

## Supporting Information

for

### **On the control of secondary carbanion structure utilising ligand effects during directed metallation**

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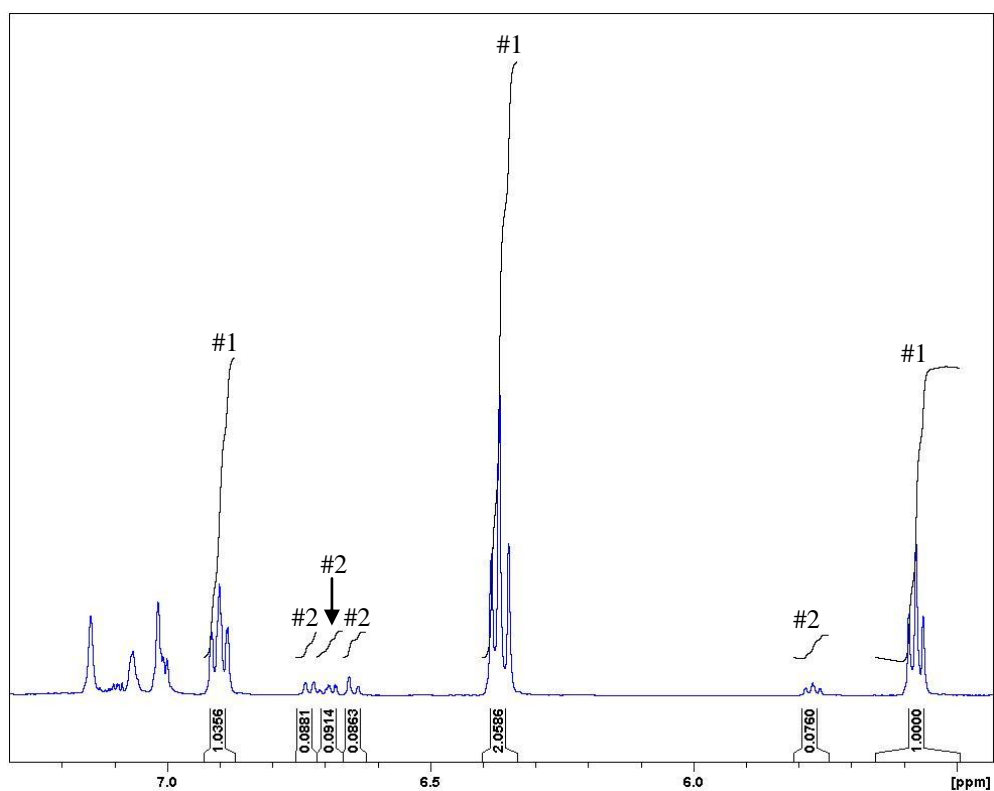
Email: Andrew Wheatley - aehw2@cam.ac.uk

\* Corresponding author

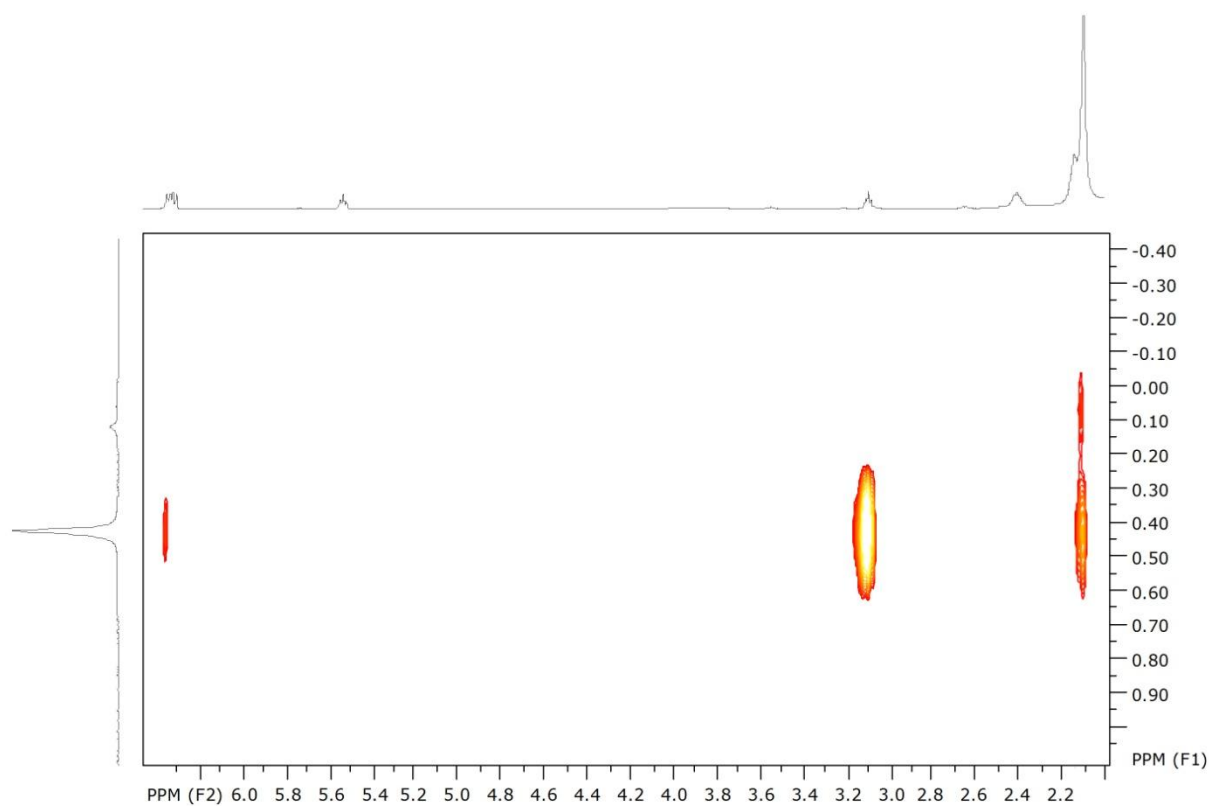
#### **NMR spectroscopic data and DFT calculations for 6-Li·L (L = PMDTA, DGME)**

#### **Contents**

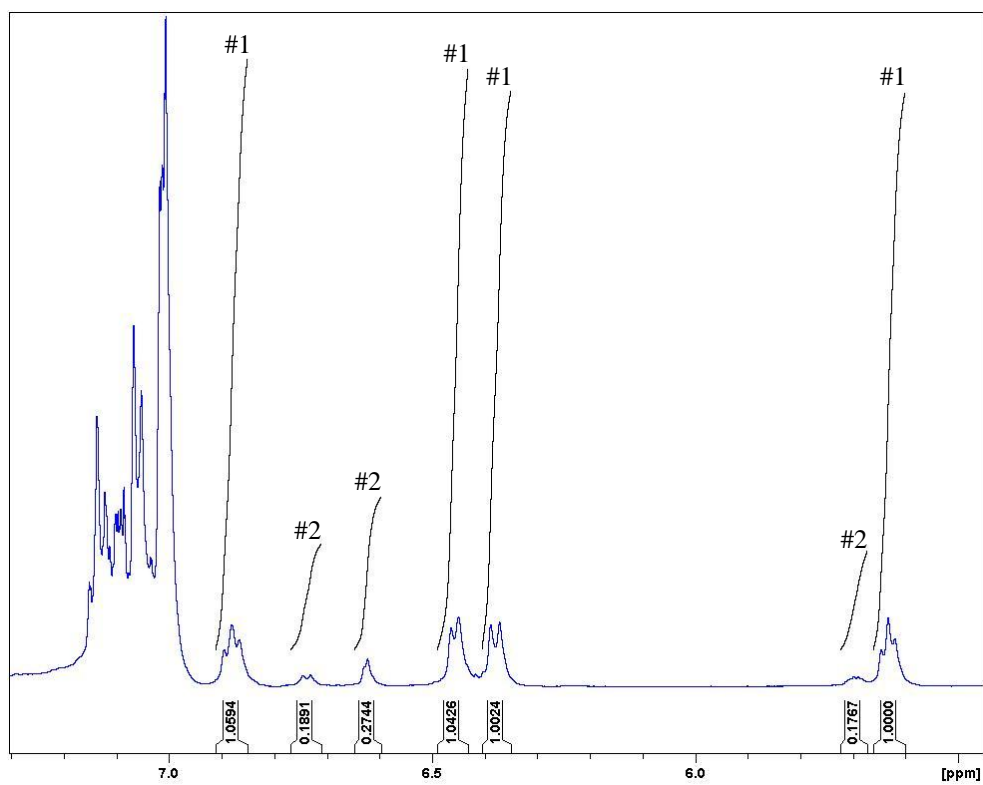
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**Figure S1:**  $^1\text{H}$  NMR spectrum of the aromatic region of  $6\text{-Li}_I\text{-PMDTA}$  in  $[\text{D}_8]\text{toluene}$  at 273 K. Unmarked signals (left) attributable to superimposed reformed  $6\text{-H}$  (#3) and  $[\text{D}_8]\text{toluene}$ .



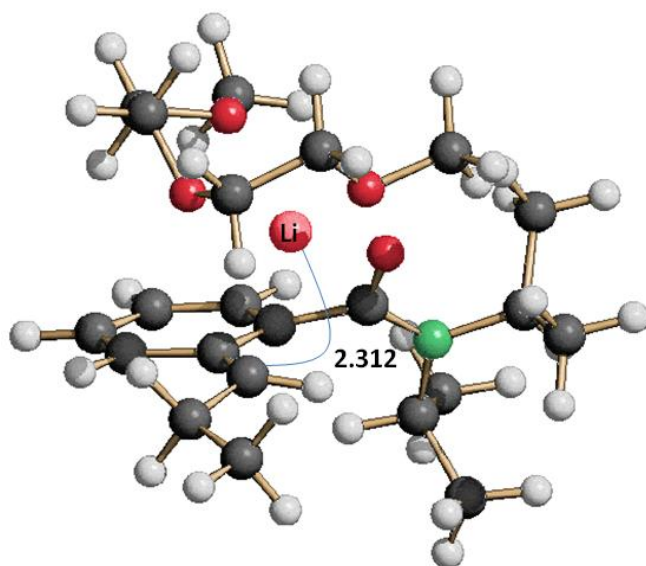
**Figure S2:**  $^1\text{H}, ^7\text{Li}$ -HOESY of  $6\text{-Li}_I\text{-PMDTA}$  in  $[\text{D}_8]\text{toluene}$  at 273 K ( $\tau = 1.5$  s).



**Figure S3:**  $^1\text{H}$  NMR spectrum of the aromatic region of  $6\text{-Li}_7\text{-DGME}$  in  $[\text{D}_8]\text{toluene}$  at 273 K. Unmarked signals (left) attributable to superimposed reformed  $6\text{-H}$  (#3) and  $[\text{D}_8]\text{toluene}$ .



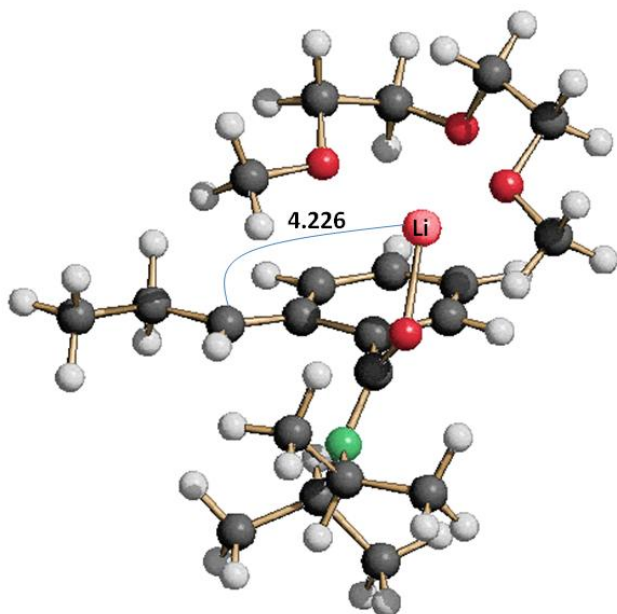
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Coordinates (Å) of *trans*-6-Li<sub>r</sub>-DGME (C<sup>-</sup>...Li<sup>+</sup> = 2.312 Å)  
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1	8	0	-0.567629	-1.019942	-0.420996
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64	6	0	4.054968	0.540146	-1.123009
65	1	0	4.383668	-0.321613	-1.709830
66	1	0	4.912996	1.200570	-0.959497

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Coordinates (Å) of *trans*-6-Li<sub>1</sub>-DGME (C<sup>-</sup>...Li<sup>+</sup> = 4.226 Å)  
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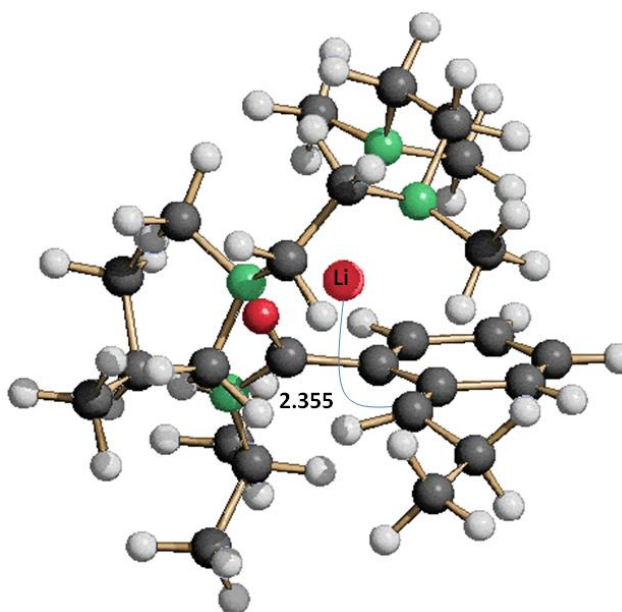


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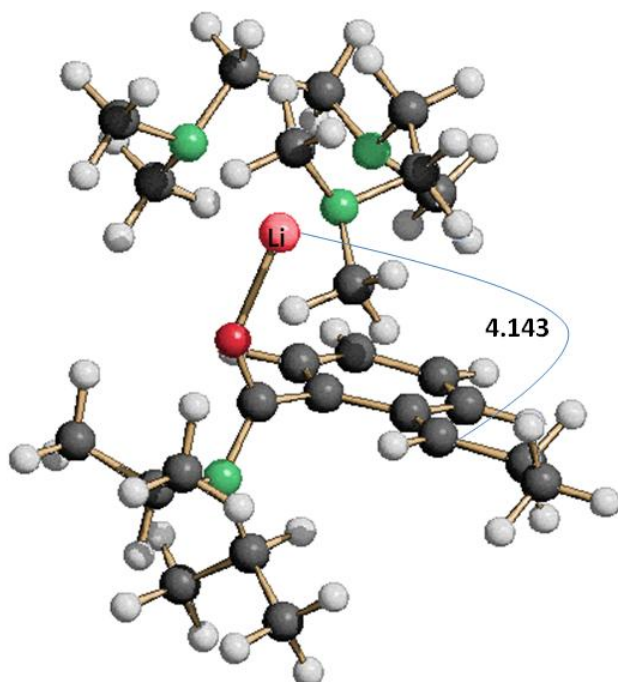
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Coordinates (Å) of *trans*-6-Li<sub>7</sub>PMDTA (C<sup>-</sup>...Li<sup>+</sup> = 2.355 Å)  
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70	1	0	-4.976597	0.665992	-1.751995
71	1	0	-0.889379	0.293668	-4.198709
72	1	0	-0.937344	-1.153342	-3.170624
73	1	0	0.316293	0.059217	-2.913662
74	1	0	2.978513	1.725007	-1.453088
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76	1	0	0.886220	5.111614	0.095629
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78	1	0	-0.391250	3.681411	1.562274

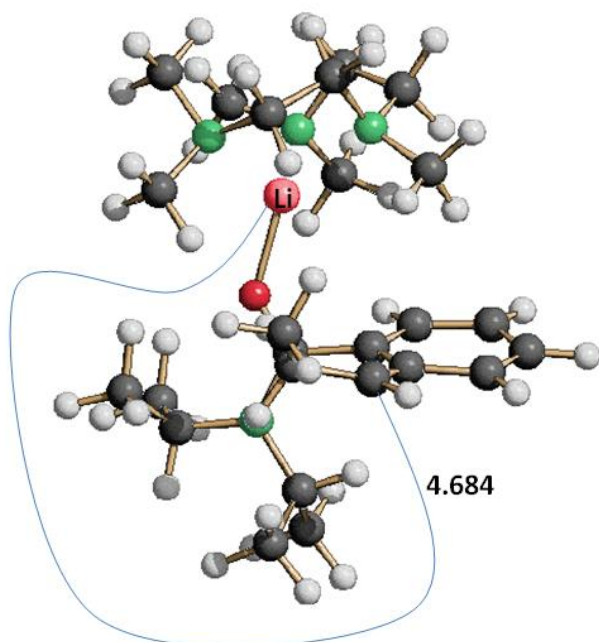
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Coordinates (Å) of *trans*-6-Li<sub>7</sub>-PMDTA (C<sup>-</sup>...Li<sup>+</sup> = 4.143 Å)  
-----



1	8	0	0.154311	-1.198500	0.318221
2	7	0	2.404545	-1.339320	0.150731
3	7	0	-2.778193	1.074129	-0.674481
4	7	0	-2.896249	-1.862505	-0.792625
5	6	0	1.226356	-0.762558	-0.176029
6	6	0	2.472386	-2.496521	1.078042
7	1	0	3.531475	-2.740274	1.127318
8	7	0	-2.220294	0.366320	2.174961
9	6	0	0.880149	0.062810	-2.470287
10	6	0	1.477742	2.687874	-1.801321
11	6	0	1.199620	0.364625	-1.153947
12	6	0	1.464010	1.727254	-0.715828
13	6	0	1.175438	2.351627	-3.100721
14	6	0	1.686549	2.083816	0.603045
15	6	0	0.838339	1.036686	-3.471448
16	6	0	3.685298	-0.859078	-0.426837
17	1	0	3.415856	0.002612	-1.028085
18	6	0	-1.066882	0.538436	3.071856
19	1	0	-1.336890	1.099653	3.977305
20	1	0	-0.273780	1.068384	2.547853
21	1	0	-0.691938	-0.438031	3.371976
22	6	0	-2.115807	-2.312448	-1.955015
23	1	0	-2.725455	-2.921567	-2.637217
24	1	0	-1.271436	-2.904839	-1.610743
25	1	0	-1.718127	-1.463005	-2.503628
26	6	0	1.758676	-3.739163	0.532364
27	1	0	0.683241	-3.588049	0.497242
28	1	0	1.969496	-4.593331	1.177997
29	1	0	2.109866	-3.980509	-0.470588
30	6	0	-3.565480	1.581158	0.464857
31	1	0	-4.408510	0.914783	0.640468
32	1	0	-3.992562	2.566557	0.235099
33	6	0	2.030296	-2.150517	2.503755
34	1	0	2.548714	-1.264414	2.867755

35	1	0	2.268384	-2.980847	3.170589
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40	1	0	-2.691369	2.935371	-1.717144
41	6	0	2.060326	3.475418	1.040921
42	1	0	1.324891	4.213218	0.690615
43	1	0	3.011659	3.802566	0.591367
44	6	0	4.662008	-0.385299	0.653571
45	1	0	4.198357	0.375885	1.277911
46	1	0	5.536243	0.058667	0.176855
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48	6	0	2.185751	3.610302	2.561258
49	1	0	1.240833	3.375851	3.057171
50	1	0	2.473855	4.621487	2.854128
51	1	0	2.939715	2.924160	2.954148
52	6	0	-2.721208	1.682440	1.731560
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54	1	0	-3.304270	2.171302	2.525483
55	3	0	-1.563302	-0.460666	0.245202
56	6	0	-4.034814	-1.020470	-1.199174
57	1	0	-4.701618	-0.938106	-0.340607
58	1	0	-4.618036	-1.498504	-2.000195
59	6	0	-3.263710	-0.402242	2.860565
60	1	0	-2.873377	-1.380109	3.138932
61	1	0	-4.124112	-0.554141	2.211716
62	1	0	-3.609733	0.102972	3.773587
63	6	0	4.310310	-1.904607	-1.355883
64	1	0	4.605927	-2.809920	-0.822339
65	1	0	5.206552	-1.491672	-1.819610
66	1	0	3.617903	-2.181691	-2.150116
67	6	0	-3.609999	0.372148	-1.664782
68	1	0	-3.024873	0.292626	-2.579142
69	1	0	-4.511562	0.946277	-1.923944
70	6	0	-3.359644	-3.030039	-0.035903
71	1	0	-4.006391	-3.684760	-0.637098
72	1	0	-3.918736	-2.709914	0.841913
73	1	0	-2.500927	-3.611308	0.296183
74	1	0	0.693788	-0.973380	-2.733527
75	1	0	1.735422	1.308819	1.358995
76	1	0	1.205614	3.125667	-3.859336
77	1	0	0.625873	0.774523	-4.497575
78	1	0	1.740034	3.712367	-1.576422

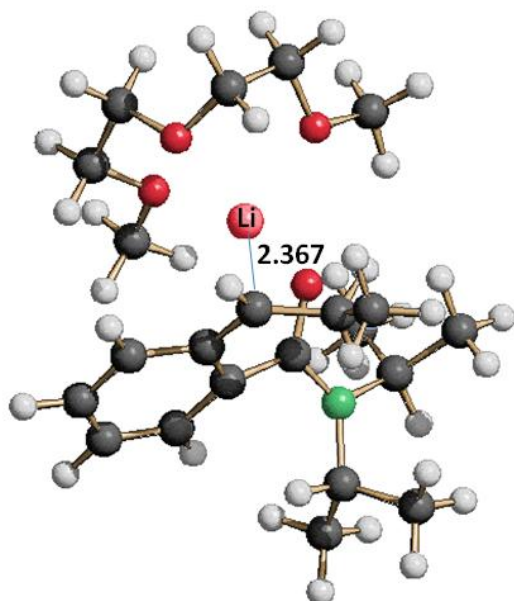
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Coordinates (Å) of *cis*-6-Li<sub>1</sub>-PMDTA (C<sup>-</sup>...Li<sup>+</sup> = 4.684 Å)  
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1	6	0	0.765208	3.268369	-1.497360
2	6	0	0.756771	1.887068	-1.406703
3	6	0	1.260102	1.183855	-0.301451
4	6	0	1.735960	1.900825	0.879780
5	6	0	1.825088	3.339198	0.685133
6	6	0	1.354447	3.983263	-0.422602
7	6	0	1.303665	-0.284676	-0.494930
8	7	0	2.497046	-0.927761	-0.608287
9	6	0	3.771038	-0.166729	-0.687476
10	6	0	4.293636	-0.097190	-2.127477
11	6	0	2.049872	1.365063	2.112883
12	1	0	2.419382	2.062213	2.858079
13	6	0	2.565499	-2.379272	-0.912087
14	6	0	2.038308	-3.251396	0.230911
15	8	0	0.229547	-0.937043	-0.658629
16	6	0	1.938161	-2.757151	-2.261748
17	6	0	4.839283	-0.689938	0.276734
18	3	0	-1.537293	-0.448169	-0.292094
19	7	0	-2.895991	-0.293695	-2.023196
20	6	0	-3.433779	-1.567004	-2.516398
21	6	0	-2.169437	0.373759	-3.114030
22	6	0	-3.976929	0.563629	-1.501685
23	6	0	-3.465382	1.703605	-0.621294
24	7	0	-2.658294	1.231352	0.517503
25	6	0	-1.834968	2.330881	1.057437
26	6	0	-3.485524	0.634049	1.584074
27	6	0	-2.745542	-0.476082	2.322979
28	7	0	-2.429879	-1.621208	1.446604
29	6	0	-3.622676	-2.434215	1.184403
30	6	0	-1.407624	-2.472714	2.071524
31	1	0	3.630025	-2.585903	-0.997297
32	1	0	3.522713	0.840590	-0.376259
33	1	0	-1.752372	-2.886163	3.029569

34	1	0	-0.501252	-1.899777	2.243774
35	1	0	-1.168548	-3.300584	1.406913
36	1	0	-2.826403	0.563087	-3.974511
37	1	0	-1.343159	-0.256538	-3.436178
38	1	0	-1.754779	1.318608	-2.775970
39	1	0	0.858751	-2.639976	-2.237807
40	1	0	2.175008	-3.797818	-2.491550
41	1	0	2.335749	-2.137974	-3.065030
42	1	0	-4.399972	0.235032	1.148644
43	1	0	-3.798136	1.399446	2.305578
44	1	0	2.528924	-2.999718	1.170067
45	1	0	2.237755	-4.301776	0.011706
46	1	0	0.967186	-3.122205	0.353196
47	1	0	-1.196092	2.732654	0.275912
48	1	0	-1.185665	1.965782	1.850292
49	1	0	-2.464080	3.135897	1.460948
50	1	0	4.466955	-0.713606	1.298132
51	1	0	5.699013	-0.020116	0.249153
52	1	0	5.198324	-1.685996	0.011243
53	1	0	-1.804677	-0.084760	2.708338
54	1	0	-3.337699	-0.797517	3.192514
55	1	0	-4.653277	-0.072450	-0.930644
56	1	0	-4.573242	0.990499	-2.321332
57	1	0	-3.367296	-3.249922	0.509845
58	1	0	-4.405796	-1.841810	0.717341
59	1	0	-4.030274	-2.868013	2.108752
60	1	0	4.573290	-1.079618	-2.511984
61	1	0	5.181601	0.534863	-2.165102
62	1	0	3.544558	0.335535	-2.789619
63	1	0	-2.834933	2.369125	-1.208271
64	1	0	-4.325104	2.303592	-0.289329
65	1	0	-4.131298	-1.425161	-3.353995
66	1	0	-3.958012	-2.088231	-1.718135
67	1	0	-2.615076	-2.197656	-2.859737
68	1	0	0.416823	1.306200	-2.255235
69	6	0	1.852527	-0.040050	2.592810
70	1	0	1.440216	5.062045	-0.481334
71	1	0	0.431565	3.772947	-2.392784
72	1	0	2.262987	3.917936	1.489604
73	6	0	1.438037	-0.104156	4.070577
74	1	0	1.090267	-0.537272	1.985917
75	1	0	2.745927	-0.674189	2.481491
76	1	0	1.326262	-1.134934	4.417324
77	1	0	2.189273	0.374732	4.701491
78	1	0	0.495472	0.420981	4.239209

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Coordinates (Å) of *cis*-6-Li<sub>1</sub>-DGME (C<sup>-</sup>...Li<sup>+</sup> = 2.367 Å)  
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1	6	0	-1.085870	3.685001	-0.029003
2	6	0	0.098263	3.829743	0.736513
3	6	0	0.686732	2.754008	1.338040
4	6	0	0.131716	1.416838	1.279383
5	6	0	-1.014454	1.271090	0.384377
6	6	0	-1.599550	2.416374	-0.193145
7	6	0	-1.354278	-0.050364	-0.159993
8	7	0	-2.658940	-0.427835	-0.363145
9	6	0	-3.778972	0.199339	0.376110
10	6	0	-4.850700	0.783969	-0.552090
11	6	0	0.679070	0.409191	2.062494
12	1	0	1.518110	0.700950	2.685651
13	6	0	-2.980286	-1.625404	-1.175800
14	6	0	-2.553409	-2.954602	-0.536557
15	8	0	-0.427119	-0.826689	-0.525078
16	6	0	-2.487164	-1.498626	-2.622147
17	6	0	-4.402127	-0.754935	1.404359
18	3	0	1.389159	-0.280706	-0.087446
19	8	0	2.361011	-2.133244	-0.149333
20	6	0	1.838503	-3.212592	-0.917784
21	6	0	3.775534	-2.156072	-0.032226
22	6	0	4.187869	-0.958715	0.808044
23	8	0	3.595331	0.243973	0.336564
24	6	0	4.180053	0.812309	-0.831285
25	6	0	3.128265	1.681755	-1.477077
26	8	0	2.018283	0.845857	-1.789734
27	6	0	1.023976	1.517341	-2.568621
28	1	0	1.575313	2.896839	1.941250
29	1	0	0.541226	4.811620	0.855182
30	1	0	-2.444854	2.284757	-0.855240
31	1	0	-4.068090	-1.637327	-1.223687
32	6	0	0.018759	-0.891556	2.431979
33	1	0	-3.331875	1.017724	0.929464
34	1	0	-1.548259	4.536763	-0.506543
35	1	0	1.446245	1.823338	-3.530254

36	1	0	0.632786	2.387117	-2.038823
37	1	0	0.220992	0.805454	-2.729098
38	1	0	4.227834	-2.129050	-1.030265
39	1	0	4.108067	-3.077413	0.459808
40	1	0	2.811906	2.478821	-0.797183
41	1	0	3.534318	2.133349	-2.388868
42	1	0	-3.646288	-1.137009	2.089478
43	1	0	-4.902066	-1.602024	0.932851
44	1	0	-5.149951	-0.219611	1.990879
45	1	0	-4.417309	1.464249	-1.283320
46	1	0	-5.580568	1.341268	0.035917
47	1	0	-5.395197	0.008117	-1.092853
48	1	0	-2.839934	-0.569506	-3.070135
49	1	0	-2.875106	-2.327937	-3.215886
50	1	0	-1.401590	-1.517950	-2.671293
51	1	0	3.817767	-1.078666	1.824801
52	1	0	5.279489	-0.880915	0.841312
53	1	0	-2.943822	-3.050716	0.475103
54	1	0	-1.472073	-3.033125	-0.490137
55	1	0	-2.944016	-3.785323	-1.127859
56	1	0	2.269815	-3.215240	-1.923333
57	1	0	0.767053	-3.057226	-0.982057
58	1	0	2.050266	-4.168854	-0.431855
59	1	0	4.490393	0.033952	-1.533170
60	1	0	5.057000	1.411019	-0.563326
61	6	0	0.372629	-1.339198	3.855345
62	1	0	-1.070440	-0.782288	2.354326
63	1	0	0.253946	-1.718234	1.745740
64	1	0	-0.103354	-2.289585	4.105939
65	1	0	1.451541	-1.472119	3.966483
66	1	0	0.058431	-0.596796	4.590518

## References

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