Supplementary Materials: Structural Study of Mismatched Disila-Crown Ether Complexes

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Supporting Information of Computations

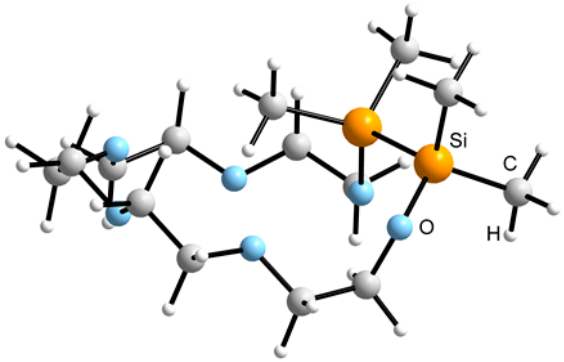

Figure S1. Calculated structure of 1,2-disila[18]crown-6.

Table S1. XYZ data of 1,2-disila[18]crown-6.

C	−4.6334893	10.0887881	13.5192227
H	−4.7059345	9.9582112	14.6164338
H	−5.0841020	11.0658949	13.2602510
C	−3.1796023	10.0681844	13.1130495
O	−5.3186703	9.0386684	12.8427772
H	−2.6103836	10.7617147	13.7617629
H	−2.7638880	9.0516487	13.2572279
O	−3.0712921	10.4598175	11.7482555
C	−6.7108500	9.0106060	13.1482443
C	−1.7350607	10.3763303	11.2634857
H	−7.1598239	10.0074398	12.9771826
H	−6.8676056	8.7425781	14.2110259
C	−7.3878999	7.9908495	12.2630768
O	−7.4846248	8.5197768	10.9443831
O	−4.5406482	10.4341573	7.5921546
O	−6.6897419	8.5151161	8.1576179
C	−1.6970114	10.8908173	9.8425775
H	−1.3801210	9.3269533	11.2843603
H	−1.0560837	10.9790395	11.8980566
H	−6.8014388	7.0521016	12.2618304
H	−8.3940021	7.7610139	12.6648720
C	−7.9123679	7.5544809	9.9903657
C	−5.3201914	9.7559709	6.6063307
Si	−4.9667759	11.8704937	8.3690322
C	−8.0003300	8.2165888	8.6363739
C	−6.7276217	9.3972261	7.0421951
O	−1.9211351	12.3040838	9.8234032
H	−0.7072790	10.6662063	9.4090276
H	−2.4587198	10.3615155	9.2424804
H	−8.9096360	7.1527684	10.2569349
H	−7.2036276	6.7042767	9.9575834

H	−4.7731075	8.8361457	6.3456822
H	−5.4005315	10.3677183	5.6900490
C	−6.0177686	12.9555725	7.2305791
Si	−2.9364072	13.0301846	8.6928064
C	−5.8828745	11.5109209	9.9640759
H	−8.5272195	7.5461562	7.9303710
H	−8.5906390	9.1485029	8.7227362
H	−7.2981053	10.3073512	7.3099407
H	−7.2469890	8.9262425	6.1833850
H	−6.1598014	13.9412103	7.7002370
H	−5.5267448	13.1158223	6.2594855
H	−7.0154141	12.5308767	7.0452910
C	−2.0511214	13.1553855	7.0323603
C	−3.2478708	14.7490366	9.3871130
H	−6.1244459	12.4537027	10.4798121
H	−5.2573624	10.9013128	10.6297263
H	−6.8141274	10.9555881	9.7848308
H	−2.6826168	13.6803161	6.2992110
H	−1.1045622	13.7092724	7.1280296
H	−1.8306392	12.1560464	6.6297349
H	−3.8544521	15.3415355	8.6861755
H	−3.7838657	14.6996023	10.3456670
H	−2.2979250	15.2815791	9.5475753

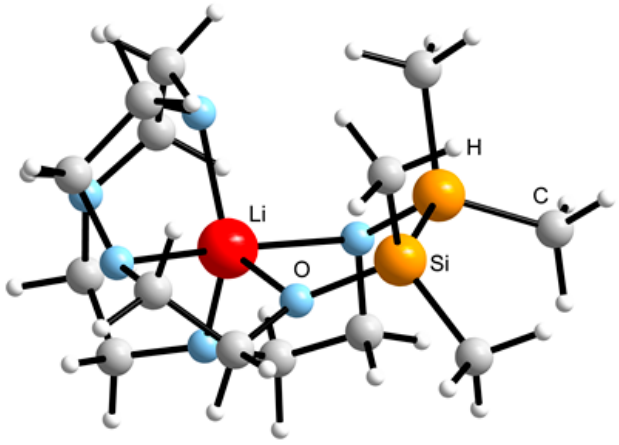

Figure S2. Calculated structure of [Li(1,2-disila[18]crown-6)]$^+$.

Table S2. XYZ data of [Li(1,2-disila[18]crown-6)]$^+$.

Si	7.4590436	10.3488264	2.0514619
Si	5.5972800	11.1376405	3.2791329
O	7.4425369	8.7608167	2.6585554
C	9.0872793	11.1772110	2.4852902
C	7.2284336	10.3077172	0.1898414
O	4.9342996	9.6980207	3.9153745
C	4.3276591	12.0203520	2.2188056
C	6.0876560	12.1569194	4.7667103
Li	6.6054146	8.3120695	4.4092285
C	8.3595509	7.7134519	2.2918653
H	9.0920486	12.2120064	2.1106334
H	9.9382322	10.6504737	2.0269323

H	9.2435723	11.2133148	3.5728750
H	6.3094794	9.7702892	−0.0839558
H	8.0794112	9.8216335	−0.3106972
H	7.1517400	11.3342049	−0.1996866
C	4.1834058	8.8307856	3.0420828
H	4.7587925	12.9626131	1.8482427
H	3.4277083	12.2625447	2.8040260
H	4.0281498	11.4238202	1.3456961
H	6.8131898	11.6118639	5.3850659
H	5.2079333	12.3981206	5.3815439
H	6.5482334	13.0988683	4.4345939
O	5.1939272	6.9646086	4.1059543
O	7.3533216	9.3071518	6.0276557
O	8.3772779	7.1176334	4.5984803
H	8.9805991	7.9967813	1.4282955
H	7.7612096	6.8327702	2.0148154
C	9.2426953	7.4086369	3.4818309
H	4.7560030	8.6305563	2.1194147
H	3.2241508	9.2944978	2.7664174
C	3.9179931	7.5355737	3.7692715
C	5.1251198	5.8029327	4.9537170
C	6.6255087	9.2467213	7.2773800
C	8.7523924	8.9675986	6.1198774
C	8.9447908	7.4814371	5.8742369
H	9.8753740	8.2807599	3.7086067
H	9.8954120	6.5448217	3.2754898
H	3.3288353	7.7296426	4.6803787
H	3.3537142	6.8435495	3.1227962
H	6.1195352	5.3425701	4.8848818
H	4.3744556	5.0945584	4.5647961
C	4.8222121	6.1524209	6.4021104
H	6.3200277	10.2681707	7.5525184
H	7.2814699	8.8530469	8.0676029
C	5.4005091	8.3758151	7.1379401
H	9.1609029	9.2619346	7.0976086
H	9.2591758	9.5646266	5.3486059
H	10.0115551	7.2102607	5.9200236
H	8.3913430	6.8969884	6.6201566
O	5.8326988	7.0286150	6.9208239
H	3.8253468	6.6065246	6.5136524
H	4.8307099	5.2234239	6.9933280
H	4.7978609	8.4539946	8.0606402
H	4.7826823	8.7335823	6.2959245

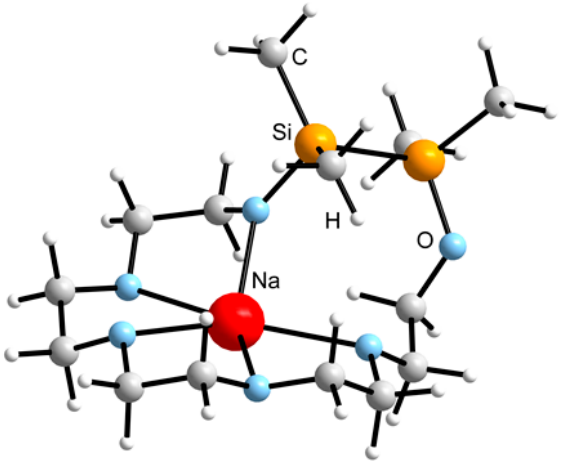

Figure S3. Calculated structure of [Na(1,2-disila[18]crown-6)]$^+$.

Table S3. XYZ data of [Na(1,2-disila[18]crown-6)]$^+$.

C	−4.8414423	9.9455011	13.3653942
H	−4.8628843	9.7407621	14.4493952
H	−5.3252457	10.9230315	13.1876816
C	−3.4105589	9.9523270	12.8900947
O	−5.5331297	8.9171985	12.6472765
H	−2.8357340	10.6987679	13.4647903
H	−2.9552478	8.9589389	13.0538502
O	−3.3749239	10.2770107	11.4913616
C	−6.9047128	8.7600140	13.0360773
Na	−5.2984934	9.2118414	10.2952143
C	−2.0336415	10.1926679	10.9802642
H	−7.4479031	9.7124089	12.8991566
H	−6.9738510	8.4663457	14.0972099
C	−7.4924755	7.6773839	12.1643321
O	−7.4353356	8.1312121	10.8047259
O	−5.2973547	10.8133286	8.6075149
O	−6.3638610	8.2973294	8.2567767
C	−1.9602406	10.7967655	9.5986034
H	−1.7180517	9.1343712	10.9401006
H	−1.3489887	10.7349867	11.6555035
H	−6.9073221	6.7473260	12.2728312
H	−8.5355645	7.4744134	12.4611751
C	−7.6684393	7.0836773	9.8527716
C	−5.1750609	10.1495873	7.3393871
Si	−5.1885858	12.5003706	8.7945713
C	−7.6489725	7.6974334	8.4745582
C	−6.3540951	9.2203144	7.1589676
O	−2.0410180	12.2231168	9.6654570
H	−0.9992500	10.5024090	9.1445365
H	−2.7648300	10.3760492	8.9702285
H	−8.6513436	6.6120242	10.0245410
H	−6.8875931	6.3081535	9.9549288
H	−4.2299057	9.5816472	7.3250156
H	−5.1522957	10.8652137	6.5022640
C	−6.3410763	13.3398349	7.5719884
Si	−2.9280280	13.1150210	8.5400398

C	−5.7429586	12.7628128	10.5651789
H	−7.8519432	6.9202730	7.7178953
H	−8.4311197	8.4728053	8.3983753
H	−7.2901185	9.8051199	7.1635413
H	−6.2762444	8.6845370	6.1968295
H	−6.3064438	14.4294403	7.7234054
H	−6.0559759	13.1415809	6.5290355
H	−7.3787979	13.0048219	7.7198986
C	−2.3114762	12.7650839	6.7971249
C	−2.6346450	14.9045371	9.0155446
H	−5.7721044	13.8363653	10.8008083
H	−5.0356250	12.2830245	11.2558266
H	−6.7492288	12.3494079	10.7328564
H	−2.8987422	13.3407075	6.0657044
H	−1.2539279	13.0512497	6.6906322
H	−2.4061747	11.7002520	6.5396389
H	−3.1923050	15.5716646	8.3417883
H	−2.9673130	15.1029452	10.0442520
H	−1.5659289	15.1554462	8.9396181