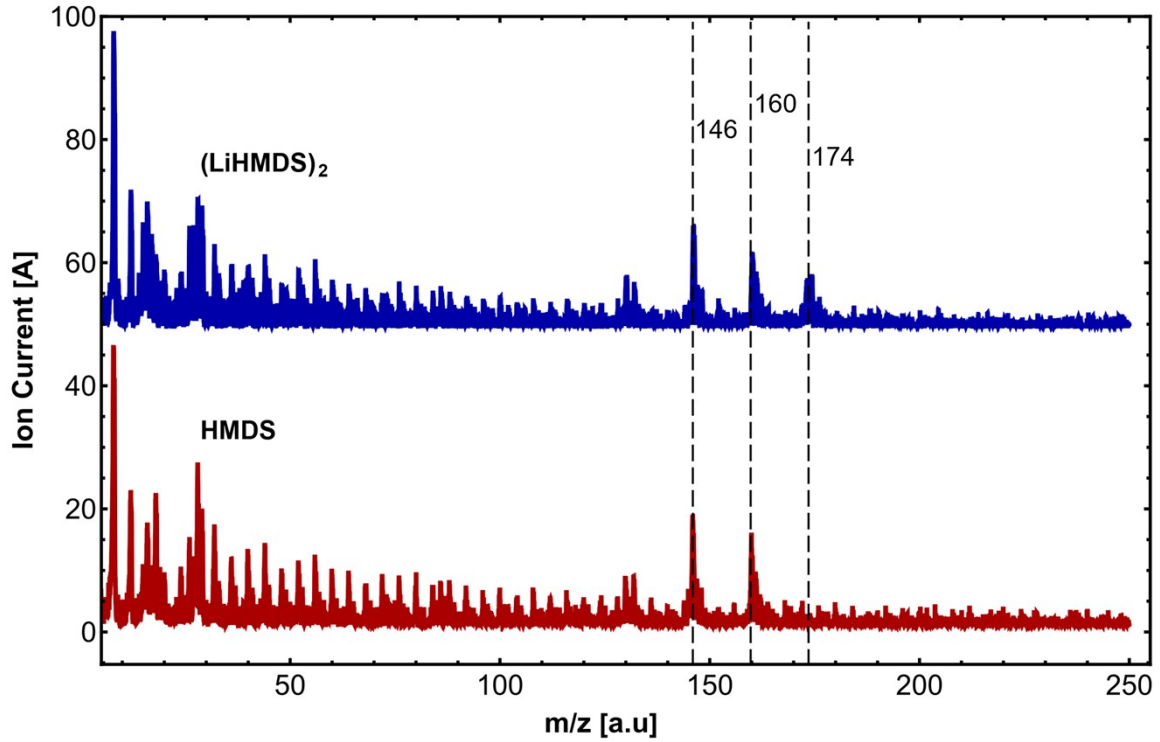

Figure S1. Mass spectra of HMDS and $(LiHMDS)_2$ in superfluid helium droplets. The nozzle was cooled to 14 K.

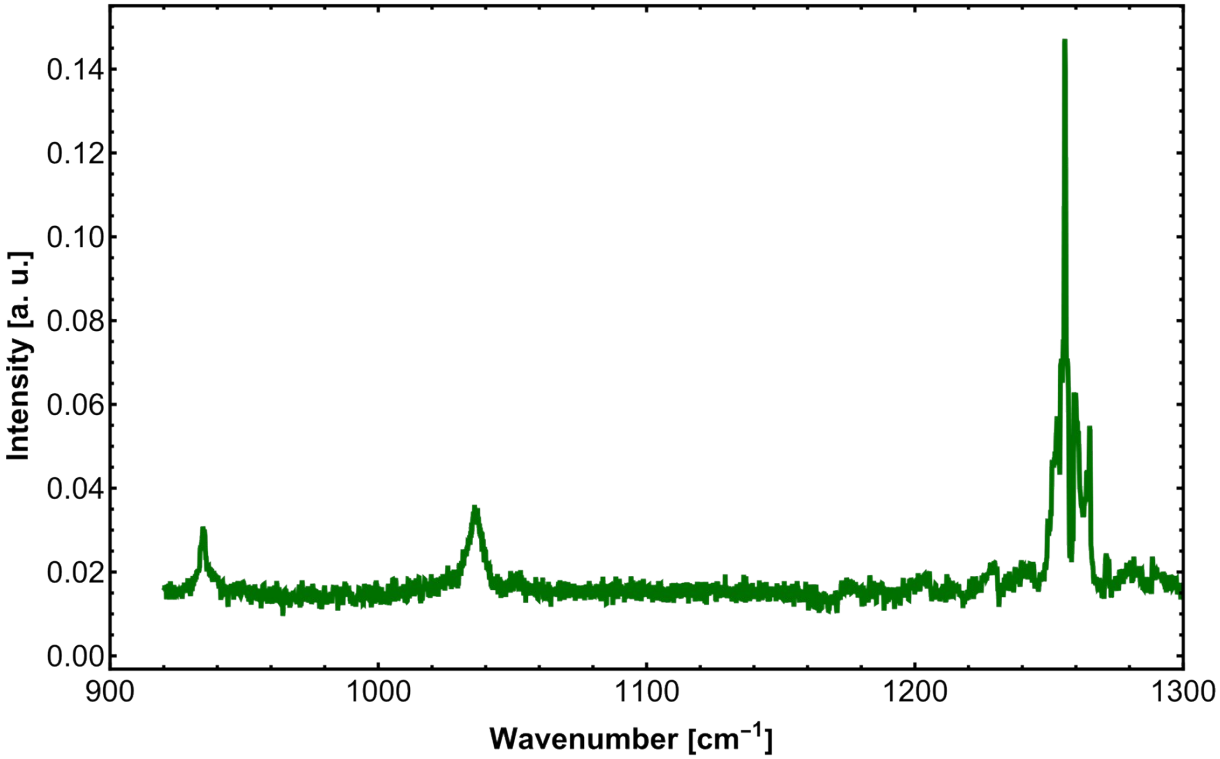

Figure S2. Experimental spectrum of HMDS-d_1, 900-1300 cm^{-1}.

Computational data for the calculated molecular structures.

H_2O C2v B3LYP-D3/def2-TZVP E = -76.4630039 ZPVE = 0.021170				
	O	0.000000	0.000000	0.116878
	H	0.000000	0.765086	-0.467514
	H	0.000000	-0.765086	-0.467514

$(LiHMDS)_2$ D2 B3LYP-D3/def2-TZVP E = -1762.300166 ZPVE = 0.458242				
	N	0.000000	1.583977	-0.000002
	Li	0.000000	0.000000	1.144532
	Si	-1.317676	2.357673	0.758492
	Si	1.317674	2.357680	-0.758494
	C	-0.845307	3.865174	1.790721
	H	-0.442639	4.667371	1.167617
	H	-1.712055	4.267235	2.322239
	H	-0.084621	3.612395	2.533703
	C	-2.676938	2.885784	-0.435262
	H	-3.065383	2.039586	-1.007007
	H	-3.517731	3.350226	0.086917
	H	-2.285735	3.613338	-1.151044
	C	-2.078841	1.097337	1.971012
	H	-1.405692	0.838432	2.799714
	H	-2.970328	1.517134	2.441814
	H	-2.394246	0.170677	1.481191
	C	0.845301	3.865183	-1.790718
	H	0.084625	3.612404	-2.533710
	H	0.442621	4.667372	-1.167612
	H	1.712050	4.267257	-2.322225
	C	2.676927	2.885795	0.435268
	H	2.285722	3.613354	1.151044
	H	3.065368	2.039600	1.007019
	H	3.517725	3.350233	-0.086908
	C	2.078845	1.097351	-1.971016
	H	2.970325	1.517157	-2.441824
	H	2.394257	0.170692	-1.481198
	H	1.405690	0.838447	-2.799713
	N	0.000000	-1.583977	-0.000002
	Li	0.000000	0.000000	-1.144537
	Si	1.317676	-2.357673	0.758492
	Si	-1.317674	-2.357680	-0.758494
	C	2.676938	-2.885784	-0.435262
	H	3.065383	-2.039586	-1.007007
	H	3.517731	-3.350226	0.086917
	H	2.285735	-3.613338	-1.151044
	C	2.078841	-1.097337	1.971012
	H	1.405692	-0.838432	2.799714
	H	2.970328	-1.517134	2.441814
	H	2.394246	-0.170677	1.481191
	C	-0.845301	-3.865183	-1.790718
	H	-0.084625	-3.612404	-2.533710
	H	-0.442621	-4.667372	-1.167612
	H	-1.712050	-4.267257	-2.322225
	C	-2.676927	-2.885795	0.435268
	H	-2.285722	-3.613354	1.151044
	H	-3.065368	-2.039600	1.007019
	H	-3.517725	-3.350233	-0.086908
	C	-2.078845	-1.097351	-1.971016
	H	-2.970325	-1.517157	-2.441824
	H	-2.394257	-0.170692	-1.481198
	H	-1.405690	-0.838447	-2.799713
	C	0.845307	-3.865174	1.790721
	H	0.442639	-4.667371	1.167617
	H	1.712055	-4.267235	2.322239
	H	0.084621	-3.612395	2.533703

1
C1
B3LYP-D3/def2-TZVP
E = -1838.789508
ZPVE = 0.483154

N	1.566069	0.002389	-0.120993
Li	-0.024127	-0.029027	1.125805
Si	2.540388	1.321154	0.367933
Si	2.151154	-1.461250	-0.772691
N	-1.630485	0.051541	-0.042145
Li	-0.060770	0.107717	-1.197101
Si	-2.627657	-1.286669	0.338336
Si	-2.234406	1.585151	-0.500555
O	0.755256	-0.620035	2.798618
H	0.468423	-1.168376	3.535651
H	1.606246	-0.965966	2.497634
C	-0.989284	2.343978	-1.734730
H	0.033335	2.421090	-1.353922
H	-0.963734	1.789530	-2.682062
H	-1.292665	3.360634	-1.994309
C	-3.881973	1.577764	-1.422625
H	-4.690775	1.161384	-0.818468
H	-4.166730	2.598513	-1.692474
H	-3.821672	0.993378	-2.343483
C	-2.421172	2.773716	0.951362
H	-2.731464	3.769897	0.624489
H	-3.182464	2.398239	1.640713
H	-1.492031	2.883054	1.514402
C	-3.486961	-2.031859	-1.169578
H	-4.185055	-1.326871	-1.624722
H	-2.757769	-2.315026	-1.933916
H	-4.049184	-2.930144	-0.899707
C	-1.602202	-2.695000	1.086449
H	-0.847235	-3.071702	0.393735
H	-1.092483	-2.403065	2.008072
H	-2.259492	-3.532157	1.335504
C	-3.956808	-0.876881	1.619858
H	-4.551475	-1.759263	1.871577
H	-3.505082	-0.503987	2.543425
H	-4.645382	-0.108099	1.261074
C	2.365368	-2.807931	0.540201
H	3.119348	-2.505939	1.274833
H	1.431599	-3.011123	1.069702
H	2.705330	-3.750675	0.103557
C	3.781145	-1.356084	-1.717419
H	4.608118	-1.032582	-1.081765
H	4.045844	-2.334968	-2.126731
H	3.711592	-0.654795	-2.552082
C	0.874396	-2.093472	-2.039660
H	-0.139599	-2.191723	-1.639638
H	0.833409	-1.448551	-2.926478
H	1.155847	-3.084635	-2.402525
C	3.303028	2.262879	-1.078754
H	3.845879	3.149031	-0.738854
H	4.003532	1.635667	-1.633979
H	2.531339	2.595365	-1.778425
C	1.505351	2.565667	1.349689
H	0.736512	3.046096	0.741974
H	1.018363	2.109001	2.216916
H	2.151794	3.358892	1.734673
C	3.953359	0.809436	1.522822
H	4.611931	0.067726	1.065358
H	4.568338	1.672606	1.791763
H	3.572892	0.385574	2.457373

2
C1
B3LYP-D3/def2-TZVP
E = -1838.789715
ZPVE = 0.480941

N	-1.756567	-0.078583	-0.067423
Li	0.069624	0.002962	0.585802
Li	1.044059	-0.070497	-1.956794
N	1.872497	0.107991	-0.230740
Si	2.864690	-1.291511	-0.218739
Si	-2.722141	1.338047	-0.235817
Si	-2.306430	-1.593129	0.527177
Si	2.277030	1.657906	0.383723
O	-0.664977	-0.385669	-2.376417
H	-1.211430	-0.291412	-1.433611
H	-1.222452	-0.828857	-3.018302
C	-4.283073	1.015877	-1.251369
H	-4.024715	0.648693	-2.248526
H	-4.872002	1.928270	-1.377902
H	-4.928020	0.269100	-0.782350
C	-3.243822	2.075517	1.420636
H	-3.923984	1.414831	1.961226
H	-3.754493	3.031497	1.275258
H	-2.379088	2.257829	2.063996
C	-1.741263	2.657744	-1.163133
H	-1.363014	2.261470	-2.108199
H	-0.890526	3.029025	-0.588413
H	-2.376984	3.517696	-1.389660
C	0.987168	2.134370	1.699606
H	1.054401	1.478706	2.574801
H	-0.047878	2.124210	1.344430
H	1.165773	3.151630	2.056106
C	2.235720	2.966523	-0.974860
H	3.020107	2.770041	-1.711682
H	2.407684	3.968678	-0.573301
H	1.277461	2.988084	-1.499832
C	3.950484	1.804077	1.240059
H	4.036377	2.785134	1.715303
H	4.776283	1.708377	0.532980
H	4.084536	1.048553	2.017563
C	4.617452	-1.011867	-0.864696
H	5.221748	-0.430687	-0.166629
H	4.613591	-0.481761	-1.821264
H	5.122931	-1.969266	-1.018910
C	2.089846	-2.562747	-1.401471
H	2.129941	-2.244871	-2.451018
H	1.047758	-2.793880	-1.169248
H	2.650524	-3.499630	-1.353304
C	3.029692	-2.096152	1.479058
H	2.065281	-2.395319	1.893893
H	3.493485	-1.402731	2.185349
H	3.661518	-2.987225	1.431254
C	-0.887716	-2.419309	1.479724
H	-0.569397	-1.831936	2.348612
H	-0.012440	-2.602546	0.851862
H	-1.201824	-3.392880	1.864240
C	-2.771393	-2.758150	-0.882479
H	-3.588216	-2.339133	-1.476226
H	-3.094860	-3.734709	-0.513252
H	-1.920191	-2.919238	-1.549267
C	-3.761513	-1.508273	1.723114
H	-4.646999	-1.061704	1.266206
H	-3.513682	-0.921861	2.610615
H	-4.033525	-2.514127	2.054717

3
C1
B3LYP-D3/def2-TZVP
E = -1838.794209
ZPVE = 0.482703

N	1.850597	-0.113332	0.159642
Li	-1.087257	0.111094	2.044406
Si	2.853587	1.326812	0.178748
Si	2.231646	-1.709891	-0.452403
C	4.431908	1.042635	1.160020
H	5.061390	0.268648	0.716810
H	5.024962	1.959028	1.219075
H	4.191201	0.735242	2.180786
C	3.288180	1.843862	-1.575606
H	2.396252	1.944873	-2.198723
H	3.790940	2.814550	-1.564058
H	3.959896	1.134198	-2.061021
C	1.875033	2.681137	1.030702
H	1.430846	2.278111	1.944098
H	2.524259	3.518920	1.296585
H	1.070769	3.076088	0.407519
C	3.856268	-1.791396	-1.388629
H	3.847117	-1.156794	-2.276381
H	4.706501	-1.499157	-0.770552
H	4.027886	-2.818658	-1.721148
C	2.220287	-2.916139	0.977410
H	3.088272	-2.755507	1.621482
H	1.327566	-2.760676	1.587164
H	2.238336	-3.953796	0.636333
C	0.873336	-2.175817	-1.685495
H	1.049695	-3.174250	-2.092848
H	-0.125715	-2.207577	-1.241566
H	0.850342	-1.485880	-2.535481
N	-1.879763	0.128593	0.248938
Li	-0.066334	0.004253	-0.437461
Si	-2.878435	-1.265818	0.202589
Si	-2.246711	1.681808	-0.372361
C	-3.211514	-1.904772	-1.544758
H	-2.287934	-2.114158	-2.089855
H	-3.793125	-2.830369	-1.515294
H	-3.781446	-1.178845	-2.129245
C	-2.036626	-2.666712	1.159246
H	-1.850056	-2.410760	2.206822
H	-2.675413	-3.554001	1.156135
H	-1.075027	-2.954977	0.729366
C	-3.930484	1.895166	-1.192208
H	-4.091423	1.179121	-2.000542
H	-4.744394	1.778805	-0.474134
H	-4.009763	2.898839	-1.619004
C	-2.112712	3.002266	0.970397
H	-2.885829	2.855233	1.730479
H	-1.141077	2.982632	1.471090
H	-2.246153	4.006703	0.559778
C	-0.960039	2.101480	-1.714929
H	-1.103259	3.120406	-2.082861
H	0.079131	2.060179	-1.371265
H	-1.060430	1.433517	-2.576775
C	-4.562427	-1.009747	1.021041
H	-5.170548	-0.284782	0.476927
H	-5.121623	-1.948724	1.056890
H	-4.458274	-0.649236	2.048495
H	1.434924	-0.194025	1.147844
O	0.540041	-0.158018	2.506944
H	1.037335	-0.374188	3.295470

4
C1
B3LYP-D3/def2-TZVP
E = -1838.809379
ZPVE = 0.484533

N	-1.980484	-0.229647	-0.452225
Li	0.050768	0.121701	-0.931841
Li	1.808191	0.701251	-2.335199
N	2.040573	0.254678	-0.464217
Si	2.242403	1.597675	0.573938
Si	-2.241801	-1.720970	0.461974
Si	-2.889948	1.280208	-0.258399
Si	2.800405	-1.268547	-0.307134
O	0.110541	0.493043	-2.697123
H	-1.927676	-0.437545	-1.450407
H	-0.445512	0.567379	-3.469599
C	-4.064258	-2.176067	0.547309
H	-4.484934	-2.308205	-0.452490
H	-4.198863	-3.114755	1.091233
H	-4.654028	-1.412714	1.058975
C	-1.568602	-1.506100	2.194536
H	-2.182210	-0.825802	2.786143
H	-1.550016	-2.469367	2.710567
H	-0.551166	-1.113973	2.183642
C	-1.331265	-3.082194	-0.450788
H	-1.664347	-3.155887	-1.489268
H	-0.251691	-2.930554	-0.457247
H	-1.521893	-4.047151	0.025200
C	2.290468	-2.198511	1.259601
H	2.528138	-1.607244	2.148285
H	1.219917	-2.409388	1.287626
H	2.818277	-3.152231	1.345918
C	2.359704	-2.350415	-1.802738
H	2.875768	-2.004763	-2.705016
H	2.682048	-3.381409	-1.633118
H	1.292533	-2.368462	-2.032157
C	4.690996	-1.208466	-0.295370
H	5.103223	-2.218023	-0.381329
H	5.072264	-0.622577	-1.136489
H	5.086639	-0.765993	0.619837
C	3.903530	1.710503	1.465970
H	4.057560	0.870843	2.148072
H	4.740259	1.726563	0.764449
H	3.946833	2.627826	2.059934
C	2.063987	3.199542	-0.424057
H	2.910134	3.328889	-1.107024
H	1.146956	3.221264	-1.018883
H	2.046804	4.074581	0.231223
C	0.927856	1.631199	1.939411
H	-0.088720	1.608130	1.541003
H	1.039001	0.762034	2.592985
H	1.016031	2.527774	2.558936
C	-1.863661	2.716135	-0.885015
H	-1.073279	2.979692	-0.179874
H	-1.389737	2.476253	-1.839402
H	-2.492370	3.599943	-1.019548
C	-4.475367	1.164995	-1.259702
H	-5.096897	0.333131	-0.921795
H	-5.063802	2.082044	-1.174216
H	-4.259462	1.011062	-2.320490
C	-3.294838	1.543650	1.553176
H	-3.972432	0.786612	1.951628
H	-2.395832	1.556776	2.171235
H	-3.785475	2.514081	1.665366

5
C1
B3LYP-D3/def2-TZVP
E = -1915.29853
ZPVE = 0.508769

N	2.103425	0.129475	-0.466043
Li	-0.003522	-0.139224	-0.793133
Li	-1.801382	-0.699889	-2.247278
N	-1.987331	-0.162266	-0.234704
Si	-2.073539	-1.350497	0.996817
Si	2.567332	1.677599	0.245618
Si	2.944148	-1.410787	-0.233001
Si	-2.579632	1.444263	-0.101106
O	-0.061144	-0.555406	-2.530737
H	1.924186	0.239862	-1.466094
H	0.458091	-0.691834	-3.320544
C	4.408431	2.011309	0.055171
H	4.701232	2.018219	-0.997539
H	4.666090	2.985784	0.478488
H	5.016117	1.260771	0.565053
C	2.119744	1.683063	2.063809
H	2.762325	1.019612	2.643925
H	2.228261	2.690826	2.472739
H	1.087662	1.367591	2.220695
C	1.621608	3.008977	-0.675582
H	1.794166	2.947199	-1.752989
H	0.546184	2.947868	-0.507188
H	1.947394	3.998456	-0.345584
C	-1.860930	2.387838	1.373096
H	-2.140423	1.907375	2.314724
H	-0.770959	2.434774	1.343629
H	-2.234778	3.414810	1.404314
C	-2.165977	2.399291	-1.682607
H	-2.768131	2.033551	-2.520261
H	-2.399503	3.460411	-1.561194
H	-1.118426	2.319858	-1.979733
C	-4.460290	1.549483	0.065966
H	-4.785626	2.593753	0.054482
H	-4.961369	1.044590	-0.764481
H	-4.817121	1.102569	0.995078
C	-3.638569	-1.299474	2.056668
H	-3.708843	-0.374739	2.634316
H	-4.544336	-1.378308	1.450136
H	-3.641224	-2.131460	2.766551
C	-2.024163	-3.074658	0.214321
H	-2.955104	-3.289248	-0.318928
H	-1.205215	-3.181786	-0.500528
H	-1.902814	-3.850447	0.974854
C	-0.628856	-1.228034	2.215780
H	0.343963	-1.235664	1.720578
H	-0.693258	-0.297681	2.785171
H	-0.638465	-2.056306	2.929492
C	1.778735	-2.827385	-0.612241
H	1.047332	-2.970772	0.184792
H	1.232609	-2.645302	-1.540764
H	2.338439	-3.760487	-0.715692
C	4.410120	-1.496877	-1.405176
H	5.113704	-0.681641	-1.224965
H	4.950413	-2.440305	-1.292696
H	4.079826	-1.429348	-2.445303
C	3.531804	-1.543036	1.542709
H	4.282747	-0.793441	1.797590
H	2.705248	-1.450522	2.249175
H	3.985950	-2.525977	1.692653
O	-3.700118	-1.130127	-2.303986
H	-4.216671	-1.939772	-2.352545
H	-3.583783	-0.902760	-1.355234

6
C1
B3LYP-D3/def2-TZVP
E = -1915.304171
ZPVE = 0.506925

N	2.937078	-0.193867	0.623738
Li	0.868387	-0.388419	0.897894
Li	-1.623542	0.302841	1.925336
N	-2.619679	0.022532	0.310637
Si	-2.926899	1.530761	-0.432411
Si	3.457370	-1.594829	-0.319556
Si	3.178078	1.523339	0.249618
Si	-3.579007	-1.393730	0.233943
O	0.067492	0.177516	2.389120
H	3.133174	-0.346388	1.610939
H	0.466583	0.304306	3.248788
C	5.280026	-1.937606	-0.030747
H	5.484561	-2.119909	1.027584
H	5.607077	-2.820766	-0.585506
H	5.896149	-1.093977	-0.348491
C	3.152531	-1.245383	-2.134762
H	3.731394	-0.394139	-2.497456
H	3.442852	-2.115991	-2.727820
H	2.097937	-1.047909	-2.332013
C	2.440632	-3.068169	0.237408
H	2.532528	-3.236619	1.313887
H	1.381745	-2.930874	0.004455
H	2.775566	-3.979440	-0.264285
C	-3.994476	-1.895196	-1.542109
H	-4.575034	-1.120535	-2.050182
H	-3.082375	-2.058670	-2.122613
H	-4.578623	-2.819031	-1.572533
C	-2.613315	-2.822233	1.007313
H	-2.383094	-2.637217	2.061064
H	-3.178575	-3.756542	0.956542
H	-1.665303	-2.969834	0.484493
C	-5.210660	-1.235371	1.173121
H	-5.776830	-2.170598	1.142379
H	-5.036990	-0.987656	2.224224
H	-5.839937	-0.450025	0.749138
C	-4.752778	1.998935	-0.541219
H	-5.313705	1.282266	-1.146195
H	-5.216184	2.029838	0.447735
H	-4.874355	2.984427	-0.999236
C	-2.052609	2.899167	0.547190
H	-2.513291	3.055537	1.528106
H	-0.994336	2.672205	0.709231
H	-2.102614	3.853210	0.015671
C	-2.229755	1.600408	-2.192312
H	-1.139236	1.519659	-2.188653
H	-2.627012	0.783041	-2.799993
H	-2.484411	2.540300	-2.689326
C	1.952790	2.040611	-1.070253
H	2.091701	1.482103	-1.997293
H	0.921550	1.895558	-0.744086
H	2.080836	3.101160	-1.300961
C	2.855149	2.451645	1.842233
H	3.572780	2.177000	2.620127
H	2.934283	3.530057	1.686805
H	1.849816	2.229857	2.208653
C	4.925809	1.853250	-0.357678
H	5.666131	1.550697	0.386666
H	5.145817	1.317530	-1.283916
H	5.067367	2.919200	-0.554193
O	-0.241988	-0.730075	-0.554039
H	-1.216542	-0.449742	-0.280981
H	-0.175399	-0.603470	-1.503142

7	Li	0.990658	-0.352686	-0.496336
Ci	Li	-0.990658	0.352686	0.496336
B3LYP-D3/def2-TZVP	O	0.258901	-0.772719	1.128925
E = -1915.316764	H	0.228501	-1.461115	1.790387
ZPVE = 0.508587	O	-0.258901	0.772719	-1.128925
	H	-2.326112	0.191305	-1.009305
	H	-0.228501	1.461115	-1.790387
	H	2.326112	-0.191305	1.009305
	N	-2.967637	0.019129	-0.227401
	N	2.967637	-0.019129	0.227401
	Si	4.010841	-1.400720	-0.038926
	Si	3.351881	1.691487	0.083849
	Si	-4.010841	1.400720	0.038926
	Si	-3.351881	-1.691487	-0.083849
	C	2.926567	-2.911782	-0.310427
	H	3.531143	-3.821141	-0.354674
	H	2.204869	-3.025928	0.501602
	H	2.364870	-2.848216	-1.246643
	C	5.119737	-1.705759	1.446350
	H	5.757584	-0.841069	1.641597
	H	4.525015	-1.889225	2.344954
	H	5.765595	-2.574075	1.292015
	C	5.064075	-1.092014	-1.561077
	H	5.676990	-1.971794	-1.772567
	H	4.447428	-0.895754	-2.440622
	H	5.740846	-0.245383	-1.429039
	C	5.014732	2.086965	0.872120
	H	5.017961	1.822123	1.932185
	H	5.831671	1.543658	0.391222
	H	5.238406	3.154103	0.792940
	C	1.990495	2.642285	0.950402
	H	2.215549	3.711424	0.970386
	H	1.045224	2.496812	0.422731
	H	1.860753	2.304399	1.981187
	C	3.405227	2.163435	-1.731590
	H	4.186335	1.626874	-2.273123
	H	2.447429	1.939654	-2.206728
	H	3.597050	3.233495	-1.845954
	C	-3.405227	-2.163435	1.731590
	H	-4.186335	-1.626874	2.273123
	H	-3.597050	-3.233495	1.845954
	H	-2.447429	-1.939654	2.206728
	C	-1.990495	-2.642285	-0.950402
	H	-2.215549	-3.711424	-0.970386
	H	-1.860753	-2.304399	-1.981187
	H	-1.045224	-2.496812	-0.422731
	C	-5.014732	-2.086965	-0.872120
	H	-5.017961	-1.822123	-1.932185
	H	-5.238406	-3.154103	-0.792940
	H	-5.831671	-1.543658	-0.391222
	C	-2.926567	2.911782	0.310427
	H	-2.204869	3.025928	-0.501602
	H	-3.531143	3.821141	0.354674
	H	-2.364870	2.848216	1.246643
	C	-5.064075	1.092014	1.561077
	H	-5.740846	0.245383	1.429039
	H	-4.447428	0.895754	2.440622
	H	-5.676990	1.971794	1.772567
	C	-5.119737	1.705759	-1.446350
	H	-4.525015	1.889225	-2.344954
	H	-5.757584	0.841069	-1.641597
	H	-5.765595	2.574075	-1.292015

TS(1→2)
C1
B3LYP-D3/def2-TZVP
E = -1838.786897
ZPVE = 0.482545

N	1.677427	-0.074156	0.071727
Li	-0.457717	0.062474	1.580046
Si	2.623345	1.325471	0.388010
Si	2.190987	-1.496704	-0.730623
N	-1.721318	0.098546	0.117512
Li	-0.035322	0.028591	-0.874809
Si	-2.715906	-1.278285	0.367997
Si	-2.271424	1.606173	-0.486205
O	0.939642	-0.654153	2.582757
H	1.136845	-1.507237	2.977820
H	1.436725	-0.585785	1.694745
C	-0.957569	2.252658	-1.704865
H	0.040264	2.353792	-1.268696
H	-0.881097	1.615841	-2.594945
H	-1.230694	3.246530	-2.066630
C	-3.879122	1.562812	-1.471522
H	-4.721930	1.197926	-0.881333
H	-4.130967	2.570219	-1.814015
H	-3.789756	0.925488	-2.353825
C	-2.480386	2.893449	0.876169
H	-2.784607	3.862667	0.472122
H	-3.250676	2.571943	1.582474
H	-1.558026	3.049948	1.441245
C	-3.365568	-2.048033	-1.227861
H	-4.059537	-1.379196	-1.740115
H	-2.552972	-2.276828	-1.922180
H	-3.896763	-2.981083	-1.020689
C	-1.708266	-2.627051	1.240465
H	-0.842818	-2.941040	0.652535
H	-1.346151	-2.319911	2.226307
H	-2.333364	-3.510204	1.395481
C	-4.197649	-0.923328	1.484341
H	-4.783700	-1.828113	1.666891
H	-3.871676	-0.538140	2.454696
H	-4.867565	-0.180291	1.046047
C	2.388977	-2.945173	0.464479
H	3.167019	-2.725956	1.201423
H	1.461637	-3.150773	1.004409
H	2.677236	-3.861760	-0.056178
C	3.782327	-1.371382	-1.732770
H	4.634082	-1.084366	-1.112610
H	4.017081	-2.338334	-2.186231
H	3.696107	-0.639734	-2.538762
C	0.831528	-1.981088	-1.980074
H	-0.150074	-2.152061	-1.525602
H	0.718834	-1.234648	-2.776695
H	1.095400	-2.915525	-2.480124
C	3.195150	2.220177	-1.173262
H	3.686429	3.164036	-0.921330
H	3.909207	1.617158	-1.737500
H	2.358744	2.450300	-1.838148
C	1.595298	2.553121	1.395264
H	0.715323	2.908606	0.854706
H	1.267469	2.111238	2.341136
H	2.191363	3.434145	1.646815
C	4.150578	0.933303	1.426499
H	4.819013	0.236460	0.915470
H	4.724566	1.835923	1.652634
H	3.858431	0.478086	2.376520

TS(2→3)
C1
B3LYP-D3/def2-TZVP
E = -1838.789684
ZPVE = 0.479379

N	-1.761723	-0.082995	-0.080462
Li	0.074107	0.001282	0.576819
Li	1.046799	-0.087505	-1.960119
N	1.877428	0.105883	-0.230169
Si	2.876850	-1.288187	-0.215378
Si	-2.730197	1.338517	-0.235712
Si	-2.311095	-1.600917	0.519265
Si	2.274135	1.659443	0.378426
O	-0.659662	-0.387647	-2.346532
H	-1.229733	-0.282861	-1.364908
H	-1.230341	-0.779968	-3.009012
C	-4.299912	1.016010	-1.235559
H	-4.051532	0.647618	-2.234692
H	-4.888438	1.929327	-1.356918
H	-4.941533	0.270787	-0.759667
C	-3.233240	2.065327	1.430174
H	-3.911367	1.404737	1.973164
H	-3.741891	3.023653	1.293539
H	-2.362731	2.242299	2.067019
C	-1.752682	2.654929	-1.167960
H	-1.371633	2.252202	-2.108959
H	-0.903655	3.031366	-0.594149
H	-2.390616	3.511655	-1.400190
C	0.978336	2.134552	1.689872
H	1.045059	1.481545	2.567111
H	-0.055524	2.120341	1.331472
H	1.151930	3.153451	2.044153
C	2.228485	2.964439	-0.983256
H	3.014377	2.769522	-1.718836
H	2.395312	3.968455	-0.584161
H	1.270754	2.979259	-1.509373
C	3.944020	1.816967	1.239803
H	4.021907	2.798271	1.715919
H	4.772454	1.727202	0.535048
H	4.080897	1.061651	2.017070
C	4.635365	-0.997300	-0.840529
H	5.231647	-0.421915	-0.130916
H	4.639304	-0.457813	-1.791811
H	5.144297	-1.952109	-0.999426
C	2.122482	-2.558444	-1.411811
H	2.183235	-2.239728	-2.460022
H	1.075656	-2.787708	-1.200156
H	2.680753	-3.496178	-1.353155
C	3.026926	-2.098823	1.481243
H	2.060180	-2.413019	1.879292
H	3.469902	-1.402145	2.197733
H	3.671487	-2.981039	1.439610
C	-0.881097	-2.433324	1.446710
H	-0.544443	-1.850147	2.311521
H	-0.018370	-2.619199	0.802619
H	-1.193523	-3.406058	1.834674
C	-2.800862	-2.753466	-0.889332
H	-3.628974	-2.331737	-1.464919
H	-3.114721	-3.733761	-0.521844
H	-1.960906	-2.904222	-1.572130
C	-3.745565	-1.503800	1.737413
H	-4.635459	-1.051528	1.295096
H	-3.479927	-0.920530	2.621747
H	-4.018417	-2.508427	2.072002

TS(3→4)
C1
B3LYP-D3/def2-TZVP
E = -1838.794162
ZPVE = 0.482527

N	-1.869652	-0.101009	-0.179241
Li	1.120530	0.125854	-2.062100
Si	-2.844326	1.357226	-0.107214
Si	-2.260933	-1.716872	0.377345
C	-4.466646	1.146183	-1.032950
H	-5.108486	0.390366	-0.577090
H	-5.025274	2.085507	-1.056916
H	-4.275159	0.846222	-2.066288
C	-3.193638	1.808501	1.684042
H	-2.270958	1.899093	2.262320
H	-3.708171	2.771593	1.735763
H	-3.828918	1.072203	2.179285
C	-1.867622	2.721883	-0.944838
H	-1.454740	2.342304	-1.882738
H	-2.508715	3.578926	-1.164866
H	-1.038838	3.082348	-0.333026
C	-3.951602	-1.859248	1.180139
H	-4.060460	-1.205175	2.046699
H	-4.755665	-1.631032	0.478891
H	-4.097677	-2.886458	1.525074
C	-2.135157	-2.885281	-1.079246
H	-2.979274	-2.736898	-1.757258
H	-1.223750	-2.686970	-1.646666
H	-2.134671	-3.931114	-0.763420
C	-0.984731	-2.182326	1.693211
H	-1.161263	-3.194782	2.064316
H	0.044221	-2.175662	1.321529
H	-1.040743	-1.509543	2.554685
N	1.886737	0.109689	-0.256239
Li	0.058055	0.003878	0.383308
Si	2.857521	-1.301205	-0.143868
Si	2.281233	1.675165	0.318026
C	3.158845	-1.866976	1.634424
H	2.223414	-2.058874	2.166070
H	3.744532	-2.790145	1.656700
H	3.710673	-1.114375	2.202466
C	1.998297	-2.728123	-1.043552
H	1.823871	-2.512267	-2.102005
H	2.621382	-3.625394	-0.998006
H	1.029928	-2.982185	-0.607579
C	4.002568	1.905553	1.051031
H	4.210366	1.194005	1.852646
H	4.781036	1.794425	0.293877
H	4.093112	2.911346	1.470596
C	2.091065	2.958355	-1.055249
H	2.839819	2.798643	-1.837256
H	1.103123	2.921019	-1.521869
H	2.231358	3.973752	-0.675119
C	1.061395	2.136771	1.705742
H	1.202074	3.173812	2.020663
H	0.006393	2.057539	1.421765
H	1.220757	1.506698	2.586336
C	4.550906	-1.109843	-0.959954
H	5.174429	-0.383872	-0.435157
H	5.088121	-2.062196	-0.967973
H	4.457673	-0.776220	-1.997567
H	-1.456858	-0.146247	-1.168134
O	-0.520902	-0.082076	-2.512488
H	-1.015787	-0.256822	-3.312962