Planar carbon radical's assembly and stabilization, a way to design spin-based molecular materials

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Supporting information

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13.(f) Gaussian03 (RevisionA.1), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda,O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Pittsburgh, PA, **2003**.

Some calculated structural, electronic and magnetic properties of our designed hetero-decked sandwich-type complexes are listed in Table S1-4.

Table S1. The calculated spin densities of the CAl_4^- units in all of the homo-decked sandwich forms of $[(CAl_4)_2M]^{q-}$ (s-s) (M=Li, Na, K, q=1; M=Be, Mg, Ca, q=0) at 6-31+G(d)-UB3LYP/UMP2 level. The spin densities of the CAl_4^- units in the hetero-decked sandwich forms P, V, P-P, P-V and V-V, are obtained at the UB3LYP/6-31+G(d) level. The equivalent of the two CAl_4-decks due to the symmetry of D_{2d} sandwich forms, we label the two CAl_4-decks as deck1 and deck2, respectively. For the hetero-decked sandwich forms P, V, P-P, P-V and V-V, the deck1, deck2 and deck3 are illustrative in Fig. 7.

Sandwich Species (s-s) D_{2d}	**Spin density of several fragments**	**UB3LYP/6-31+G(d)**		**UMP2/6-31+G(d)**	
		singlet	**triplet**	**singlet**	**triplet**
$[(CAl_4)_2Li]^-$	deck1	0.9921	0.9917	0.8929	0.9066
	deck2	–0.9921	0.9917	–0.8929	0.9066
$[(CAl_4)_2Na]^-$	deck1	0.9918	1.0029	0.9643	1.0223
	deck2	–0.9918	1.0029	–0.9643	1.0223
$[(CAl_4)_2K]^-$	deck1	0.9993	0.9998	0.9864	0.9874
	deck2	–0.9993	0.9998	–0.9864	0.9874
$[(CAl_4)_2Be]$	deck1	1.0275	1.0189	1.2101	1.1060
	deck2	–1.0275	1.0189	–1.2101	1.1060
$[(CAl_4)_2Mg]$	deck1	1.0231	1.0226	1.0258	1.0427
	deck2	–1.0231	1.0226	–1.0258	1.0427
$[(CAl_4)_2Ca]$	deck1	0.9904	0.9945	1.0528	1.1231
	deck2	–0.9904	0.9945	–1.0528	1.1231
		singlet	**triplet**		
P	deck1	-1.0072	1.0067		
	deck2	1.0071	1.0066		
V	deck1	1.0025	1.0025		
	deck2	-1.0024	1.0024		
		doublet	**quartet**		
P-V	deck1	1.0110	1.0106		
	deck2	-0.9671	0.9665		
	deck3	1.0062	1.0061		
P-P	deck1	1.0107	1.0103		
	deck2	-0.9632	0.9622		
	deck3	1.0081	1.0081		
V-V	deck1	1.0053	1.0056		
	deck2	-0.9574	0.9574		
	deck3	1.0056	1.0057		

Table S2. The calculated spin densities of the CAl_4^- units in all of the hetero-decked sandwich forms (f-f, f-s and f-c) of $[CpM(CAl_4)]^{q-}$ and in the ground states of saturated sandwich-type compounds $(Li^+)_q[CpLi(CAl_4)]^{q-}$

(M=Li, Na, K, q=1; M=Be, Mg, Ca, q=0) and in the low-lying structures of extended sandwich-like compounds $[(CpLi)_n(CAl_4)]^-$ (n=2, 3, 4 and 6) at UB3LYP/6-31+G(d) level.

	Spin densities of the CAl_4^- units in all kinds of designed sandwich-type species				
Ref specie: CAl_4^-	1.0000			Saturated sandwiches	
Sandwich species	Face-face (f-f)	Face-side (f-s)	Face-corner (f-c)	$(Li^+)[CpLi(CAl_4)]^-$	0.9591
$[CpLi(CAl_4)]^-$	1.2827	0.9899	0.7892	$(Li^+)[CpNa(CAl_4)]^-$	0.9625
$[CpNa(CAl_4)]^-$	1.1462	0.9974	1.0067	$(Li^+)[CpK(CAl_4)]^-$	0.9652
$[CpK(CAl_4)]^-$	1.0227	0.9986	1.0000	$[(CpLi)_2(CAl_4)]^-$	1.1483
$[CpBe(CAl_4)]$	1.0048	0.9730		$[(CpLi)_3(CAl_4)]^-$	1.0587
$[CpMg(CAl_4)]$	1.2043	1.0304		$[(CpLi)_4(CAl_4)]^-$	1.0716
$[CpCa(CAl_4)]$	1.0386	0.9983		$[(CpLi)_6(CAl_4)]^-$	1.0802

Table S3. The natural charge distribution of the CAl_4^- units in all of the sandwich-like species with more than one ptC-radical CAl_4^--decks (including homo-decked sandwich forms (s-s) of $[(CAl_4)_2M]^{q-}$ and hetero-decked extended sandwich forms of P, V, P-V, P-P and V-V) at UB3LYP/6-31+G(d) level.

Sandwich Species (s-s) D_{2d}	**Charge distribution of several fragments**	**UB3LYP/6-31+G(d)**		**UMP2/6-31+G(d)**	
		singlet	**triplet**	**singlet**	**triplet**
$[(CAl_4)_2Li]^-$	deck1	-0.8284	-0.8373	-0.8328	-0.8336
	deck2	-0.8284	-0.8373	-0.8328	-0.8336
$[(CAl_4)_2Na]^-$	deck1	-0.8500	-0.8655	-0.8807	-0.8812
	deck2	-0.8500	-0.8655	-0.8807	-0.8812
$[(CAl_4)_2K]^-$	deck1	-0.9311	-0.9312	-0.9382	-0.9384
	deck2	-0.9311	-0.9312	-0.9382	-0.9384
$[(CAl_4)_2Be]$	deck1	-0.3910	-0.3992	-0.3808	-0.3882
	deck2	-0.3910	-0.3992	-0.3808	-0.3882
$[(CAl_4)_2Mg]$	deck1	-0.5551	-0.5655	-0.5932	-0.6091
	deck2	-0.5551	-0.5655	-0.5932	-0.6091
$[(CAl_4)_2Ca]$	deck1	-0.7485	-0.7482	-0.7447	-0.7445
	deck2	-0.7485	-0.7482	-0.7447	-0.7445
		singlet	**triplet**		
P	deck1	-0.8469	-0.8469		
	deck2	-0.8468	-0.8467		
V	deck1	-0.9239	-0.9240		
	deck2	-0.9241	-0.9241		
		doublet	**quartet**		
P-V	deck1	-0.8021	-0.8021		
	deck2	-0.9096	-0.9095		
	deck3	-0.8368	-0.8369		
P-P	deck1	-0.7984	-0.7995		
	deck2	-0.9074	-0.9124		
	deck3	-0.8231	-0.8232		

V-V	deck1	-0.8796	-0.8796		
	deck2	-1.0617	-1.0621		
	deck3	-0.8803	-0.8804		

Table S4. The natural charge distribution of the hetero-decked unsaturated, saturated and extended sandwich-like species with one ptC-radical CAl_4^--deck are obtained at the UB3LYP/6-31+G(d) level.

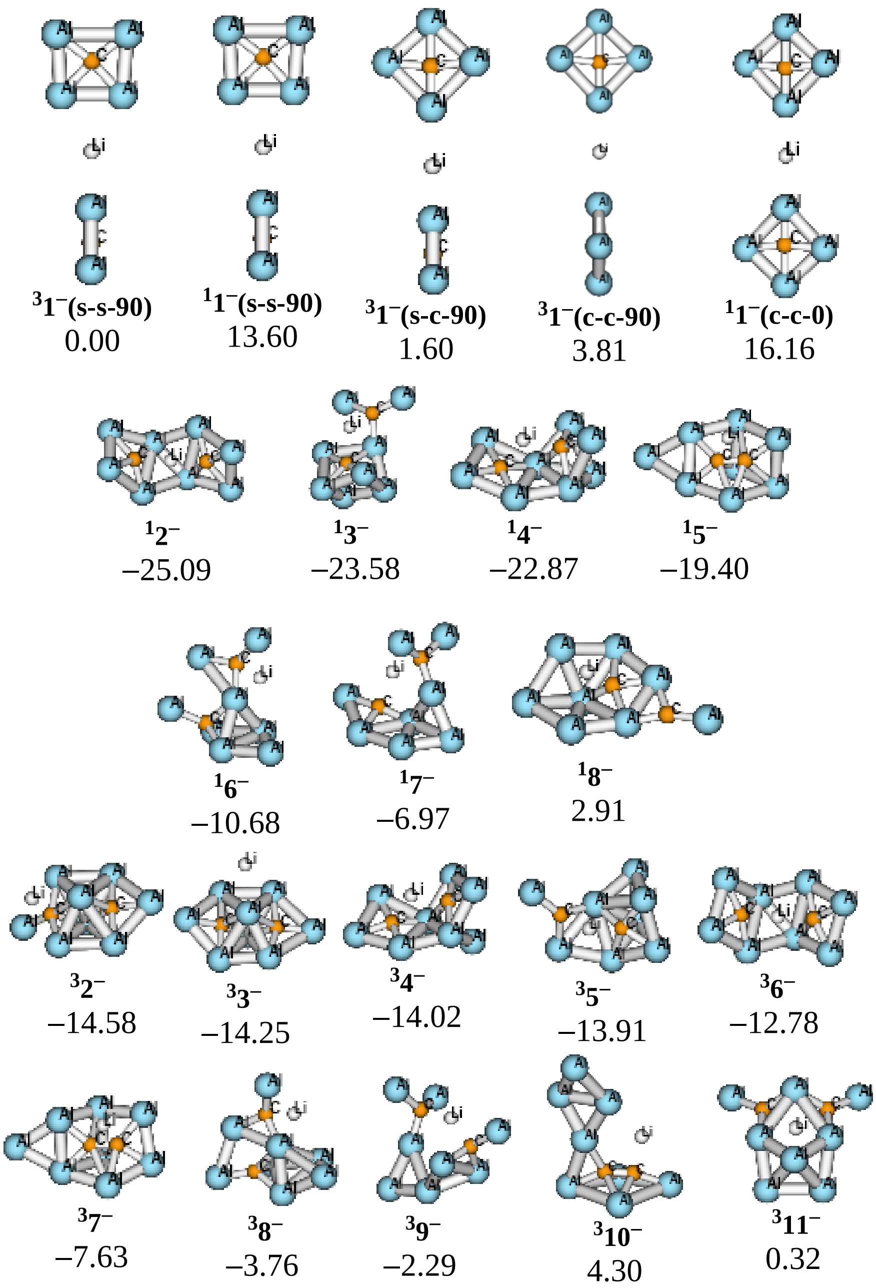
	Natural charge distribution of the CAl_4^- units in all kinds of designed sandwich-type species				
Ref specie: CAl_4^-	-1.0000			Saturated sandwiches	
Sandwich species	Face-face (f-f)	Face-side (f-s)	Face-corner (f-c)	$(Li^+)[CpLi(CAl_4)]^-$	-0.7315
$[CpLi(CAl_4)]^-$	-1.0006	-0.9087	-0.9362	$(Li^+)[CpNa(CAl_4)]^-$	-0.7468
$[CpNa(CAl_4)]^-$	-1.2355	-1.1969	-0.8354	$(Li^+)[CpK(CAl_4)]^-$	-0.8284
$[CpK(CAl_4)]^-$	-0.9907	-0.9784	-0.9755	$[(CpLi)_2(CAl_4)]^-$	-0.9483
$[CpBe(CAl_4)]$	-0.8759	-0.4221		$[(CpLi)_3(CAl_4)]^-$	-0.9688
$[CpMg(CAl_4)]$	-0.8800	-0.5886		$[(CpLi)_4(CAl_4)]^-$	-0.9783
$[CpCa(CAl_4)]$	-0.9039	-0.7898		$[(CpLi)_6(CAl_4)]^-$	-0.9817

1. An imaginary frequency indicates the existence of a vibrational mode that is dynamically unstable and leads to a more stable structure. Transition states of a chemical reaction are saddle points exhibiting only one imaginary frequency. Saddle points with more dynamical systems with sufficiently high vibrational energy but are generally not of chemical significance. The criteria of SCF converge is 10^{-6} used in the present systems.

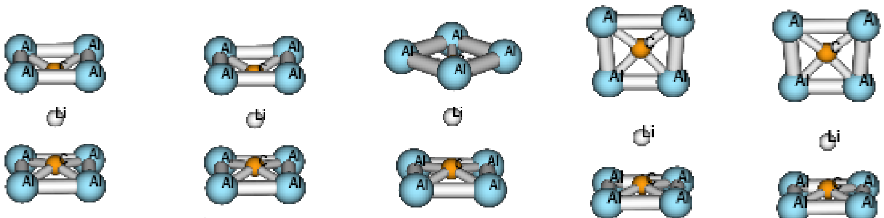
In this report, **NIMAG** means the number of imaginary frequency of saddle point.[S50]

$^{m}N^{q-}$: "m" means spin electron state (singlet, triplet), **"N"** means the energy order of various isomers, superscript **"q–"** means the charge of the total system**.**

1. The calculated properties of $C_2Al_8Li^-$



Supplementary Material (ESI) for PCCP



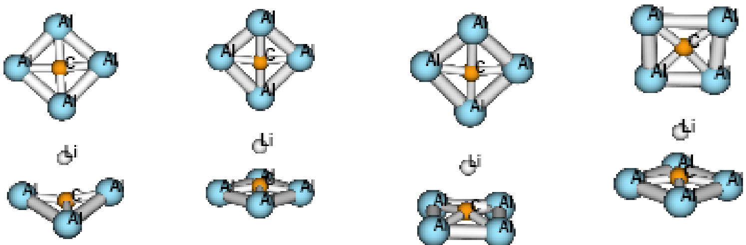
^{3}1(f-f-0) (NIMAG=5) 6.58

^{1}1(f-f-0) (NIMAG=4) 15.61

^{3}1(f-f-90) (NIMAG=4) 6.44

^{3}1(f-s-0) (NIMAG=3) 2.59

^{1}1(f-s-0) (NIMAG=3) 14.52

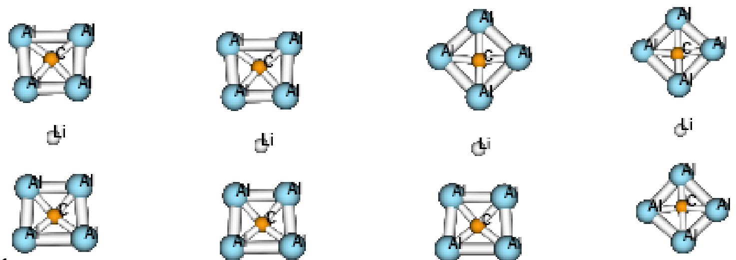


^{1}1(f-c-90) (NIMAG=3) 30.84

^{3}1(f-c-90) (NIMAG=3) 4.64

^{3}1(f-c-0) (NIMAG=2) 4.63

^{3}1(f-s-90) (NIMAG=2) 2.52



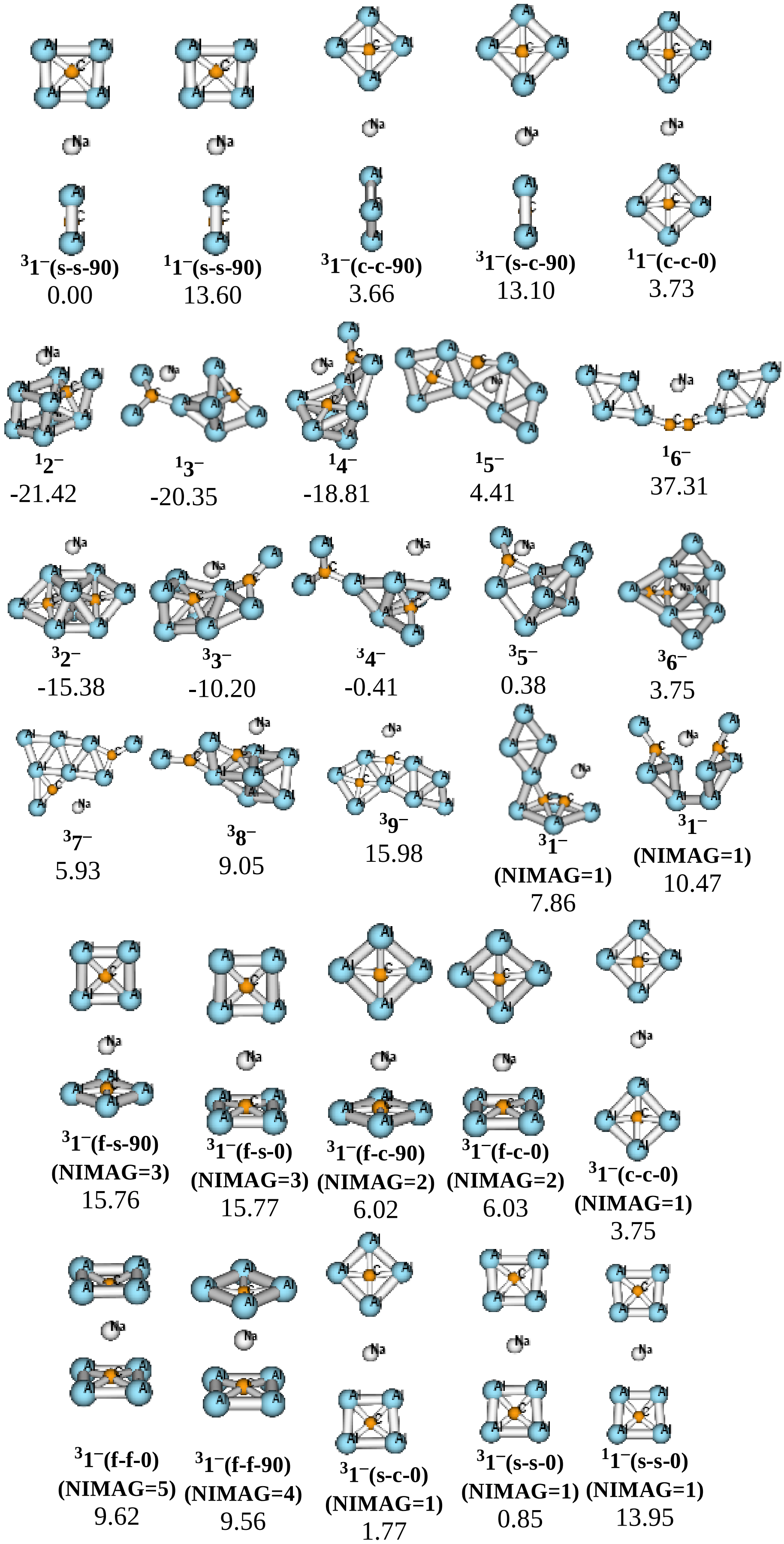
^{1}1(s-s-0) (NIMAG=1) 14.53

^{3}1(s-s-0) (NIMAG=1) 1.63

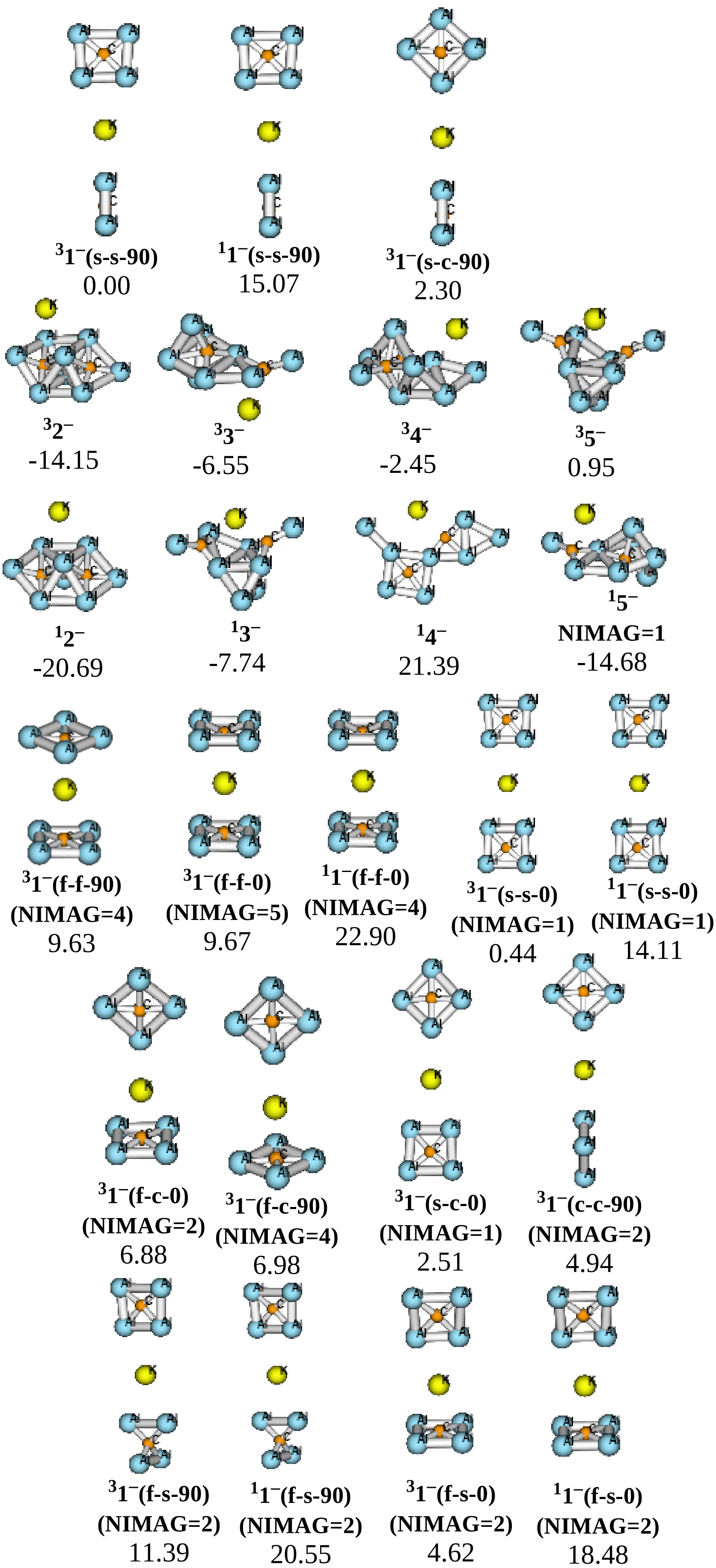
^{3}1(s-c-0) (NIMAG=1) 1.90

^{3}1(c-c-0) (NIMAG=1) 3.93

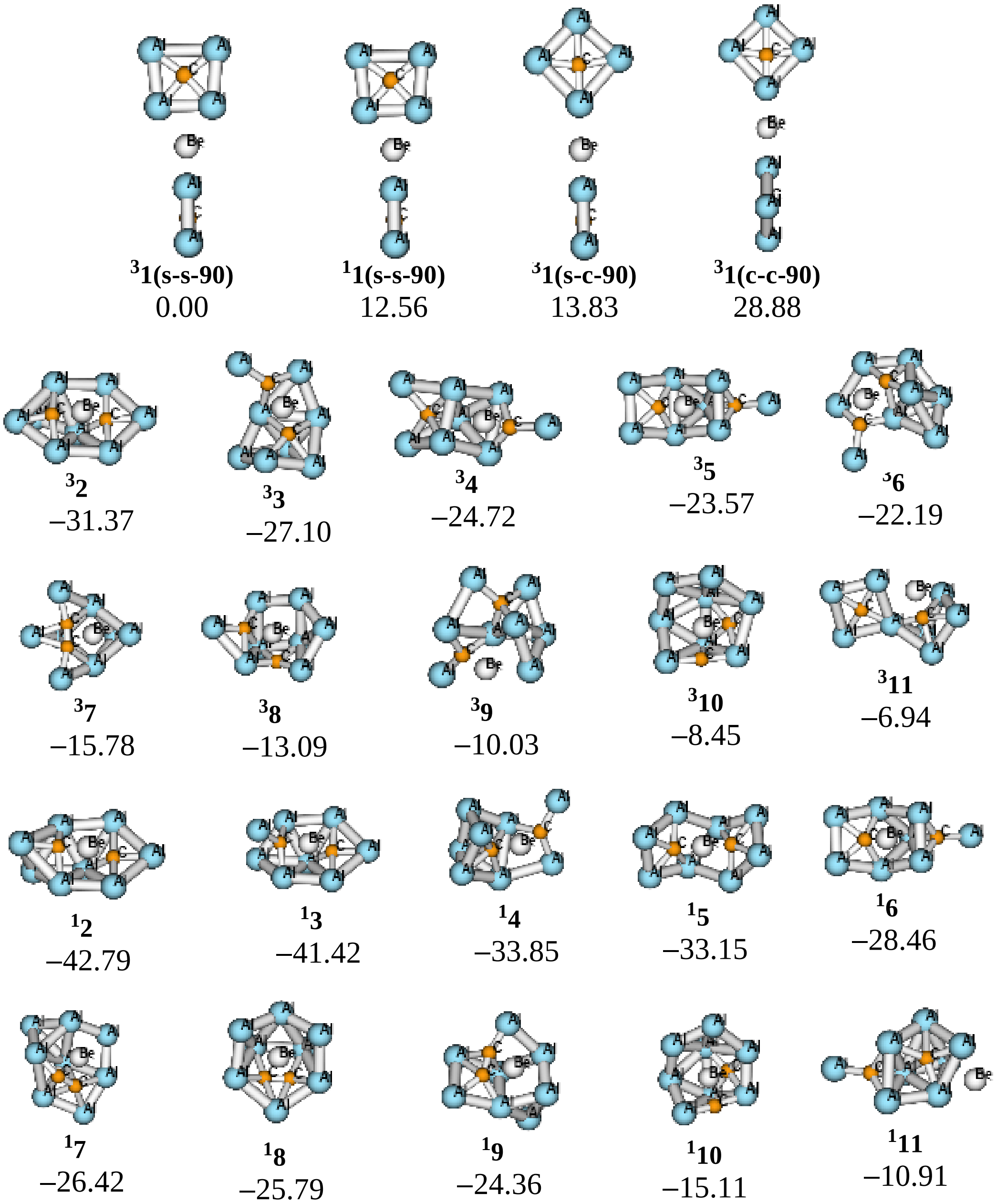
2. The calculated properties of $C_2Al_8Na^-$



3. The calculated properties of $C_2Al_8K^-$


$^{3}1^{-}$(s-s-90)
0.00
$^{1}1^{-}$(s-s-90)
15.07
$^{3}1^{-}$(s-c-90)
2.30
$^{3}2^{-}$
-14.15
$^{3}3^{-}$
-6.55
$^{3}4^{-}$
-2.45
$^{3}5^{-}$
0.95
$^{1}2^{-}$
-20.69
$^{1}3^{-}$
-7.74
$^{1}4^{-}$
21.39
$^{1}5^{-}$
NIMAG=1
-14.68
$^{3}1^{-}$(f-f-90)
(NIMAG=4)
9.63
$^{3}1^{-}$(f-f-0)
(NIMAG=5)
9.67
$^{1}1^{-}$(f-f-0)
(NIMAG=4)
22.90
$^{3}1^{-}$(s-s-0)
(NIMAG=1)
0.44
$^{1}1^{-}$(s-s-0)
(NIMAG=1)
14.11
$^{3}1^{-}$(f-c-0)
(NIMAG=2)
6.88
$^{3}1^{-}$(f-c-90)
(NIMAG=4)
6.98
$^{3}1^{-}$(s-c-0)
(NIMAG=1)
2.51
$^{3}1^{-}$(c-c-90)
(NIMAG=2)
4.94
$^{3}1^{-}$(f-s-90)
(NIMAG=2)
11.39
$^{1}1^{-}$(f-s-90)
(NIMAG=2)
20.55
$^{3}1^{-}$(f-s-0)
(NIMAG=2)
4.62
$^{1}1^{-}$(f-s-0)
(NIMAG=2)
18.48

4. The calculated properties of C_2Al_8Be



^{3}**1(s-s-90)** 0.00; ^{1}**1(s-s-90)** 12.56; ^{3}**1(s-c-90)** 13.83; ^{3}**1(c-c-90)** 28.88

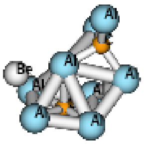
^{3}**2** –31.37; ^{3}**3** –27.10; ^{3}**4** –24.72; ^{3}**5** –23.57; ^{3}**6** –22.19

^{3}**7** –15.78; ^{3}**8** –13.09; ^{3}**9** –10.03; ^{3}**10** –8.45; ^{3}**11** –6.94

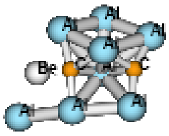
^{1}**2** –42.79; ^{1}**3** –41.42; ^{1}**4** –33.85; ^{1}**5** –33.15; ^{1}**6** –28.46

^{1}**7** –26.42; ^{1}**8** –25.79; ^{1}**9** –24.36; ^{1}**10** –15.11; ^{1}**11** –10.91

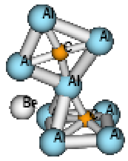
Supplementary Material (ESI) for PCCP



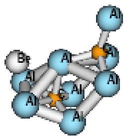
^{3}**12**
–0.77



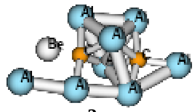
^{3}**13**
0.34



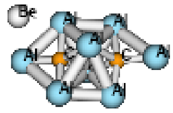
^{3}**14**
0.38



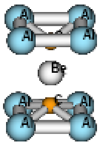
^{3}**15**
2.39



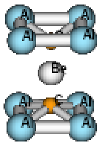
^{3}**16**
3.78



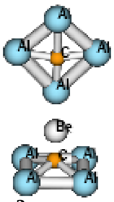
^{3}**17**
18.35



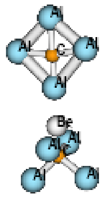
^{3}1(f-f-0)
(NIMAG=5)
0.24



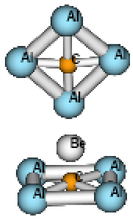
^{1}1(f-f-0)
(NIMAG=5)
5.61



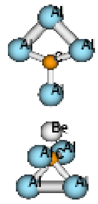
^{3}1(f-c-0)
(NIMAG=3)
11.28



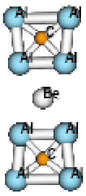
^{3}1(f-c-90)
(NIMAG=2)
17.87



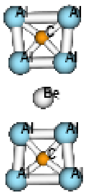
^{1}1(f-c-0)
(NIMAG=5)
33.44



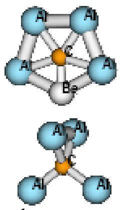
^{1}1(f-c-90)
(NIMAG=3)
20.19



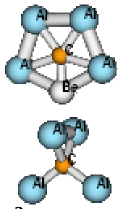
^{1}1(s-s-0)
(NIMAG=2)
20.76



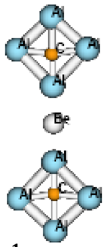
^{3}1(s-s-0)
(NIMAG=1)
11.56



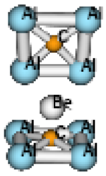
^{1}1(f-s-90)
(NIMAG=3)
7.70



^{3}1(f-s-90)
(NIMAG=4)
10.81

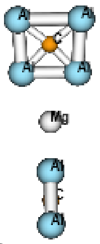


^{1}1(c-c-0)
(NIMAG=1)
33.83

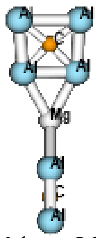


^{1}1(f-s-0)
(NIMAG=5)
7.66

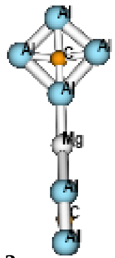
5. The calculated properties of C_2Al_8Mg



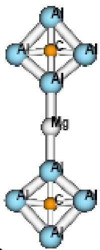
^{3}**1(s-s-90)**
0.00



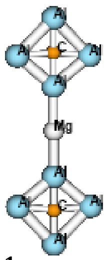
^{1}**1(s-s-90)**
13.14



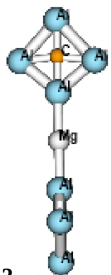
^{3}**1(s-c-90)**
10.66



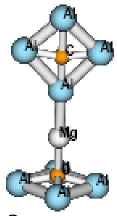
^{3}**1(c-c-0)**
(NIMAG=3)
21.75



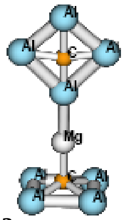
^{1}**1(c-c-0)**
(NIMAG=3)
34.09



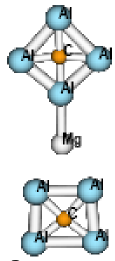
^{3}**1(c-c-90)**
(NIMAG=2)
21.28



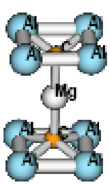
^{3}**1(f-c-90)**
(NIMAG=3)
22.78



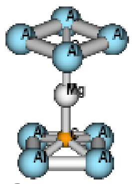
^{3}**1(f-c-0)**
(NIMAG=2)
22.78



^{3}**1(s-c-0)**
(NIMAG=2)
11.14

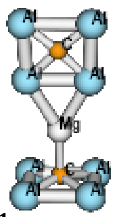


^{3}**1(f-f-0)**
(NIMAG=5)
22.72

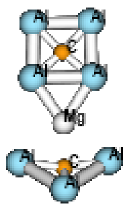


^{3}**1(f-f-90)**
(NIMAG=4)
22.53

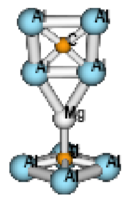
^{1}**1(s-s-0)**
(NIMAG=1)
15.31



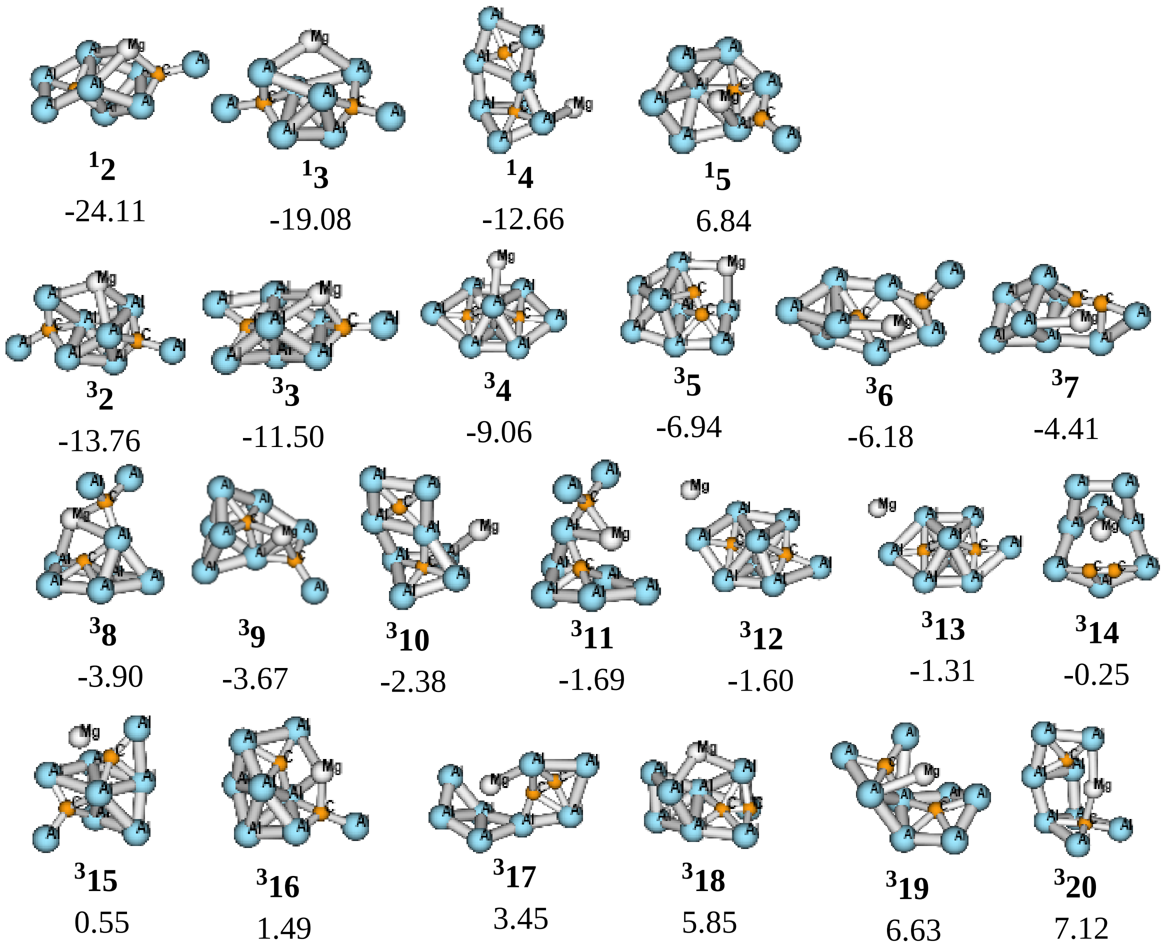
^{1}**1(f-s-0)**
(NIMAG=3)
22.01



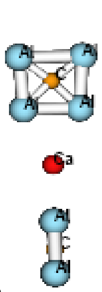
28.90
^{1}**1(f-s-90)**
(NIMAG=3)
28.90



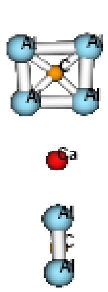
^{3}**1(f-s-90)**
(NIMAG=2)
10.63


^{1}**2** -24.11
^{1}**3** -19.08
^{1}**4** -12.66
^{1}**5** 6.84
^{3}**2** -13.76
^{3}**3** -11.50
^{3}**4** -9.06
^{3}**5** -6.94
^{3}**6** -6.18
^{3}**7** -4.41
^{3}**8** -3.90
^{3}**9** -3.67
^{3}**10** -2.38
^{3}**11** -1.69
^{3}**12** -1.60
^{3}**13** -1.31
^{3}**14** -0.25
^{3}**15** 0.55
^{3}**16** 1.49
^{3}**17** 3.45
^{3}**18** 5.85
^{3}**19** 6.63
^{3}**20** 7.12

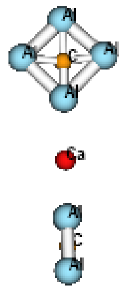
6. The calculated properties of C_2Al_8Ca



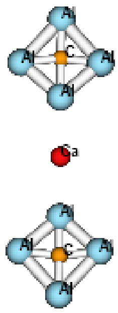
^{3}1(s-s-90)
0.00



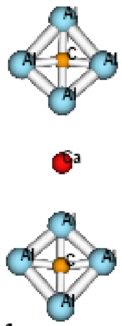
^{1}1(s-s-90)
13.26



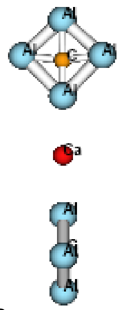
^{3}1(s-c-90)
11.25



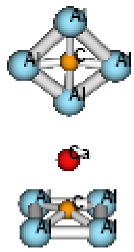
^{3}1(c-c-0)
(NIMAG=3)
21.15



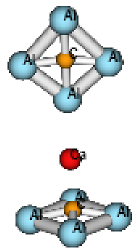
^{1}1(c-c-0)
(NIMAG=3)
35.34



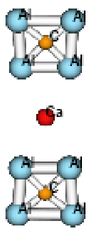
^{3}1(c-c-90)
(NIMAG=2)
23.66



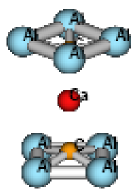
^{3}1(f-c-0)
(NIMAG=4)
22.22



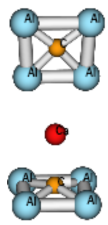
^{3}1(f-c-90)
(NIMAG=4)
22.21



^{1}1(s-c-0)
(NIMAG=1)
13.87



^{3}1(f-f-90)
(NIMAG=4)
22.87

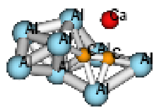


^{1}1(f-s-0)
(NIMAG=2)
24.26

^{1}1(f-s-90)
(NIMAG=1)
17.44

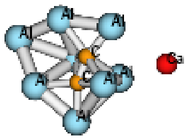
^{3}1(f-s-90)
(NIMAG=2)
9.02

Supplementary Material (ESI) for PCCP



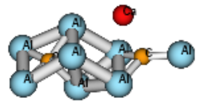
^{3}**2**

-17.58



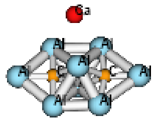
^{3}**3**

-12.13



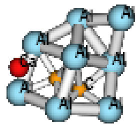
^{3}**4**

-11.48



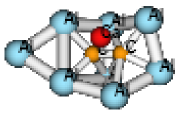
^{3}**5**

-9.66



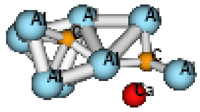
^{3}**6**

-9.62



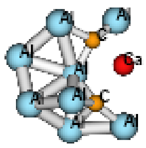
^{3}**7**

-9.34



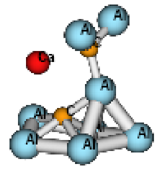
^{3}**8**

-7.10



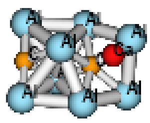
^{3}**9**

-5.30



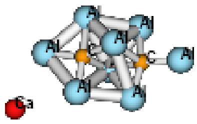
^{3}**10**

-4.39



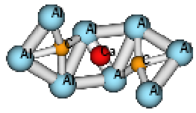
^{3}**11**

-3.73



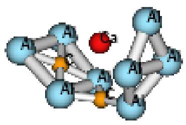
^{3}**12**

-3.45



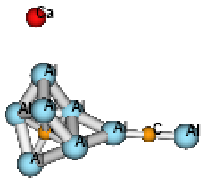
^{3}**13**

2.07



^{3}**14**

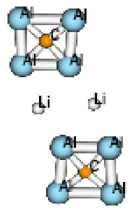
27.22



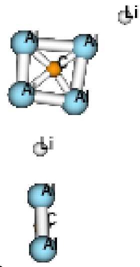
^{3}**15**

47.30

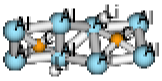
7. The calculated properties of $C_2Al_8Li_2$



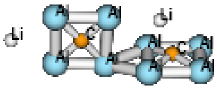
^{3}**1(s-s-0)**
0.00



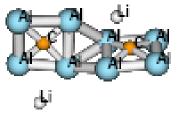
^{3}**1(s-s-90)**
22.84



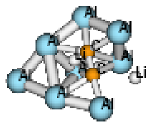
^{1}**2**
–33.58



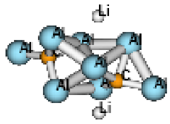
^{1}**3**
–31.56



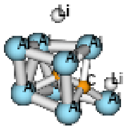
^{1}**4**
–27.55



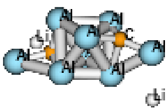
^{1}**5**
–27.35



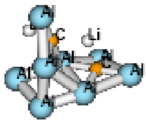
^{1}**6**
–27.14



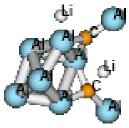
^{1}**7**
–25.86



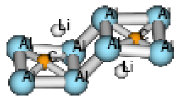
^{1}**8**
–25.42



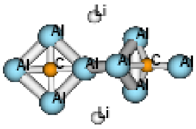
^{1}**9**
–19.29



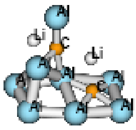
^{1}**10**
–17.65



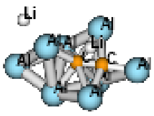
^{1}**11**
–16.39



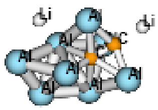
^{1}**12**
–16.26



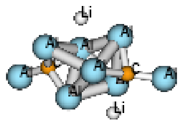
^{1}**13**
–12.45



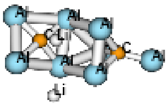
^{3}**2**
–20.69



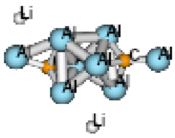
^{3}**3**
–19.13



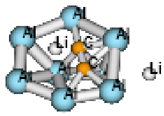
^{3}**4**
–19.01



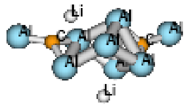
^{3}**5**
–17.05



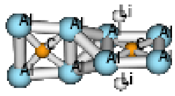
^{3}**6**
–15.42



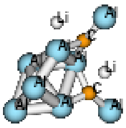
^{3}**7**
–15.10



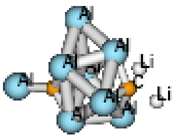
^{3}**8**
–14.52



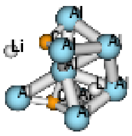
^{3}**9**
–12.64



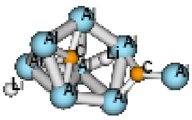
^{3}**10**
–11.67



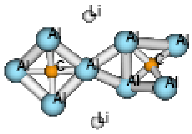
^{3}**11**
–11.42



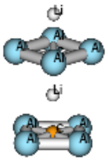
^{3}**12**
–8.14



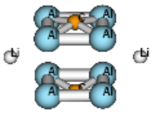
^{3}**13**
–7.65



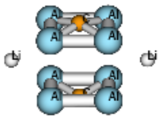
^{3}**14**
–6.66



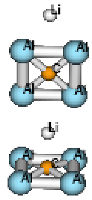
^{3}1(f-f-90)
(NIMAG=7)
36.76



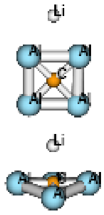
^{3}1(f-f-0)
(NIMAG=4)
9.52



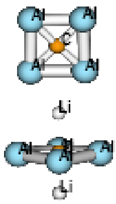
^{1}1(f-f-0)
(NIMAG=4)
14.23



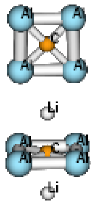
^{3}1(f-s-0)
(NIMAG=4)
22.60



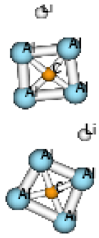
^{3}1(f-s-90)
(NIMAG=5)
21.57



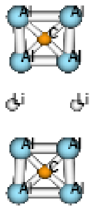
^{3}1(f-s-90)
(NIMAG=5)
40.77



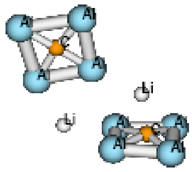
^{3}1(f-s-0)
(NIMAG=6)
40.89



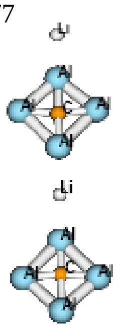
^{3}1(s-c-0)
(NIMAG=1)
12.38



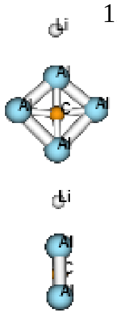
^{3}1(s-s-0)
(NIMAG=1)
1.11



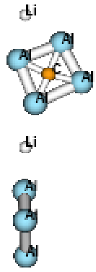
^{3}1(f-s-90)
(NIMAG=2)
-0.57



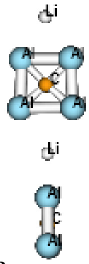
^{3}1(c-c-0)
(NIMAG=1)
28.17



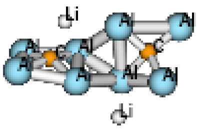
^{3}1(s-c-90)
(NIMAG=1)
22.76



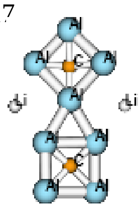
^{3}1(c-c-90)
(NIMAG=1)
20.70



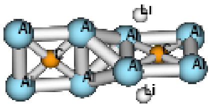
^{3}1(s-s-90)
(NIMAG=2)
18.65



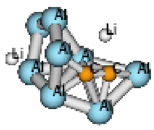
^{1}14
(NIMAG=1)
-26.76



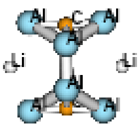
^{1}15
(NIMAG=2)
-20.60



^{1}16
(NIMAG=1)
-18.31

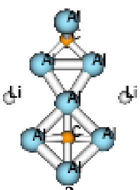


^{1}17
(NIMAG=1)
-17.15

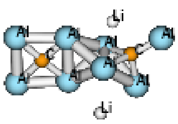


^{1}18
(NIMAG=5)
15.61

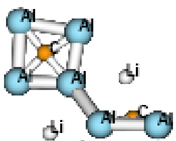
^{3}15
(NIMAG=2)
-9.80



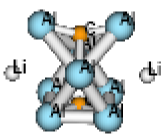
^{3}16
(NIMAG=2)
-6.16



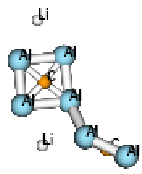
^{3}17
(NIMAG=1)
-4.68



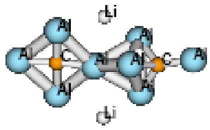
^{3}18
(NIMAG=1)
-3.65



^{3}19
(NIMAG=2)
-1.38

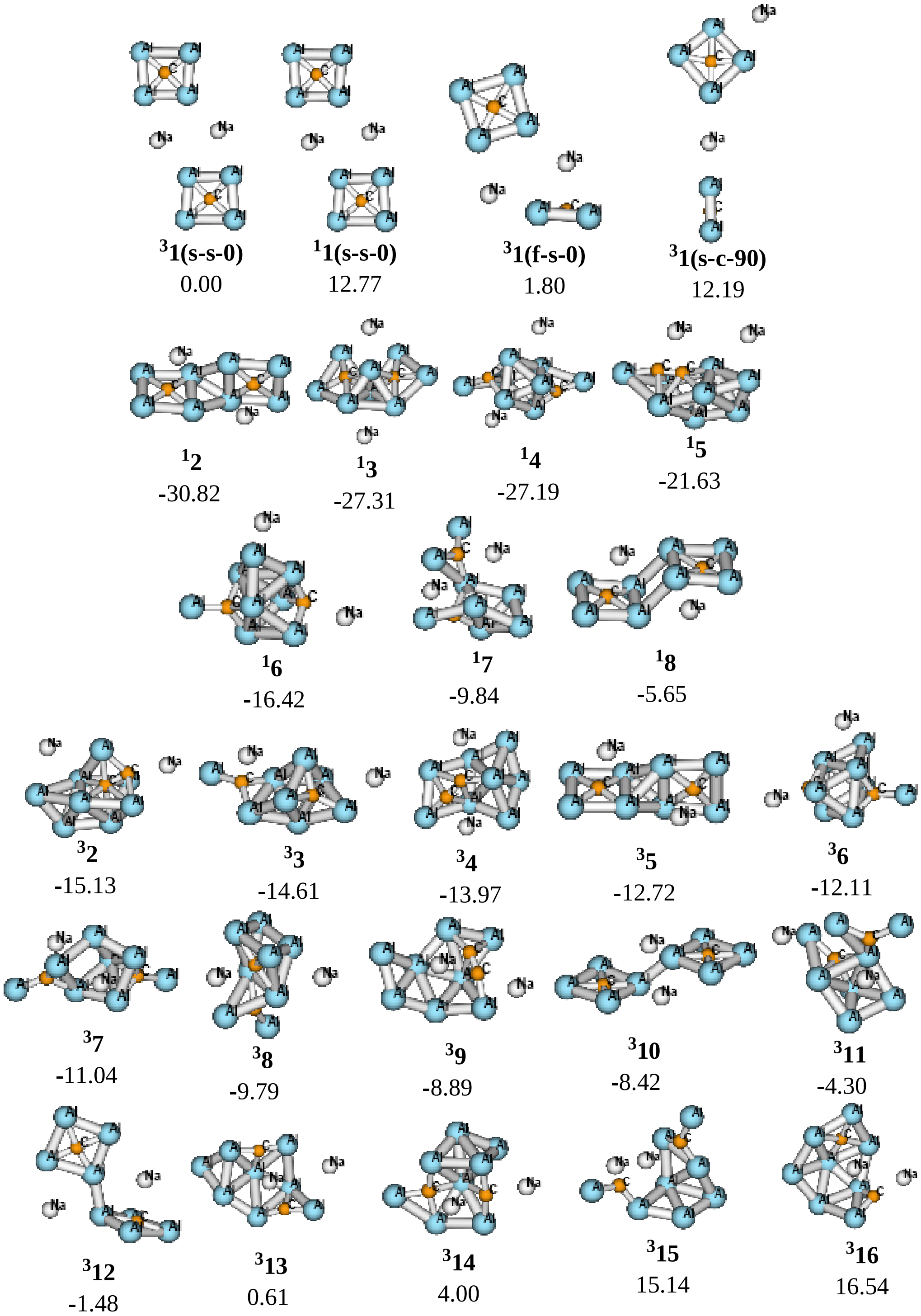


^{3}20
(NIMAG=1)
0.84



^{3}21
(NIMAG=2)
0.96

8. The calculated properties of $C_2Al_8Na_2$



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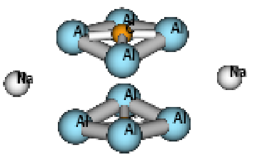
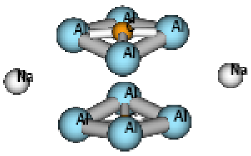
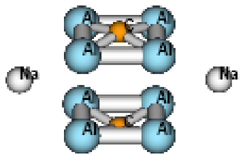


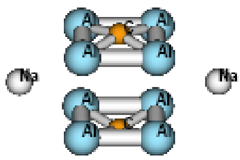
^{1}1(f-f-0)
(NIMAG=5)
14.54



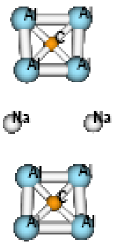
^{3}1(f-f-0)
(NIMAG=5)
7.55



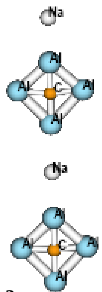
^{3}1(f-f-0)
(NIMAG=6)
9.14



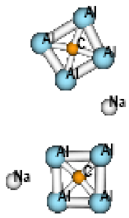
^{1}1(f-f-0)
(NIMAG=4)
17.80



^{3}1(s-s-0)
(NIMAG=1)
0.76

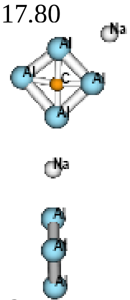


^{3}1(c-c-0)
(NIMAG=2)
23.03

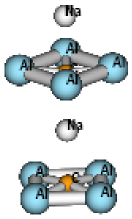


^{3}1(s-c-0)
(NIMAG=1)
12.13

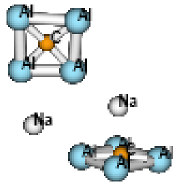
^{3}1(s-c-90)
(NIMAG=2)
18.09



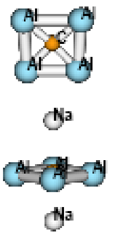
^{3}1(c-c-90)
(NIMAG=1)
17.12



^{3}1(f-f-90)
(NIMAG=6)
35.35

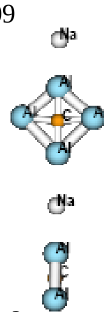


^{3}1(f-s-90)
(NIMAG=1)
4.76

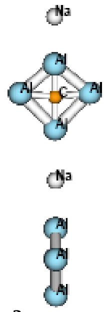


^{3}1(f-s-90)
(NIMAG=3)
28.71

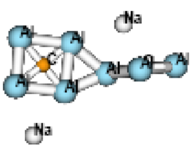
^{3}1(f-s-0)
(NIMAG=4)
28.74



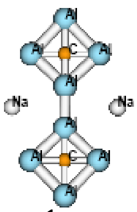
^{3}1(s-c-90)
(NIMAG=1)
18.30



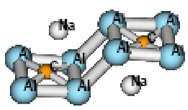
^{3}1(c-c-90)
(NIMAG=2)
23.26



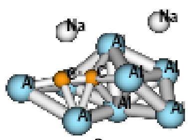
^{1}9
(NIMAG=1)
-17.89



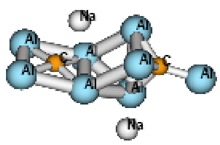
^{1}10
(NIMAG=3)
-11.94



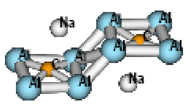
^{3}11
(NIMAG=2)
-1.51



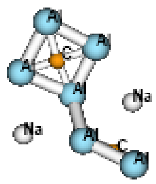
^{3}17
(NIMAG=1)
-16.85



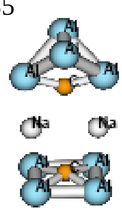
^{3}18
(NIMAG=1)
-13.60



^{3}19
(NIMAG=1)
-5.36

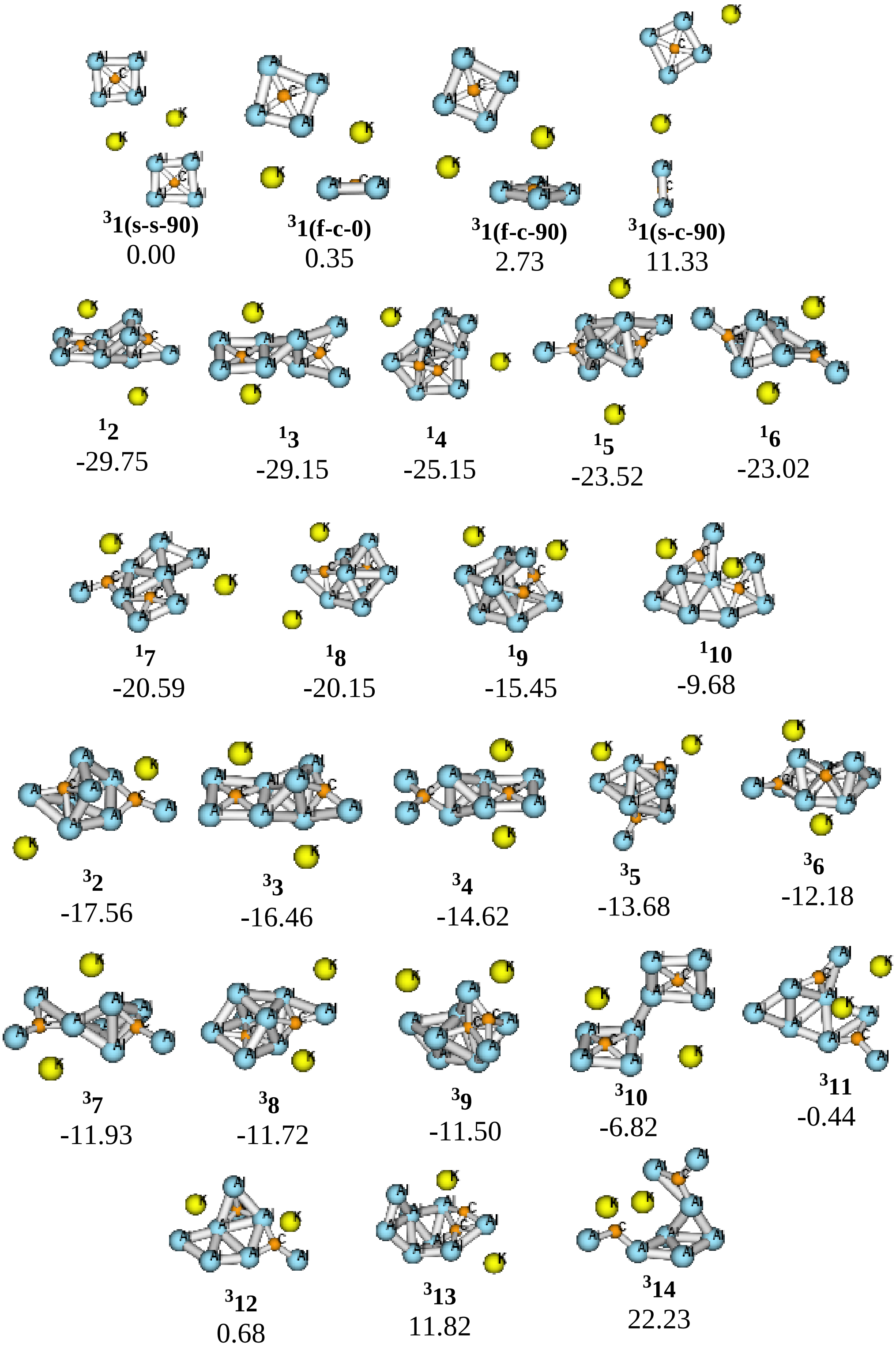


^{3}20
(NIMAG=1)
-3.19



^{3}21
(NIMAG=7)
59.32

9. The calculated properties of $C_2Al_8K_2$



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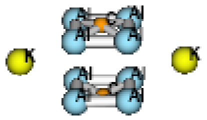
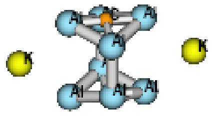
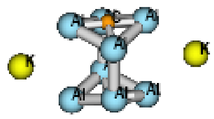


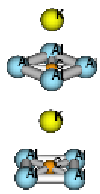
^{3}1(f-f-0)
(NIMAG=7)
9.74



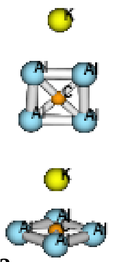
^{3}1
(NIMAG=5)
5.85



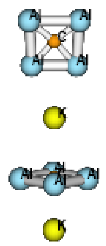
^{1}1
(NIMAG=5)
12.53



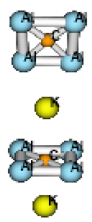
^{3}1(f-f-90)
(NIMAG=4)
29.47



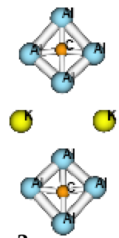
^{3}1(f-s-90)
(NIMAG=3)
18.75



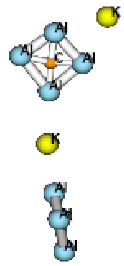
^{3}1(f-s-90)
(NIMAG=2)
24.54



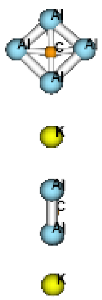
^{3}1(f-s-0)
(NIMAG=2)
24.54



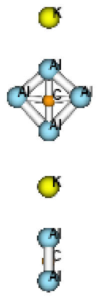
^{3}1(c-c-0)
(NIMAG=2)
1.37



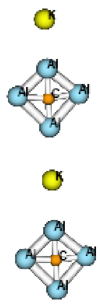
^{3}1(c-c-90)
(NIMAG=2)
15.79



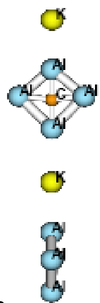
^{3}1(s-c-90)
(NIMAG=1)
16.53



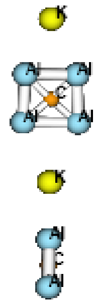
^{3}1(s-c-90)
(NIMAG=1)
16.11



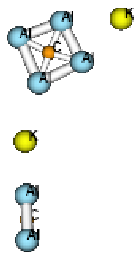
^{3}1(c-c-0)
(NIMAG=2)
20.49



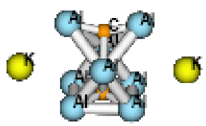
^{3}1(c-c-90)
(NIMAG=2)
20.47



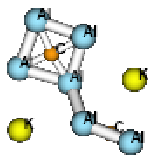
^{3}1(s-s-90)
(NIMAG=1)
12.70



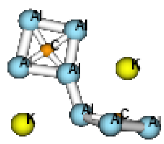
^{3}1(s-c-90)
(NIMAG=1)
11.33



^{1}11
(NIMAG=2)
-17.83



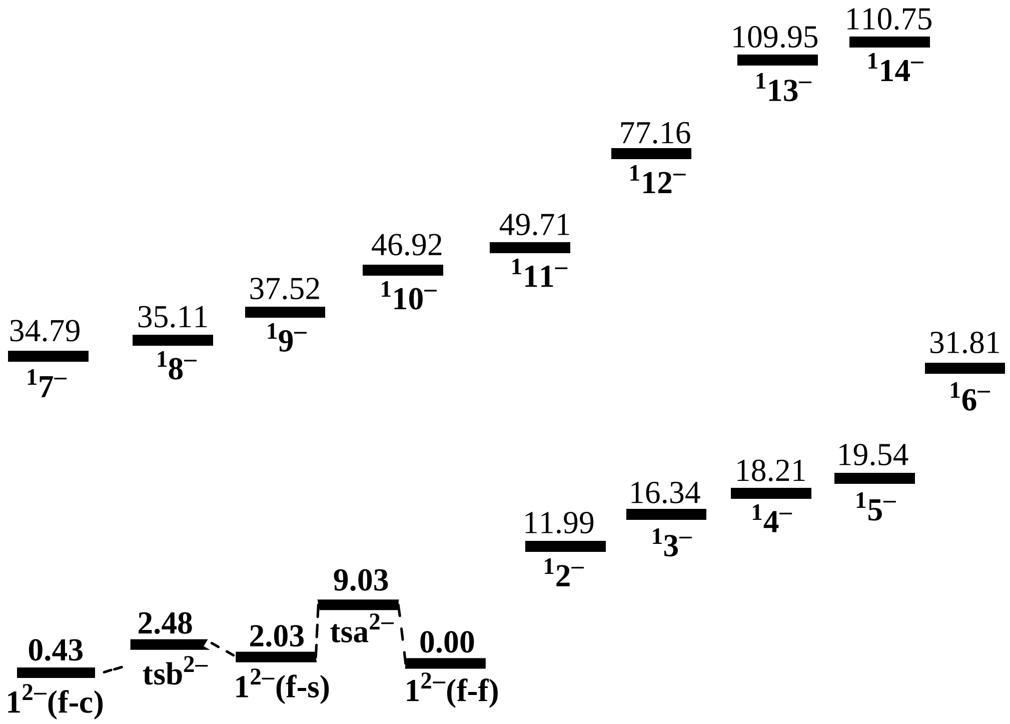
^{3}15
(NIMAG=1)
-6.62



^{3}16
(NIMAG=1)
-5.04

Supplementary Material (ESI) for PCCP

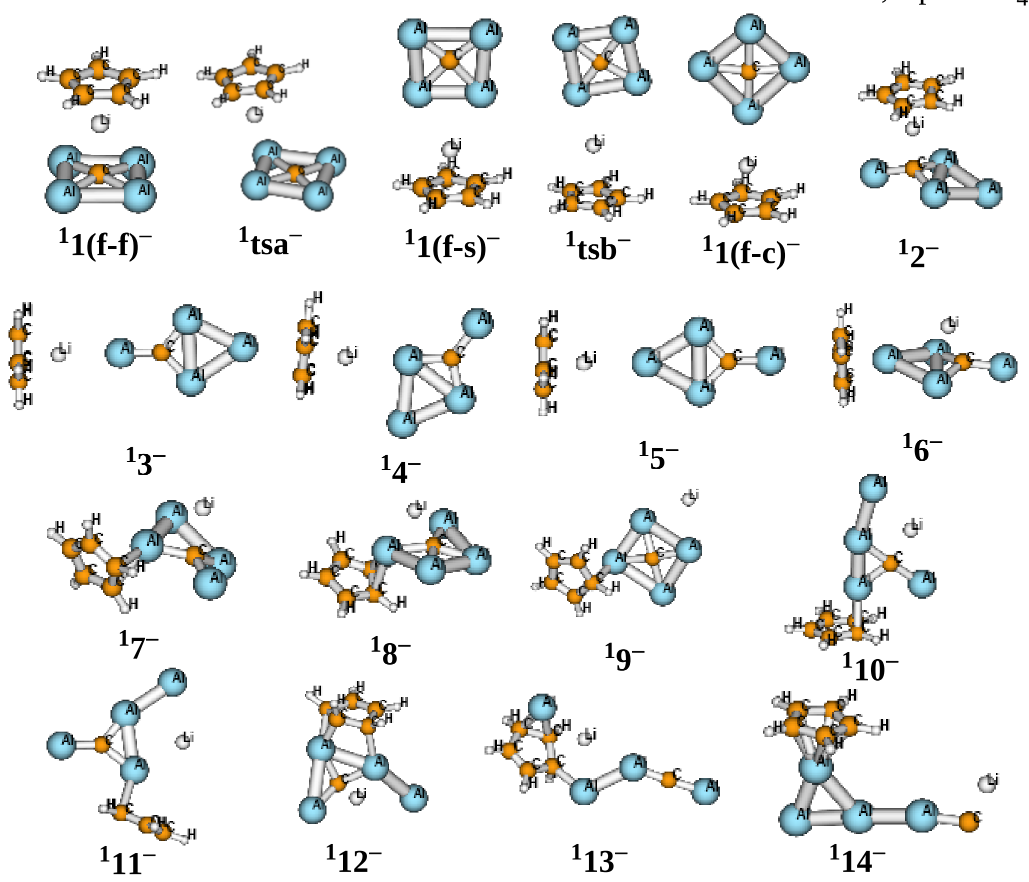
10. The calculated properties of $^{1}CAl_4LiCp^{-}$



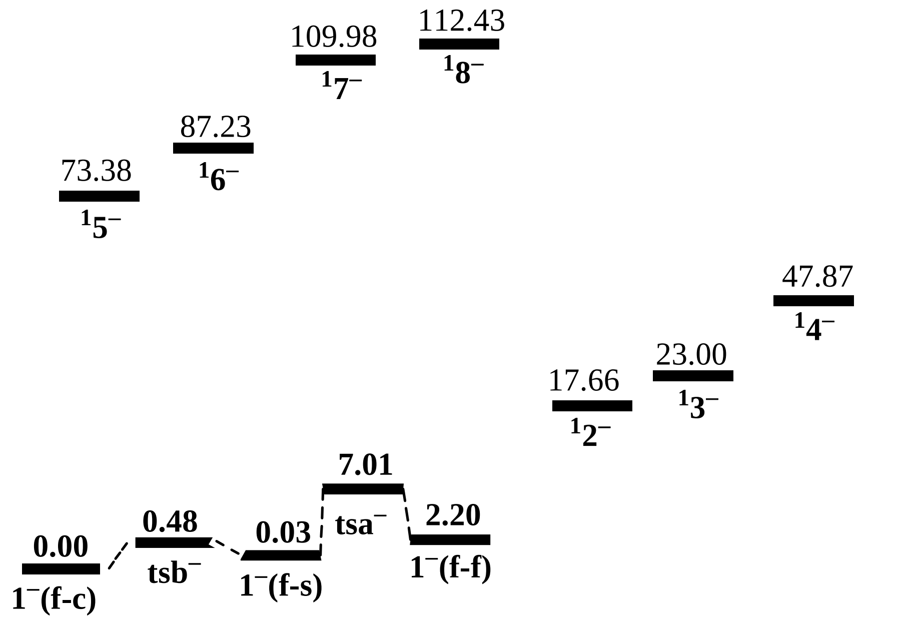
"f-f" stands for face-to-face sandwich form,

"f-s" stands for face-to-side sandwich form,

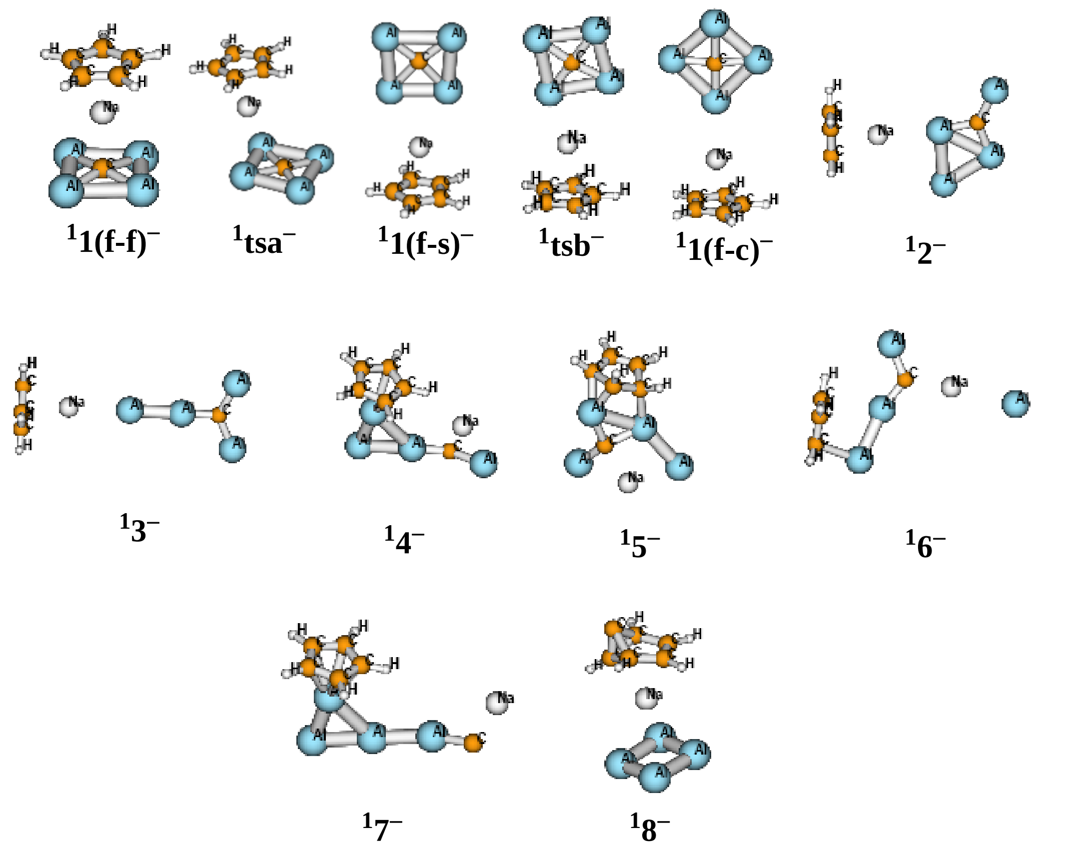
"f-c" stands for face-to-corner sandwich form, $CpLiCAl_4^{-}$



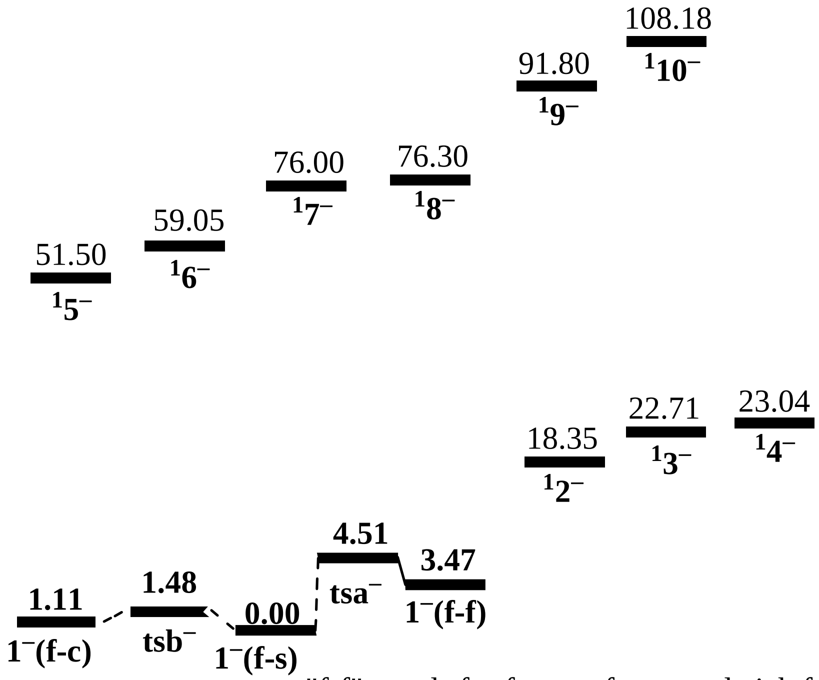
11. The calculated properties of $^{1}CAl_4NaCp^-$



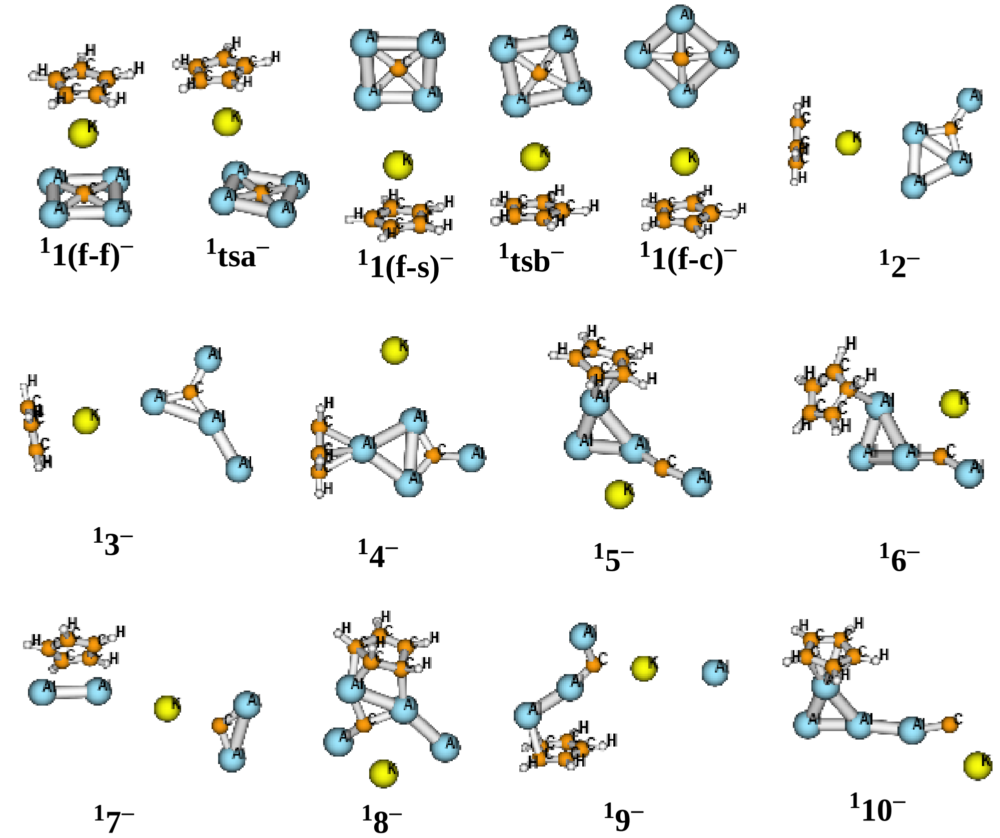
"f-f" stands for face-to-face sandwich form,
"f-s" stands for face-to-side sandwich form,
"f-c" stands for face-to-corner sandwich form, $CpNaCAl_4^-$



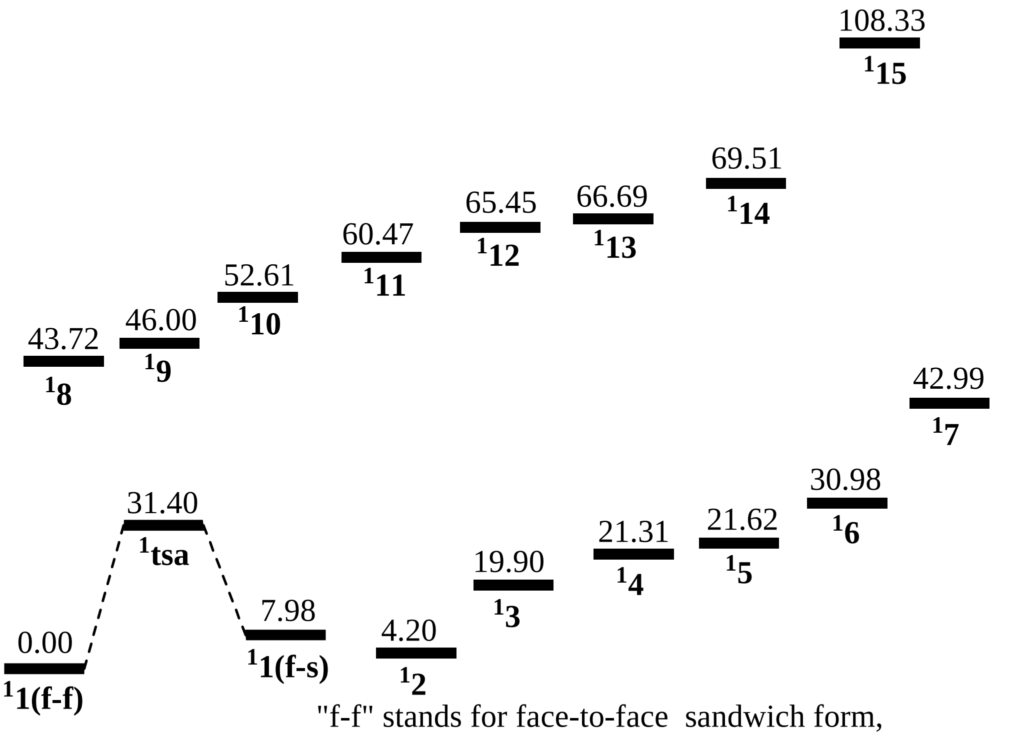
12. The calculated properties of $^{1}CAl_4KCp^{-}$



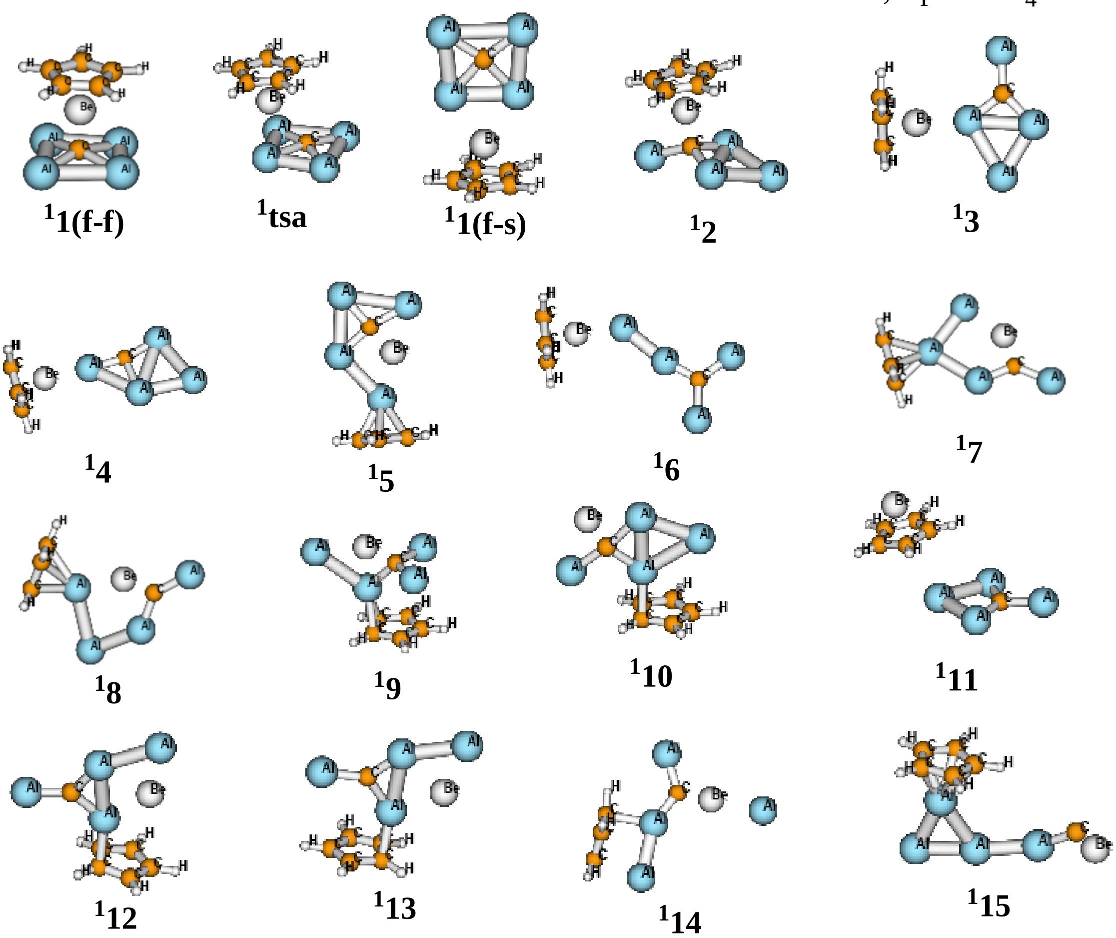
"f-f" stands for face-to-face sandwich form,
"f-s" stands for face-to-side sandwich form,
"f-c" stands for face-to-corner sandwich form, $CpKCAl_4^{-}$



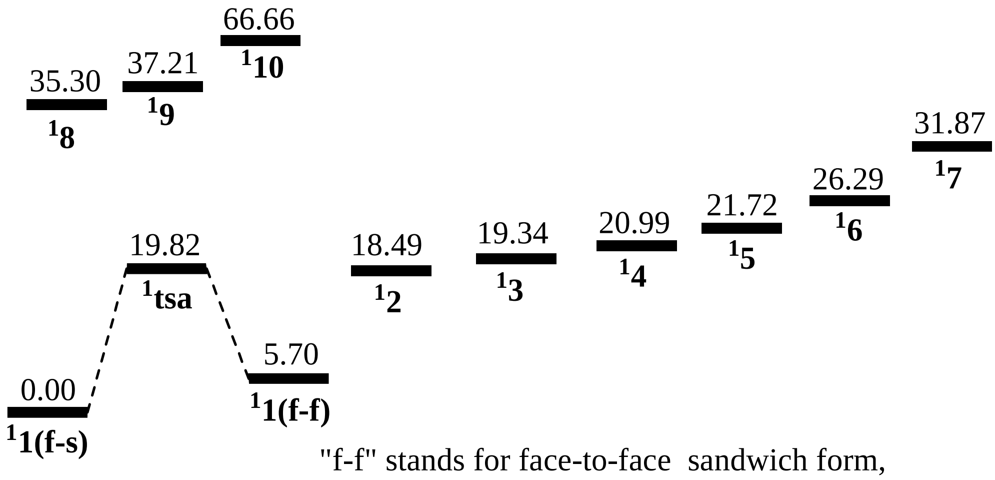
13. The calculated properties of $^{1}CAl_4BeCp$



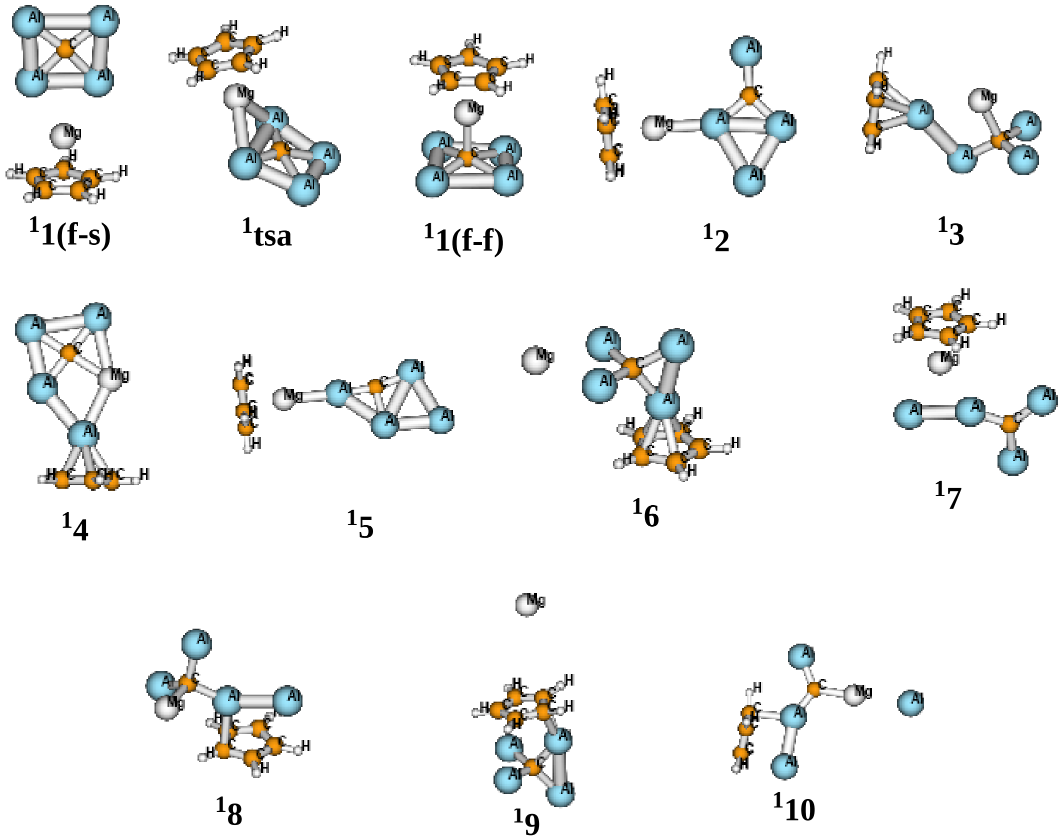
"f-f" stands for face-to-face sandwich form,
"f-s" stands for face-to-side sandwich form, $CpBeCAl_4$



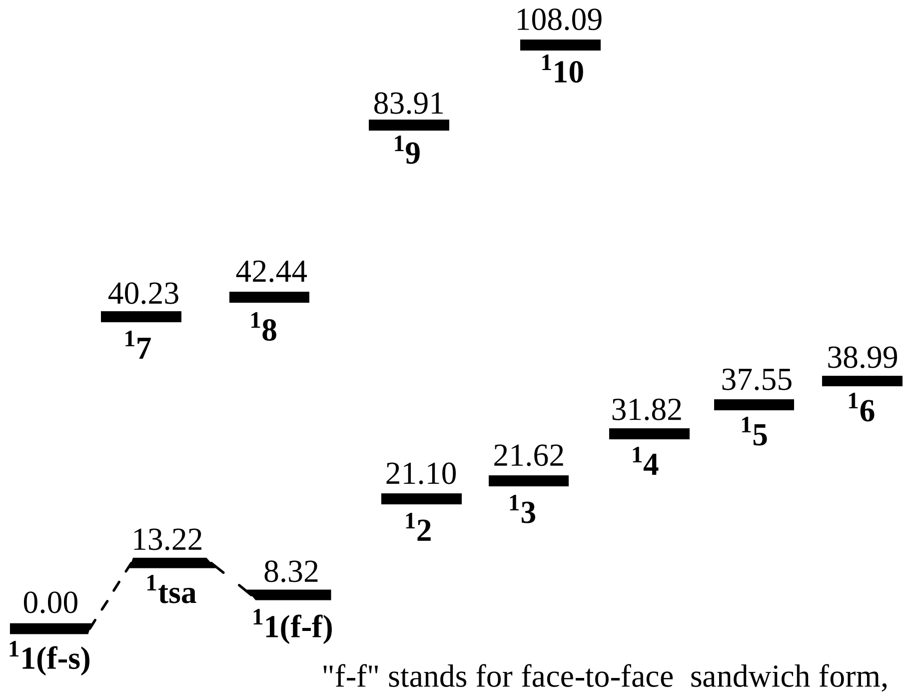
14. The calculated properties of $^{1}CAl_4MgCp$



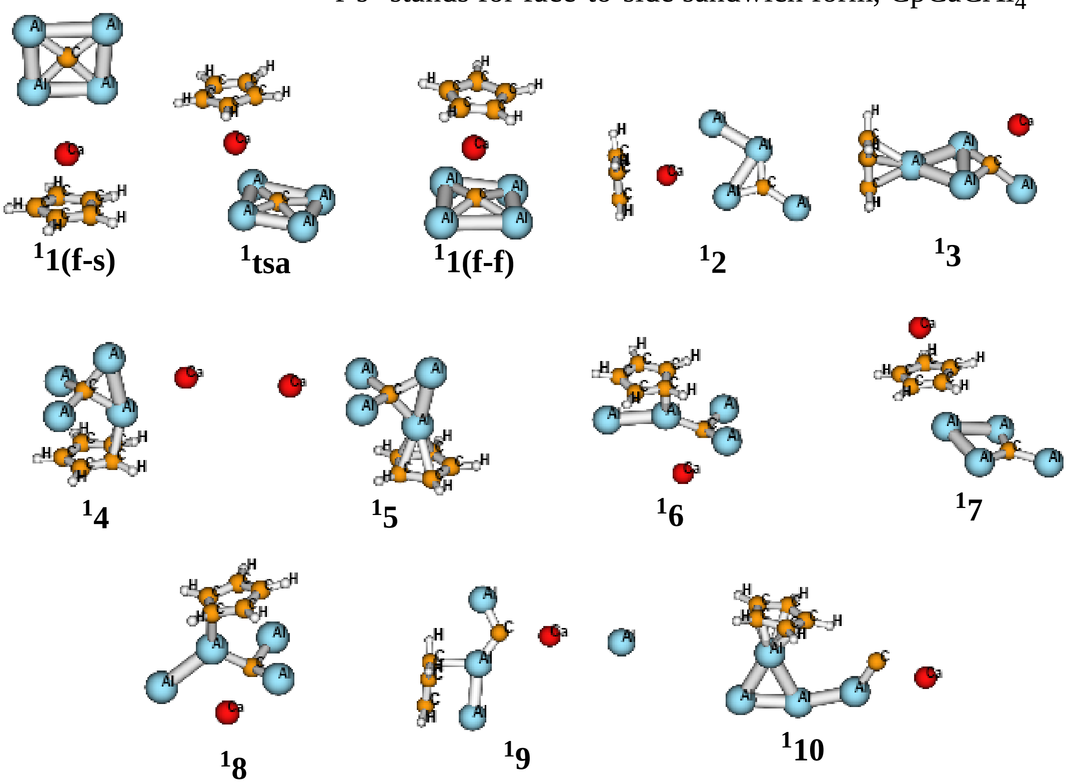
"f-f" stands for face-to-face sandwich form,
"f-s" stands for face-to-side sandwich form, $CpMgCAl_4$



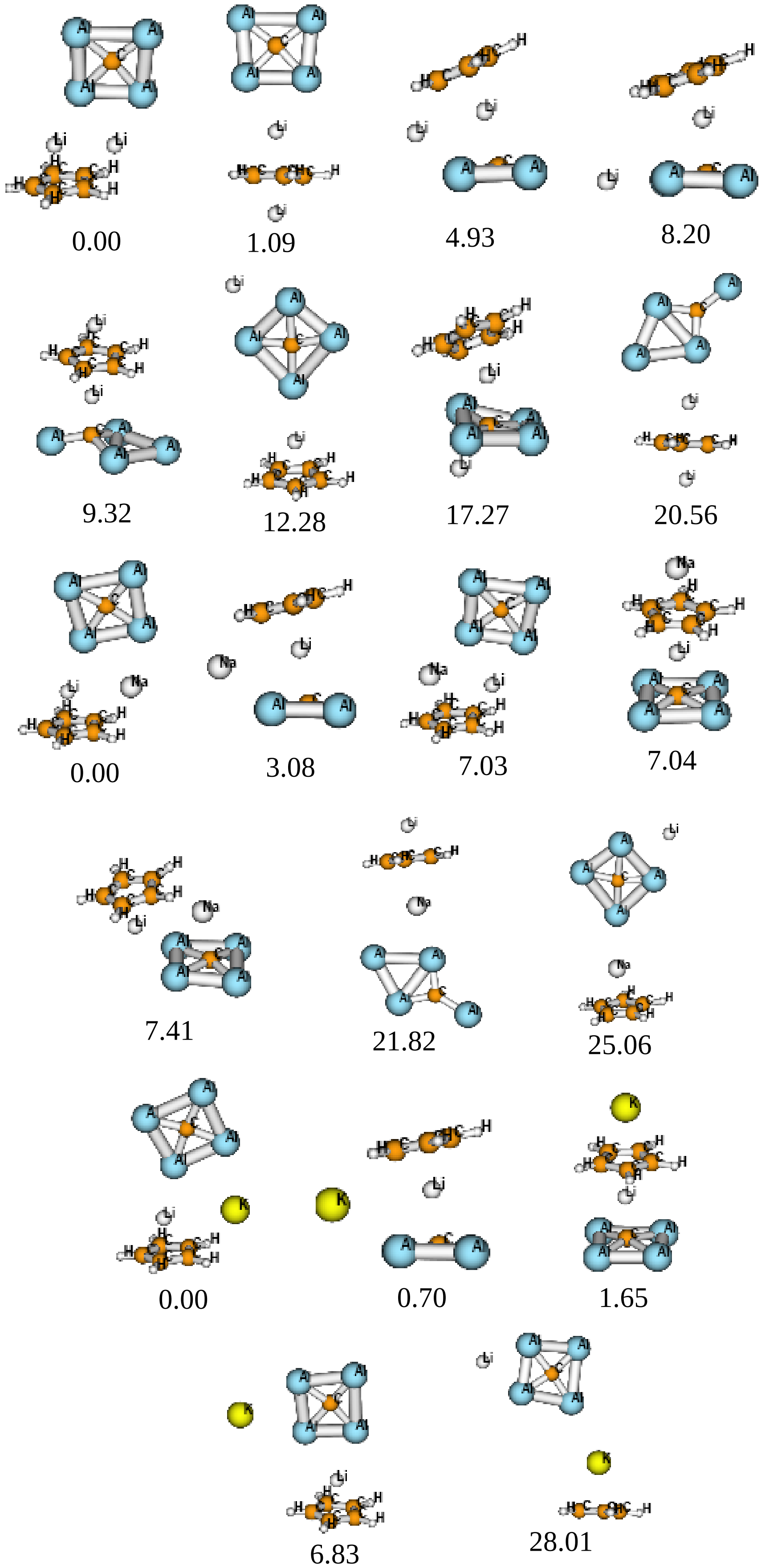
15. The calculated properties of $^{1}CAl_4CaCp$



"f-f" stands for face-to-face sandwich form,
"f-s" stands for face-to-side sandwich form, $CpCaCAl_4$



16. The calculated properties of $(Li)^{+}CAl_4MCp^{-}$ (M=Li, Na, K)



17. The calculated properties of various extend system