Supporting information for:

BAl$_4$Mg$^{-/0/+}$: Global Minima with A Planar Tetracoordinate or Hypercoordinate Boron Atom

Maya Khatun,[†] Saikat Roy,[†] Sandip Giri,[†] Sasanka Sankhar Reddy CH,[‡] Anakuthil Anoop,[*,†] and Venkatesan S. Thimmakondu[*,¶]

[†]Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur 721 302, West Bengal, India.

[‡]Department of Electrical and Electronics Engineering, Birla Institute of Technology and Science, Pilani K K Birla Goa Campus, Goa - 403 726, India.

[¶]Department of Chemistry and Biochemistry, San Diego State University, San Diego, CA 92182-1030, USA.

E-mail: anoop@chem.iitkgp.ac.in; vthimmakondusamy@sdsu.edu

Contents

List of Figures

List of Tables

1a; C_{2v}
0.00 (0.00)
NImag = 0

2a; C_{2v}
0.46 (0.92)*
NImag = 0

3a; C_{2v}
4.47 (10.27)
NImag = 0

4a; C_s
17.08 (15.08)
NImag = 0

5a; C_{2v}
18.50 (21.03)
NImag = 1

6a; C_s
19.57 (20.54)
NImag = 0

7a; C_s
19.85 (16.73)
NImag = 1

8a; C_s
20.08 (15.84)*
NImag = 1

9a; C_s
21.07 (22.77)
NImag = 1

Figure S1: Isomers **1a-9a** of BAl_4Mg^- in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory. Relative energies obtained at the CBS-QB3 level are shown in parentheses.

10a; C_s
21.19
NImag = 1

11a; C_s
23.91
NImag = 0

12a; C_{2v}
25.27
NImag = 3

13a; C_{2v}
31.10
NImag = 0

14a; C_1
32.59
NImag = 0

15a; C_s
39.03
NImag = 0

16a; C_{2v}
39.67
NImag = 2

17a; C_{2v}
40.35
NImag = 2

18a; C_s
45.09
NImag = 0

19a; C_1
46.88
NImag = 0

Figure S2: Isomers **10a-19a** of BAl_4Mg^- in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

20a; C_1
50.03
NImag = 1

21a; C_{2v}
51.89
NImag = 1

22a; C_s
65.08
NImag = 0

23a; C_1
67.03
NImag = 0

24a; C_s
68.05
NImag = 2

25a ; C_1
70.22
NImag = 0

26a; C_{2v}
79.33
NImag = 3

27a; C_{2v}
80.43
NImag = 1

28a; C_{2v}
87.09
NImag = 3

29a; C_{2v}
111.14
NImag = 2

30a; C_{2v}
111.86
NImag = 3

31a; C_{2v}
113.21
NImag = 1

32a; C_{2v}
136.32
NImag = 3

33a; C_{2v}
154.24
NImag = 1

Figure S3: Isomers **20a-33a** of BAl_4Mg^- in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

1n; C_{2v}
0.00 (0.00)
NImag = 0

2n; C_{2v}
0.98 (2.14)
NImag = 0

3n; C_s
5.99 (6.90)
NImag = 0

4n; C_{2v}
6.82 (11.58)
NImag = 0

5n; C_1
10.89 (11.16)
NImag = 0

6n; C_s
14.46 (14.12)
NImag = 0

7n; C_{2v}
15.33 (17.35)
NImag = 0

8n; C_s
16.43 (15.37)
NImag = 0

9n; C_s
18.13 (15.86)
NImag = 0

Figure S4: Isomers **1n**-**9n** of BAl_4Mg in their respective doublet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory. Relative energies obtained at the CBS-QB3 level are shown in parentheses.

10n; C_{2v}
20.99
NImag = 3

11n; C_s
22.04
NImag = 1

12n; C_s
22.11
NImag = 0

13n; C_1
23.04
NImag = 0

14n; C_s
35.13
NImag = 1

15n; C_{2v}
35.42
NImag = 2

16n; C_1
36.94
NImag = 1

17n; C_{3v}
37.74
NImag = 0

18n; C_{2v}
38.73
NImag = 2

19n; C_s
39.33
NImag = 2
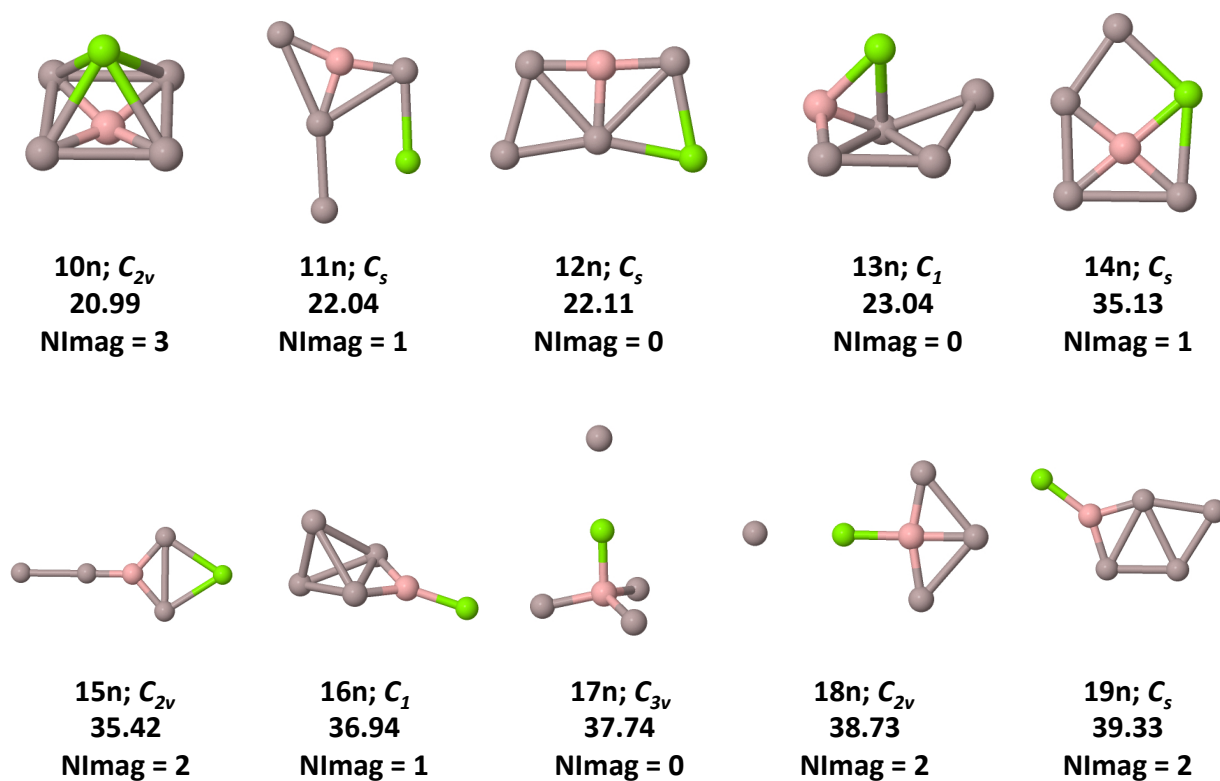
Figure S5: Isomers **10n**-**19n** of BAl_4Mg in their respective doublet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

20n; C_s
47.29
NImag = 1

21n; C_s
50.59
NImag = 2

22n; C_{2v}
53.11
NImag = 1

23n; C_s
53.34
NImag = 1

24n; C_s
53.83
NImag = 0

25n; C_{2v}
54.19
NImag = 0

26n; C_{2v}
64.92
NImag = 4

27n; C_{2v}
71.43
NImag = 0

28n; C_{2v}
85.39
NImag = 4

29n; C_s
101.96
NImag = 1

30n; C_{2v}
104.50
NImag = 3

31n; C_{2v}
110.01
NImag = 2

32n; C_{2v}
120.07
NImag = 2

33n; C_{2v}
121.65
NImag = 1
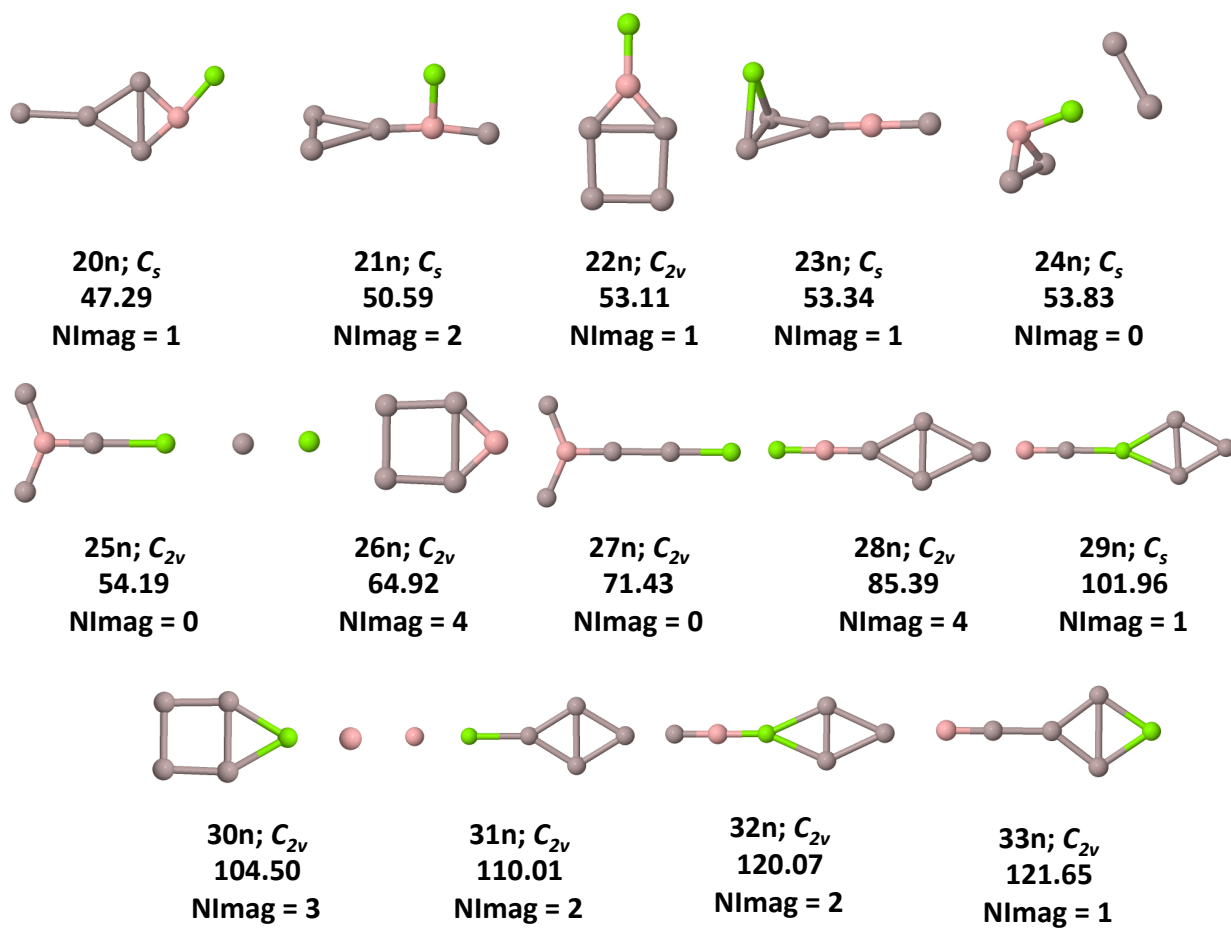
Figure S6: Isomers **20n**-**33n** of BAl$_4$Mg in their respective doublet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

1c; C_{2v}
0.00 (0.00)
NImag = 0

2c; C_s
1.99 (6.72)
NImag = 0

3c; C_{2v}
3.89 (3.09)
NImag = 0

4c; C_s
7.52 (18.66)
NImag = 0

5c; C_{2v}
11.41 (16.80)
NImag = 0

6c; C_s
11.50 (12.50)*
NImag = 0

7c; C_s
14.09 (14.69)
NImag = 0

8c; C_1
14.62 (16.29)*
NImag = 0
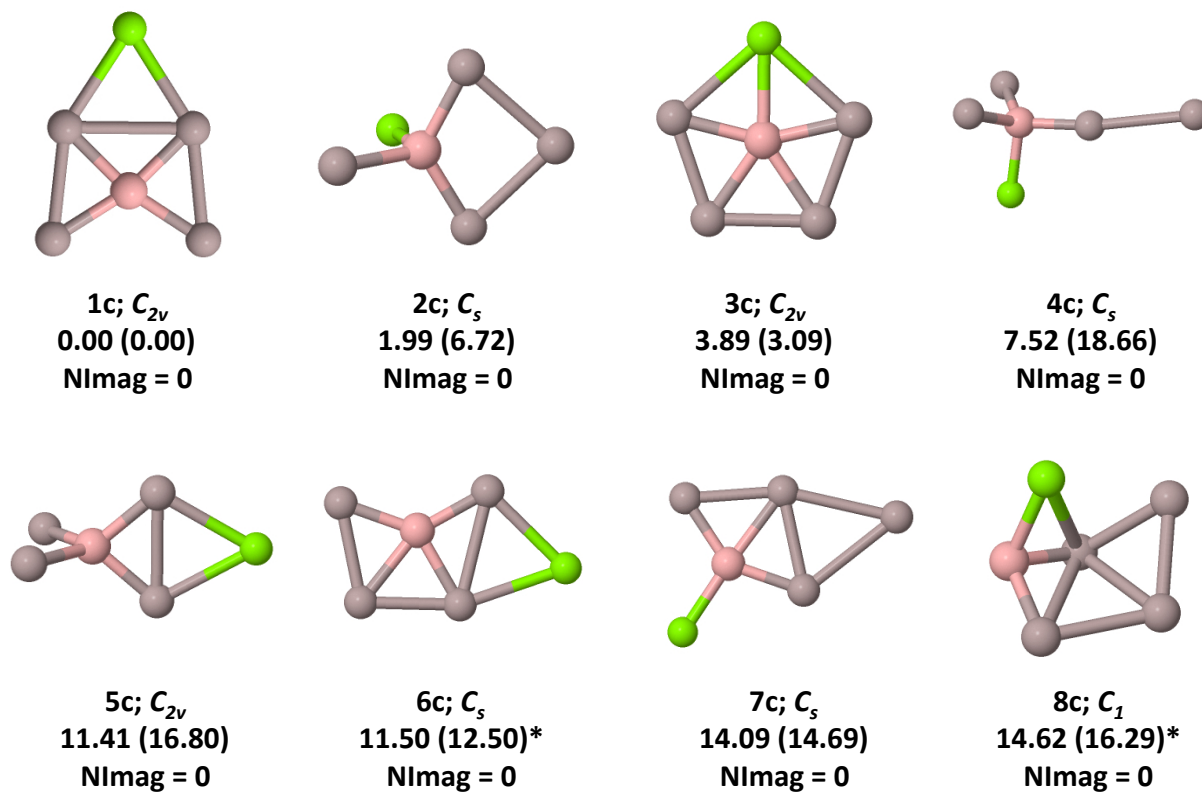
Figure S7: Isomers **1c**-**8c** of BAl_4Mg^+ in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory. Relative energies obtained at the CBS-QB3 level are shown in parentheses.

9c; C_1
14.91
NImag = 0

10c; C_s
15.52
NImag = 0

11c; C_{2v}
16.09
NImag = 0

12c; C_{3v}
16.64
NImag = 0

13c; C_{2v}
18.90
NImag = 2

14c; C_s
19.52
NImag = 0

15c; C_{2v}
19.64
NImag = 1

16c; C_s
21.38
NImag = 0

17c; C_{2v}
23.95
NImag = 1

18c; C_s
27.09
NImag = 0
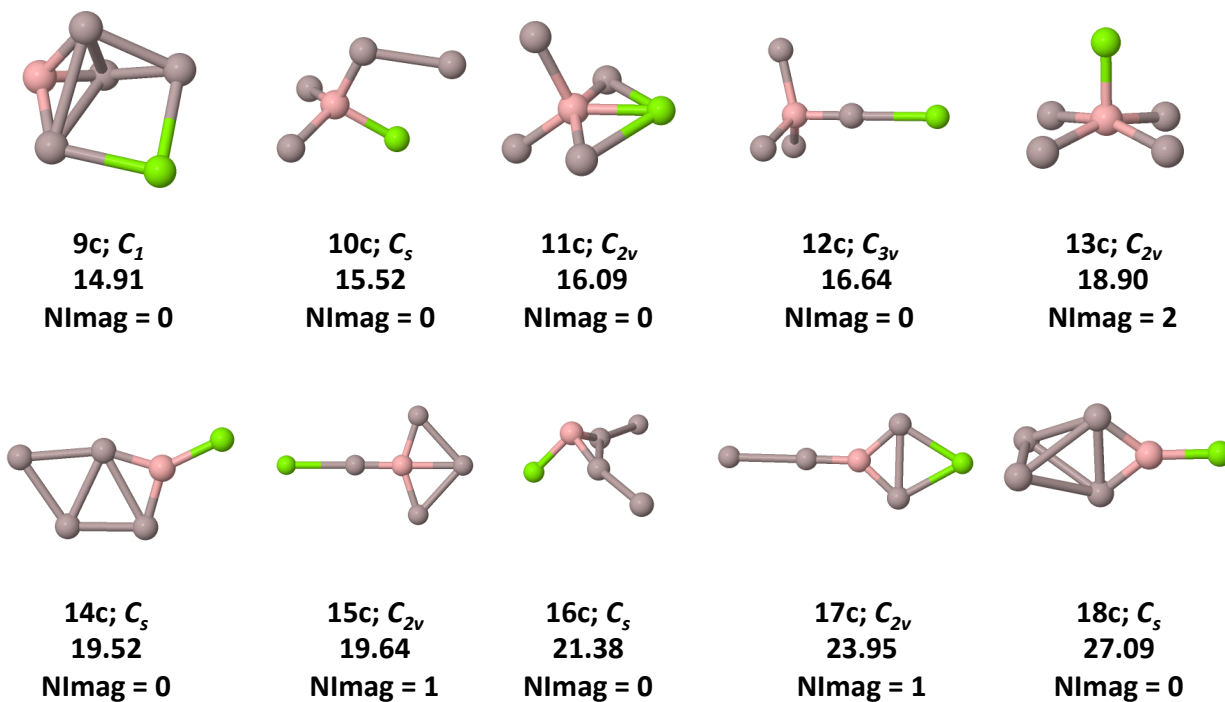
Figure S8: Isomers **9c-18c** of BAl_4Mg^+ in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

19c; C_{2v}
30.44
NImag = 0

20c; C_{2v}
32.47
NImag = 1

21c; C_1
35.34
NImag = 0

22c; C_{2v}
53.88
NImag = 1

23c; C_{3v}
54.22
NImag = 2

24c; C_1
55.68
NImag = 0

25c; C_{2v}
63.50
NImag = 1

26c; C_{2v}
68.60
NImag = 3

27c; C_{2v}
70.36
NImag = 4

28c; C_{2v}
82.48
NImag = 2

29c; C_{2v}
104.37
NImag = 2

30c; C_{2v}
109.81
NImag = 2

31c; C_{2v}
110.64
NImag = 2

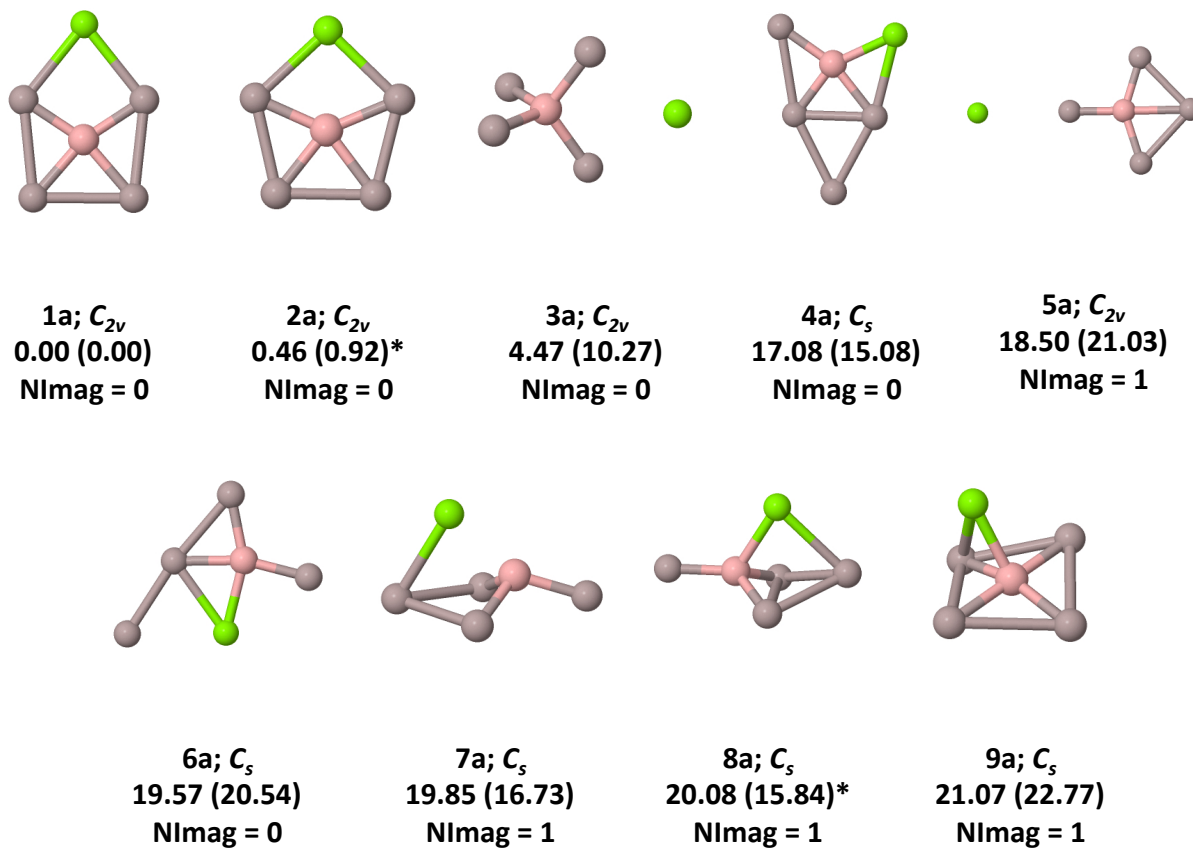32c; C_{2v}
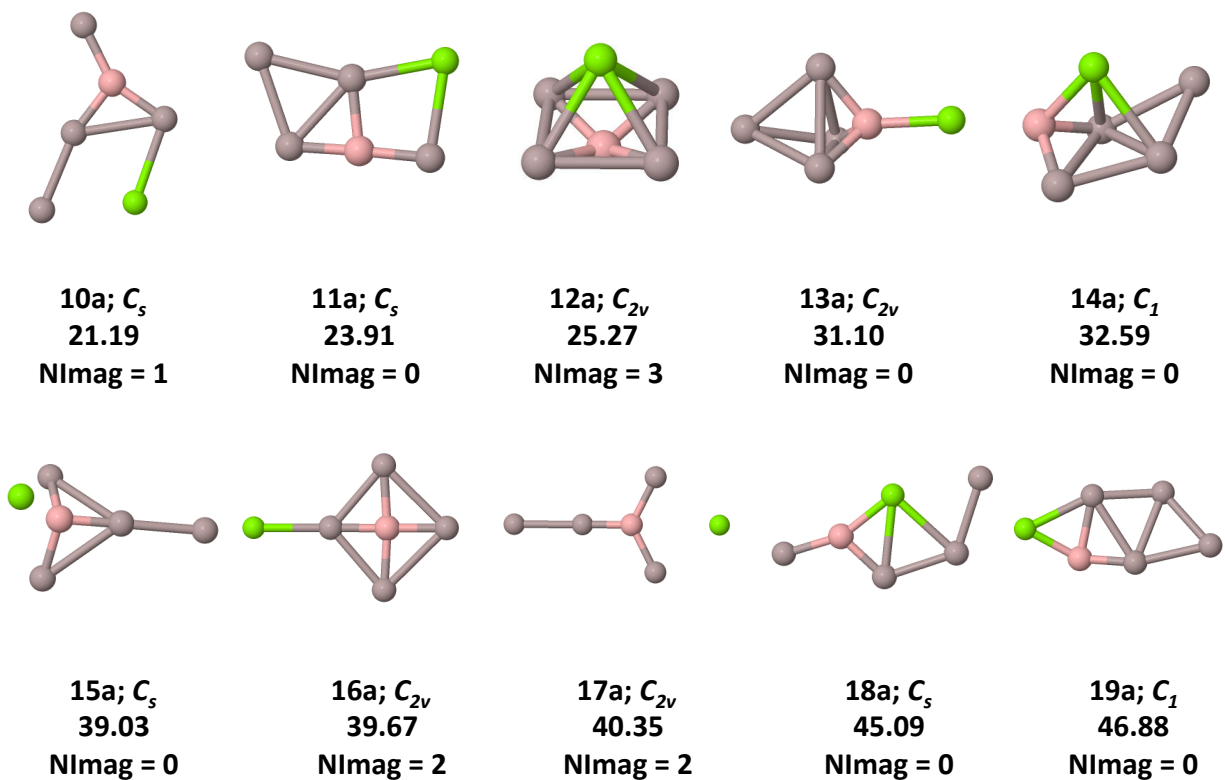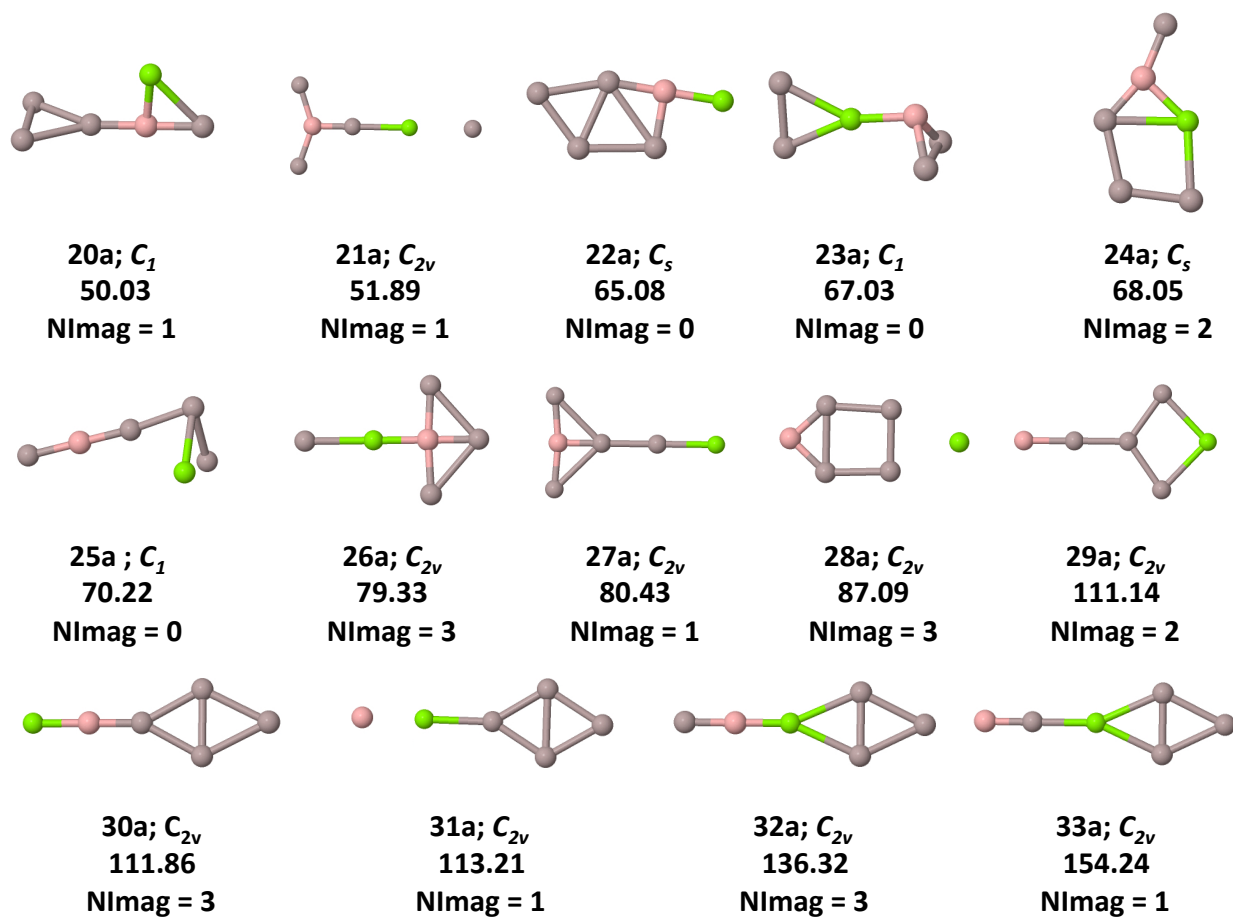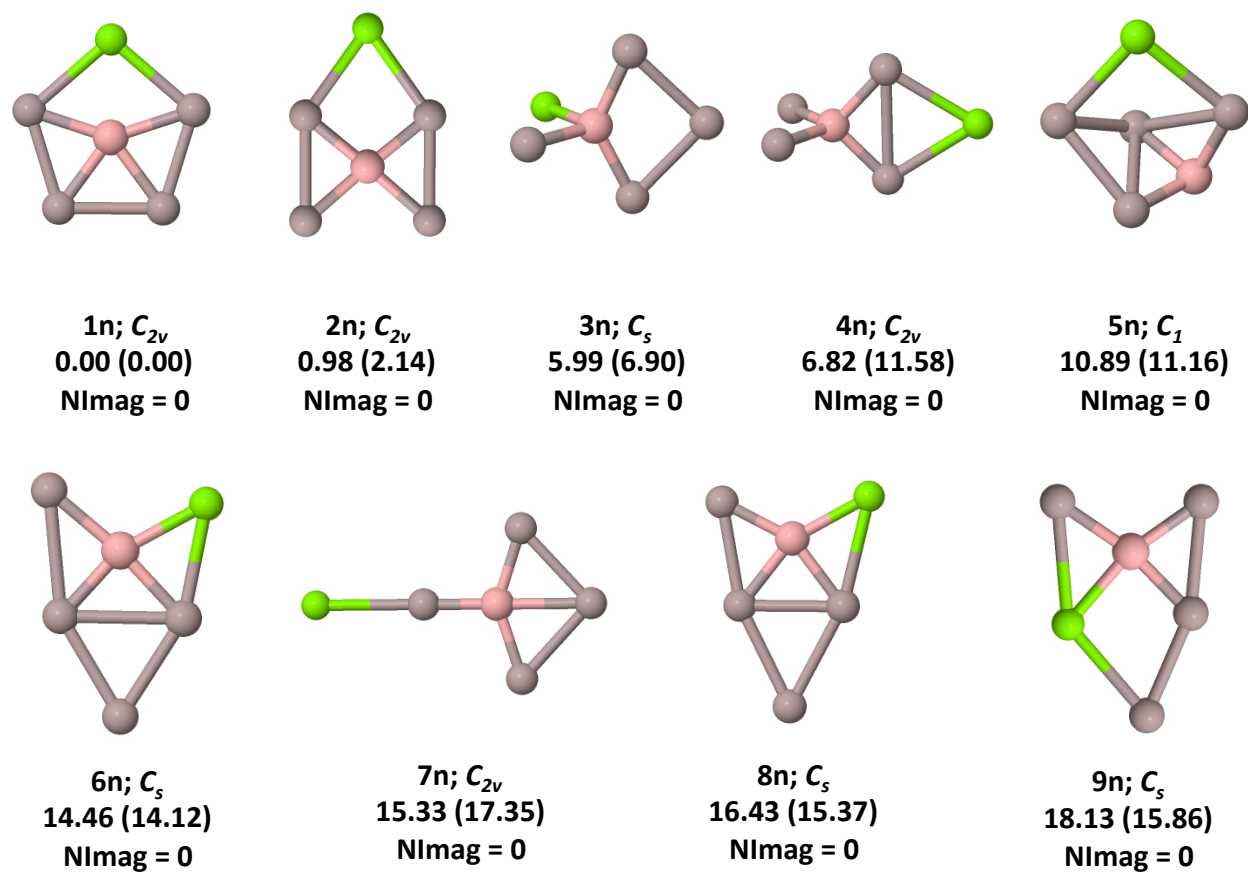121.56
NImag = 1

33c; C_{2v}
140.38
NImag = 1
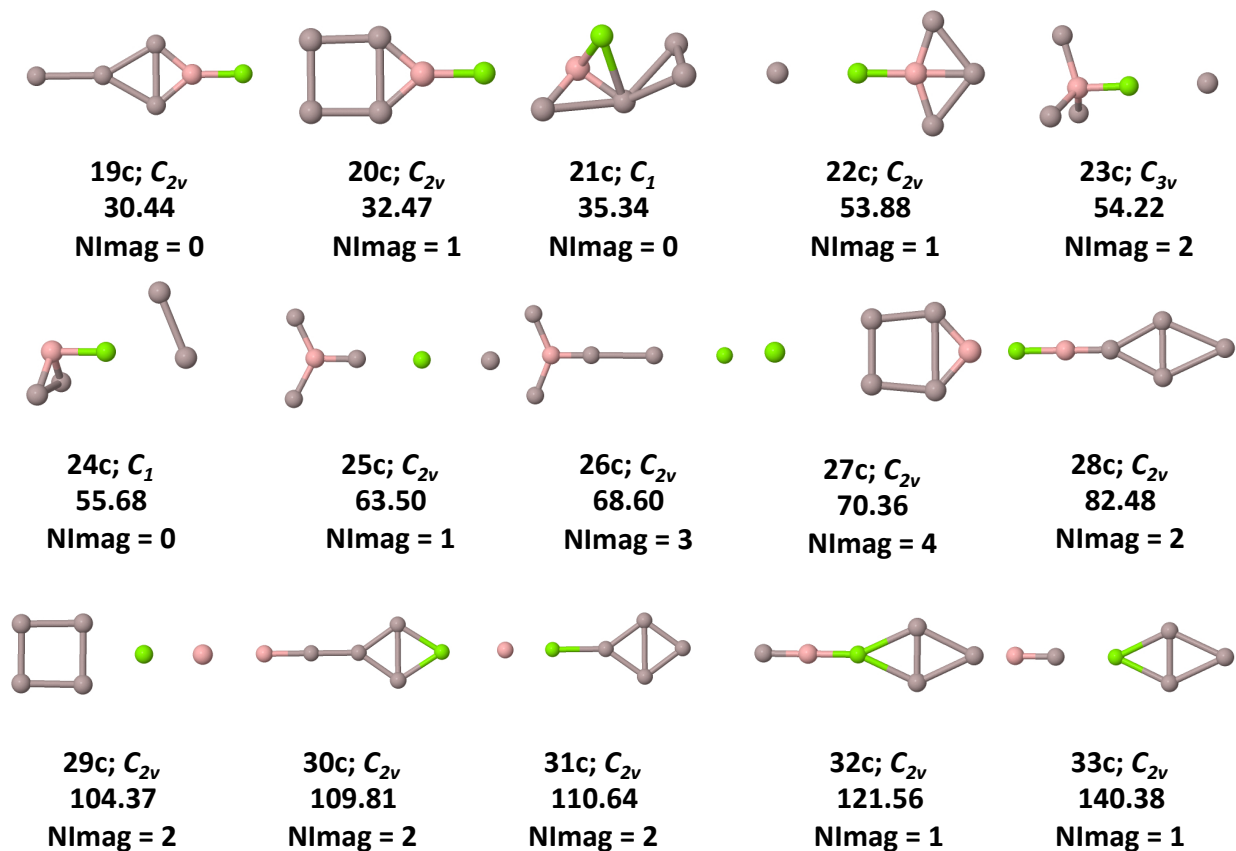
Figure S9: Isomers **19c**-**33c** of BAl_4Mg^+ in their respective singlet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

Table S1: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl_4Mg^- isomers in their respective singlet ground electronic states calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag
	a.u			Debye	kcal mol^{-1}		
1a	-1194.6156199	0.007695	-1194.607925	4.98	0.00	0.00	0
2a	-1194.6150628	0.007872	-1194.607191	2.71	0.35	0.46	0
3a	-1194.6080430	0.007245	-1194.600798	1.95	4.75	4.47	0
4a	-1194.5884849	0.007786	-1194.580699	3.25	17.03	17.09	0
5a	-1194.5848979	0.006450	-1194.578448	1.90	19.28	18.50	1
6a	-1194.5841398	0.007403	-1194.576737	1.62	19.75	19.57	0
7a	-1194.5833045	0.007010	-1194.576295	0.91	20.28	19.85	1
8a	-1194.5829304	0.007004	-1194.575927	0.91	20.51	20.08	1
9a	-1194.5813822	0.007030	-1194.574352	4.86	21.48	21.06	1
10a	-1194.5811322	0.007135	-1194.573997	3.94	21.64	21.29	1
11a	-1194.5772924	0.007471	-1194.569821	3.27	24.05	23.91	0
12a	-1194.5747421	0.007083	-1194.567659	1.09	25.65	25.27	3
13a	-1194.5651873	0.006828	-1194.55836	0.93	31.65	31.11	0
14a	-1194.5636561	0.007667	-1194.555989	1.75	32.61	32.59	0
15a	-1194.5524624	0.006734	-1194.545729	6.02	39.63	39.03	0
16a	-1194.5523552	0.007644	-1194.544711	7.17	39.70	39.67	2
17a	-1194.5499537	0.006336	-1194.543618	5.65	41.21	40.36	2
18a	-1194.5430381	0.006968	-1194.53607	2.05	45.55	45.09	0
19a	-1194.5405068	0.007294	-1194.533213	2.11	47.13	46.88	0
20a	-1194.5351146	0.006919	-1194.528196	4.02	50.52	50.03	1
21a	-1194.5319045	0.006665	-1194.525239	11.37	52.53	51.88	1
22a	-1194.5133046	0.009089	-1194.504215	5.93	64.20	65.07	0
23a	-1194.5077799	0.006672	-1194.501108	5.05	67.67	67.03	0
24a	-1194.5065692	0.007086	-1194.499484	4.08	68.43	68.05	2
25a	-1194.5021766	0.006150	-1194.496027	5.23	71.19	70.22	0
26a	-1194.4881854	0.006681	-1194.481504	2.33	79.97	79.33	3
27a	-1194.4863652	0.006611	-1194.479755	8.96	81.11	80.43	1
28a	-1194.4756250	0.006479	-1194.469146	3.29	87.85	87.09	3
29a	-1194.4358077	0.005000	-1194.430808	4.50	112.83	111.14	2
30a	-1194.4354175	0.005750	-1194.429667	6.22	113.08	111.86	3
31a	-1194.4321770	0.004668	-1194.427509	2.82	115.11	113.21	1
32a	-1194.3961804	0.005499	-1194.390682	5.00	137.70	136.32	3
33a	-1194.3676189	0.005490	-1194.362129	9.58	155.62	154.24	1

Table S2: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl_4Mg isomers in their respective doublet ground electronic states calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag	$<S^2>$
		a.u		Debye	kcal mol^{-1}			
1n	-1194.5336974	0.007292	-1194.526406	6.03	0.00	0.00	0	0.797305
2n	-1194.5257394	0.007321	-1194.518418	1.63	4.99	5.01	0	0.758181
3n	-1194.5246042	0.007512	-1194.517092	5.21	5.71	5.85	0	0.807541
4n	-1194.5186755	0.008075	-1194.510601	3.25	9.43	9.92	0	0.796030
5n	-1194.5125226	0.007613	-1194.504910	3.41	13.29	13.49	0	0.774463
6n	-1194.5106080	0.007073	-1194.503535	6.22	14.49	14.35	0	0.762152
7n	-1194.5089735	0.007202	-1194.501772	4.66	15.51	15.45	0	0.905247
8n	-1194.5063576	0.007294	-1194.499064	3.00	17.16	17.16	0	0.931497
9n	-1194.4995268	0.005016	-1194.494511	1.96	21.44	20.01	3	1.180257
10n	-1194.4995693	0.006731	-1194.492838	1.70	21.42	21.07	1	0.785372
11n	-1194.5004499	0.007725	-1194.492725	4.06	20.86	21.13	0	0.834877
12n	-1194.4990253	0.007787	-1194.491239	2.16	21.76	22.07	0	0.814272
13n	-1194.4790494	0.007072	-1194.471978	2.18	34.29	34.15	1	1.485627
14n	-1194.4784580	0.006948	-1194.47151	1.45	34.66	34.44	2	0.810084
15n	-1194.4756012	0.006508	-1194.469093	5.17	36.46	35.97	1	0.934291
16n	-1194.4746819	0.006869	-1194.467813	9.39	37.03	36.76	0	0.815897
17n	-1194.4714365	0.005200	-1194.466236	3.47	39.07	37.76	2	1.735140
18n	-1194.4723819	0.007101	-1194.465281	4.04	38.48	38.36	2	1.651501
19n	-1194.4593909	0.006787	-1194.452604	1.72	46.63	46.31	1	1.285082
20n	-1194.4535963	0.006255	-1194.447342	5.37	50.26	49.61	2	0.767085
21n	-1194.4535129	0.010194	-1194.443319	5.32	50.32	52.14	1	0.822814
22n	-1194.4487132	0.005763	-1194.44295	7.41	53.33	52.37	0	1.776772
23n	-1194.4488860	0.006715	-1194.442171	1.80	53.22	52.86	0	0.765920
24n	-1194.4486190	0.007011	-1194.441608	7.75	53.39	53.21	0	0.895698
25n	-1194.4305410	0.006042	-1194.424499	4.25	64.73	63.95	4	0.786752
26n	-1194.4211906	0.007055	-1194.414135	11.93	70.60	70.45	0	1.596845
27n	-1194.3970563	0.005177	-1194.391879	9.46	85.74	84.41	4	1.697244
28n	-1194.3713196	0.005837	-1194.365483	4.88	101.89	100.98	1	2.742919
29n	-1194.3663925	0.004968	-1194.361425	3.31	104.99	103.53	3	1.058016
30n	-1194.3577752	0.005120	-1194.352655	0.77	110.39	109.03	2	0.773237
31n	-1194.3425329	0.005918	-1194.336615	0.21	119.96	119.10	2	1.011501
32n	-1194.3528095	0.018716	-1194.334094	8.47	113.51	120.68	1	2.782482

Table S3: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected to-tal energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl_4Mg^+ isomers in their respective singlet ground electronic states calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag
		a.u		Debye	kcal mol^{-1}		
1c	-1194.3105651	0.007701	-1194.302864	6.11	0.00	0.00	0
2c	-1194.3066723	0.006981	-1194.299691	5.96	2.44	1.99	0
3c	-1194.3041293	0.007469	-1194.296660	4.42	4.04	3.89	0
4c	-1194.2976791	0.006794	-1194.290885	6.41	8.09	7.52	0
5c	-1194.2922057	0.007517	-1194.284688	7.59	11.52	11.40	0
6c	-1194.2922500	0.007785	-1194.284465	6.08	11.49	11.54	0
7c	-1194.2875655	0.007155	-1194.280410	7.67	14.43	14.09	0
8c	-1194.2876975	0.008136	-1194.279562	3.27	14.35	14.62	0
9c	-1194.2874644	0.008348	-1194.279117	4.7	14.50	14.91	0
10c	-1194.2849899	0.006861	-1194.278129	4.79	16.05	15.52	0
11c	-1194.2835385	0.006308	-1194.277230	4.02	16.96	16.09	0
12c	-1194.2829208	0.006576	-1194.276345	12.03	17.35	16.64	0
13c	-1194.2769276	0.004176	-1194.272752	6.46	21.11	18.90	2
14c	-1194.2790827	0.007320	-1194.271763	8.05	19.76	19.52	0
15c	-1194.2781299	0.006562	-1194.271568	13.26	20.35	19.64	1
16c	-1194.2758487	0.007060	-1194.268789	4.05	21.78	21.38	0
17c	-1194.2719989	0.007298	-1194.264701	2.09	24.20	23.95	1
18c	-1194.2666647	0.006970	-1194.259695	7.01	27.55	27.09	0
19c	-1194.2615976	0.007246	-1194.254352	5.69	30.73	30.44	0
20c	-1194.2588454	0.007739	-1194.251107	7.14	32.45	32.47	1
21c	-1194.2534199	0.006869	-1194.246551	3.24	35.86	35.34	0
22c	-1194.2257063	0.008702	-1194.217005	7.44	53.25	53.88	1
23c	-1194.2226979	0.006236	-1194.216462	11.31	55.14	54.22	2
24c	-1194.2203676	0.006238	-1194.214130	8.05	56.60	55.68	0
25c	-1194.2066849	0.005008	-1194.201677	9.09	65.19	63.50	1
26c	-1194.1977622	0.004225	-1194.193537	12.0	70.78	68.60	3
27c	-1194.1967993	0.006054	-1194.190746	4.39	71.39	70.36	4
28c	-1194.1773282	0.005907	-1194.171421	10.73	83.61	82.48	2
29c	-1194.1411329	0.004597	-1194.136536	1.15	106.32	104.37	2
30c	-1194.1333514	0.005488	-1194.127864	2.62	111.20	109.81	2
31c	-1194.1315951	0.005040	-1194.126555	0.31	112.31	110.64	2
32c	-1194.1141220	0.004983	-1194.109138	4.53	123.27	121.56	1
33c	-1194.0839056	0.004758	-1194.079148	2.74	142.23	140.38	1

1at; C_{2v}; $^3A_1$
0.00
NImag = 0

2at; C_s; $^3A''$
2.33
NImag = 0

3at; C_1; ^3A
2.35
NImag = 0

4at; C_{2v}; $^3B_2$
12.39
NImag = 1

5at; C_1; ^3A
18.74
NImag = 0

6at; C_{2v}; $^3A_2$
19.47
NImag = 0

7at; C_{2v}; $^3B_1$
22.42
NImag = 1

8at; C_s; $^3A''$
26.25
NImag = 1
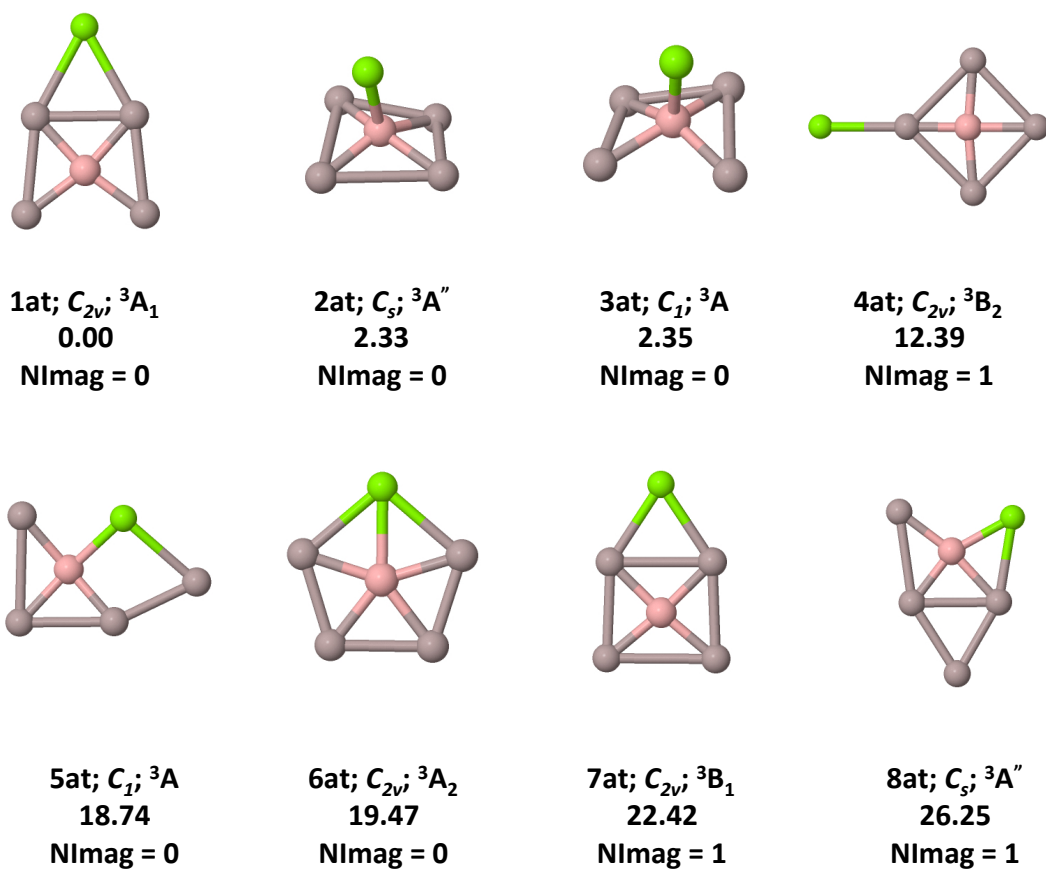
Figure S10: Isomers **1at**-**8at** of BAl_4Mg^- in their respective triplet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

1nq; C_1; ^4A
0.00
NImag = 0

2nq; C_1; ^4A
0.52
NImag = 0

3nq; C_s; $^4A''$
15.91
NImag = 2

4nq; C_1; ^4A
17.15
NImag = 0

5nq; C_{2v}; $^4B_2$
17.18
NImag = 2

6nq; C_{2v}; $^4B_1$
19.79
NImag = 0

7nq; C_s; $^4A''$
21.55
NImag = 0
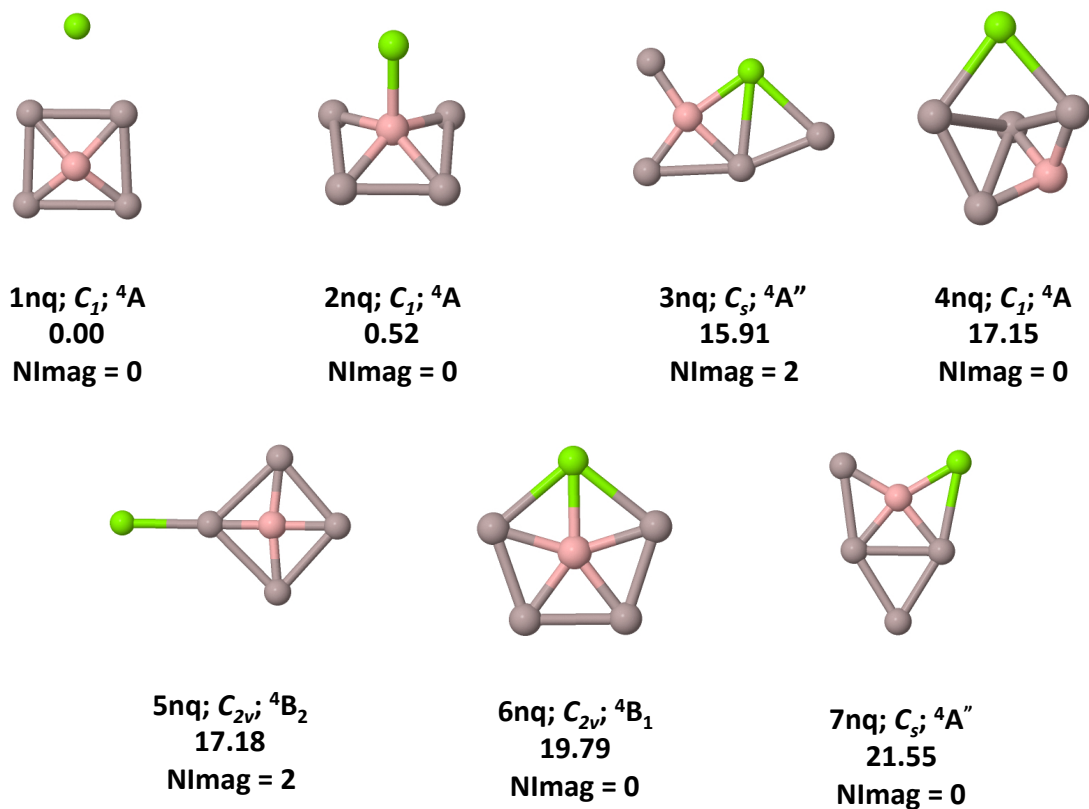
Figure S11: Isomers **1nq-7nq** of BAl_4Mg in their respective quartet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

1ct; C_{2v}; $^3B_2$
0.00
NImag = 0

2ct; C_{2v}; $^3B_2$
3.52
NImag = 0

3ct; C_1; ^3A
8.91
NImag = 0

4ct; C_s; $^3A'$
9.39
NImag = 0

5ct; C_1; ^3A
11.55
NImag = 0

6ct; C_s; $^3A'$
12.27
NImag = 1

7ct; C_1; ^3A
16.50
NImag = 0

8ct; C_1; ^3A
33.05
NImag = 0
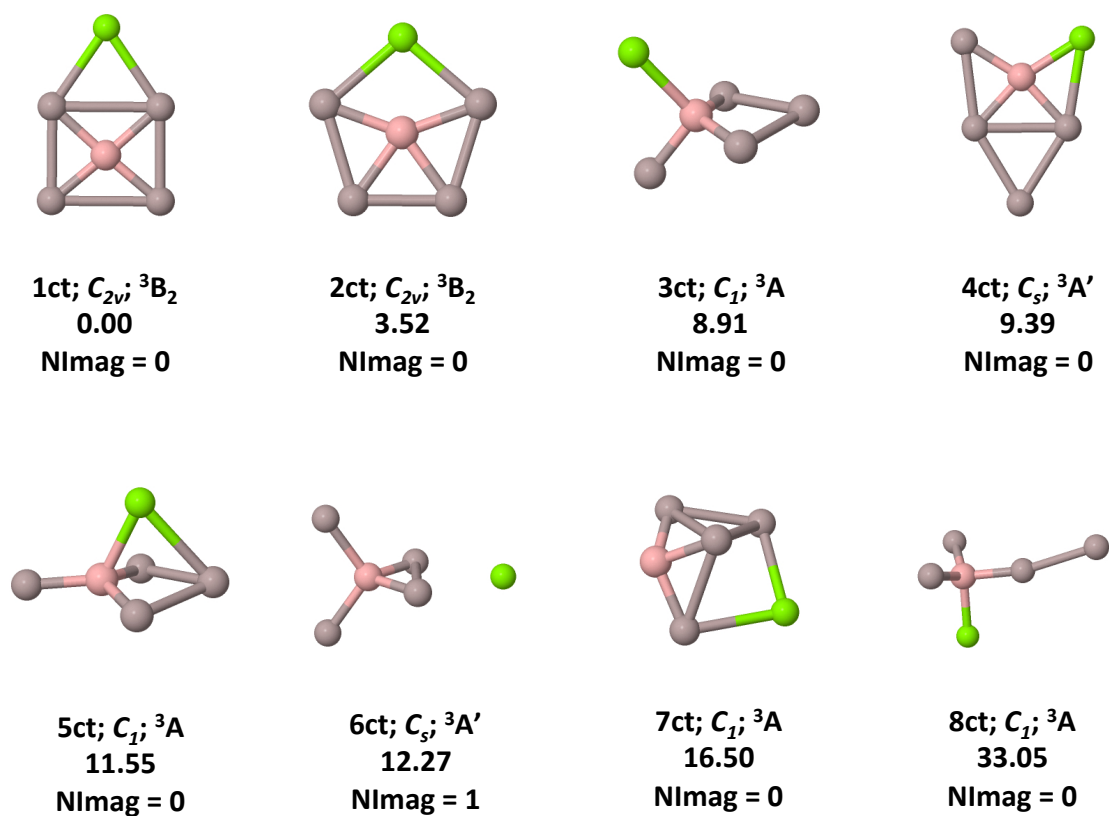
Figure S12: Isomers **1ct-8ct** of BAl_4Mg^+ in their respective triplet ground electronic states. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Table S4: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl_4Mg^- isomers in their respective triplet ground electronic states calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag	$<S^2>$
	a.u			Debye	kcal mol^{-1}			
1at	-1194.6090575	0.007308	-1194.601749	1.61	0.0	0.0	0	2.040891
2at	-1194.6048604	0.006832	-1194.598028	2.32	2.63	2.33	0	2.035347
3at	-1194.6048616	0.006851	-1194.598010	2.32	2.63	2.35	0	2.035546
4at	-1194.5888312	0.00683	-1194.582001	5.82	12.69	12.39	1	2.042446
5at	-1194.5789162	0.007026	-1194.571890	3.50	18.91	18.74	0	2.054027
6at	-1194.5787969	0.008081	-1194.570716	1.71	18.99	19.47	0	2.086528
7at	-1194.573345	0.007326	-1194.566019	3.98	22.41	22.42	1	2.070890
8at	-1194.5674607	0.007539	-1194.559922	3.28	26.10	26.25	1	2.030094

Table S5: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl$_4$Mg isomers in their respective quartet ground electronic states calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag	$<S^2>$
	a.u			Debye	kcal mol^{-1}			
1nq	-1194.5186133	0.007083	-1194.511530	0.63	0.00	0.00	0	3.792889
2nq	-1194.5172344	0.006522	-1194.510713	1.73	0.87	0.52	0	3.803457
3nq	-1194.4928275	0.006652	-1194.486176	2.34	16.18	15.91	2	3.792782
4nq	-1194.4917139	0.007506	-1194.484208	3.71	16.88	17.15	0	3.791863
5nq	-1194.4920503	0.007901	-1194.484149	4.04	16.67	17.18	2	3.788159
6nq	-1194.4875504	0.007567	-1194.479983	2.71	19.49	19.79	0	3.836763
7nq	-1194.4851523	0.007954	-1194.477198	5.02	21.00	21.55	0	3.899811

Table S6: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy ($E+ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE_e), ZPVE-corrected relative energy (ΔE_0), and number of imaginary frequencies of BAl_4Mg^+ isomers in their respective triplet ground electronic states calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	E	$ZPVE$	$E+ZPVE$	μ	ΔE_e	ΔE_0	NImag	$<S^2>$
		a.u		Debye	kcal mol^{-1}			
1ct	-1194.3112215	0.007210	-1194.304012	5.01	0.00	0.00	0	2.035598
2ct	-1194.3053276	0.006924	-1194.298403	3.43	3.70	3.52	0	2.064882
3ct	-1194.2965511	0.006726	-1194.289825	1.14	9.21	8.91	0	2.019328
4ct	-1194.2966025	0.007560	-1194.289042	5.23	9.17	9.39	0	2.037799
5ct	-1194.2923763	0.006762	-1194.285614	3.20	11.83	11.55	0	2.028067
6ct	-1194.2909792	0.006527	-1194.284452	6.49	12.70	12.27	1	2.013184
7ct	-1194.2852007	0.007479	-1194.277722	4.47	16.33	16.50	0	2.049800
8ct	-1194.2580803	0.006726	-1194.251354	6.13	33.35	33.05	0	2.039504

Figure S13: Energy evolution of ptB BAl$_4$Mg (**2n**) at 298 K for 2000 fs time in the ADMP simulation performed at the UωB97XD/6-311++G(2d,2p) level.
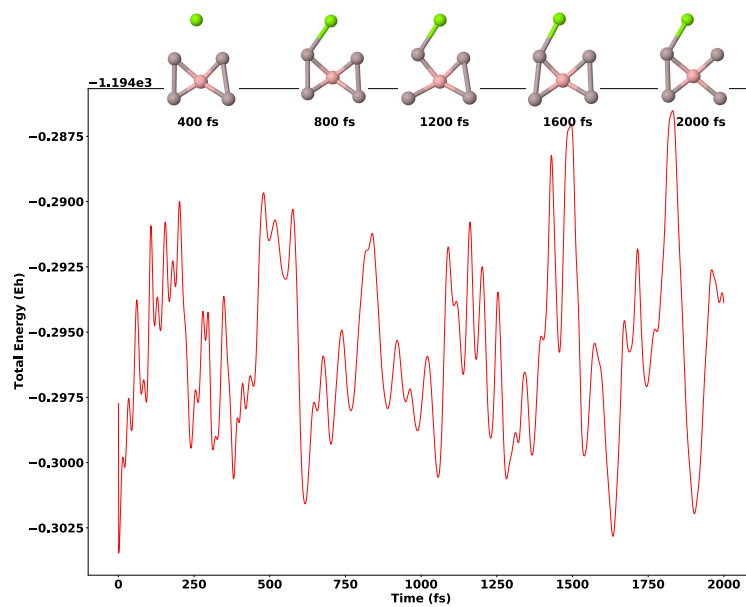
Figure S14: Energy evolution of ptB BAl$_4$Mg$^+$ (**1c**) at 298 K for 2000 fs time in the ADMP simulation performed at the ωB97XD/6-311++G(2d,2p) level.
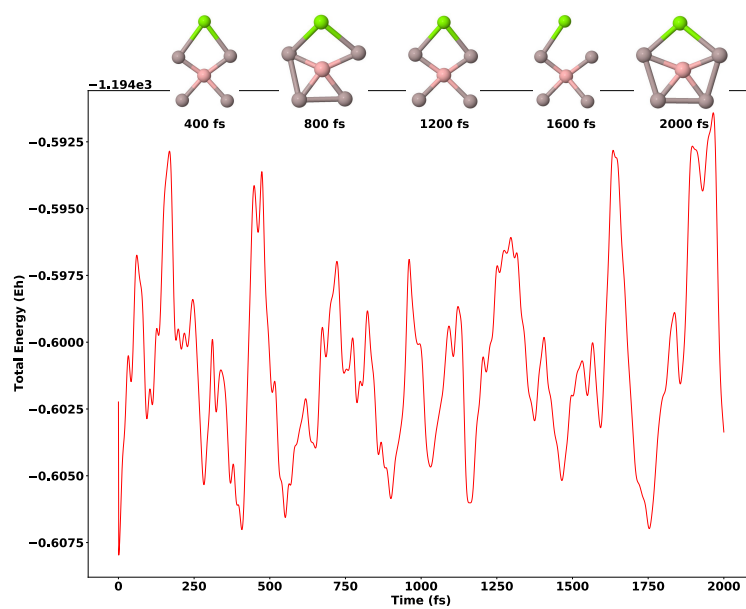
Figure S15: Energy evolution of ppB BAl_4Mg^- (**2a**) at 298 K for 2000 fs time in the ADMP simulation performed at the ωB97XD/6-311++G(2d,2p).
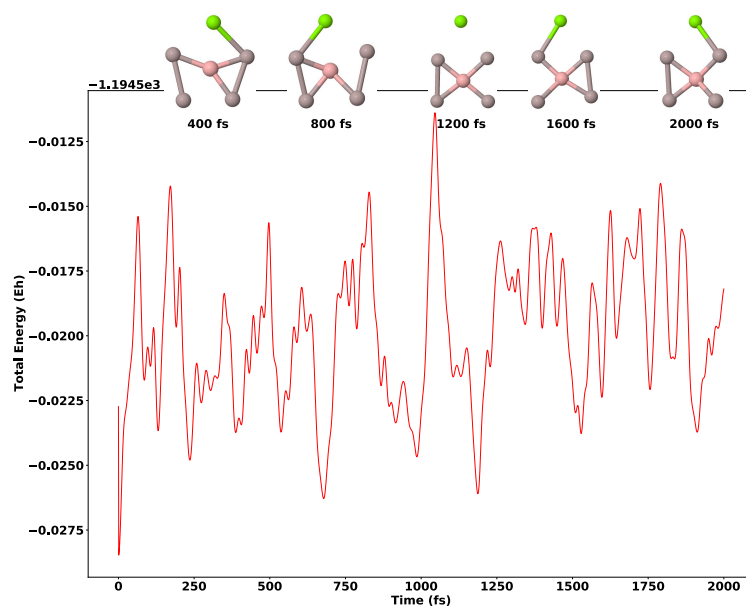
Figure S16: Energy evolution of ppB BAl$_4$Mg (**1n**) at 298 K for 2000 fs time in the ADMP simulation performed at the UωB97XD/6-311++G(2d,2p) level.
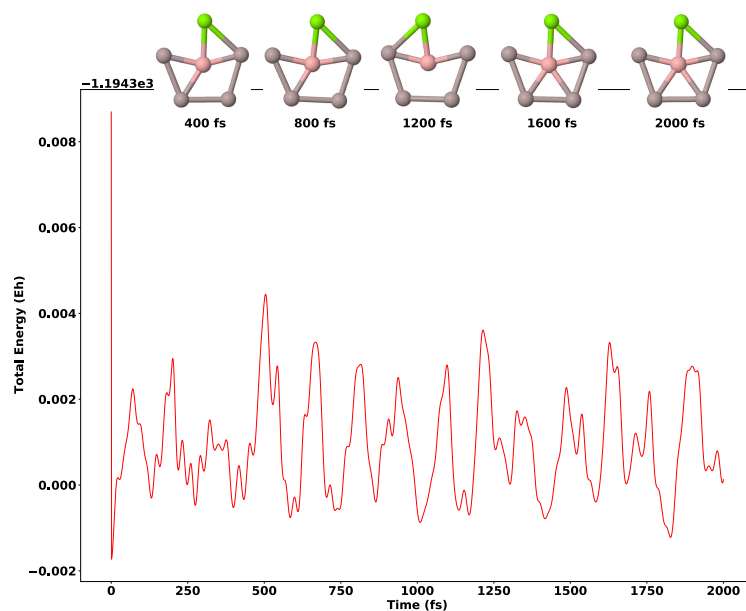
Figure S17: Energy evolution of ptB BAl$_4$Mg$^+$ (**3c**) at 100 K for 2000 fs time in the ADMP simulation performed at the ωB97XD/6-311++G(2d,2p) level.
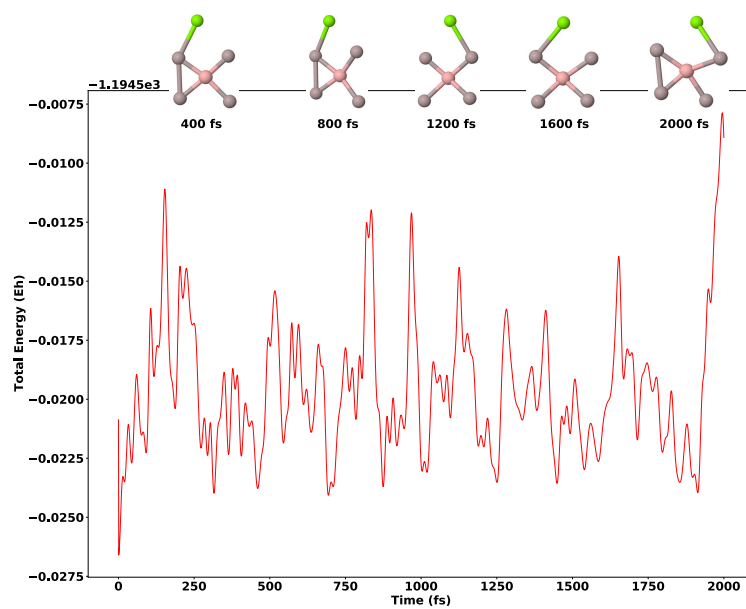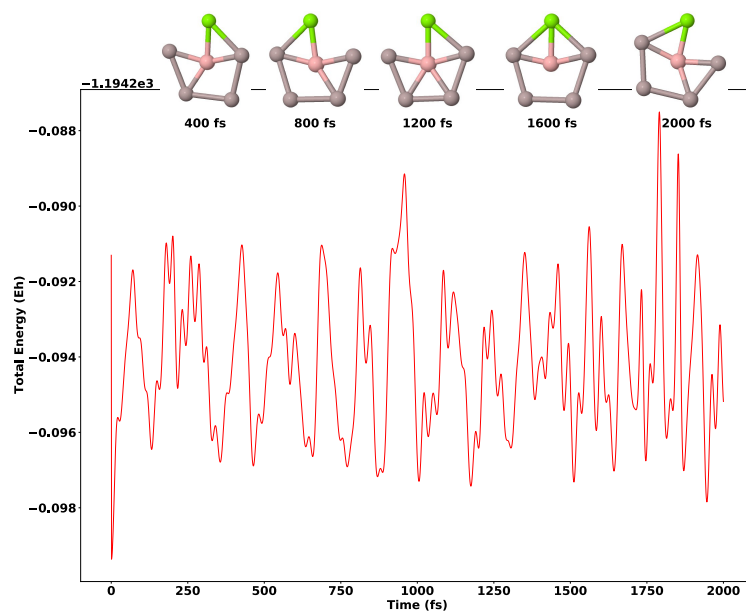
Figure S18: Energy evolution of ptB BAl$_4$Mg$^+$ (**3c**) at 200 K for 2000 fs time in the ADMP simulation performed at the ωB97XD/6-311++G(2d,2p) level.

Table S7: Molecular orbital composition analysis by NAO method. Major atomic orbital contributions (%) are given

Type	Species	HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4	LUMO
ptB	**1n**	1B($2p_z$ 26.3)	1B($2p_y$ 20.2)	2Mg(3s 22.6)	1B($2p_x$ 65.5) (3,4)Al($3p_x$ 10.2)	(3,4)Al(3s 18.6 ,$3p_z$ 11.7) (5,6)Al(3s 14.8)	2Mg(3s 21.0) (5,6)Al($3p_y$ 10.3)
		(5,6)Al($3p_z$ 12.5)	(5,6)Al(3s 15.3)	(3,4)Al(3s 8.6, $3p_{y/z}$ 17.1)			
	2n	1B($2p_z$ 20.0)	1B($2p_y$ 19.8)	2Mg (3s 19.0)	1B($2p_x$ 68.6) (3,4)Al($3p_x$ 10.7)	(3,4)Al(3s 22.5, $3p_z$ 10.7) (5,6)Al(3s 12.3)	2Mg(3s 33.9)
		(5,6)Al(3s 9.6, $3p_z$ 13.8)	(5,6)Al(3s 19.3)	(3,4)Al (3s 5.2, $3p_{y/z}$ 16.8)			(3,4)Al(3s 7.9, $3p_z$ 7.0)
	1c	1B($2p_y$ 21.6)	1B($2p_x$ 67.6)	1B($2p_z$ 15) 2Mg(3s 14.3)	(3,4)Al(3s 26.0, $3p_z$ 9.8) (5.6)Al(3s 9.4)	1B(2s 13.0, $2p_z$ 16.6) 2Mg(3s 15.7)	1B($2p_z$ 9.6) (3,4)Al($3p_y$ 14.7)
		(5,6)Al(3s 22.0)	(3,4)Al($3p_x$ 12.0)	(3,4)Al ($3p_{y/z}$ 17.7)		(5,6)Al(3s 15.5)	(5,6)Al($3p_z$ 13.7)
ppB	**2a**	1B($2p_z$ 29.3)	1B($2p_y$ 23.4)	2Mg (3s 19.7)	1B($2p_x$ 62.9) (3,4)Al($3p_x$ 9.2) (5,6)Al($3p_x$ 8.5)	(3,4)Al(3s 15.9, $3p_z$ 14.2) (5,6)Al(3s 15.8)	2Mg(3s 23.8)
		2Mg(3s 16.7)	(5,6)Al(3s 10.2)	(3,4)Al (3s 6.5, $3p_{y/z}$ 13.2)			(5,6)Al($3p_y$ 12.2)
	1n	1B($2p_z$ 34.0)	1B($2p_y$ 24.5)	2Mg(3s 20.9)	1B($2p_x$ 66.9) (3,4)Al($3p_x$ 7.0)	(3,4)Al(3s 12.5, $3p_z$ 14.8) (5,6)Al(3s 18.6)	2Mg(3s 35.9)
		2Mg(3s 13.9)	(3,4)Al(3s 10.7, $3p_y$ 10.8)	(3,4)Al ($3p_z$ 8.0) (5,6)Al ($3p_z$ 10.9)	(5,6)Al($3p_x$ 8.8)		(5,6)Al($3p_y$ 11.6)
	3c	1B($2p_y$ 23.6) (3,4)Al(3s 16.9, $3p_z$ 10.1)	1B($2p_x$ 69.4) (3,4)Al($3p_x$ 6.1) (5,6)Al($3p_x$ 8.3)	1B($2p_z$ 10.5) 2Mg(3s 14.3) (5,6)Al (3s 7.1 , $3p_y$ 7.9 ,$3p_z$ 11.7)	(3,4)Al($3p_z$ 14.4) (5,6)Al(3s 22.0)	1B(2s 21.6) 2Mg(3s 15.7) (3,4)Al(3s 20.8)	1B($2p_z$ 23.8) 2Mg(3s 20.7) (3,4)Al($3p_z$ 9.1)

S30

Optimized geometries of BAl4Mg− (singlet) obtained at the wB97XD/6-311++G(2d,2p) level

```
      6
scf done: −1194.615620
 B       0.000000    −0.000000    −0.390761
Mg      −0.000000     0.000000     2.838681
Al      −0.000000     1.687714     0.713812
Al      −0.000000    −1.687714     0.713812
Al       0.000000     1.394426    −2.003367
Al       0.000000    −1.394426    −2.003367


      6
scf done: −1194.615063
 B      −0.201305    −0.000000     1.000000
Mg       2.434306    −0.000000     1.000000
Al       0.626657     0.000000     2.909221
Al       0.626657    −0.000000    −0.909221
Al      −1.893157     0.000000     2.303229
Al      −1.893157    −0.000000    −0.303229


      6
scf done: −1194.608043
 B       0.155774     0.606159     1.965698
Al       1.884890     0.655864     0.840966
Al       0.630554     0.424568     3.972205
Mg      −0.918066    −2.085923     4.096217
Al      −0.844924     2.381585     1.645537
Al      −1.028070    −0.980408     1.360919


      6
scf done: −1194.588485
 B       0.000000     0.000000     0.000000
Al       0.000000     0.000000     2.130340
Al       2.529536    −0.000000     3.196310
Al       1.986775    −0.000000     0.495270
Al       0.606258     0.000000    −1.973659
Mg      −2.123508     0.000000     0.514726


      7
scf done: −1194.584898
Al      −0.934321    −0.000000     1.000000
Mg       2.530897    −0.000000     1.000000
 B      −2.941742     0.000000     1.000000
Al      −3.546097     0.000000     2.926912
Al      −3.546097     0.000000    −0.926912
Al      −5.358408     0.000000     1.000000
XX      −0.934321    −0.000000     2.000000


      6
scf done: −1194.584140
 B      −0.319817     0.371396     0.038395
Al      −1.491845     1.052939     1.547079
Al      −0.997575    −1.462024     0.862623
Al      −0.293456    −3.864197    −0.088499
```

```
Mg      0.662696    −1.211542    −1.248792
Al      0.582290     1.802185    −1.081795


        6
scf done: −1194.583305
 B      0.873185    −0.204738     0.514190
Mg     −0.182430     0.313530     2.608268
Al      2.669812    −0.182418     1.465006
Al      1.797886     2.245747     2.430912
Al      0.629993     1.745312    −0.010503
Al      1.115522    −1.316305    −1.153434


        6
scf done: −1194.582930
Al     −1.270090    −2.006794     0.277596
 B     −0.295696    −0.251244     0.235671
Al      1.478568     0.058761     1.195716
Al     −1.216415     1.537600     0.579293
Mg      0.614260     0.587324    −1.714338
Al      1.290793     2.587153     0.112071


        6
scf done: −1194.581382
 B      0.000000    −0.259756    −0.089583
Al      0.000000     0.798796     1.744637
Mg      0.000000     1.927388    −0.525754
Al     −0.000000    −1.938575    −1.401885
Al      2.146505    −0.259549    −0.089396
Al     −2.146505    −0.259549    −0.089396


        6
scf done: −1194.581132
 B     −0.687703    −0.000000    −0.029862
Al      0.348563    −0.000000     1.678351
Mg      3.006656     0.000000     0.945716
Al      3.456853     0.000000    −1.974916
Al      0.958738    −0.000000    −1.133242
Al     −2.471059    −0.000000    −1.053208


        6
scf done: −1194.577292
Al      1.439709     1.522402     1.905636
Al     −0.491400    −0.067737     1.095747
 B      1.248092     0.560401     0.159184
Al      1.109868    −0.384922    −1.621236
Mg     −1.292333    −1.573370    −0.992923
Al     −0.646446     1.059385     3.630346


        6
scf done: −1194.574742
 B      0.000000     0.000000    −0.911315
Mg      0.000000     0.000000     1.634421
Al      0.000000     2.009573    −0.289532
Al     −0.000000    −2.009573    −0.289532
Al      2.009548    −0.000000    −0.289563
```

```
Al    -2.009548      0.000000     -0.289563


      6
scf done: -1194.565187
 B     0.165800      0.436137      0.764788
Al     0.992048     -1.416276      1.068346
Al     0.662444      0.958272      2.684914
Al     3.275023     -0.197385      2.326507
Al     1.985851      1.126950      0.120262
Mg    -1.906674      0.863904     -0.265072


      6
scf done: -1194.563656
 B    -0.215797     -0.038101     -0.144456
Mg     0.024443      0.015981      2.141050
Al     2.795050      0.035245      1.455199
Al     2.045932      2.260507      2.684831
Al     0.939696      1.596314      0.125830
Al     1.314644     -1.268818     -0.408014


      6
scf done: -1194.552462
 B    -0.023990      0.000000      0.101141
Mg    -0.343683     -0.000000      2.556456
Al     1.765767     -0.000000     -0.637531
Al    -0.807025     -1.708248     -0.774931
Al    -0.807025      1.708248     -0.774931
Al     4.195029     -0.000000     -1.747146


      6
scf done: -1194.552355
Al    -1.154318     -0.000000      1.000000
Mg     1.525128     -0.000000      1.000000
 B    -3.094051      0.000000      1.000000
Al    -2.979595     -0.000000      3.124204
Al    -2.979595      0.000000     -1.124204
Al    -5.112966      0.000000      1.000000


      7
scf done: -1194.549954
Al    -0.000000     -0.000000      1.639187
Al    -0.000000     -0.000000      4.326761
 B     0.000000      0.000000     -0.272705
Al     0.000000      1.823779     -1.198481
Al    -0.000000     -1.823779     -1.198481
Mg     0.000000      0.000000     -3.652475
XX    -0.000000     -1.000000      1.639187


      6
scf done: -1194.543038
 B     1.404944     -0.257272     -0.170268
Mg     0.968631     -0.443030      2.015332
Al     1.044202     -0.237619     -2.215226
Al     3.140110      0.386348      0.561053
Al     3.424536      0.569457      3.073214
```

```
Al      1.630800      −0.017884      4.866853


        6
scf done: −1194.540507
 B      0.043654       0.430142      2.701508
Mg     −1.565583      −0.324278      1.420724
Al      1.274727       0.102707      4.256258
Al      2.139820      −0.316305      6.745750
Al     −0.383111      −0.533917      6.287733
Al     −1.336518      −0.804619      3.983583


        6
scf done: −1194.535115
Al      0.715722      −2.981951      0.310623
Mg      1.863798      −0.661818     −0.820329
Al     −0.850759       0.739549     −0.193234
 B     −0.064075      −1.108181      0.054700
Al     −1.211073       3.220886      0.552667
Al     −2.048221       2.572336     −1.625087


        7
scf done: −1194.531905
Mg      0.193366      −0.000000      1.000000
Al      3.170660      −0.000000      1.000000
Al     −2.532066       0.000000      1.000000
Al     −5.089884       0.000000      2.929843
Al     −5.089884      −0.000000     −0.929843
 B     −4.448623       0.000000      1.000000
XX     −2.532066       0.000000      0.000000


        6
scf done: −1194.513305
 B     −0.472023      −0.000000      0.219146
Mg      0.820063      −0.000000      1.883403
Al      1.125751      −0.000000     −1.029539
Al     −1.726045       0.000000     −1.369271
Al     −2.585367       0.000000     −3.768625
Al     −0.168710      −0.000000     −3.437403


        6
scf done: −1194.507780
Al      1.101298      −1.720414      0.836205
Mg     −0.210842       1.337383      0.110281
 B     −0.559856      −0.681356      1.210585
Al     −1.304918      −1.871392     −0.206722
Al      0.543652       3.152252     −1.882426
Al     −0.401922       4.132577      0.104864


        6
scf done: −1194.506569
 B      1.054112      −0.000000      0.041617
Al      0.408493       0.000000      1.903685
Al      1.030100      −0.000000     −2.007700
Mg      3.052615      −0.000000      0.866484
Al      4.206102       0.000000      3.349947
```

```
Al      1.861800        0.000000        3.976924


        6
scf done: -1194.502177
  B     -0.123694       0.224903        1.134985
 Al      1.870747       0.783598        0.810970
 Al     -2.056184      -0.264014        1.478288
 Al     -4.371508      -1.003158        2.096422
 Al     -4.604099      -1.165288       -0.510687
 Mg     -4.511030       1.423962        0.990021


        7
scf done: -1194.488185
 Mg     -0.961301      -0.000000        1.000000
 Al      1.750873      -0.000000        1.000000
  B     -3.100740       0.000000        1.000000
 Al     -3.207543       0.000000        3.137454
 Al     -3.207543      -0.000000       -1.137454
 Al     -5.069513       0.000000        1.000000
 XX     -0.961301      -0.000000        0.000000


        7
scf done: -1194.486365
 Al     -0.057409      -0.000000        1.000000
 Mg      2.534062      -0.000000        1.000000
 Al     -2.538846       0.000000        1.000000
 Al     -4.628705       0.000000        3.074473
 Al     -4.628705      -0.000000       -1.074473
  B     -4.476163       0.000000        1.000000
 XX     -0.057409      -0.000000       -0.000000


        6
scf done: -1194.475625
  B      0.551581      -0.000000        1.000000
 Al     -0.918506      -0.000000        2.309599
 Al     -0.918506       0.000000       -0.309599
 Al     -3.515814      -0.000000        2.196967
 Al     -3.515814       0.000000       -0.196967
 Mg     -6.221953       0.000000        1.000000


        7
scf done: -1194.435808
 Al     -0.018490      -0.000000        1.000000
  B      2.208983      -0.000000        1.000000
 Al     -2.390271      -0.000000        1.000000
 Al     -3.869651       0.000000        3.097369
 Al     -3.869651      -0.000000       -1.097369
 Mg     -5.856689       0.000000        1.000000
 XX     -0.018490       0.000000        0.000000


        7
scf done: -1194.433985
  B      0.208374       0.000000        1.000000
 Mg      2.334417       0.000000        1.000000
 Al     -1.785858       0.000000        1.000000
```

```
Al     -4.033554      0.000000      2.231379
Al     -4.033554      0.000000     -0.231379
Al     -6.485594      0.000000      1.000000
XX      0.208374      0.000000      2.000000


       7
scf done: -1194.424551
Mg      0.511574      0.000000      1.000000
 B      3.007899      0.000000      1.000000
Al     -2.193291      0.000000      1.000000
Al     -4.319778      0.000000      2.309585
Al     -4.319778      0.000000     -0.309585
Al     -6.482393      0.000000      1.000000
XX      0.511574      0.000000      2.000000


       7
scf done: -1194.396180
 B     -0.000000     -0.000000      3.068342
Al     -0.000000     -0.000000      4.981545
Mg     -0.000000     -0.000000      0.988749
Al      0.000000      1.177586     -1.637622
Al     -0.000000     -1.177586     -1.637622
Al      0.000000      0.000000     -4.034358
XX      1.000000      0.000000      3.068342


       6
scf done: -1194.367619
Al     -0.000000      0.012556     -3.566147
 B     -0.000000      0.016540     -5.461707
Mg     -0.000000      0.007034     -1.033382
Al      0.000000      1.179239      1.575747
Al      0.000000     -1.175882      1.571017
Al      0.000000     -0.002973      3.986217
```

Optimized geometries of BAl4Mg− (triplet) obtained at the UwB97XD/6-311++G(2d,2p) level

```
       6
scf done: -1194.609058
 B      0.612326      0.575158      2.109187
Al      1.936668      0.106942      0.604075
Al      1.264623      2.328898      2.967607
Mg     -2.674912     -1.552763      3.176873
Al     -0.909106      0.698286      3.497371
Al     -0.349440     -1.154675      1.526427


       6
scf done: -1194.604860
 B     -0.000000      0.004346     -0.016064
Al     -0.000000      0.714452      1.946423
Mg     -0.000000      2.073228     -0.812898
Al      0.000000     -1.751092     -1.397487
Al      2.047400     -0.516101     -0.085739
Al     -2.047400     -0.516101     -0.085739
```

```
     6
scf done: −1194.604862
 B      1.149828      0.407128      0.921874
Mg    −0.540576     −0.433907      2.082650
Al     2.855721     −0.492150      1.800730
Al     2.294974      2.168784      1.679912
Al     0.217353      2.009738     −0.084111
Al     0.926669     −1.058466     −0.546616


     6
scf done: −1194.588831
Al    −1.067838     −0.000000      1.000000
Mg     1.731143     −0.000000      1.000000
 B    −3.001254      0.000000      1.000000
Al    −3.158704      0.000000      3.071871
Al    −3.158704      0.000000     −1.071871
Al    −5.140410      0.000000      1.000000


     6
scf done: −1194.578916
 B    −0.528274      0.108006     −0.082350
Al    −1.394856      1.228219      1.455898
Al    −1.003051     −1.475581      1.105618
Al    −0.312245     −3.610725     −0.297191
Mg     0.866784     −1.237111     −1.217895
Al     0.513935      1.675949     −0.935068


     6
scf done: −1194.578797
 B    −0.093124     −0.000000      1.000000
Mg     2.280594     −0.000000      1.000000
Al     0.546320      0.000000      3.055576
Al     0.546320     −0.000000     −1.055576
Al    −1.790054      0.000000      2.322613
Al    −1.790054     −0.000000     −0.322613


     6
scf done: −1194.573345
 B     0.000000     −0.000000     −0.679801
Mg    −0.000000      0.000000      2.994911
Al    −0.000000      1.470129      0.773524
Al    −0.000000     −1.470129      0.773524
Al     0.000000      1.571164     −1.996674
Al     0.000000     −1.571164     −1.996674


     6
scf done: −1194.567461
 B     0.072967      0.000000      0.058523
Al    −0.018515     −0.000000      2.204153
Al     2.399458     −0.000000      3.073098
Al     2.059952     −0.000000      0.484130
Al     0.538619      0.000000     −1.940029
Mg    −2.053420      0.000000      0.483112
```

Optimized geometries of BAl4Mg (doublet) obtained at the UwB97XD/6-311++G(2d,2p) level

6
1n   scf done: -1194.533697
 B   -0.059261   -0.000000   1.000000
Mg   3.462181   -0.000000   1.000000
Al   1.238856   -0.000000   2.580014
Al   1.238856   -0.000000   -0.580014
Al   -1.441392   0.000000   2.581367
Al   -1.441392   0.000000   -0.581367

6
2n   scf done: -1194.525739
Al   0.775233   1.069224   1.798800
Al   -1.789846   0.286022   -0.227325
 B   0.301660   0.568934   -0.139295
Al   1.170937   -0.827597   -1.373933
Al   2.474177   -0.702467   0.891809
Mg   0.398699   2.499303   -1.288036

6
3n   scf done: -1194.524604
 B   -0.121493   -0.000000   0.951941
Mg   3.656418   0.000000   1.016646
Al   1.314459   0.000000   -0.489289
Al   1.264261   0.000000   2.441504
Al   -1.354461   -1.698472   0.930603
Al   -1.354461   1.698472   0.930603

6
4n   scf done: -1194.518675
Al   -0.416125   -1.447220   -0.393157
Al   -0.682499   1.315321   -0.904537
 B   0.557291   -0.140663   -1.591647
Al   2.140213   0.489540   -0.505785
Al   -1.380106   0.328436   1.343485
Mg   1.054736   1.443067   1.897012

6

5n   scf done: -1194.512600
 B   -0.151075   0.007393   0.434333
Al   -0.180587   -0.008174   2.553123
Mg   1.924995   0.000406   -0.330784
Al   -2.163028   0.005017   0.471935
Al   -2.987025   -0.004150   -2.056940
Al   -0.372046   -0.000492   -1.649739

     7
6n   scf done: -1194.510608
Al   -0.880254   -0.000000   1.000000
Mg   1.965586   -0.000000   1.000000
 B   -2.804155   0.000000   1.000000
Al   -3.427905   -0.000000   2.946949
Al   -3.427905   0.000000   -0.946949
Al   -5.221135   0.000000   1.000000
XX   -0.880254   0.000000   0.000000

     6
7n   scf done: -1194.508973
 B   -0.190467   0.435400   0.020808
Al   -1.198642   2.132574   0.306156
Mg   0.949781   -0.022537   -1.768345
Al   -1.003049   0.094263   1.965729
Al   0.496787   -1.475857   0.582033
Al   -0.343201   -2.376453   3.143269
     6
8n   scf done: -1194.506358
Al   -0.973395   -1.609257   0.839785
Mg   1.690905   -1.366461   -0.319472
Al   1.328653   1.481706   -0.554392
 B   0.016990   0.062466   0.195169
Al   -1.732846   0.930725   0.815718
Al   0.448862   -3.800890   0.534845

     6
9n   scf done: -1194.499527
 B   0.000000   0.000000   -0.779575
Mg   0.000000   0.000000   1.657830
Al   0.000000   2.090572   -0.307238
Al   -0.000000   -2.090572   -0.307238

Al   2.091073   -0.000000   -0.307996
Al   -2.091073   0.000000   -0.307996

    6
10n   scf done: -1194.499569
 B   1.635223   -0.303857   -0.000000
Al   0.769989   -2.128599   -0.000000
Mg -1.932048   -1.395941   0.000000
Al   -2.577224   1.512913   0.000000
Al   0.000000   0.846983   -0.000000
Al   2.961732   1.174132   -0.000000

    6
11n   scf done: -1194.500450
Al   1.500794   1.585011   1.956798
Al   -0.531388   -0.110035   1.059534
 B   1.225371   0.598490   0.267303
Al   1.042809   -0.365911   -1.495598
Mg -1.317313   -1.600542   -1.017045
Al   -0.552784   1.009147   3.405760

    6
12n   scf done: -1194.499025
 B   -0.165549   0.003279   -0.099345
Mg -0.087419   0.048802   2.132114
Al   2.914317   0.081034   1.333393
Al   1.966853   2.099621   2.622567
Al   0.949351   1.664760   0.142870
Al   1.326414   -1.296369   -0.277159

    6
13n   scf done: -1194.479049
Al   1.420926   2.090205   -0.000000
Al   -1.644365   1.811423   -0.000000
 B   0.000000   0.627761   -0.000000
Mg   1.840015   -0.700873   0.000000
Al   -1.536305   -0.788410   0.000000
Al   0.061269   -2.707704   0.000000

6

14n   scf done: -1194.478458
Al   0.000000   -0.000000   1.810889
Al   0.000000   -0.000000   4.596579
 B   -0.000000   0.000000   -0.106097
Al   -0.000000   1.491955   -1.437911
Al   -0.000000   -1.491955   -1.437911
Mg   -0.000000   0.000000   -3.781742

6

15n   scf done: -1194.475601
 B   -0.133208   0.334063   0.214837
Al   0.487741   -0.873067   1.677159
Al   1.822125   0.869690   3.486629
Al   3.293077   -0.417132   1.806027
Al   1.435536   1.453694   0.731417
Mg   -1.730778   0.404352   -1.216324

6

16n   scf done: -1194.474682
Al   0.000000   0.000000   4.061598
Mg   0.000000   0.000000   1.010483
 B   0.000000   0.000000   -1.109900
Al   -0.000000   2.062961   -1.522489
Al   1.786577   -1.031481   -1.522489
Al   -1.786577   -1.031481   -1.522489

7

17n scf done: -1194.471437
Mg   -0.853059   -0.000000   1.000000
Al   2.101023   -0.000000   1.000000
 B   -3.066379   0.000000   1.000000
Al   -3.417876   0.000000   3.043171
Al   -3.417876   -0.000000   -1.043171
Al   -5.141601   0.000000   1.000000
XX   -0.853059   -0.000000   2.000000

6

18n   scf done: -1194.472382
 B   0.054905   -0.000000   0.049480
Mg   0.017976   -0.000000   2.216744

```
Al    1.265963   -0.000000   -1.542378
Al   -1.491855    0.000000   -1.180967
Al   -2.658169    0.000000   -3.442710
Al   -0.195150    0.000000   -3.602458


   6
19n   scf done: -1194.459391
 B   -0.224887   -0.096815    2.297360
Mg   -2.192548   -0.382095    1.378733
Al    1.455506    0.119027    3.360545
Al    1.470141   -0.384989    8.448994
Al    0.786214   -0.250999    5.788337
Al   -1.121436   -0.450398    4.121585


   6
20n   scf done: -1194.453596
Al    0.549547   -3.093145    0.408516
Mg    1.890957   -0.529142   -0.870578
Al   -0.713039    0.697113   -0.233856
 B    0.040530   -1.106734    0.013347
Al   -1.247522    3.242247    0.610011
Al   -2.115082    2.570482   -1.648100


   6
21n   scf done: -1194.453513
 B    0.243940   -0.000000    1.000000
Mg    2.402685   -0.000000    1.000000
Al   -1.251011   -0.000000    2.307326
Al   -1.251011   -0.000000   -0.307326
Al   -3.695514    0.000000    2.205331
Al   -3.695514    0.000000   -0.205331


   6
22n   scf done: -1194.448713
 B   -0.130095    0.212082    1.009934
Al    1.947501    0.711610    0.983379
Al   -2.064438   -0.240208    1.048685
Al   -4.415515   -1.039513    2.262066
Al   -4.409691   -1.058241   -0.303921
Mg   -4.723530    1.414271    0.999856
```

6

23n   scf done: -1194.448886
Al   1.109231   -1.660091   0.801185
Mg -0.204478   1.220039   0.128991
 B   -0.581063   -0.730290   1.286440
Al   -1.308786   -1.801622   -0.224208
Al   0.573467   3.174538   -1.915134
Al   -0.420960   4.146476   0.095513

7

24n scf done: -1194.448619
Mg   0.258483   -0.000000   1.000000
Al   3.236629   -0.000000   1.000000
Al   -2.514868   0.000000   1.000000
Al   -5.183603   0.000000   2.888896
Al   -5.183603   -0.000000   -0.888896
 B   -4.409468   0.000000   1.000000
XX -2.514868   0.000000   -0.000000

6

25n scf done: -1194.430541
 B   0.494980   -0.000000   1.000000
Al   -0.956586   -0.000000   2.385154
Al   -0.956586   0.000000   -0.385154
Al   -3.433493   -0.000000   2.299549
Al   -3.433493   0.000000   -0.299549
Mg -6.253835   0.000000   1.000000

8

26n scf done: -1194.421191
Al   0.148020   -0.000000   1.000000
Mg   2.676507   -0.000000   1.000000
Al   -2.276448   -0.000000   1.000000
Al   -5.055315   0.000000   2.952999
Al   -5.055315   -0.000000   -0.952999
 B   -4.233216   0.000000   1.000000
XX -2.276448   -0.000000   0.000000
XX   0.148020   0.000000   0.000000

```
    7
27n  scf done: -1194.397056
 B    0.208374   -0.000000   1.000000
Mg   2.334417   -0.000000   1.000000
Al   -1.785858   -0.000000   1.000000
Al   -4.033554    0.000000   2.231379
Al   -4.033554    0.000000  -0.231379
Al   -6.485594    0.000000   1.000000
XX   0.208374   -0.000000   2.000000


    6
28n  scf done: -1194.371320
Al   0.000000    0.017916  -3.552287
 B   0.000000    0.061158  -5.513258
Mg   0.000000   -0.069080  -0.873666
Al   0.000000    1.288236   1.540615
Al   0.000000   -1.238056   1.667965
Al   0.000000   -0.023661   3.802377


    6
29n   scf done: -1194.366392
Mg  -0.000000   -0.000000   2.495378
 B  -0.000000   -0.000000   4.961763
Al   0.000000    1.333839   0.181849
Al  -0.000000   -1.333839   0.181849
Al   0.000000    1.273372  -2.287747
Al  -0.000000   -1.273372  -2.287747


    7
30n   scf done: -1194.357775
Mg   0.511574    0.000000   1.000000
 B   3.007899    0.000000   1.000000
Al  -2.193291    0.000000   1.000000
Al  -4.319778   -0.000000   2.309585
Al  -4.319778    0.000000  -0.309585
Al  -6.482393    0.000000   1.000000
XX   0.511574    0.000000   2.000000


    7
```

31n scf done: -1194.342533
```
 B   -0.000000   -0.000000    3.123545
 Al  -0.000000   -0.000000    5.046300
 Mg  -0.000000   -0.000000    0.971685
 Al   0.000000    1.177172   -1.640350
 Al  -0.000000   -1.177172   -1.640350
 Al   0.000000   -0.000000   -4.131795
 XX   1.000000    0.000000    3.123545
```

```
    7
```
32n scf done: -1194.352810
```
 Al   0.376393   -0.000000    1.000000
 B    2.339761   -0.000000    1.000000
 Al  -2.107511   -0.000000    1.000000
 Al  -4.065542    0.000000    2.500489
 Al  -4.065542   -0.000000   -0.500489
 Mg  -6.273326    0.000000    1.000000
 XX   0.376393   -0.000000    2.000000
```

Optimized geometries of BAl4Mg (quartet) obtained at the UwB97XD/6-311++G(2d,2p) level

```
    6
scf done: -1194.518613
 B     0.836003    0.000026    0.438452
 Mg   -3.289232   -0.002000   -0.130151
 Al   -0.689426   -1.385420    0.032123
 Al   -0.691277    1.384493    0.036329
 Al    2.053396   -1.501239   -0.176778
 Al    2.051137    1.504768   -0.172740

    6
scf done: -1194.517234
 Al    0.484976    1.220182    1.901332
 Al   -1.498562    0.219718   -0.361857
 B     0.542846    0.513077   -0.058044
 Al    0.804791   -1.247908   -1.344845
 Al    2.442629   -0.423101    0.523304
 Mg    0.554180    2.611450   -0.997869

    6
scf done: -1194.477098
 Al   -0.841714    1.203961    0.000471
 Al   -3.028299   -0.005736   -0.001100
 Mg   -0.743829   -1.583615    0.001291
 B     0.936482   -0.020731    0.002332
 Al    1.922134    1.733731    0.002721
```

```
Al      2.275632     -1.462428      0.003870


      6
scf done: -1194.491714
Al    -0.736832     -1.447013     -0.604885
Al    -0.569587      1.483900     -1.103606
 B     0.536403     -0.169038     -1.556964
Al     1.966497      0.344963     -0.217182
Al    -0.884173     -0.085142      1.509753
Mg     0.961201      1.860811      1.818254


      6
scf done: -1194.492050
Al    -1.078018     -0.000000      1.000000
Mg     1.677238     -0.000000      1.000000
 B    -3.004361      0.000000      1.000000
Al    -3.196865      0.000000      3.071735
Al    -3.196865      0.000000     -1.071735
Al    -4.996897      0.000000      1.000000


      6
scf done: -1194.487550
 B     0.471152     -0.000000      1.000000
Mg     2.816057     -0.000000      1.000000
Al     1.109268      0.000000      3.074519
Al     1.109268     -0.000000     -1.074519
Al    -1.253949      0.000000      2.286315
Al    -1.253949     -0.000000     -0.286315


      6
scf done: -1194.485152
 B    -0.133447      0.000000     -0.025460
Al     0.089974     -0.000000      2.079449
Al     2.563801     -0.000000      2.686107
Al     1.978777     -0.000000      0.176204
Al     0.393909      0.000000     -1.936418
Mg    -2.223424      0.000000      0.505311
```

Optimized geometries of BAl4Mg+ (singlet) obtained at the wB97XD/6-311++G(2d,2p) level

```
   6
1c   scf done: -1194.310565
B   -0.244364    0.000000     1.000000
Mg   3.540667   -0.000000     1.000000
Al   1.218688    0.000000     2.485248
Al   1.218688   -0.000000    -0.485248
Al  -1.367916    0.000000     2.746933
Al  -1.367916   -0.000000    -0.746933


   6
```

2c   scf done: -1194.306672
B   0.199978   -0.137949   0.226507
Al   -0.390570   0.023455   2.242489
Al   2.200657   0.168746   -0.358732
Al   -0.848058   -1.712351   -0.908100
Mg   -0.591167   1.696447   -0.456129
Al   2.265373   0.512711   2.320355

    6
3c   scf done: -1194.304129
B   0.013577   -0.000000   1.000000
Mg   2.328626   -0.000000   1.000000
Al   0.502784   0.000000   3.069258
Al   0.502784   -0.000000   -1.069258
Al   -1.823885   0.000000   2.267144
Al   -1.823885   -0.000000   -0.267144

    6
4c   scf done: -1194.297679
B   0.005541   0.013045   -0.104760
Al   2.135377   0.306543   -0.468740
Mg -0.047112   -1.689123   1.143606
Al   -1.281996   -0.541145   -1.775217
Al   -0.808012   1.312898   1.180490
Al   -1.949748   3.506932   2.744310

    6
5c   scf done: -1194.292206
B   -0.152171   0.000000   0.951311
Mg   3.731117   -0.000000   1.017982
Al   1.409264   -0.000000   -0.339435
Al   1.364036   -0.000000   2.294894
Al   -1.473762   -1.711642   0.928628
Al   -1.473762   1.711642   0.928628

    6
6c   scf done: -1194.292247
Al   0.000000   0.000000   0.000000
Mg   0.000000   0.000000   2.769192
Al   2.402650   0.000000   1.536359
B   2.052929   0.000000   -0.420628
Al   0.839277   0.000000   -2.302549
Al   3.287909   0.000000   -1.995515

6

7c   scf done: -1194.287565
B   0.000000   0.000000   -0.000000
Al   0.000000   0.000000   2.038923
Al   2.531152   -0.000000   3.666203
Al   2.216566   -0.000000   0.697047
Al   1.229152   -0.000000   -1.612660
Mg -2.021036   0.000000   -0.519600

6

8c   scf done: -1194.287698
B   -0.118278   0.006877   0.018199
Mg -0.430845   0.150545   2.168227
Al   3.173310   0.136296   1.152256
Al   1.905027   1.869642   2.533495
Al   0.956585   1.704274   0.157567
Al   1.418168   -1.266507   -0.175304

6

9c   scf done: -1194.287464
Al   -0.386244   -1.327075   -0.335821
Al   -0.898642   1.130951   -1.179580
B   0.616749   -0.140709   -1.646784
Al   2.013354   0.566259   -0.434483
Al   -1.274583   0.476905   1.302344
Mg 1.202876   1.282152   2.139696

6

10c   scf done: -1194.284990
Al   -1.301025   0.351854   -1.838324
B   -0.211195   0.131125   0.020415
Mg 0.586852   -1.882867   0.088708
Al   1.433431   1.510275   0.312084
Al   -1.373471   -0.121445   1.634531
Al   -1.067880   -2.538922   2.544554

6

11c   scf done: -1194.283539
Al   1.873762   0.780400   0.911126
Al   -0.909630   -1.150507   1.726601
B   -0.056316   0.296888   0.113167
Al   -1.840122   1.057523   -0.800523
Al   0.616110   -0.951461   -1.546479

Mg   -0.222614   2.552688   0.837018

   6
12c   scf done: -1194.282921
 B   -0.210463   -0.108520   0.040930
Al   0.400833   -0.792055   2.052682
Al   -1.885755   -1.248324   -0.842320
Al   1.276158   -0.554991   -1.063012
Al   -0.382966   2.085083   -0.168144
Mg   3.460502   -1.209803   -2.686616

   6
13c   scf done: -1194.276928
 B   -0.000000   0.000000   -0.161268
Mg   -0.000000   0.000000   1.957588
Al   -0.000000   2.264685   -0.554011
Al   0.000000   -2.264685   -0.554011
Al   2.275790   0.000000   -0.520006
Al   -2.275790   -0.000000   -0.520006

   6
14c   scf done: -1194.279083
 B   -0.043288   -0.000000   0.090391
Mg   0.217909   -0.000000   2.208168
Al   1.283277   -0.000000   -1.418057
Al   -1.537145   0.000000   -1.208691
Al   -2.823463   0.000000   -3.628231
Al   -0.103620   0.000000   -3.545868

   7
15c scf done: -1194.278130
Al   -0.883985   -0.000000   1.000000
Mg   1.892953   -0.000000   1.000000
 B   -2.780749   0.000000   1.000000
Al   -3.415327   0.000000   2.987628
Al   -3.415327   0.000000   -0.987628
Al   -5.193332   0.000000   1.000000
XX   -0.883985   0.000000   -0.000000

   6
16c   scf done: -1194.275849
 B   0.969630   -0.202643   0.769762
Al   1.439701   -1.616493   -0.569203
Mg   -0.339110   -1.479236   1.841067

```
Al   -0.527887    0.717567   -0.191207
Al   -2.207856    2.720004   -1.424291
Al    2.887382   -3.317309   -2.403297


    7
17c  scf done: -1194.271999
Al   -0.000000    0.000000    1.887911
Al   -0.000000    0.000000    4.803045
 B   -0.000000   -0.000000   -0.077664
Al    0.000000    1.326147   -1.555581
Al   -0.000000   -1.326147   -1.555581
Mg    0.000000   -0.000000   -3.858322
XX    0.000000    1.000000    1.887911


    6
18c  scf done: -1194.266665
 B   -0.208663    0.338220    0.148958
Al    0.483780   -0.801633    1.620107
Al    1.911947    0.873785    3.588461
Al    3.402757   -0.429600    1.883787
Al    1.375482    1.384852    0.730470
Mg   -1.790810    0.405976   -1.272039



    6
19c   scf done: -1194.261598
 B   -0.740824   -0.215405    2.509572
Mg   -1.606222   -0.189911    0.566413
Al    1.020587    0.063961    3.400270
Al    1.960572   -0.307331    8.555629
Al    0.796523   -0.264544    5.955431
Al   -1.257646   -0.533040    4.408239


    6
20c   scf done: -1194.258845
 B   -0.000000   -0.000000    1.687301
Mg   -0.000000   -0.000000    3.853690
Al   -0.000000    1.294828    0.175702
Al   -0.000000   -1.294828    0.175702
Al    0.000000    1.266850   -2.278809
Al   -0.000000   -1.266850   -2.278809
```

6

21c   scf done: -1194.253420
 B   -1.138135   0.830372   1.730863
Al   0.412961   0.845553   0.470994
Al   -1.726291   -0.987715   1.073405
Al   -4.213731   -0.990853   2.355157
Al   -4.227556   -1.188848   -0.151351
Mg -2.903015   1.491493   0.520930

7

22c   scf done: -1194.225706
Mg   -0.773500   -0.000000   1.000000
Al   2.302743   -0.000000   1.000000
 B   -2.970485   0.000000   1.000000
Al   -3.608698   0.000000   2.959760
Al   -3.608698   -0.000000   -0.959760
Al   -5.137131   0.000000   1.000000
XX   -0.773500   -0.000000   2.000000

7

23c scf done: -1194.222698
Al   -0.000000   -0.000000   4.237516
Mg -0.000000   -0.000000   1.074310
 B   -0.000000   -0.000000   -1.034132
Al   0.000000   2.111275   -1.627647
Al   1.828418   -1.055638   -1.627647
Al   -1.828418   -1.055637   -1.627647
XX   -0.000000   1.000000   1.074310

6

24c scf done: -1194.220368
Al   1.092206   -1.697819   0.883285
Mg -0.128353   1.032493   -0.028848
 B   -0.586337   -0.694822   1.303120
Al   -1.364001   -1.839798   -0.141565
Al   0.638604   3.380228   -2.061200
Al   -0.484708   4.168767   0.217996

7

25c   scf done: -1194.206685
Mg   0.399081   -0.000000   1.000000
Al   3.468982   -0.000000   1.000000

```
Al   -2.530585    0.000000    1.000000
Al   -5.357331    0.000000    2.846705
Al   -5.357331   -0.000000   -0.846705
 B   -4.419246    0.000000    1.000000
XX   -2.530585    0.000000    2.000000


   7
26c  scf done: -1194.197762
Al    0.334793   -0.000000    1.000000
Mg    3.603555   -0.000000    1.000000
Al   -2.616115    0.000000    1.000000
Al   -5.308572    0.000000    2.940958
Al   -5.308572   -0.000000   -0.940958
 B   -4.500857    0.000000    1.000000
XX   -2.616115    0.000000    0.000000


   6
27c  scf done: -1194.196799
 B    0.501382   -0.000000    1.000000
Al   -0.813241   -0.000000    2.470209
Al   -0.813241    0.000000   -0.470209
Al   -3.232068   -0.000000    2.240208
Al   -3.232068    0.000000   -0.240208
Mg   -6.949778    0.000000    1.000000


   7
28c  scf done: -1194.177328
 B    0.235562   -0.000000    1.000000
Mg    2.381322   -0.000000    1.000000
Al   -1.737638   -0.000000    1.000000
Al   -4.000164    0.000000    2.217388
Al   -4.000164    0.000000   -0.217388
Al   -6.674686    0.000000    1.000000
XX    0.235562   -0.000000    2.000000


   6
29c  scf done: -1194.141133
Mg   -0.000000    0.000000    2.745252
 B   -0.000000    0.000000    5.257579
Al   -0.000000    1.287145    0.130458
```

```
Al   -0.000000   -1.287145    0.130458
Al    0.000000    1.249745   -2.509201
Al    0.000000   -1.249745   -2.509201


    7
30c   scf done: -1194.133351
Al    0.297125   -0.000000    1.000000
 B    2.702041   -0.000000    1.000000
Al   -2.146975   -0.000000    1.000000
Al   -4.140416    0.000000    2.403816
Al   -4.140416   -0.000000   -0.403816
Mg   -6.367126    0.000000    1.000000
XX    0.297125   -0.000000    2.000000


    7
31c   scf done: -1194.131595
Mg    0.504145    0.000000    1.000000
 B    3.017439    0.000000    1.000000
Al   -2.297783    0.000000    1.000000
Al   -4.341679   -0.000000    2.452998
Al   -4.341679    0.000000   -0.452998
Al   -6.336210   -0.000000    1.000000
XX    0.504145    0.000000    2.000000


    7
 32c   scf done: -1194.114122
 B   -0.000000    0.000000    3.185630
Al   -0.000000    0.000000    5.234467
Mg  -0.000000    0.000000    0.915889
Al    0.000000    1.204622   -1.704680
Al   -0.000000   -1.204622   -1.704680
Al    0.000000   -0.000000   -4.197592
XX    1.000000    0.000000    3.185630


    6
33c   scf done: -1194.083906
Al   -0.000000    0.005377   -3.813183
 B   -0.000000    0.043237   -5.834498
Mg  -0.000000   -0.009422   -0.879605
Al    0.000000    1.195384    1.671108
```

```
Al    0.000000   -1.201442    1.677361
Al    0.000000    0.003379    4.250563
```

Optimized geometries of BAl4Mg+ (triplet) obtained at the UwB97XD/6-311++G(2d,2p) level

```
      6
scf done: -1194.311221
 B    -0.000000     0.000000    -0.665823
Mg     0.000000    -0.000000     2.988586
Al    -0.000000     1.535595     0.730475
Al    -0.000000    -1.535595     0.730475
Al    -0.000000     1.554246    -1.981780
Al    -0.000000    -1.554246    -1.981780

      6
scf done: -1194.305328
 B    -0.127014    -0.000000     1.000000
Mg     2.351059    -0.000000     1.000000
Al     0.602534    -0.000000     3.033072
Al     0.602534    -0.000000    -1.033072
Al    -1.864556     0.000000     2.265965
Al    -1.864556     0.000000    -0.265965

      6
scf done: -1194.296551
 B     0.246239     0.110252     0.286849
Al    -0.414557    -0.119029     2.287832
Al     2.253188     0.032191    -0.391042
Al    -0.554445    -1.493264    -0.602334
Mg    -0.938584     1.832373    -0.795827
Al     2.244373     0.188537     2.280912

      6
scf done: -1194.296603
 B     0.289964     0.000000     0.031046
Al    -0.187236     0.000000     2.051350
Al     2.176415    -0.000000     3.348721
Al     2.269588    -0.000000     0.691408
Al     1.283411    -0.000000    -1.751536
Mg    -1.876309     0.000000    -0.101076

      6
scf done: -1194.292376
 B     1.155211     0.024019     0.426754
Mg    -0.072647     0.032009     2.400384
Al     2.860789    -0.204874     1.657817
Al     1.815369     2.210766     2.265448
Al     0.292872     1.919643     0.053040
Al     0.852373    -1.380435    -0.949001

      6
```

```
scf done: −1194.290979
 B     −0.191178      0.000000      0.950644
Mg     3.928803     −0.000000      1.021375
Al     1.304522     −0.000000     −0.416787
Al     1.256704     −0.000000      2.368607
Al    −1.447064     −1.832980      0.929084
Al    −1.447064      1.832980      0.929084

      6
scf done: −1194.285201
Al     0.059388     −1.108715      0.046527
Al    −1.343879      0.872623     −1.496101
 B     0.522214      0.081269     −1.547426
Al     2.190372      0.575097     −0.469371
Al    −1.367980      0.909248      1.144765
Mg     1.213395      0.658961      2.166979

      6
scf done: −1194.258080
 B     0.031270     −0.046545     −0.132366
Al     2.153444      0.526934     −0.272149
Mg    −0.062840     −1.703171      1.190926
Al    −1.508184     −0.382514     −1.671661
Al    −0.788094      1.246315      1.171385
Al    −1.771545      3.268132      2.433555
```