

Theoretical investigation of boron-doped lithium clusters $B\text{Li}_n$ ($n=3-6$) activating CO_2 : An example of the carboxylation of C-H bond

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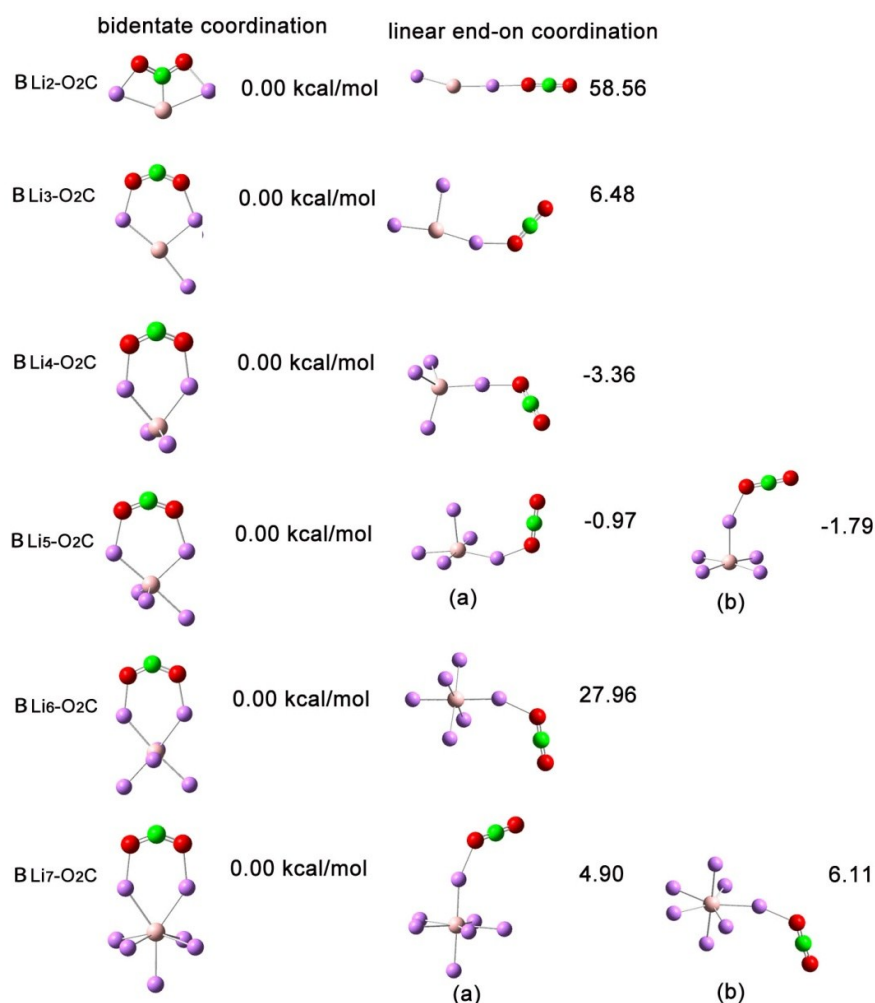


Fig S1. Comparisons of the structures and their energies between two coordination modes.

Molecular coordinates

1. C-C bond formation TS1

n=3

3	-2.549284	1.885583	0.609602
3	-3.474013	-1.092884	-0.235537
3	-6.359350	-0.387505	0.752146
5	-4.486368	0.794503	0.704871
6	-0.869006	-0.073605	-0.480007
8	-1.641074	-1.023511	-0.615802
8	-1.028425	1.074221	-0.085132
6	1.467480	-1.378118	0.252552
6	1.114455	-0.626039	-0.914717
6	1.837876	0.583382	-1.153823
6	2.659746	1.114452	-0.178524
6	2.877540	0.429559	1.026359
6	2.293260	-0.832018	1.216870
1	1.029891	-2.359193	0.399001
1	0.732735	-1.173482	-1.769866
1	1.689241	1.114211	-2.087537
1	3.160513	2.060934	-0.354721
1	3.525314	0.851823	1.785646
1	2.509959	-1.393737	2.119689

n=4

3	2.674393	-1.349410	0.219925
3	3.042792	1.259434	-0.249521
3	5.704217	-0.094444	2.237502
3	6.472813	-0.673473	-0.416623
5	4.573272	-0.206988	0.438669
6	0.594409	0.182074	-0.602233
8	1.240643	1.242407	-0.678046
8	0.940630	-0.967780	-0.295626
6	-2.593612	0.835458	1.183659
6	-1.878007	1.336199	0.110467
6	-1.505187	0.482615	-0.972718
6	-2.076083	-0.822944	-1.010060
6	-2.791059	-1.307350	0.071037
6	-3.039484	-0.494682	1.186082
1	-2.831762	1.483835	2.020772
1	-1.547940	2.368636	0.105837
1	-1.201431	0.946828	-1.904754
1	-1.901400	-1.455373	-1.873121
1	-3.178981	-2.320612	0.048187
1	-3.603526	-0.879938	2.027852

n=5

3	3.025552	-1.324491	-0.434838
3	2.426785	1.536044	-0.190999
3	5.542172	-0.970247	1.258650
3	4.923798	1.939677	1.517120
3	5.144572	0.704107	-1.409516
5	4.171414	0.350987	0.359866
6	0.463774	-0.379158	-0.384338
8	0.679464	0.801722	-0.175559
8	1.125193	-1.409163	-0.350532
6	-2.682014	-0.340156	1.389927
6	-3.153430	0.869176	0.859999
6	-2.908099	1.178438	-0.486879
6	-2.168616	0.324586	-1.281087
6	-1.560712	-0.840649	-0.721779
6	-1.938775	-1.206318	0.609081
1	-2.917297	-0.606846	2.414787
1	-3.734601	1.544770	1.476685
1	-3.320875	2.087570	-0.911545
1	-1.997510	0.563041	-2.324962
1	-1.240589	-1.628974	-1.394422
1	-1.584855	-2.145751	1.018057

n=6

3	-2.327820	1.294042	-0.014010
3	-2.808572	-1.398723	-0.260733
3	-3.477668	-0.123373	2.466741
3	-5.786731	-1.091937	0.930280
3	-5.269029	1.823797	1.193383
3	-4.979148	0.492080	-1.401329
5	-4.158039	0.172936	0.502797
6	-0.373692	-0.382868	-0.926409
8	-1.045580	-1.425922	-0.884077
8	-0.657481	0.796793	-0.681555
6	3.432785	-0.084683	0.616926
6	2.915016	-1.385237	0.517302
6	2.085688	-1.734880	-0.533368
6	1.670735	-0.753629	-1.485691
6	2.310908	0.520008	-1.441262
6	3.138921	0.852568	-0.383753
1	4.086687	0.181364	1.439723
1	3.186207	-2.129775	1.259129
1	1.697130	-2.743523	-0.612402
1	1.272058	-1.102074	-2.432781
1	2.100227	1.248346	-2.215963
1	3.580433	1.842966	-0.337995

2. H-direct transfer transition states

n=3

3	3.110687	-0.001428	1.601610
3	3.260979	0.001044	-1.354333
3	6.459800	0.001442	-1.268472
6	0.764697	-0.000374	0.312805
8	1.460041	0.000549	-0.813986
8	1.236845	-0.001352	1.445589
6	-1.433732	1.226890	-0.016530
6	-0.689270	0.000014	-0.090425
6	-1.433916	-1.226850	-0.018277
6	-2.810401	-1.211323	-0.120004
6	-3.514405	0.000304	-0.197723
6	-2.810218	1.211714	-0.118273
1	-0.901378	2.168219	0.060841
1	0.219286	0.000964	-1.351701
1	-0.901700	-2.168368	0.057731
1	-3.353642	-2.150191	-0.122924
1	-4.594582	0.000443	-0.276428
1	-3.353318	2.150666	-0.119837
5	4.875864	-0.000147	0.250728

n=5

3	-2.832330	-0.941930	-1.014394
3	-2.793528	0.681480	1.221220
3	-6.000460	-1.134116	-0.958656
3	-4.844300	1.493043	-0.973563
3	-5.929227	0.603073	1.526673
5	-4.482101	-0.202261	0.198424
6	-0.366971	-0.153710	-0.123247
8	-0.947027	0.628270	0.777143
8	-0.946624	-0.886086	-0.916641
6	3.174391	1.186776	-0.452960
6	3.939547	0.092187	-0.012079
6	3.292424	-1.078665	0.411862
6	1.915042	-1.157983	0.440971
6	1.114363	-0.004566	0.124361
6	1.797739	1.140389	-0.432555
1	3.670926	2.073705	-0.830995
1	5.021333	0.139836	-0.034095
1	3.882206	-1.940738	0.704549
1	1.423367	-2.076796	0.738690
1	0.348588	0.641570	1.183897
1	1.213615	1.985033	-0.780147

3. One H₂O molecules assisting H transfer transition states

n=3

3	-3.142760	-1.585680	0.180400
3	-3.178660	0.916864	-0.616150
3	-7.176266	-0.732599	-0.544365
6	-0.735059	-0.141697	0.028580
8	-1.361250	0.999370	-0.212546
8	-1.363202	-1.189892	0.309434
6	1.464986	0.640758	-0.970844
6	0.745035	-0.091687	0.063091
6	1.473400	-1.163772	0.713652
6	2.823974	-1.325460	0.504752
6	3.522541	-0.516966	-0.413017
6	2.813808	0.443434	-1.159636
1	0.927779	1.373034	-1.561706
1	0.677178	1.117245	0.938327
1	0.932915	-1.820690	1.383739
1	3.355015	-2.105846	1.040061
1	4.583794	-0.660644	-0.573317
1	3.331715	1.025329	-1.914797
5	-5.026966	-0.410806	-0.420102
8	0.208337	2.202936	1.206780
1	-0.615448	1.930341	0.573736
1	-0.088249	2.232538	2.125998

n=4

3	2.971207	0.872824	0.513033
3	2.958903	-1.492093	-0.511155
3	6.744954	-0.125191	-0.551113
3	5.807137	-1.160238	1.907901
6	0.532282	-0.074029	-0.099096
8	1.215197	-1.044896	-0.521611
8	1.147963	1.068069	0.247902
6	-2.986855	0.300878	1.216921
6	-1.657549	0.569690	1.008467
6	-0.927137	-0.060187	-0.100096
6	-1.642461	-1.124586	-0.799433
6	-2.974877	-1.357955	-0.560909
6	-3.684556	-0.640011	0.426435
1	-3.505052	0.808522	2.024559
1	-1.135949	1.282297	1.636273
1	-0.876664	1.230636	-0.863752
1	-1.099975	-1.712756	-1.529519
1	-3.488231	-2.125682	-1.131974
1	-4.733773	-0.839096	0.605964
5	4.766432	-0.416160	0.231684
8	-0.444300	2.352358	-1.005000
1	-0.160636	2.484492	-1.917890
1	0.417550	1.979437	-0.382147

n=5

3	-2.824700	-1.577921	0.142901
3	-2.867897	1.012203	-0.506008
3	-5.955734	-1.963652	-0.523591
3	-6.003482	0.983759	-1.206461
3	-5.164985	0.053779	1.410582
5	-4.540860	-0.384208	-0.503802
6	-0.408875	-0.119454	-0.002409
8	-1.009861	1.024230	-0.226609
8	-1.027012	-1.172550	0.255174
6	3.150080	-1.330431	0.510626
6	3.856666	-0.535692	-0.410645
6	3.166960	0.433268	-1.160195
6	1.817327	0.642356	-0.977181
6	1.086865	-0.084674	0.044524
6	1.799023	-1.151662	0.710662
1	3.671954	-2.110657	1.054473
1	4.916953	-0.692605	-0.566517
1	3.696486	1.010540	-1.910347
1	1.288352	1.380680	-1.567950
1	1.043266	1.080404	0.917606
1	1.246713	-1.796931	1.382572
8	0.589981	2.181231	1.244343
1	0.289954	2.176866	2.163042
1	-0.232113	1.962697	0.618305

n=6

3	2.705853	0.989784	0.487481
3	2.681420	-1.444688	-0.575051
3	4.957885	0.424541	-1.586415
3	5.864958	-1.876885	-0.041098
3	5.879218	0.863155	1.152554
3	4.064238	-1.204965	2.171058
5	4.422130	-0.376732	0.275936
6	0.241735	-0.049196	-0.179384
8	0.910527	-1.014398	-0.619406
8	0.864811	1.090115	0.173999
6	-3.942520	-0.693130	0.473240
6	-3.223173	0.213129	1.286562
6	-1.911179	0.520912	1.033826
6	-1.221761	-0.022777	-0.148857
6	-1.951782	-1.065112	-0.871294
6	-3.266520	-1.338782	-0.585941
1	-4.978660	-0.923014	0.688507
1	-3.711700	0.662088	2.145984
1	-1.374820	1.208654	1.676943
1	-1.206490	1.289306	-0.827564
1	-1.434472	-1.601710	-1.657528
1	-3.792307	-2.083442	-1.176185
8	-0.777085	2.434195	-0.920226
1	0.133764	1.986032	-0.343189
1	-0.541507	2.623353	-1.836083

4. Two H₂O molecules assisting H transfer transition states

n=3

3	-3.127578	0.107376	-1.115703
3	-3.099851	-1.643924	0.790198
3	-7.147873	-1.266393	-0.413446
5	-4.992296	-0.969645	-0.325546
6	-0.728365	-0.366949	-0.033460
8	-1.351247	-1.179749	0.714457
8	-1.356861	0.534008	-0.742412
6	3.526998	-0.828181	-0.467115
6	2.821592	0.062120	-1.298045
6	1.466949	0.263266	-1.141667
6	0.743131	-0.390588	-0.069774
6	1.467869	-1.390225	0.687396
6	2.823424	-1.561448	0.507670
1	4.591166	-0.977142	-0.602500
1	3.346992	0.584204	-2.091020
1	0.927112	0.929032	-1.802971
1	0.850251	0.766658	0.931125
1	0.919921	-1.980984	1.410595
1	3.351476	-2.292478	1.111406
8	0.877388	1.727667	1.574793
1	0.237016	2.363344	1.055055
1	0.509076	1.529277	2.446300
8	-0.663712	2.924546	0.012819
1	-0.999321	2.069873	-0.407269
1	-1.420428	3.485507	0.206574

n=4

3	-2.864045	0.253863	-0.545225
3	-2.960307	-1.679563	0.881066
3	-6.847897	-0.228666	0.558183
3	-5.783468	-1.748507	-1.552050
5	-4.819987	-0.771303	0.041593
6	-0.583692	-0.156159	-0.152439
8	-1.413469	-0.909913	0.487741
8	-1.086936	0.862852	-0.817486
6	3.581627	-1.163521	-0.308024
6	3.056831	-0.154599	-1.144314
6	1.733673	0.215466	-1.081067
6	0.839163	-0.385458	-0.098924
6	1.378580	-1.503408	0.662496
6	2.709833	-1.839495	0.572380
1	4.626202	-1.442461	-0.370941
1	3.704539	0.326227	-1.870833
1	1.339703	0.969424	-1.751203
1	1.016890	0.791354	0.966522
1	0.711170	-2.048526	1.318299
1	3.091764	-2.656542	1.177041
8	1.125980	1.732985	1.562131
1	0.622008	2.446575	0.938399
1	0.656898	1.619723	2.399130
8	-0.048125	3.063994	-0.133484
1	-0.509208	2.234999	-0.542316
1	-0.708578	3.748059	0.010155

n=5

3	-2.877623	0.487754	-0.923372
3	-2.855981	-1.587311	0.716189
3	-4.933994	-1.751034	-1.595409
3	-6.091722	0.816256	-0.764088
5	-4.606070	-0.493700	-0.011429
6	-0.440588	-0.327110	-0.077261
8	-1.076770	-1.176971	0.601267
8	-1.020949	0.630899	-0.730716
6	3.818799	-0.874809	-0.465896
6	3.154510	0.083089	-1.251920
6	1.803763	0.314101	-1.098552
6	1.046581	-0.373736	-0.074404
6	1.729882	-1.437782	0.628060
6	3.082446	-1.640814	0.456613
1	4.879785	-1.048803	-0.597429
1	3.706268	0.629793	-2.009547
1	1.288331	1.021959	-1.735258
1	1.152992	-2.049242	1.310346
1	3.580650	-2.420162	1.023660
8	1.131403	1.608796	1.711090
1	0.597829	2.307404	1.173121
1	0.640680	1.394682	2.516222
8	-0.297152	2.996967	0.156283
1	-0.615660	2.183715	-0.336099
1	0.084525	3.604669	-0.484676
3	-6.063245	-1.548517	1.108468
1	1.118030	0.657878	0.968200

n=6

3	2.717010	0.514602	0.834248
3	2.784326	-1.232829	-1.098048
3	5.129474	0.843532	-1.168132
3	5.970315	-1.891317	-0.649802
3	5.898917	0.127228	1.552936
5	4.500555	-0.632831	0.178710
6	0.332449	-0.134221	-0.101192
8	1.052975	-0.778662	-0.934901
8	0.891466	0.808547	0.654137
6	-3.781695	-1.230458	0.465411
6	-3.156607	-0.319858	1.345550
6	-1.853803	0.081454	1.160127
6	-1.089162	-0.376592	0.006158
6	-1.717415	-1.407714	-0.809405
6	-3.024304	-1.779470	-0.592912
1	-4.808753	-1.535063	0.625091
1	-3.708225	0.058416	2.201040
1	-1.382183	0.758295	1.861861
1	-1.435610	0.907503	-0.902392
1	-1.132568	-1.858748	-1.601482
1	-3.475312	-2.528064	-1.237795
8	-1.619393	1.894320	-1.375600
1	-0.997118	2.538111	-0.744424
1	-1.279042	1.855100	-2.278652
8	-0.194336	3.017658	0.245746
1	0.301973	2.129043	0.523168
1	0.461069	3.689476	0.036235
3	4.050133	-2.155771	1.550902