Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Material

CAl_4Be and $CAl_3Be_2^-$: Global minima with a planar pentacoordinate carbon atom

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Cartesian coordinates of all the species studied in this work calculated at CCSD(T)/aug-cc-pVTZ level.

CAl_4Be clusters

1a

C	0.00000000	0.00000000	0.22529475
Be	0.00000000	0.00000000	1.91807898
Al	0.00000000	2.05833477	1.02973571
Al	0.00000000	-1.26220664	-1.39039053
Al	0.00000000	-2.05833477	1.02973571
Al	0.00000000	1.26220664	-1.39039053

2a

C	-0.65360653	-1.07771756	0.00000000
Be	-1.47856540	0.32171428	0.00000000
Al	0.20614371	-1.24538399	1.72884138
Al	0.19228426	1.45084163	-1.27867802
Al	0.19228426	1.45084163	1.27867802
Al	0.20614371	-1.24538399	-1.72884138

3a

Al	0.00000000	1.91610961	-1.18186826
C	0.00000000	0.00004716	-0.64490420
Al	-1.65939364	-0.95803954	-1.18155379
Al	1.65939364	-0.95803954	-1.18155379

Be	0.00000000	0.00010556	1.01689277
Al	0.00000000	-0.00018423	3.51937427

4a

C	0.00000000	0.00000000	0.02251030
Be	0.00000000	0.00000000	-2.84745039
Al	0.00000000	1.56989217	-1.12582766
Al	0.00000000	-1.56989217	-1.12582766
Al	0.00000000	1.36975356	1.56154071
Al	0.00000000	-1.36975356	1.56154071

5a

C	-0.01963400	0.85143341	0.00000000
Be	-1.12392427	-0.41062108	0.00000000
Al	1.07237325	-0.98768451	0.00000000
Al	-1.50048476	2.12993825	0.00000000
Al	-0.96819970	-2.97910750	0.00000000
Al	1.79043047	1.58784842	0.00000000

6a

C	1.04498785	-0.49250572	0.00000000
Be	1.13308762	-2.12367415	0.00000000
Al	-0.91049426	-1.31974455	0.00000000
Al	-2.82401031	0.83317071	0.00000000
Al	2.89313122	0.24040660	0.00000000

Al	0.00775187	1.16256210	0.00000000

7a

Al	0.81877750	-1.52797365	0.00000000
Al	-2.51868764	0.72275743	0.00000000
Al	2.83338105	0.51222581	0.00000000
Al	0.01759731	1.09288951	0.00000000
C	-0.90712986	-0.70611161	0.00000000
Be	-2.33364935	-1.48606647	0.00000000

8a

C	1.36925901	-0.14194991	0.00000000
Be	-0.00968203	0.71127817	0.00000000
Al	0.34185651	-1.71904489	0.00000000
Al	-2.10217618	-0.71132082	0.00000000
Al	3.27359996	0.29847019	0.00000000
Al	-2.14442928	1.97110625	0.00000000

$CAl_3Be_2^-$ clusters

1b

Be	0.00000000	1.60108880	0.78194487
Be	0.00000000	-1.60108880	0.78194487
C	0.00000000	0.00000000	0.15572797

Al	0.00000000	0.00000000	2.37375828
Al	0.00000000	-1.29787359	-1.46892500
Al	0.00000000	1.29787359	-1.46892500

2b

Be	0.00000000	0.96818486	-2.01790271
Be	0.00000000	-0.96818486	-2.01790271
C	0.00000000	0.00000000	-0.50660659
Al	0.00000000	0.00000000	1.52097579
Al	0.00000000	-2.05310406	-0.00708839
Al	0.00000000	2.05310406	-0.00708839

3b

Be	2.40165260	1.63548736	0.00000000
Be	0.38401131	1.91080491	0.00000000
C	0.03335591	0.28294120	0.00000000
Al	-0.75778754	-1.57218819	0.00000000
Al	-1.85987145	0.96727560	0.00000000
Al	1.76729118	-0.64750288	0.00000000

4b

Be	-0.52924986	-2.43843377	0.00000000
Be	0.96498681	-1.08361674	0.00000000
C	-0.72977377	-0.80450882	0.00000000
Al	-2.57306069	-0.16784616	0.00000000

Al	2.76677485	0.61218725	0.00000000
Al	0.01660067	1.06108525	0.00000000

5b

Be	-0.97403443	-0.67486335	1.06397235
Be	-0.97403443	-0.67486335	-1.06397235
C	-0.51271828	0.56563534	0.00000000
Al	-0.84686028	2.43844783	0.00000000
Al	1.48276906	0.12042731	0.00000000
Al	0.26982135	-2.34484578	0.00000000

6b

Be	1.04241316	-2.11696525	0.00000000
Be	0.01081314	0.90761983	0.00000000
C	0.95876622	-0.47727922	0.00000000
Al	2.64824315	0.46738595	0.00000000
Al	-1.03556685	-1.18263283	0.00000000
Al	-2.39553481	1.29697351	0.00000000

7b

Be	0.00000000	0.97903977	0.05803728
Be	0.00000000	-0.97903977	0.05803728
C	0.00000000	0.00000000	1.36518956
Al	0.00000000	0.00000000	3.25324650
Al	-1.24216473	0.00000000	-1.96006530

Al	1.24216473	0.00000000	-1.96006530

8b

Be	0.58734194	-1.51209209	0.00000000
Be	-0.01418554	0.56084015	0.00000000
C	1.45231272	-0.13295220	0.00000000
Al	-1.72969258	-1.27623254	0.00000000
Al	3.29835026	0.31707293	0.00000000
Al	-2.41157278	1.30402575	0.00000000

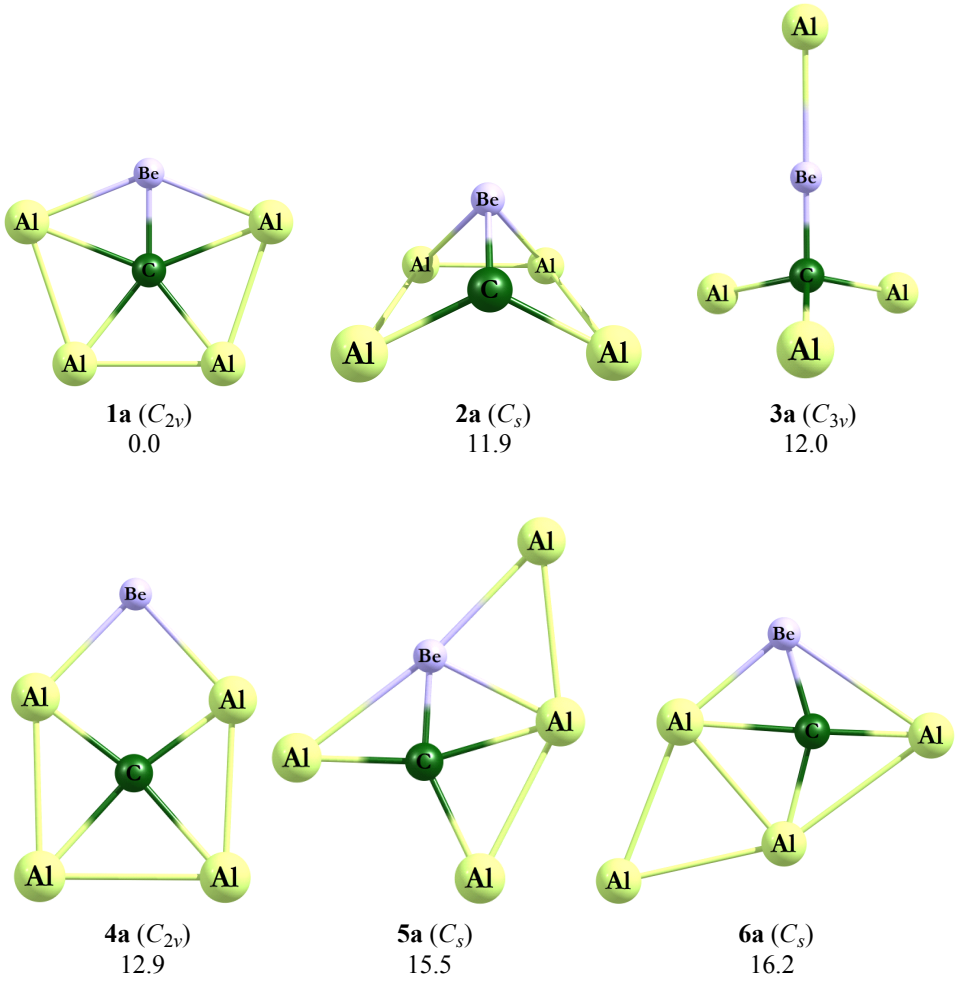

Figure SM-1. Most stable isomers of CAl_4Be optimized at the CCSD(T)/aug-cc-pVTZ level of theory.

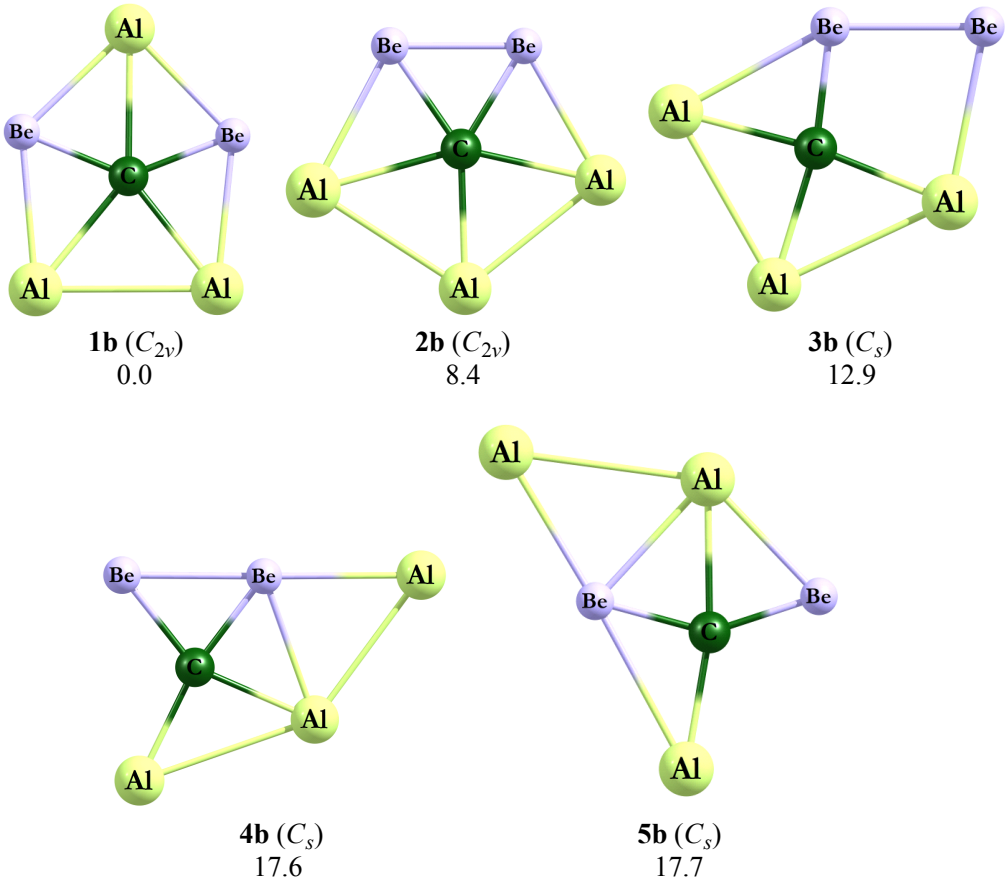

Figure SM-2. Most stable isomers of $CAl_3Be_2^-$ optimized at the CCSD(T)/aug-cc-pVTZ level of theory.