Supplementary Information (ESI)

Isovalent Effects on the Structural and Electronic Features of Scandium-doped Aluminum Clusters $Sc_mAl_{n-m}^{+/0/-}$ with m = 1 – 2, n = 3-15

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Content

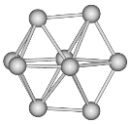
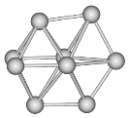
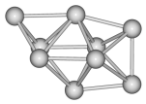
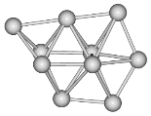
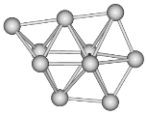
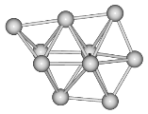
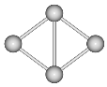
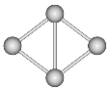
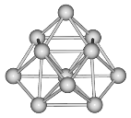
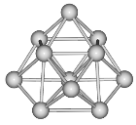
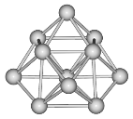
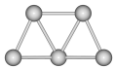
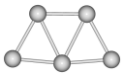
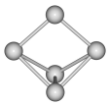
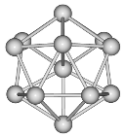
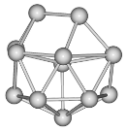
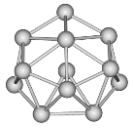
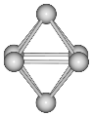
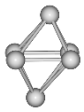
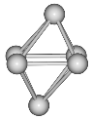
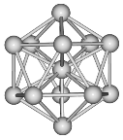
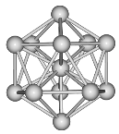
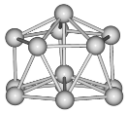
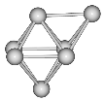
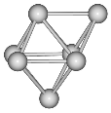
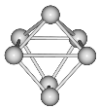
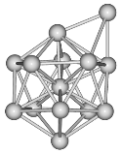
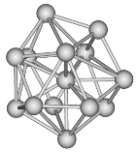
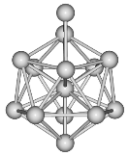
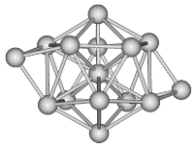
n	Anion	Neutral	Cation	n	Anion	Neutral	Cation
2	 a.2.A.1	 n.2.A.1	 C.2.A.1	9	 a.9.A.1	 n.9.A.1	 c.9.A.1
3	 a.3.A.1	 n.3.A.1	 c.3.A.1	10	 a.10.A.1	 n.10.A.1	 c.10.A.1
4	 a.4.A.1	 n.4.A.1	 c.4.A.1	11	 a.11.A.1	 n.11.A.1	 c.11.A.1
5	 a.5.A.1	 n.5.A.1	 c.5.A.1	12	 a.12.A.1	 n.12.A.1	 c.12.A.1
6	 a.6.A.1	 n.6.A.1	 c.6.A.1	13	 a.13.A.1	 n.13.A.1	 c.13.A.1
7	 a.7.A.1	 n.7.A.1	 c.7.A.1	14	 a.14.A.1	 n.14.A.1	 c.14.A.1
8	 a.8.A.1	 n.8.A.1	 c.8.A.1	15	 a.15.A.1	n.15.A.1	c.15.A.1

Figure S1: Structures of the lowest-lying cationic, neutral and anionic $Al_n^{+/0/-}$ clusters with n = 1-15 calculated at the PBE/ Def2-TZVP+ ZPE method.

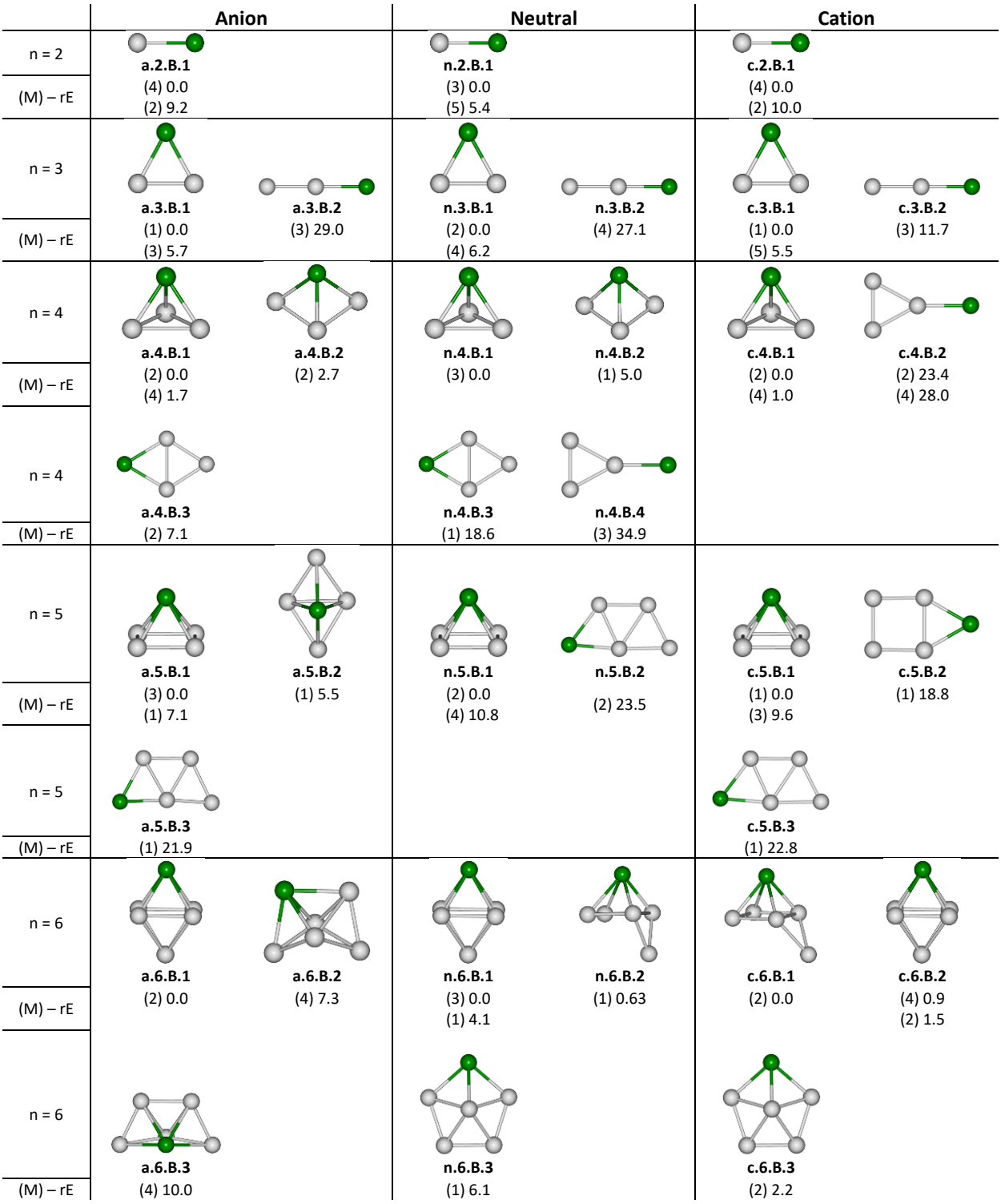


Figure S2: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_{n-1}^{+/0/-}$ clusters with n = 2-6 calculated at the PBE/ Def2-TZVP+ ZPE method.

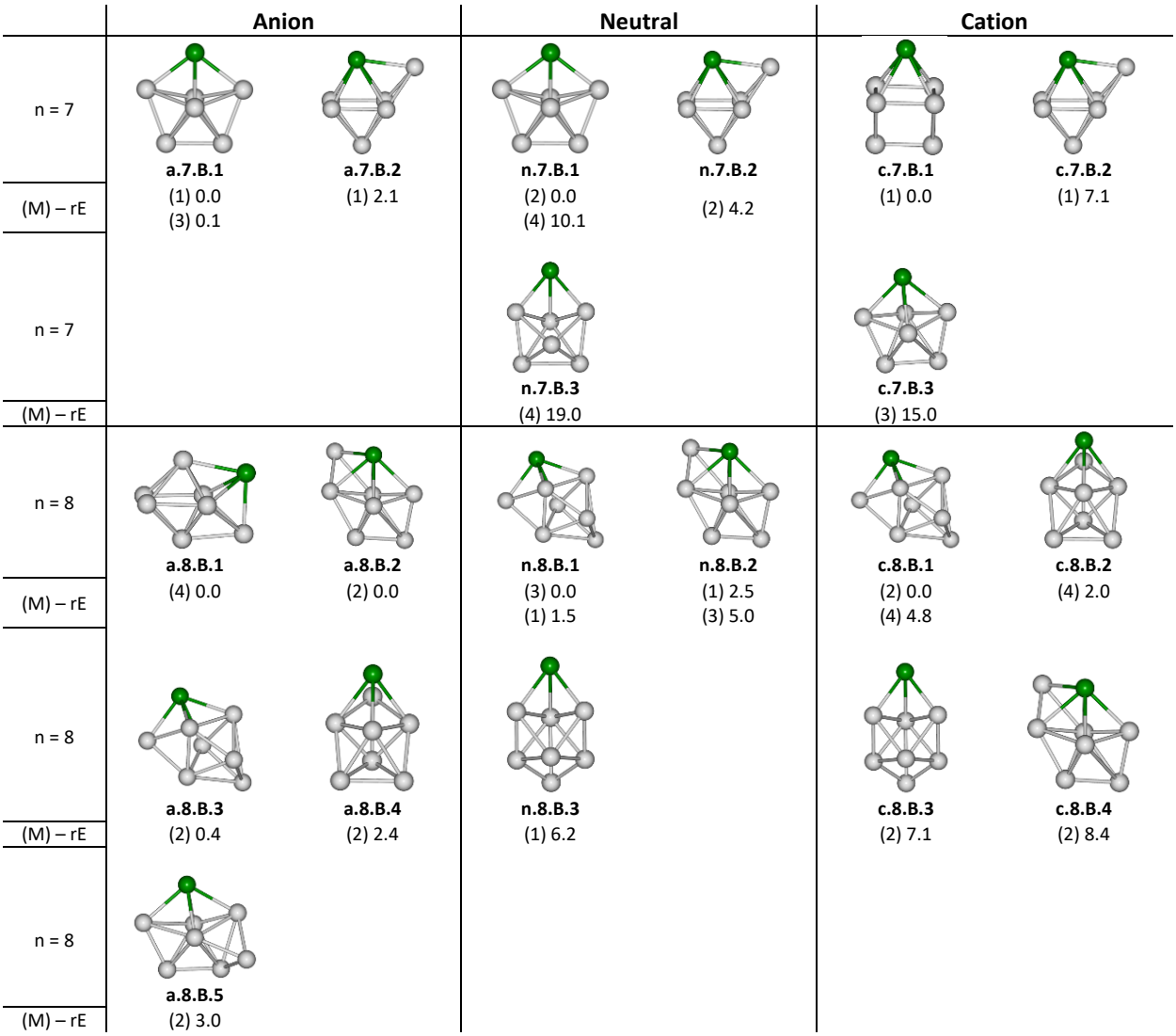


Figure S3: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_6^{+/0/-}$ and $ScAl_7^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

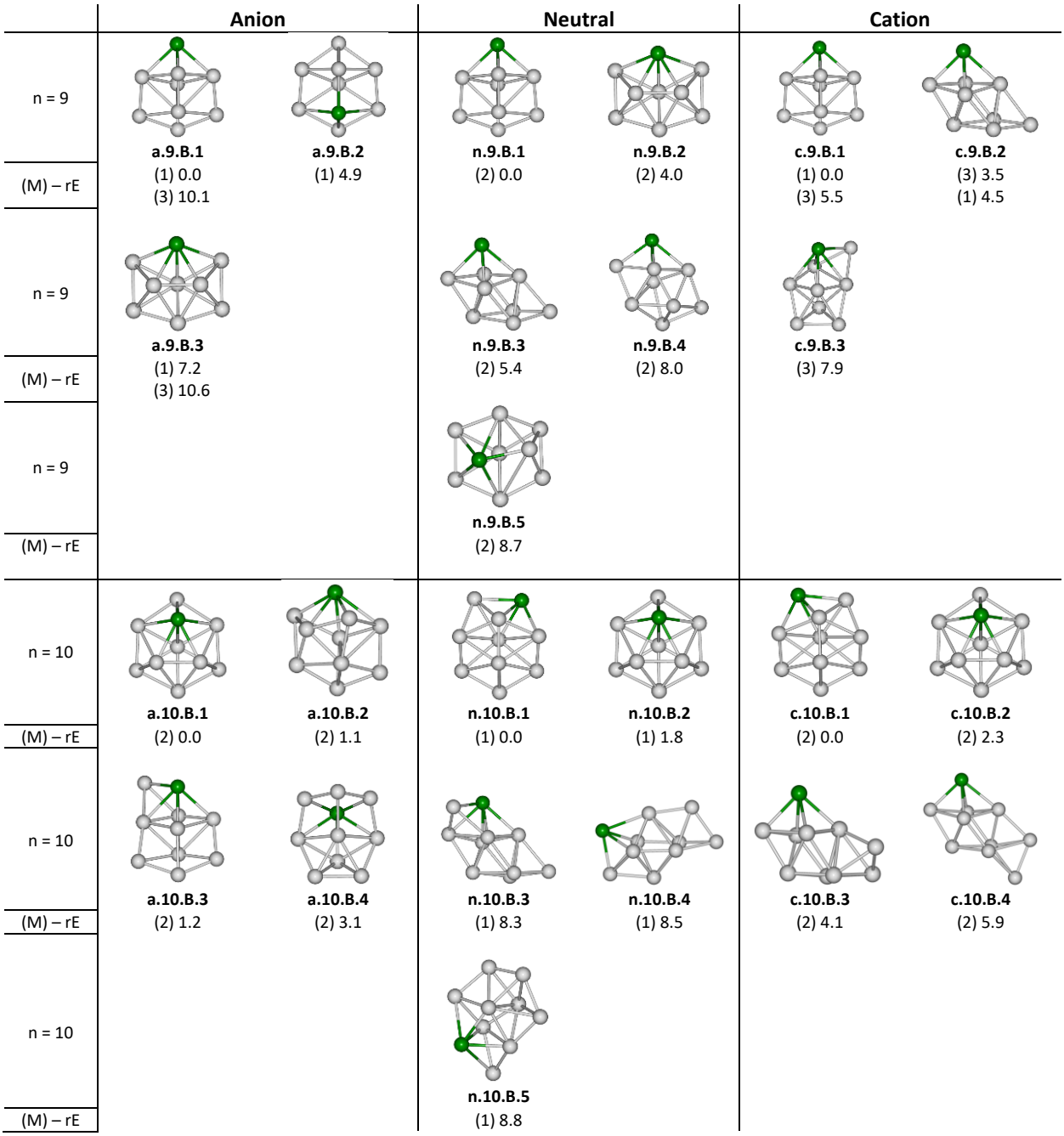


Figure S4: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_8^{+/0/-}$ and $ScAl_9^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

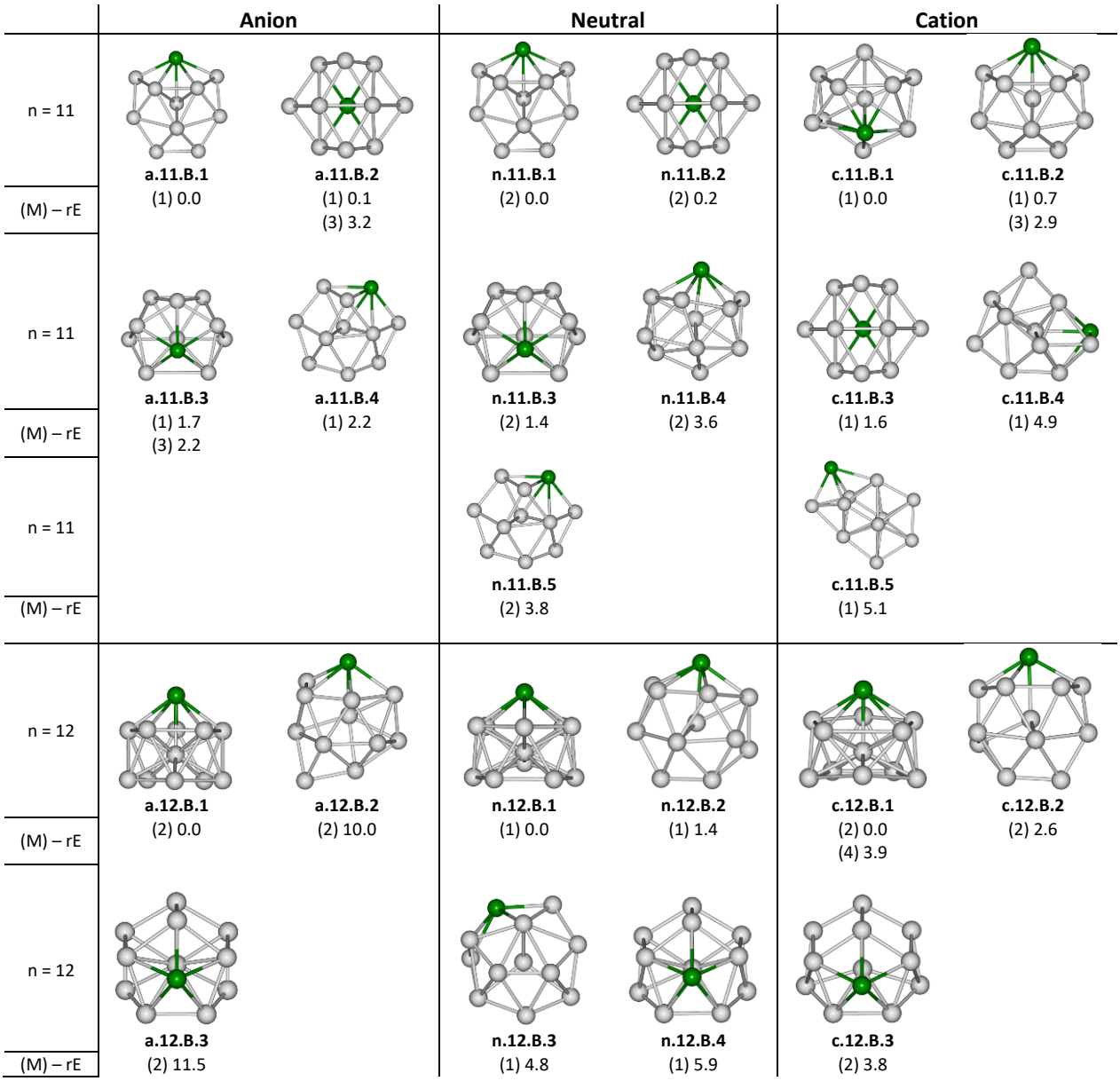


Figure S5: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_{10}^{+/0/-}$ and $ScAl_{11}^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

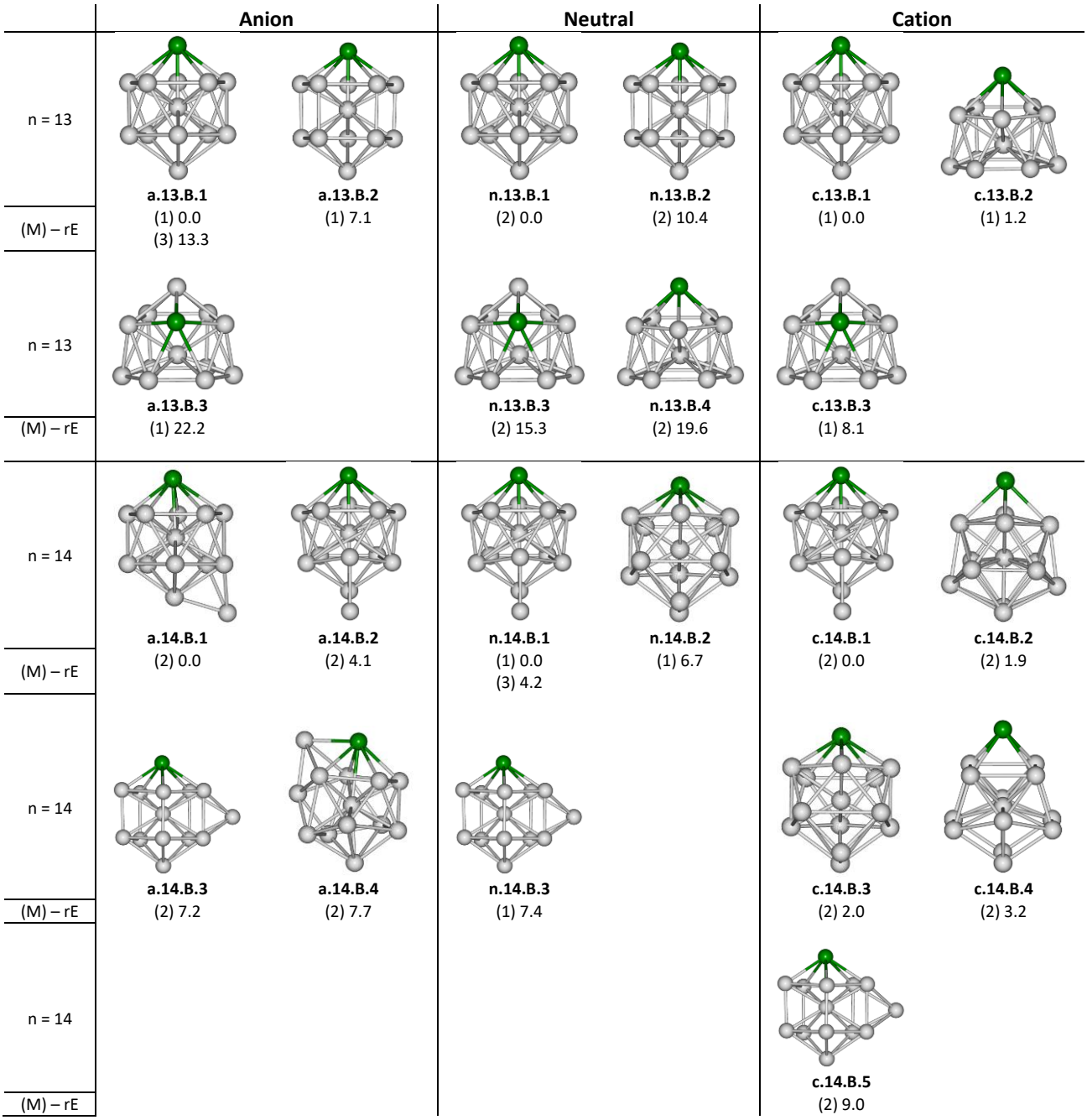


Figure S6: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_{12}^{+/0/-}$ and $ScAl_{13}^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

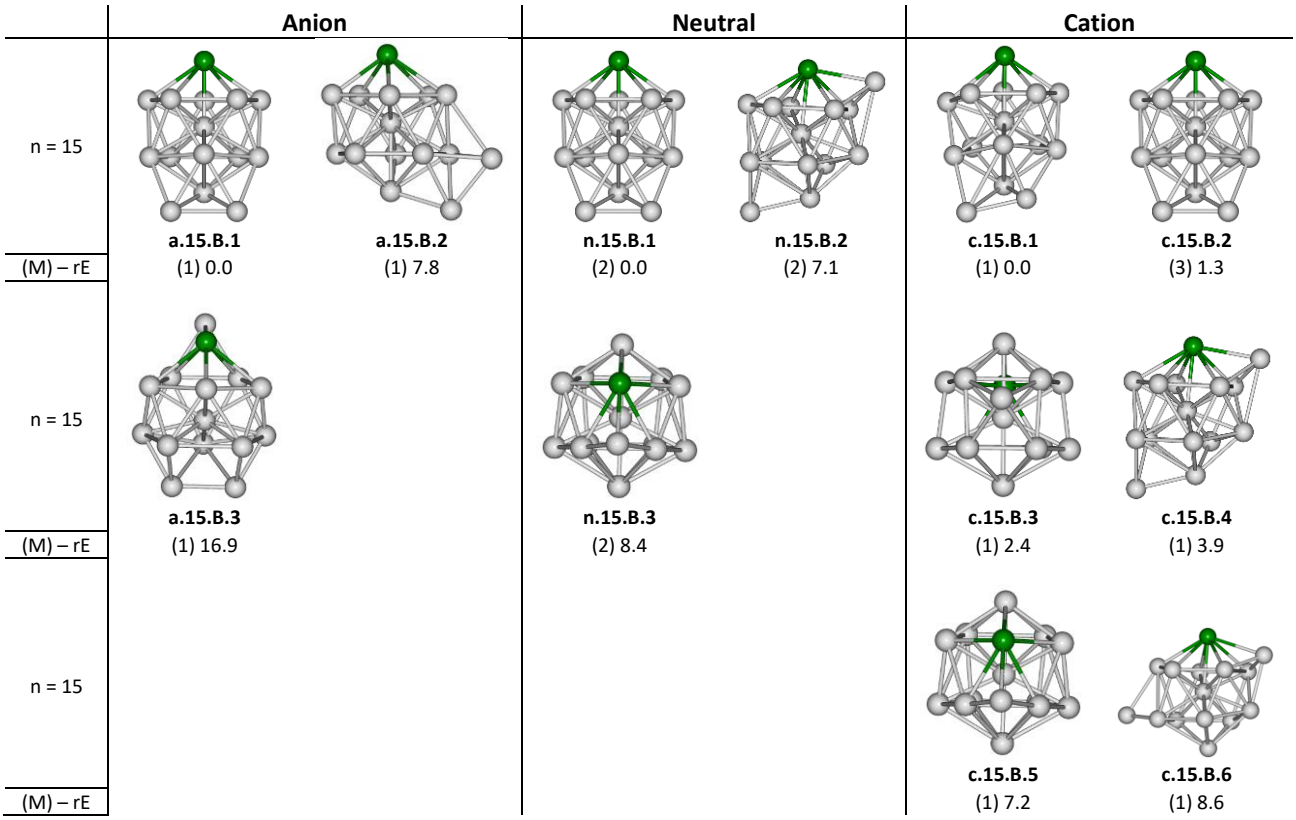


Figure S7: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $ScAl_{14}^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

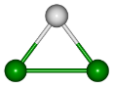
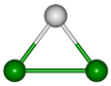
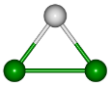
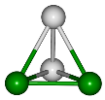
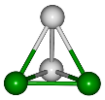
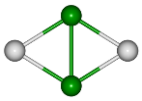
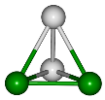
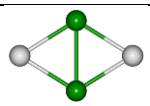
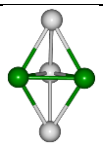
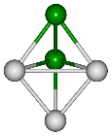
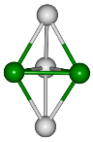
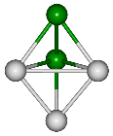
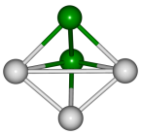
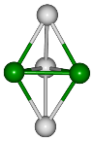
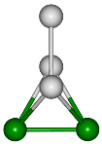
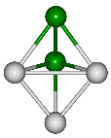
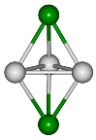
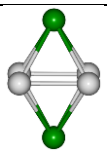
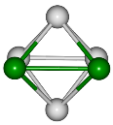
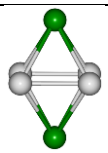
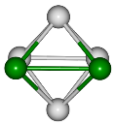
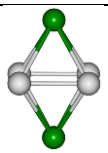
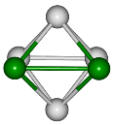
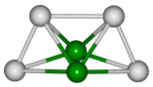
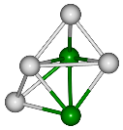
	Anion		Neutral		Cation	
n = 3						
(M) – rE	**a.3.C.1** (1) 0.0 (3) 3.7		**n.3.C.1** (2) 0.0 (4) 3.2		**c.3.C.1** (1) 0.0 (5) 0.0 (3) 3.7	
n = 4						
(M) – rE	**a.4.C.1** (4) 0.0 (2) 0.1		**n.4.C.1** (3) 0.0 (1) 7.7 (5) 11.2	**n.4.C.2** (3) 21.0	**c.4.C.1** (2) 0.0 (4) 1.9	**c.4.C.2** (2) 8.9
n = 5						
(M) – rE	**a.5.C.1** (1) 0.0 (3) 1.4	**a.5.C.2** (3) 3.3	**n.5.C.1** (4) 0.0 (2) 1.2	**n.5.C.2** (2) 0.2 (4) 4.8	**c.5.C.1** (3) 0.0	**c.5.C.2** (3) 0.7
n = 5						
(M) – rE	**a.5.C.3** (1) 11.3				**c.5.C.3** (1) 1.3	**c.5.C.4** (3) 1.4
n = 6						
(M) – rE	**a.6.C.1** (2) 0.0	**a.6.C.2** (2) 0.6	**n.6.C.1** (1) 0.0 (3) 5.3	**n.6.C.2** (3) 6.8	**c.6.C.1** (2) 0.0 (4) 3.1	**c.6.C.2** (2) 11.9 (4) 18.0
n = 6						
(M) – rE	**a.6.C.3** (2) 2.3	**a.6.C.4** (2) 2.9				

Figure S8: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_{n-2}^{+/0/-}$ clusters with n = 3-6 calculated at the PBE/ Def2-TZVP+ ZPE method.

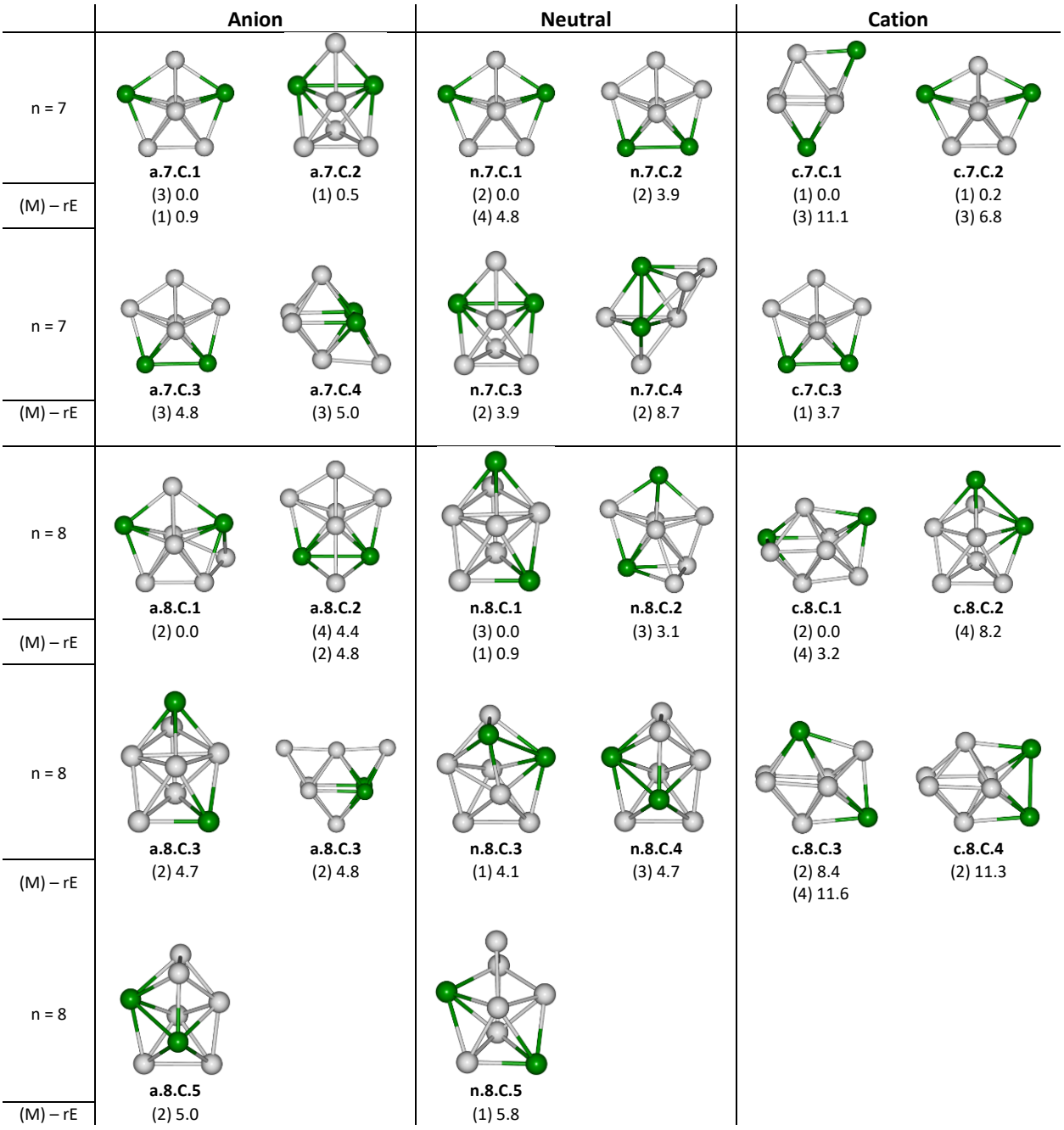


Figure S9: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_5^{+/0/-}$ and $Sc_2Al_6^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

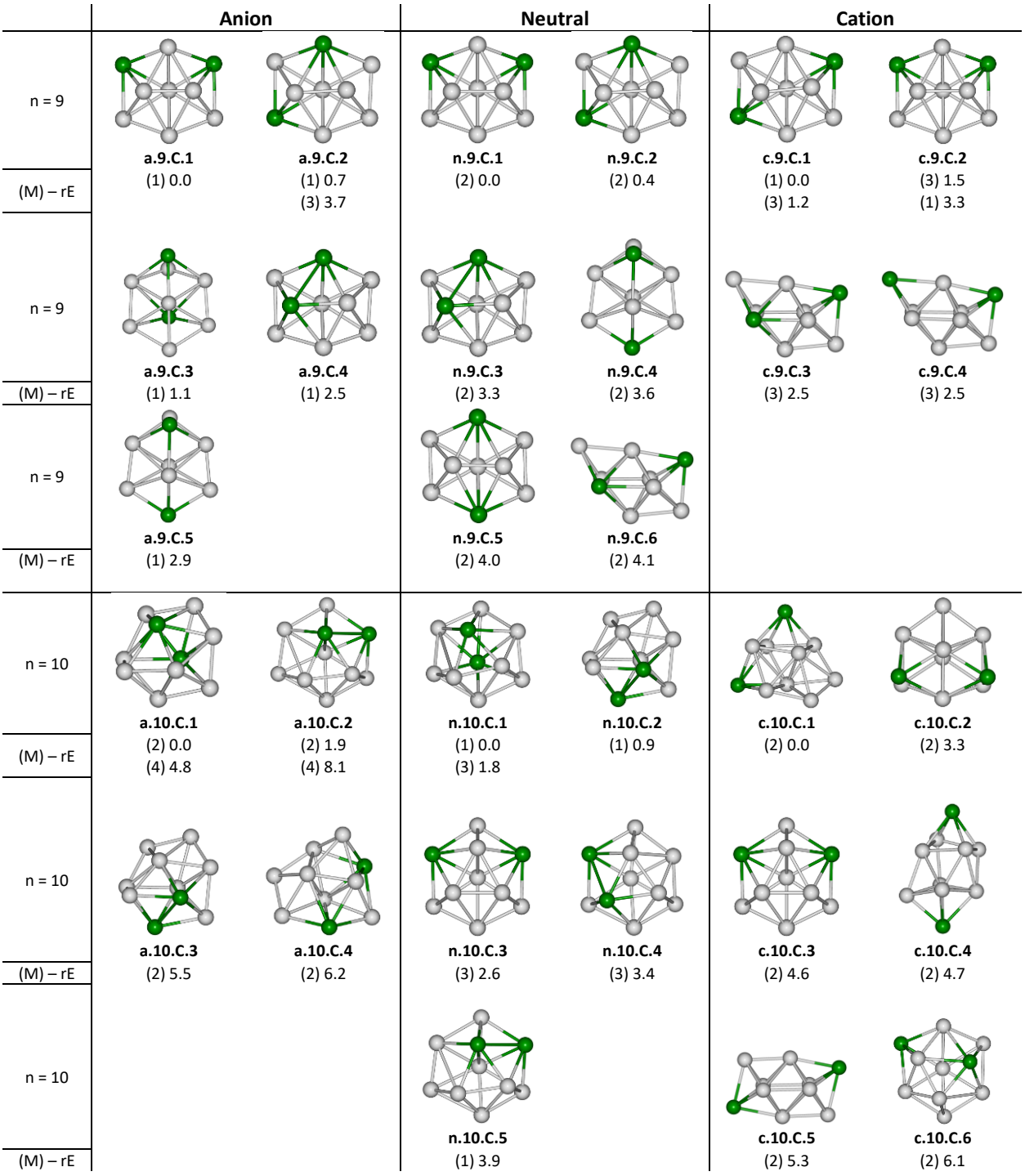


Figure S10: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_7^{+/0/-}$ and $Sc_2Al_8^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

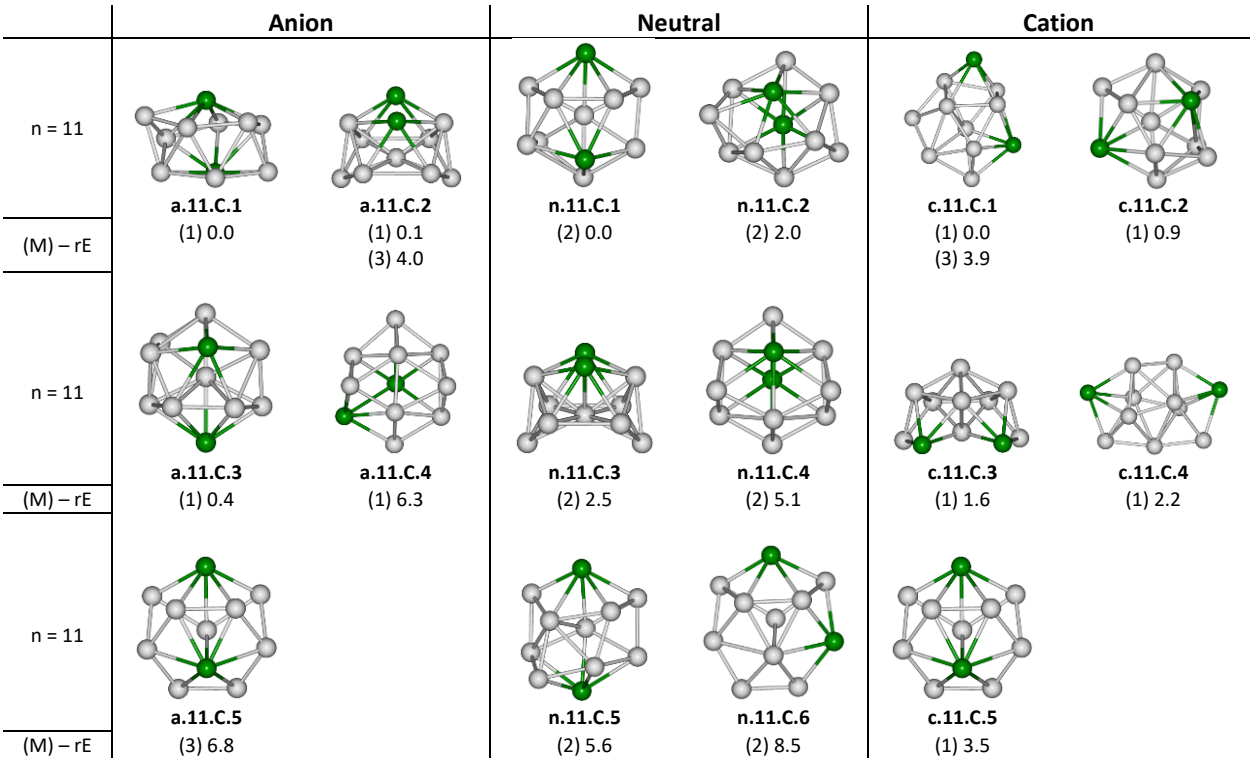


Figure S11: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_9^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

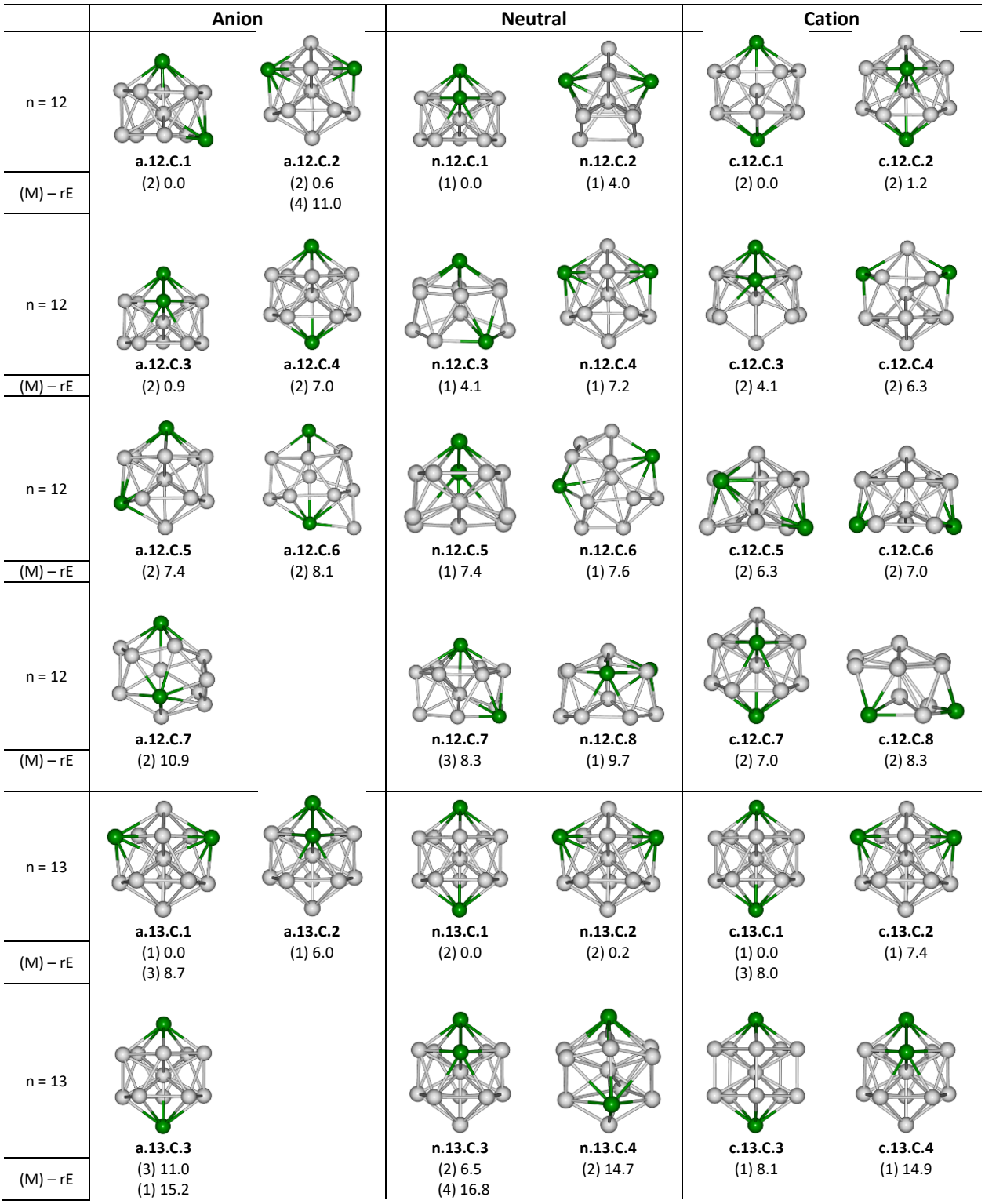


Figure S12: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_{10}^{+/0/-}$ and $Sc_2Al_{11}^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

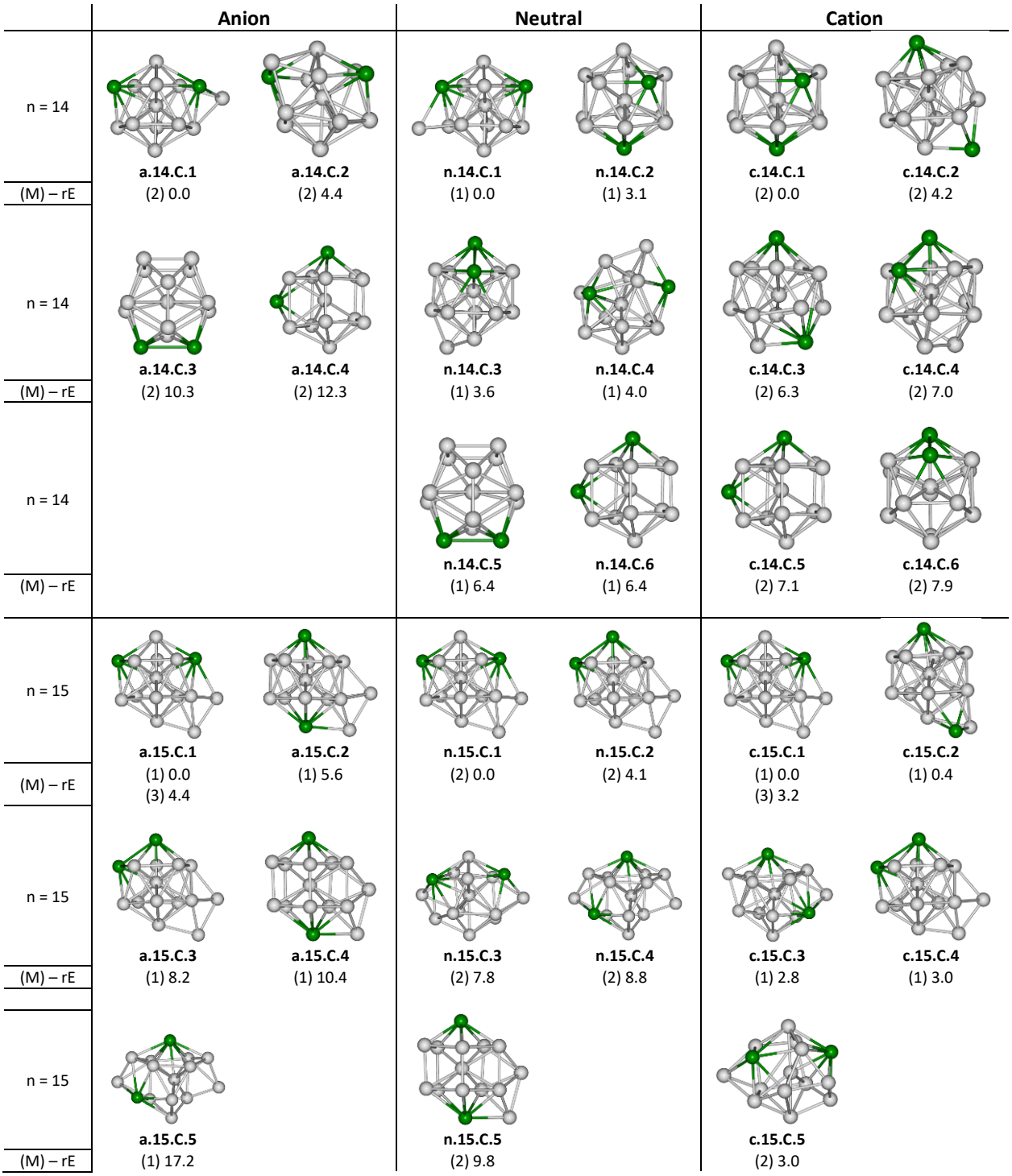


Figure S13: Structures, multiplicities (M, in bracket) and relative energies (rE, kcal.mol^{-1}) of the low-lying cationic, neutral and anionic $Sc_2Al_{12}^{+/0/-}$ and $Sc_2Al_{13}^{+/0/-}$ clusters calculated at the PBE/ Def2-TZVP+ ZPE method.

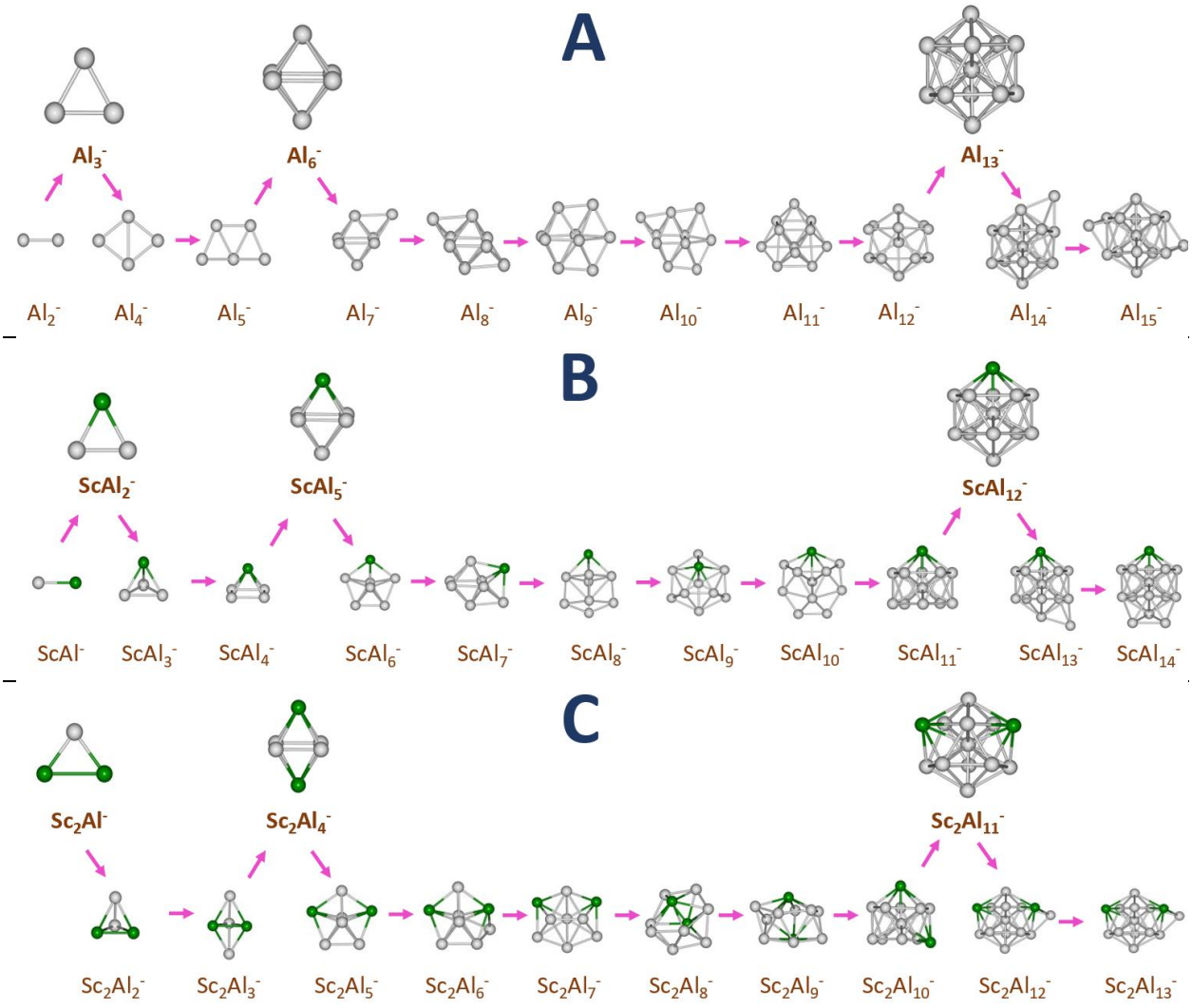


Figure S14: Structural evolution of the anionic **A)** Al_n^-, **B)** $ScAl_{n-1}^-$ and **C)** $Sc_2Al_{n-2}^-$ clusters with n = 3-15.

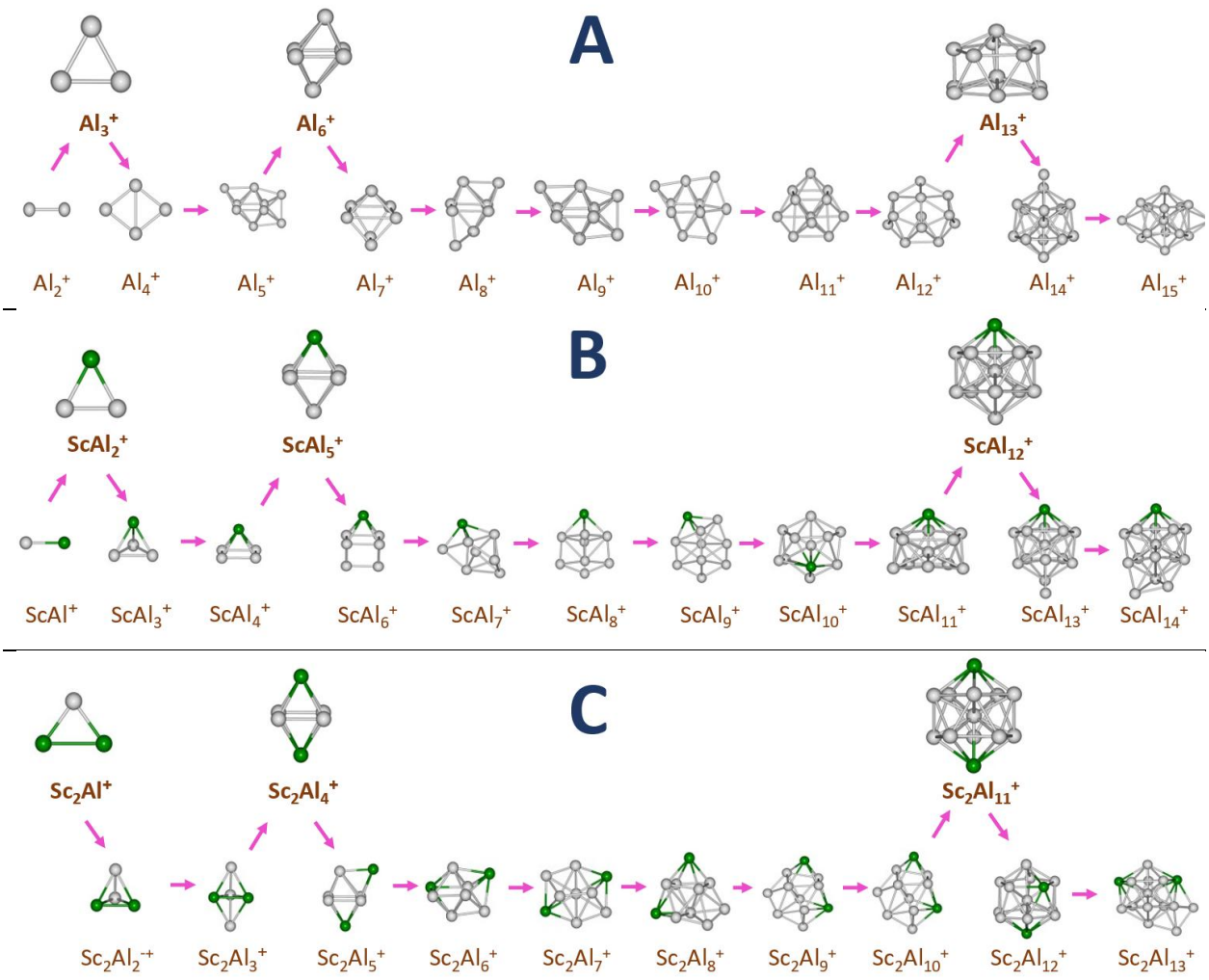


Figure S15: Structural evolution of the cationic **A)** Al_n^+, **B)** $ScAl_{n-1}^+$ and **C)** $Sc_2Al_{n-2}^+$ clusters with n = 3-15.

Table S1: Average binding energy values (E_b, eV) of the anionic and cationic $ScAl_{n-1}^{+/-}$ clusters (n = 2-15) calculated at the PBE/def2-TZVP level.

Isomer	Eb (Al^-)	Eb (Sc^-)	Isomer	Eb (Al^+)	Eb (Sc^+)
a.2.B.1	1.24	1.30	**c.2.B.1**	1.01	1.12
a.3.B.1	1.86	1.90	**c.3.B.1**	1.48	1.56
a.4.B.1	2.07	2.10	**c.4.B.1**	1.80	1.86
a.5.B.1	2.33	2.35	**c.5.B.1**	2.08	2.12
a.6.B.1	2.41	2.43	**c.6.B.1**	2.12	2.16
a.7.B.1	2.53	2.55	**c.7.B.1**	2.37	2.40
a.8.B.1	2.56	2.57	**c.8.B.1**	2.40	2.43
a.9.B.1	2.65	2.66	**c.9.B.1**	2.45	2.48
a.10.B.1	2.65	2.66	**c.10.B.1**	2.49	2.51
a.11.B.1	2.70	2.71	**c.11.B.1**	2.54	2.56
a.12.B.1	2.75	2.76	**c.12.B.1**	2.59	2.61
a.13.B.1	2.85	2.86	**c.13.B.1**	2.68	2.69
a.14.B.1	2.83	2.83	**c.14.B.1**	2.72	2.74
a.15.B.1	2.84	2.85	**c.15.B.1**	2.72	2.73

Table S2: Average binding energy values (E_b, eV) of the anionic and cationic $Sc_2Al_{n-2}^{+/-}$ clusters (n = 3-15) calculated at the PBE/def2-TZVP level.

Isomer	Eb (Al^-)	Eb (Sc^-)	Isomer	Eb (Al^+)	Eb (Sc^+)
a.3.C.1	1.76	1.80	**c.3.C.1**	1.59	1.67
a.4.C.1	2.15	2.18	**c.4.C.1**	2.02	2.07
a.5.C.1	2.33	2.35	**c.5.C.1**	2.12	2.17
a.6.C.1	2.44	2.47	**c.6.C.1**	2.38	2.42
a.7.C.1	2.58	2.60	**c.7.C.1**	2.44	2.48
a.8.C.1	2.63	2.64	**c.8.C.1**	2.54	2.57
a.9.C.1	2.67	2.68	**c.9.C.1**	2.55	2.57
a.10.C.1	2.71	2.73	**c.10.C.1**	2.60	2.62
a.11.C.1	2.76	2.77	**c.11.C.1**	2.62	2.65
a.12.C.1	2.79	2.81	**c.12.C.1**	2.68	2.70
a.13.C.1	2.89	2.90	**c.13.C.1**	2.79	2.81
a.14.C.1	2.87	2.88	**c.14.C.1**	2.79	2.81
a.15.C.1	2.89	2.90	**c.15.C.1**	2.79	2.81

Table S3. Dissociation Energies (D_e, eV) for Various Fragmentation Channels of $ScAl_{n-1}$ clusters at three charge states (n = 3–15), calculated at the PBE/def2-TZVP level.*

n	$ScAl_{n-1}$		$ScAl_{n-1}^-$				$ScAl_{n-1}^+$			
	$D_e(1)$	$D_e(2)$	$D_e(3)$	$D_e(4)$	$D_e(5)$	$D_e(6)$	$D_e(7)$	$D_e(8)$	$D_e(9)$	$D_e(10)$
3	2.73	2.71	4.04	2.71	3.89	3.10	3.01	3.21	2.76	2.42
4	3.02	2.72	4.32	2.77	3.89	2.71	3.33	3.45	2.80	2.76
5	4.09	3.10	5.64	3.40	4.52	3.35	4.49	4.41	3.27	3.19
6	3.60	2.39	5.57	3.57	4.24	2.82	3.94	4.04	2.51	2.33
7	3.91	3.43	5.75	3.33	5.14	3.30	4.67	4.96	3.96	3.84
8	3.10	2.67	4.99	2.96	4.43	2.72	3.81	3.32	3.15	2.63
9	3.74	3.03	5.98	3.95	5.14	3.38	4.32	4.23	3.37	2.89
10	3.80	2.84	5.87	3.33	4.77	2.66	4.35	4.14	3.16	2.81
11	3.98	2.97	6.26	3.78	5.12	3.18	4.57	4.48	3.32	3.01
12	4.18	3.27	6.54	3.96	5.50	3.35	4.68	4.57	3.54	3.19
13	4.86	3.82	7.36	4.86	6.19	3.96	5.25	5.01	3.98	3.70
14	3.94	2.87	6.12	2.85	4.92	2.56	4.74	4.47	3.44	3.29
15	3.84	2.82	6.29	3.86	5.14	3.08	4.51	3.95	3.26	2.70

(*)

For neutral : (1) $ScAl_{n-1} \rightarrow Al_{n-1} + Sc$; (2) $ScAl_{n-1} \rightarrow ScAl_{n-2} + Al$;

For anion : (3) $ScAl_{n-1}^- \rightarrow Al_{n-1} + Sc^-$; (4) $ScAl_{n-1}^- \rightarrow Al_{n-1}^- + Sc$;

(5) $ScAl_{n-1}^- \rightarrow ScAl_{n-2} + Al^-$; (6) $ScAl_{n-1}^- \rightarrow ScAl_{n-2}^- + Al$;

For cation : (7) $ScAl_{n-1}^+ \rightarrow Al_{n-1} + Sc^+$; (8) $ScAl_{n-1}^+ \rightarrow Al_{n-1}^+ + Sc$;

(9) $ScAl_{n-1}^+ \rightarrow ScAl_{n-2} + Al^+$; (10) $ScAl_{n-1}^+ \rightarrow ScAl_{n-2}^+ + Al$;

Table S4. Dissociation Energies (D_e, eV) for Various Fragmentation Channels of Sc_2Al_{n-2} clusters at three charge states (n = 3–15), calculated at the PBE/def2-TZVP level.*

n	Sc_2Al_{n-2}		$Sc_2Al_{n-2}^-$				$Sc_2Al_{n-2}^+$			
	D_e(11)	D_e(12)	D_e(13)	D_e(14)	D_e(15)	D_e(16)	D_e(17)	D_e(18)	D_e(19)	D_e(20)
3	2.60	2.64	3.72	2.80	3.64	3.01	3.33	2.76	3.15	2.21
4	3.23	3.34	4.32	3.02	4.31	3.32	3.90	3.63	3.79	3.29
5	3.05	2.54	4.64	3.35	4.01	3.04	3.72	3.41	2.98	2.54
6	3.24	3.29	4.58	3.03	4.50	3.04	4.28	3.88	4.09	3.66
7	3.82	2.97	5.57	3.60	4.59	3.38	4.73	4.39	3.65	2.84
8	3.38	3.00	5.13	3.28	4.61	2.99	4.51	3.75	3.89	3.21
9	3.56	2.85	5.44	3.55	4.60	2.99	4.46	3.75	3.52	2.63
10	3.50	2.97	5.52	3.28	4.86	3.11	4.47	3.89	3.70	3.04
11	3.79	3.12	5.93	3.87	5.14	3.25	4.52	3.97	3.62	2.89
12	4.05	3.23	6.13	3.85	5.18	3.16	4.82	4.23	3.77	3.27
13	4.64	3.86	6.84	4.48	5.94	3.98	5.73	5.22	4.72	4.18
14	3.61	2.80	5.68	3.19	4.74	2.66	4.72	4.33	3.67	2.81
15	3.78	3.04	6.01	3.83	5.14	3.20	4.63	3.83	3.65	2.78

(*)

(11) $Sc_2Al_{n-2} \rightarrow ScAl_{n-2} + Sc$;

(12) $Al_{n-2}Sc_2 \rightarrow Sc_2Al_{n-3} + Al$;

(13) $Sc_2Al_{n-2}^- \rightarrow ScAl_{n-2} + Sc^-$;

(14) $Al_{n-2}Sc_2^- \rightarrow ScAl_{n-2}^- + Sc$;

(15) $Sc_2Al_{n-2}^- \rightarrow Sc_2Al_{n-3} + Al^-$;

(16) $Al_{n-2}Sc_2^- \rightarrow Sc_2Al_{n-3}^- + Al$;

(17) $Sc_2Al_{n-2}^+ \rightarrow ScAl_{n-2} + Sc^+$;

(18) $Al_{n-2}Sc_2^+ \rightarrow ScAl_{n-2}^+ + Sc$;

(19) $Sc_2Al_{n-2}^+ \rightarrow Sc_2Al_{n-3} + Al^+$;

(20) $Al_{n-2}Sc_2^+ \rightarrow Sc_2Al_{n-3}^+ + Al$

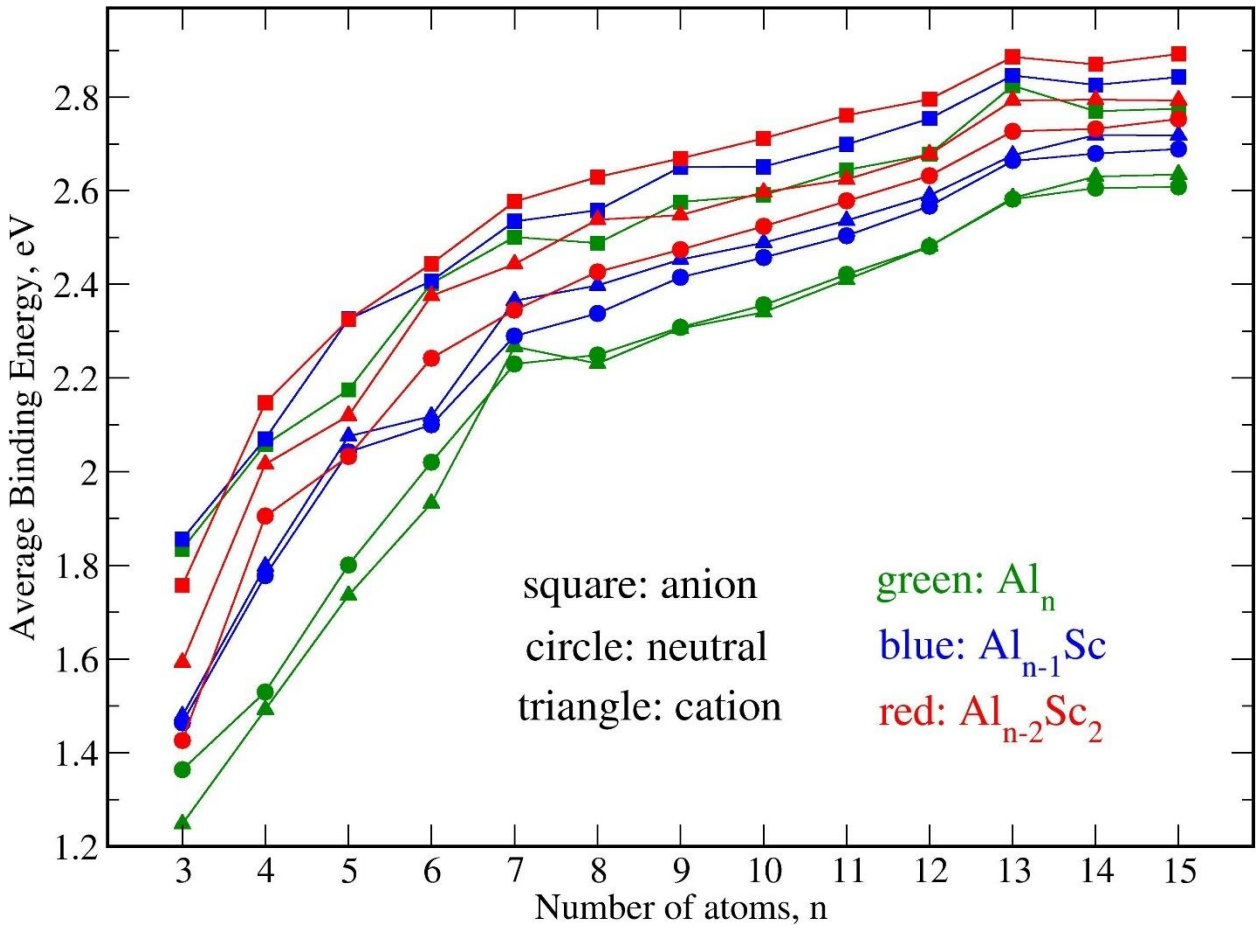


Figure S16: Average binding energies of the anionic, neutral and cationic $Al_n^{+/0/-}$, $ScAl_{n-1}^{+/0/-}$ and $Sc_2Al_{n-2}^{+/0/-}$ clusters (n = 3-15).

Table S5: Natural Electron Configuration (NEC) and Natural Charge of **da.6.A.1**, **a.6.A.1**, **n.6.A.1** and **c.6.A.1** isomers at their most stable spin state.

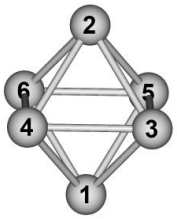
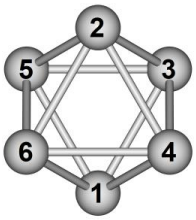
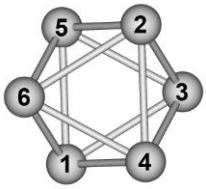
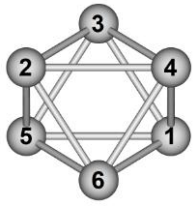
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **da.6.A.1** singlet	1	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
	2	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
	3	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
	4	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
	5	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
	6	Al	-0.33	3S(1.42)3p(1.85)3d(0.04)
 **a.6.A.1** doublet	1	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
	2	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
	3	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
	4	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
	5	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
	6	Al	-0.17	3S(1.47)3p(1.63)3d(0.05)
 **n.6.A.1** singlet	1	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
	2	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
	3	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
	4	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
	5	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
	6	Al	0.00	3S(1.51)3p(1.42)3d(0.06)
 **c.6.A.1** doublet	1	Al	0.20	3S(1.53)3p(1.19)3d(0.06)
	2	Al	0.20	3S(1.53)3p(1.19)3d(0.06)
	3	Al	0.09	3S(1.56)3p(1.26)3d(0.07)
	4	Al	0.20	3S(1.53)3p(1.19)3d(0.06)
	5	Al	0.20	3S(1.53)3p(1.19)3d(0.06)
	6	Al	0.09	3S(1.56)3p(1.26)3d(0.07)

Table S6: Natural Electron Configuration (NEC) and Natural Charge of **da.6.B.1**, **a.6.B.1**, **n.6.B.1** and **c.6.B.2** isomers at their most stable spin state.

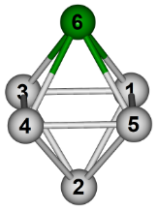
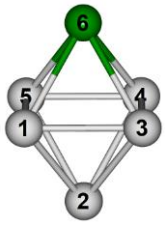
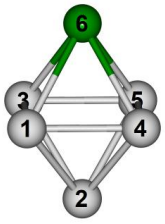
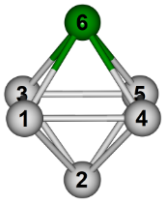
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **da.6.B.1** singlet	1	Al	-0.26	3S(1.39)3p(1.83)3d(0.03)
	2	Al	-0.36	3S(1.44)3p(1.88)3d(0.03)
	3	Al	-0.26	3S(1.39)3p(1.83)3d(0.03)
	4	Al	-0.26	3S(1.39)3p(1.83)3d(0.03)
	5	Al	-0.26	3S(1.39)3p(1.83)3d(0.03)
	6	Sc	-0.58	4S(1.19)3d(1.80)4p(0.52)
 **a.6.B.1** doublet	1	Al	-0.12	3S(1.42)3p(1.65)3d(0.04)
	2	Al	-0.11	3S(1.57)3p(1.51)3d(0.03)
	3	Al	-0.12	3S(1.42)3p(1.65)3d(0.04)
	4	Al	-0.11	3S(1.42)3p(1.64)3d(0.04)
	5	Al	-0.11	3S(1.42)3p(1.64)3d(0.04)
	6	Sc	-0.42	4S(1.02)3d(1.95)4p(0.42)
 **n.6.B.1** triplet	1	Al	0.05	3S(1.41)3p(1.50)3d(0.04)
	2	Al	0.03	3S(1.38)3p(1.53)3d(0.04)
	3	Al	0.05	3S(1.41)3p(1.50)3d(0.04)
	4	Al	0.05	3S(1.41)3p(1.50)3d(0.04)
	5	Al	0.05	3S(1.41)3p(1.50)3d(0.04)
	6	Sc	-0.24	4S(0.57)3d(2.21)4p(0.45)
 **c.6.B.2** doublet	1	Al	0.26	3S(1.39)3p(1.31)3d(0.03)
	2	Al	0.11	3S(1.28)3p(1.54)3d(0.06)
	3	Al	0.26	3S(1.39)3p(1.31)3d(0.03)
	4	Al	0.26	3S(1.39)3p(1.31)3d(0.03)
	5	Al	0.26	3S(1.39)3p(1.31)3d(0.03)
	6	Sc	-0.14	4S(0.21)3d(2.42)4p(0.50)

Table S7: Natural Electron Configuration (NEC) and Natural Charge of **da.6.C.1**, **da.6.C.2**, **a.6.C.1**, **n.6.C.1** and **c.6.C.1** isomers at their most stable spin state.

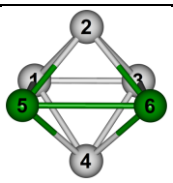
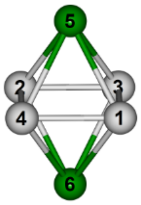
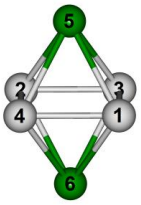
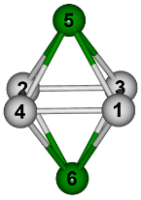
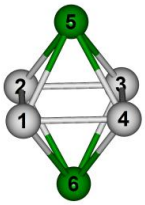
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **da.6.C.1** singlet	1	Al	-0.28	3S(1.39)3p(1.85)3d(0.03)
	2	Al	-0.18	3S(1.35)3p(1.81)3d(0.02)
	3	Al	-0.28	3S(1.39)3p(1.85)3d(0.03)
	4	Al	-0.18	3S(1.35)3p(1.81)3d(0.02)
	5	Sc	-0.53	4S(1.10)3d(1.90)4p(0.45)
	6	Sc	-0.53	4S(1.10)3d(1.90)4p(0.45)
 **da.6.C.2** singlet	1	Al	-0.27	3S(1.37)3p(1.86)3d(0.02)
	2	Al	-0.27	3S(1.37)3p(1.86)3d(0.02)
	3	Al	-0.27	3S(1.37)3p(1.86)3d(0.02)
	4	Al	-0.27	3S(1.37)3p(1.86)3d(0.02)
	5	Sc	-0.46	4S(1.18)3d(1.65)4p(0.55)
	6	Sc	-0.46	4S(1.18)3d(1.65)4p(0.55)
 **a.6.C.1** doublet	1	Al	-0.14	3S(1.34)3p(1.76)3d(0.02)
	2	Al	-0.14	3S(1.34)3p(1.76)3d(0.02)
	3	Al	-0.14	3S(1.34)3p(1.76)3d(0.02)
	4	Al	-0.14	3S(1.34)3p(1.76)3d(0.02)
	5	Sc	-0.23	4S(0.79)3d(1.86)4p(0.54)
	6	Sc	-0.23	4S(0.79)3d(1.86)4p(0.54)
 **n.6.C.1** singlet	1	Al	-0.02	3S(1.32)3p(1.66)3d(0.02)
	2	Al	-0.02	3S(1.32)3p(1.66)3d(0.02)
	3	Al	-0.02	3S(1.32)3p(1.66)3d(0.02)
	4	Al	-0.02	3S(1.32)3p(1.66)3d(0.02)
	5	Sc	0.03	4S(0.44)3d(2.07)4p(0.44)
	6	Sc	0.03	4S(0.44)3d(2.07)4p(0.44)
 **c.6.C.1** doublet	1	Al	0.19	3S(1.36)3p(1.42)3d(0.02)
	2	Al	0.19	3S(1.36)3p(1.42)3d(0.02)
	3	Al	0.19	3S(1.36)3p(1.42)3d(0.02)
	4	Al	0.19	3S(1.36)3p(1.42)3d(0.02)
	5	Sc	0.11	4S(0.41)3d(2.06)4p(0.40)
	6	Sc	0.11	4S(0.41)3d(2.06)4p(0.40)

Table S8: Natural Electron Configuration (NEC) and Natural Charge of **a.13.A.1**, **n.13.A.1** and **c.13.A.1** isomers at their most stable spin state.

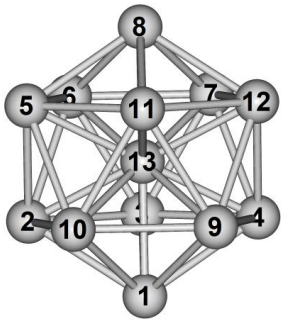
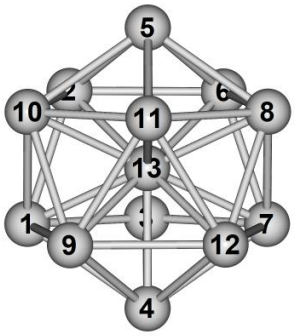
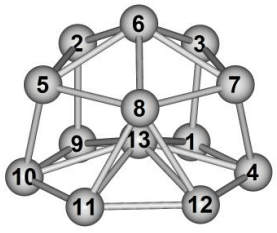
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **a.13.A.1** singlet	1	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	2	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	3	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	4	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	5	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	6	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	7	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	8	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	9	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	10	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	11	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	12	Al	0.04	3S(1.33)3p(1.54)3d(0.06)
	13	Al	-1.48	3S(0.84)3p(3.56)3d(0.04)
 **n.13.A.1** doublet	1	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	2	Al	0.18	3S(1.34)3p(1.39)3d(0.06)
	3	Al	0.18	3S(1.34)3p(1.39)3d(0.06)
	4	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	5	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	6	Al	0.18	3S(1.34)3p(1.40)3d(0.06)
	7	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	8	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	9	Al	0.18	3S(1.34)3p(1.39)3d(0.06)
	10	Al	0.09	3S(1.34)3p(1.47)3d(0.07)
	11	Al	0.18	3S(1.34)3p(1.40)3d(0.06)
	12	Al	0.18	3S(1.34)3p(1.40)3d(0.06)
	13	Al	-1.62	3S(0.89)3p(3.66)3d(0.04)
 **c.13.A.1** singlet	1	Al	0.20	3S(1.31)3p(1.43)3d(0.04)
	2	Al	0.24	3S(1.29)3p(1.39)3d(0.05)
	3	Al	0.23	3S(1.29)3p(1.41)3d(0.05)
	4	Al	0.24	3S(1.32)3p(1.38)3d(0.04)
	5	Al	0.18	3S(1.27)3p(1.48)3d(0.06)
	6	Al	-0.16	3S(1.07)3p(1.89) 3d(0.16)
	7	Al	0.15	3S(1.26)3p(1.51)3d(0.06)
	8	Al	0.13	3S(1.24)3p(1.54)3d(0.06)
	9	Al	0.19	3S(1.31)3p(1.45)3d(0.04)
	10	Al	0.23	3S(1.32)3p(1.39)3d(0.04)
	11	Al	0.25	3S(1.33)3p(1.37)3d(0.04)
	12	Al	0.25	3S(1.33)3p(1.36)3d(0.05)
	13	Al	-1.14	3S(0.96)3p(3.08)3d(0.05)

Table S9: Natural Electron Configuration (NEC) and Natural Charge of **a.13.B.1**, **n.13.B.1** and **c.13.B.1** isomers at their most stable spin state.

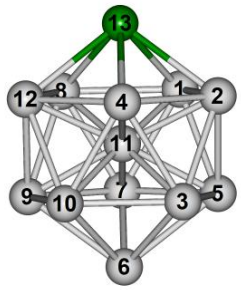
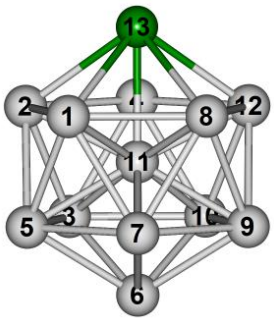
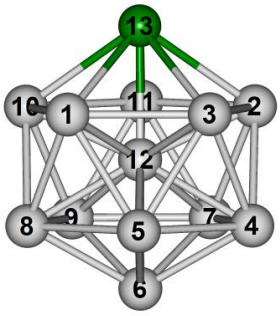
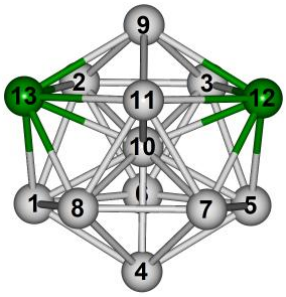
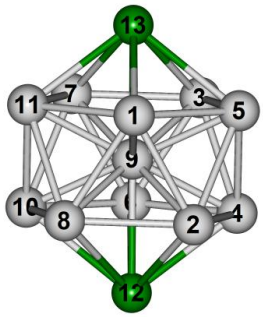
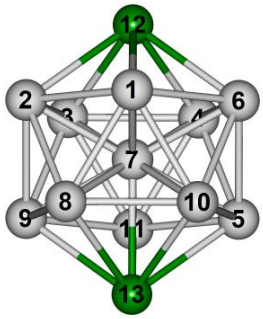
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **a.13.B.1** singlet	1	Al	0.08	3S(1.26)3p(1.58)3d(0.06)
	2	Al	0.08	3S(1.26)3p(1.58)3d(0.06)
	3	Al	0.05	3S(1.31)3p(1.56)3d(0.06)
	4	Al	0.08	3S(1.26)3p(1.58)3d(0.06)
	5	Al	0.05	3S(1.31)3p(1.56)3d(0.06)
	6	Al	-0.01	3S(1.46)3p(1.48)3d(0.04)
	7	Al	0.05	3S(1.31)3p(1.56)3d(0.06)
	8	Al	0.08	3S(1.26)3p(1.58)3d(0.06)
	9	Al	0.05	3S(1.31)3p(1.56)3d(0.06)
	10	Al	0.05	3S(1.31)3p(1.56)3d(0.06)
	11	Al	-1.22	3S(0.82)3p(3.32)3d(0.04)
	12	Al	0.08	3S(1.26)3p(1.58)3d(0.06
	13	Sc	-0.47	4S(0.70)3d(2.06)4p(0.64)
 **n.13.B.1** doublet	1	Al	0.17	3S(1.26)3p(1.50)3d(0.06)
	2	Al	0.17	3S(1.26)3p(1.50)3d(0.06)
	3	Al	0.15	3S(1.29)3p(1.48)3d(0.06)
	4	Al	0.17	3S(1.26)3p(1.50)3d(0.06)
	5	Al	0.15	3S(1.29)3p(1.48)3d(0.06)
	6	Al	0.01	3S(1.23)3p(1.67)3d(0.08)
	7	Al	0.15	3S(1.29)3p(1.48)3d(0.06)
	8	Al	0.17	3S(1.26)3p(1.50)3d(0.06)
	9	Al	0.15	3S(1.29)3p(1.48)3d(0.06)
	10	Al	0.15	3S(1.29)3p(1.48)3d(0.06)
	11	Al	-1.24	3S(0.83)3p(3.33)3d(0.05)
	12	Al	0.17	3S(1.26)3p(1.50)3d(0.06)
	13	Sc	-0.35	4S(0.39)3d(2.24)4p(0.67)
 **c.13.B.1** singlet	1	Al	0.27	3S(1.25)3p(1.41)3d(0.06)
	2	Al	0.27	3S(1.25)3p(1.41)3d(0.06)
	3	Al	0.27	3S(1.25)3p(1.41)3d(0.06)
	4	Al	0.25	3S(1.26)3p(1.41)3d(0.06)
	5	Al	0.25	3S(1.26)3p(1.41)3d(0.06)
	6	Al	0.00	3S(1.14)3p(1.75)3d(0.10)
	7	Al	0.25	3S(1.26)3p(1.41)3d(0.06)
	8	Al	0.25	3S(1.26)3p(1.41)3d(0.06)
	9	Al	0.25	3S(1.26)3p(1.41)3d(0.06)
	10	Al	0.27	3S(1.25)3p(1.41)3d(0.06)
	11	Al	0.27	3S(1.25)3p(1.41)3d(0.06)
	12	Al	-1.25	3S(0.84)3p(3.32)3d(0.04)
	13	Sc	-0.31	4S(0.15)3d(2.41)4p(0.71)

Table S10: Natural Electron Configuration (NEC) and Natural Charge of **a.13.C.1**, **n.13.C.1** and **c.13.C.1** isomers at their most stable spin state.

Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **a.13.C.1** singlet	1	Al	0.05	3S(1.31)3p(1.58)3d(0.05)
	2	Al	0.11	3S(1.23)3p(1.60)3d(0.05)
	3	Al	0.11	3S(1.23)3p(1.60)3d(0.05)
	4	Al	0.10	3S(1.31)3p(1.53)3d(0.06)
	5	Al	0.05	3S(1.31)3p(1.58)3d(0.05)
	6	Al	0.10	3S(1.31)3p(1.53)3d(0.06)
	7	Al	0.11	3S(1.23)3p(1.60)3d(0.05)
	8	Al	0.11	3S(1.23)3p(1.60)3d(0.05)
	9	Al	0.07	3S(1.20)3p(1.68)3d(0.05)
	10	Al	-1.00	3S(0.80)3p(3.11)3d(0.05)
	11	Al	0.07	3S(1.20)3p(1.68)3d(0.05)
	12	Sc	-0.42	4S(0.62)3d(2.15)4p(0.60)
	13	Sc	-0.42	4S(0.62)3d(2.15)4p(0.60)
 **n.13.C.1** doublet	1	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	2	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	3	Al	0.16	3S(1.23)3p(1.54)3d(0.05)
	4	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	5	Al	0.16	3S(1.23)3p(1.55)3d(0.05)
	6	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	7	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	8	Al	0.16	3S(1.23)3p(1.54)3d(0.05)
	9	Al	-1.05	3S(0.82)3p(3.15)3d(0.04)
	10	Al	0.16	3S(1.23)3p(1.55)3d(0.05)
	11	Al	0.15	3S(1.22)3p(1.56)3d(0.05)
	12	Sc	-0.25	4S(0.33)3d(2.23)4p(0.65)
	13	Sc	-0.25	4S(0.33)3d(2.23)4p(0.65)
 **c.13.C.1** singlet	1	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	2	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	3	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	4	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	5	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	6	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	7	Al	-1.11	3S(0.85)3p(3.19)3d(0.03)
	8	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	9	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	10	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	11	Al	0.24	3S(1.23)3p(1.47)3d(0.05)
	12	Sc	-0.12	4S(0.33)3d(2.10)4p(0.65)
	13	Sc	-0.12	4S(0.33)3d(2.10)4p(0.65)

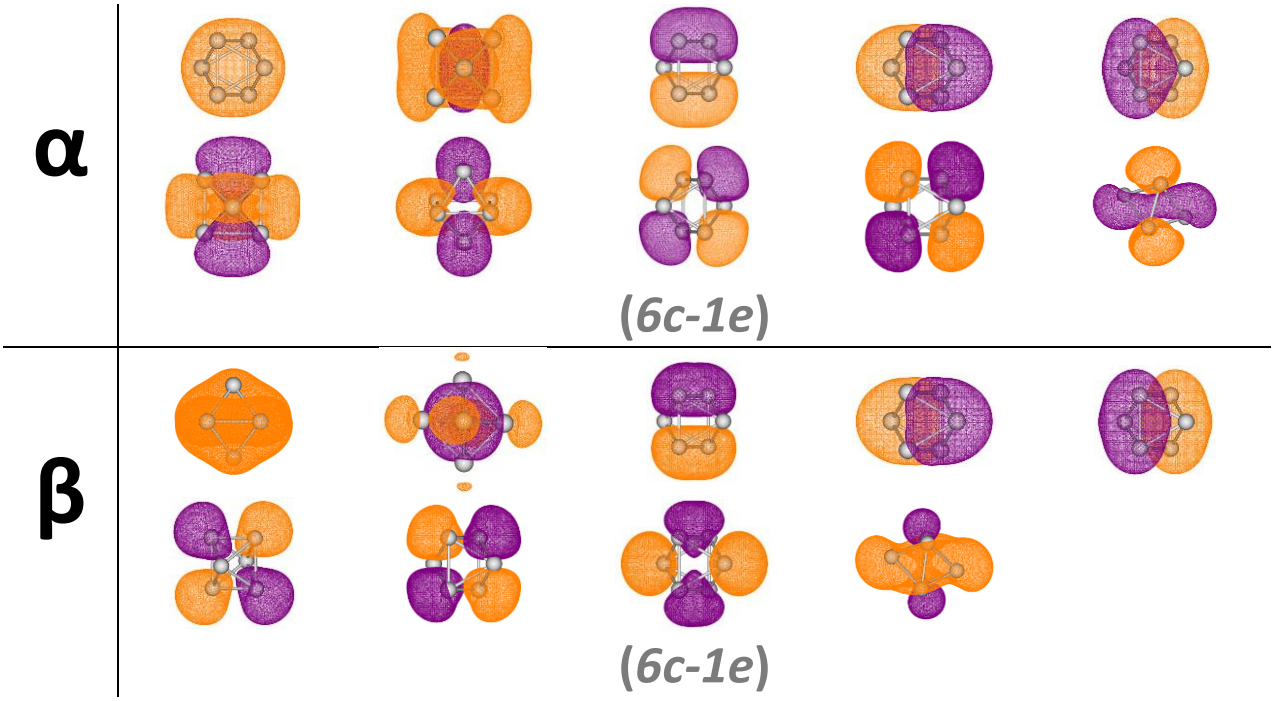


Figure S17: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the anionic octahedral **a.6.A.1** isomer via AdNDP analysis.

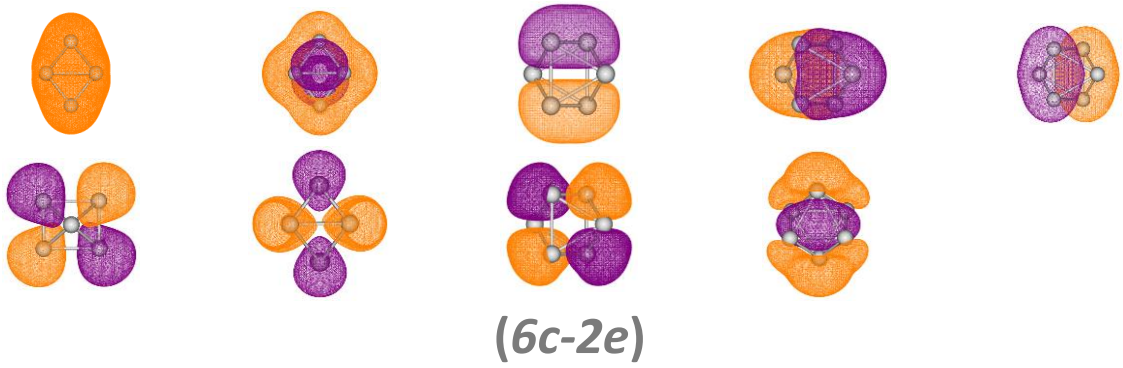


Figure S18: The metallic aromaticity arising from *(6c-2e)* delocalized bonds in the neutral octahedral **n.6.A.1** isomer via AdNDP analysis.

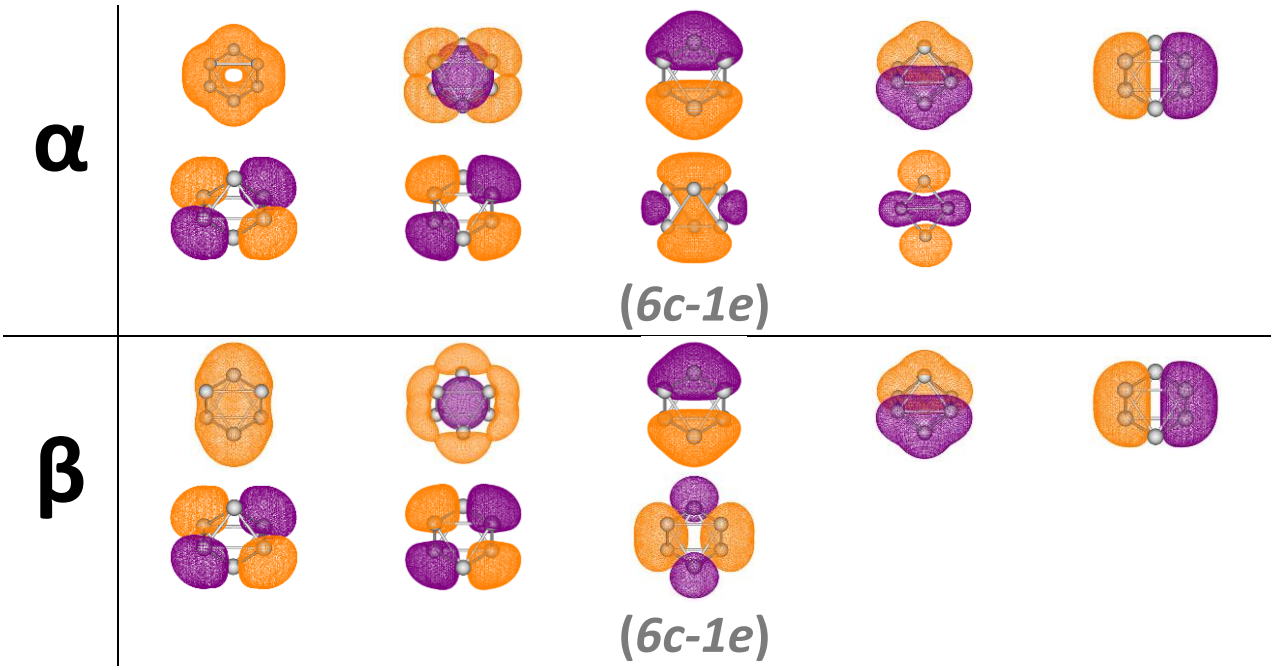


Figure S19: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the cationic octahedral **c.6.A.1** isomer via AdNDP analysis.

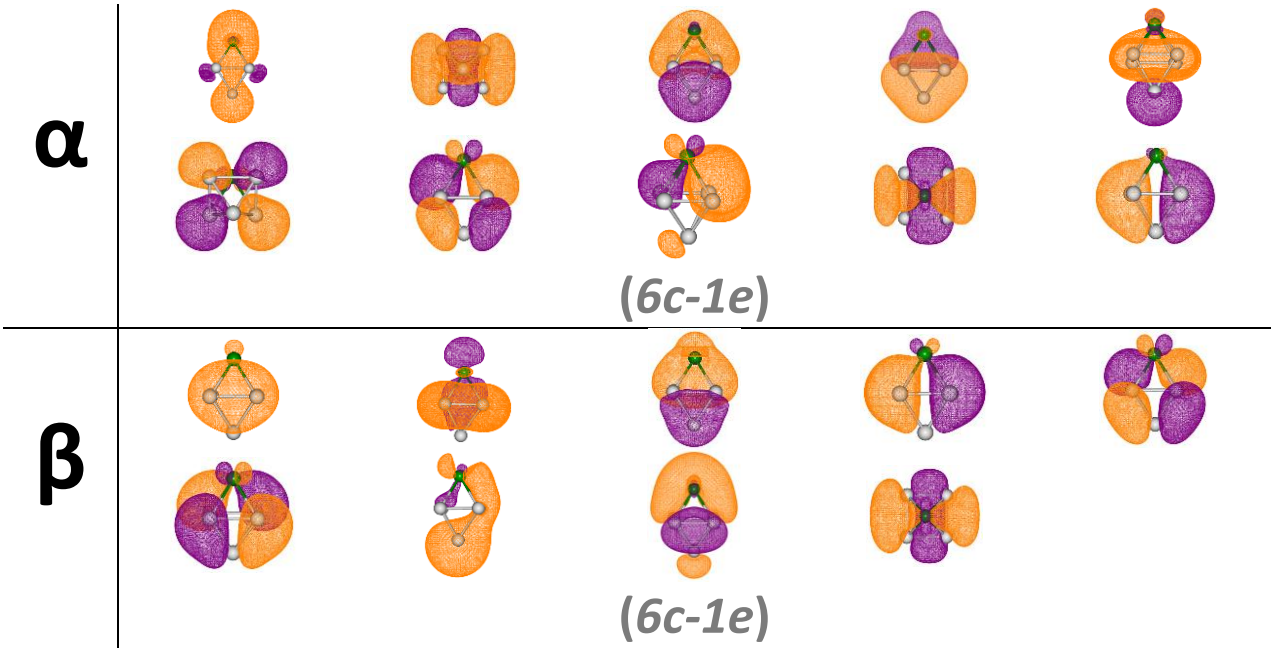


Figure S20: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the anionic octahedral **a.6.B.1** isomer via AdNDP analysis.

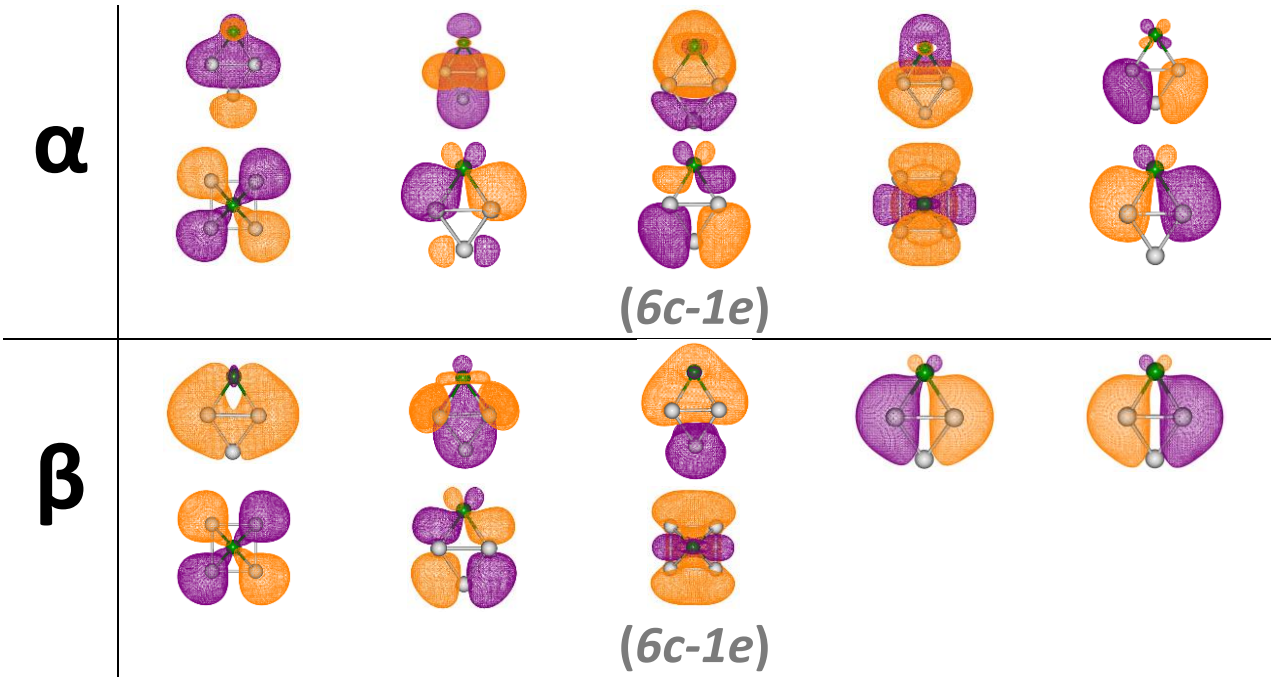


Figure S21: The metallic aromaticity arising from *(6c-2e)* delocalized bonds in the neutral octahedral **n.6.B.1** isomer via AdNDP analysis.

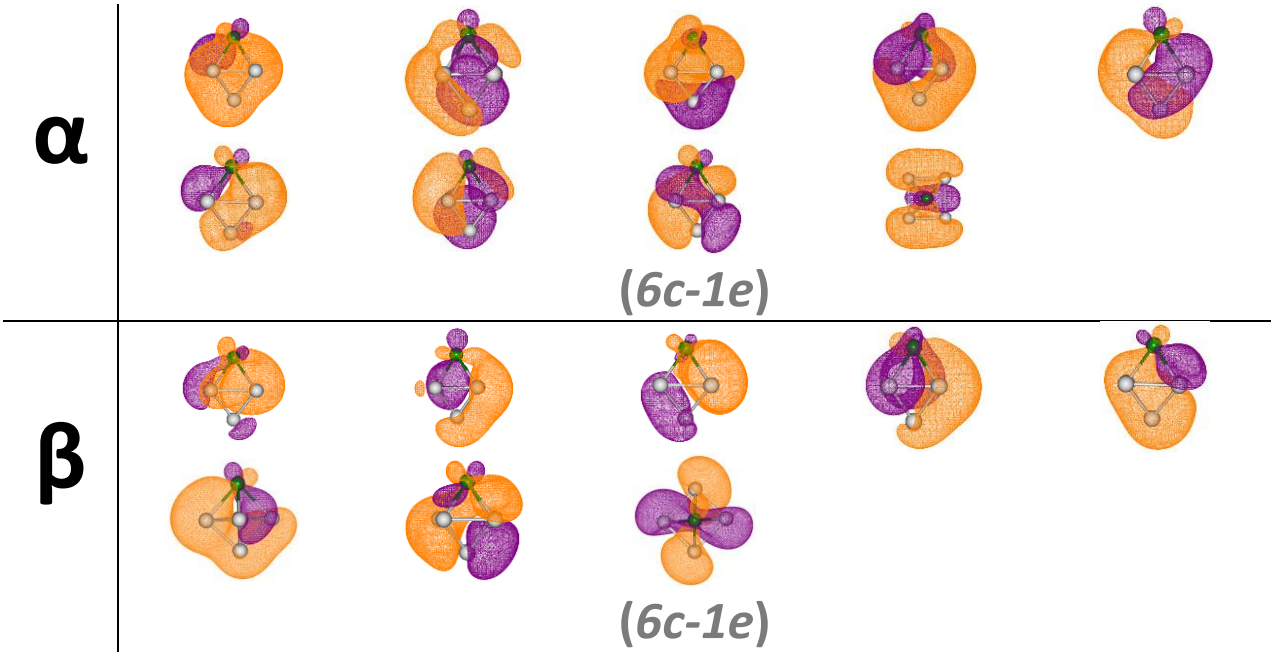


Figure S22: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the cationic octahedral **c.6.B.2** isomer via AdNDP analysis.

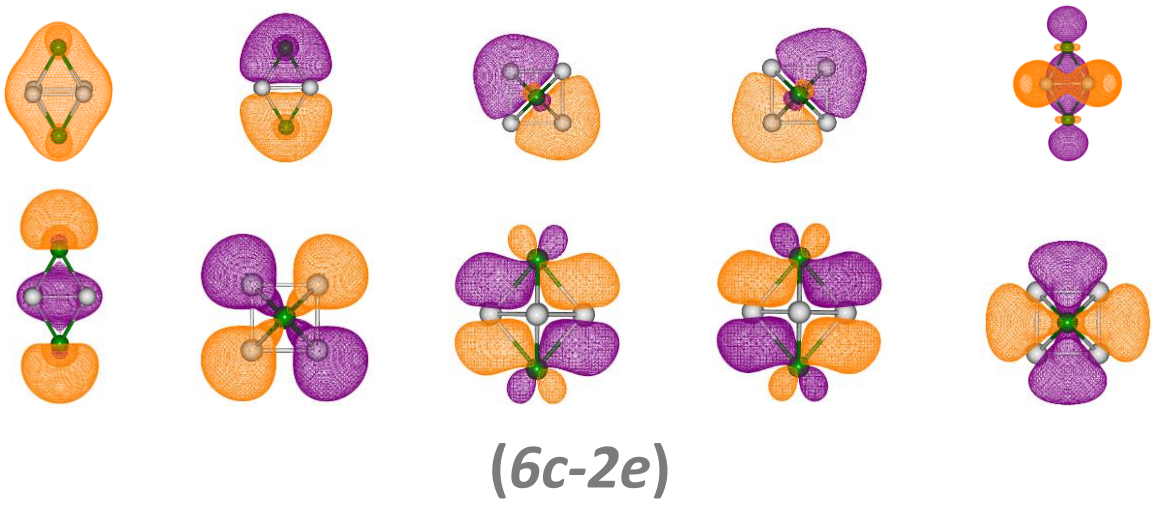


Figure S23: The metallic aromaticity arising from *(6c-2e)* delocalized bonds in the di-anionic octahedral **da.6.C.2** isomer via AdNDP analysis.

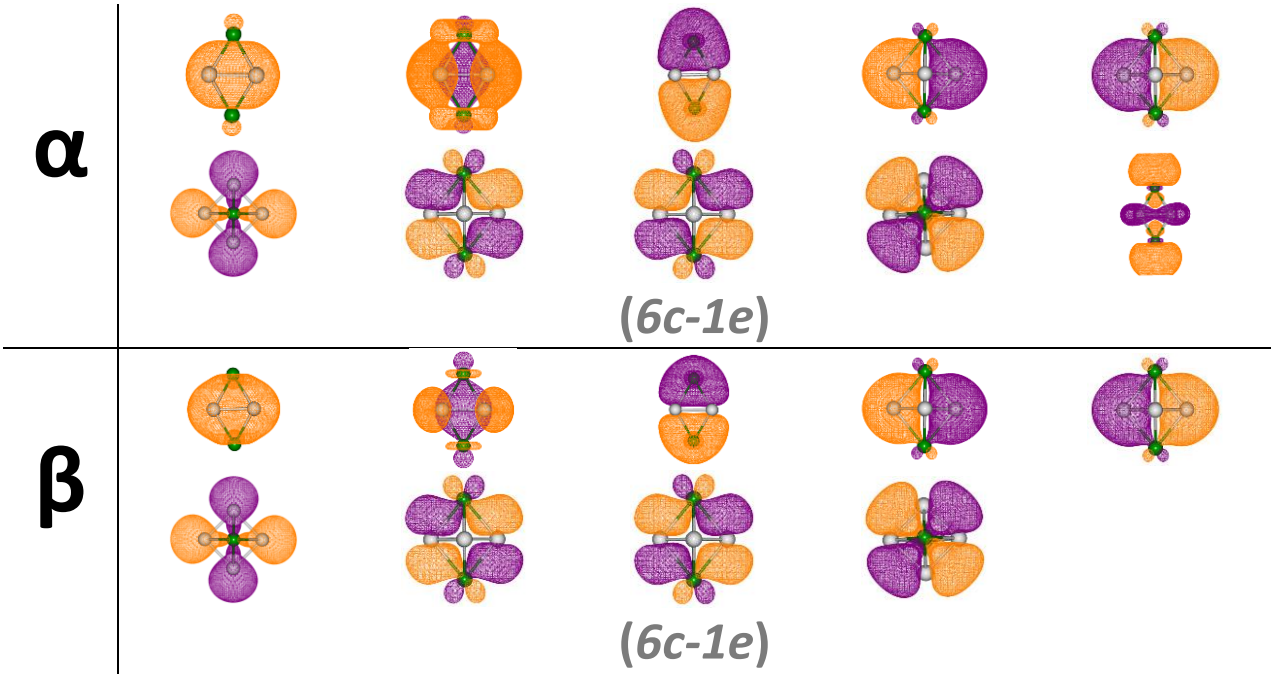


Figure S24: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the anionic octahedral **a.6.C.1** isomer via AdNDP analysis.

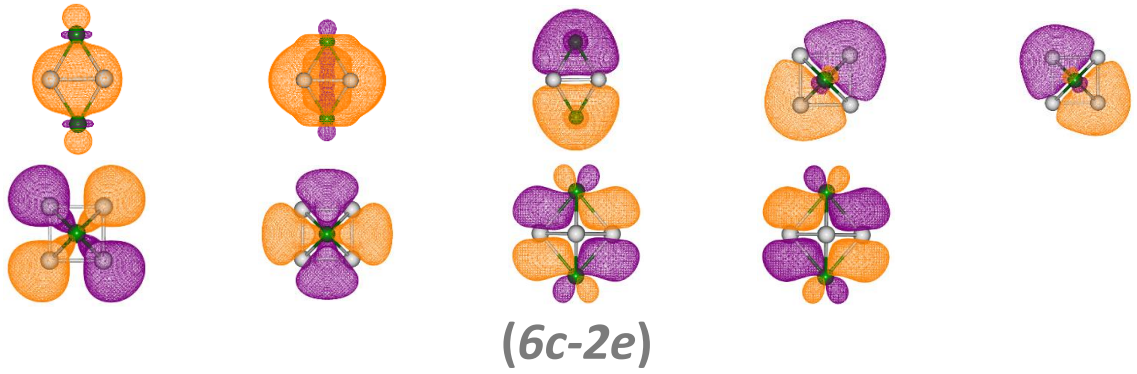


Figure S25: The metallic aromaticity arising from *(6c-2e)* delocalized bonds in the neutral octahedral **n.6.C.1** isomer via AdNDP analysis.

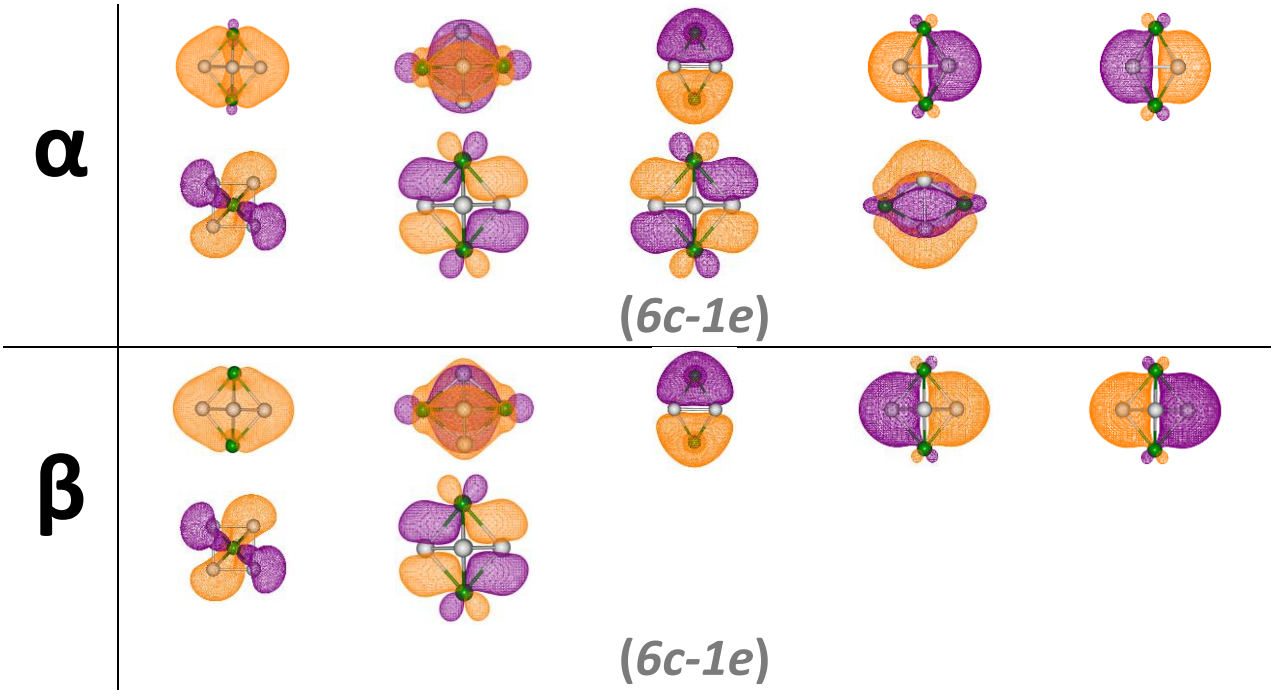


Figure S26: The metallic aromaticity arising from *(6c-1e)* delocalized bonds in the cationic octahedral **c.6.C.1** isomer via AdNDP analysis.

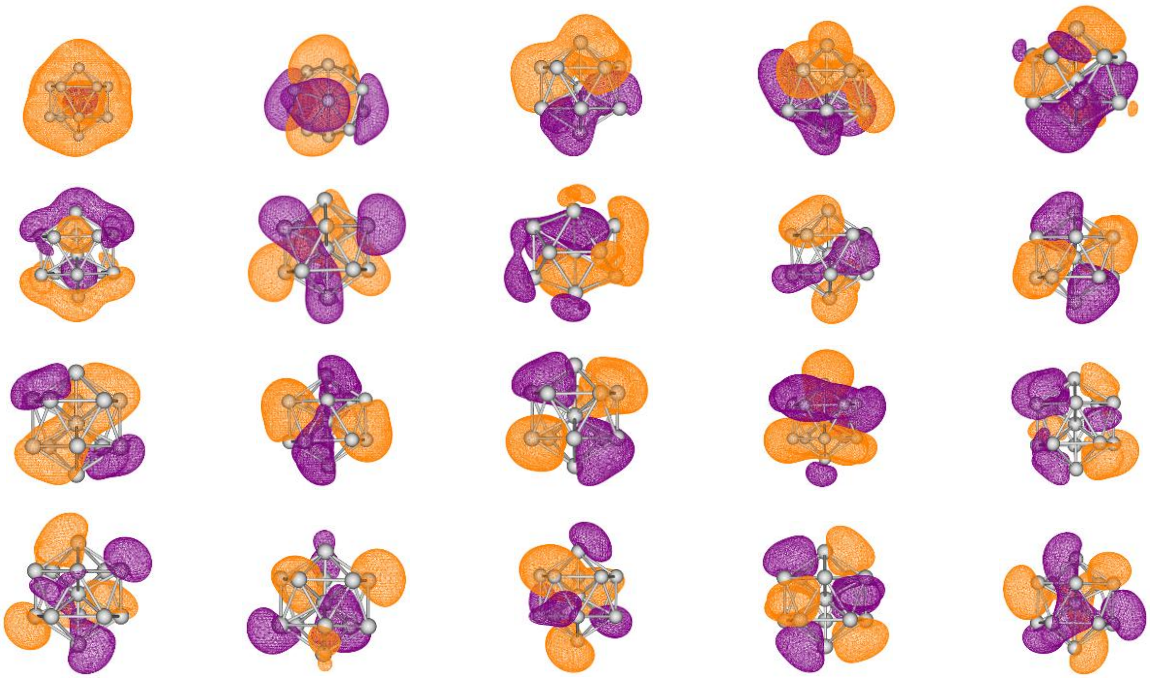


Figure S27: The metallic aromaticity arising from *(6c-2e)* delocalized bonds in the anionic icosahedral **a.13.A.1** isomer via AdNDP analysis.

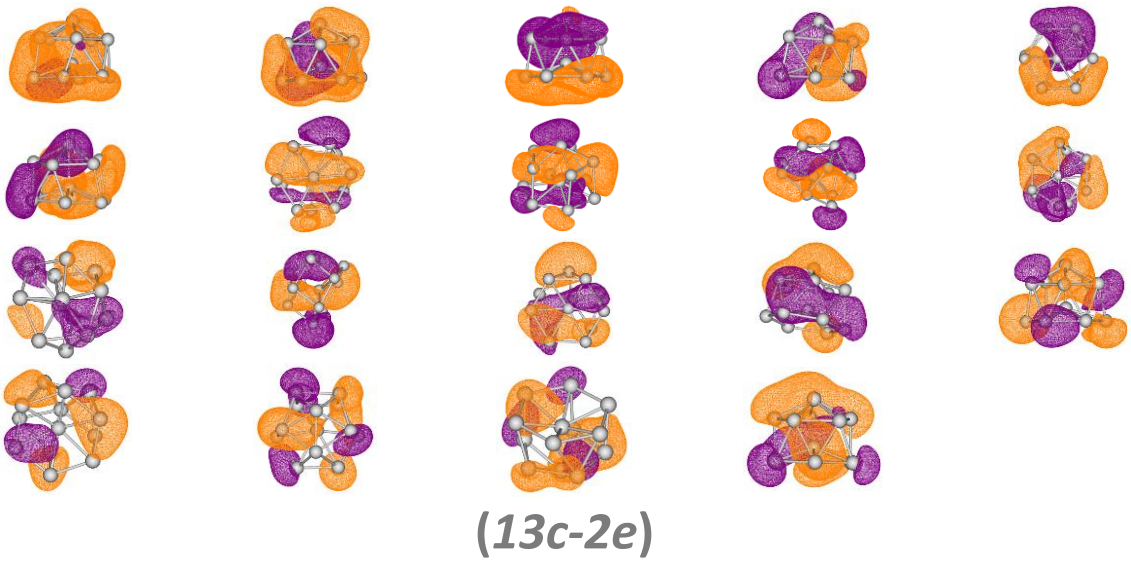


Figure S28: The metallic aromaticity arising from *(13c-2e)* delocalized bonds in the cationic **c.13.A.1** isomer cluster via AdNDP analysis.

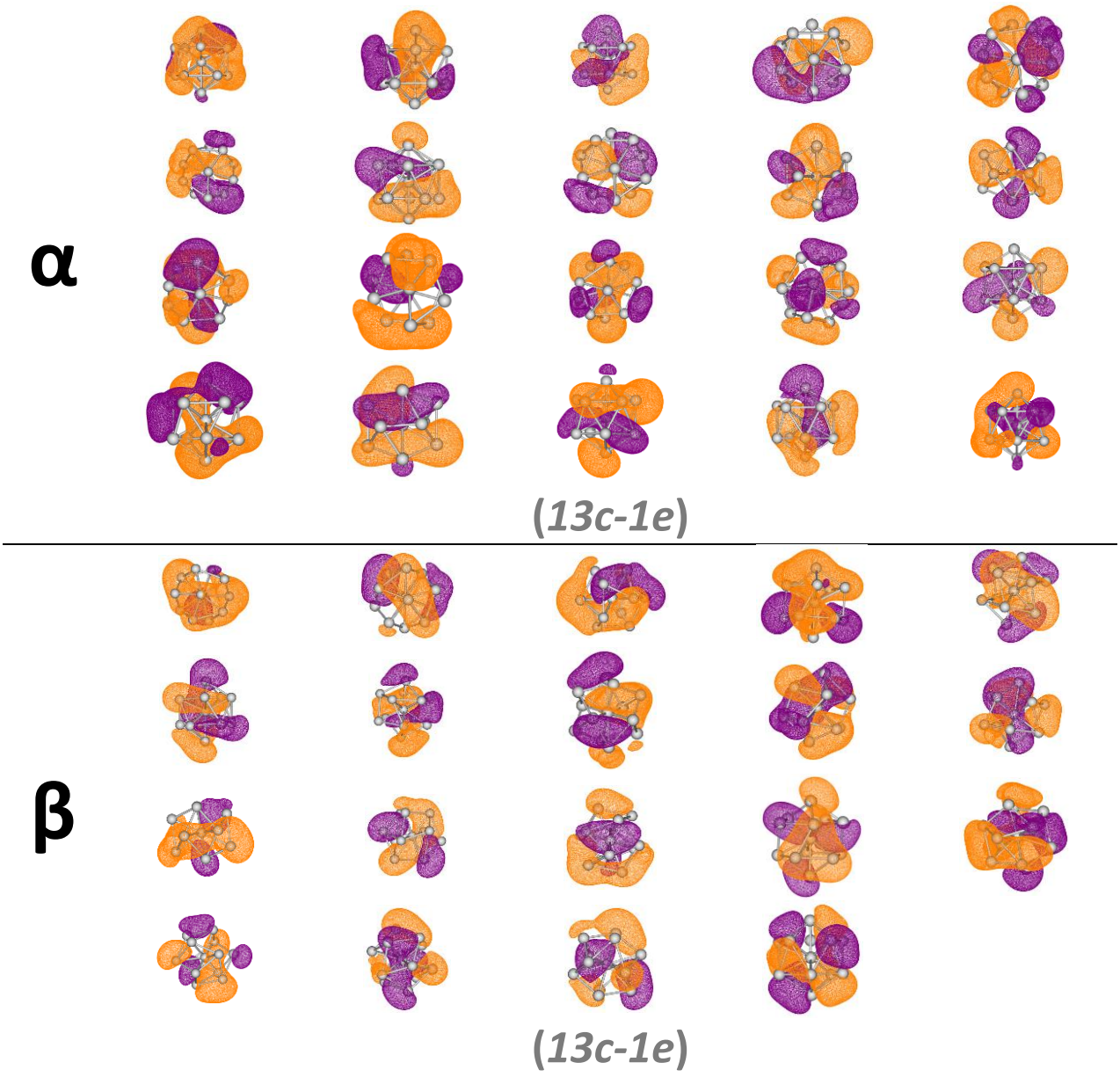


Figure S29: The metallic aromaticity arising from *(13c-1e)* delocalized bonds in the neutral icosahedral **n.13.A.1** isomer via AdNDP analysis.

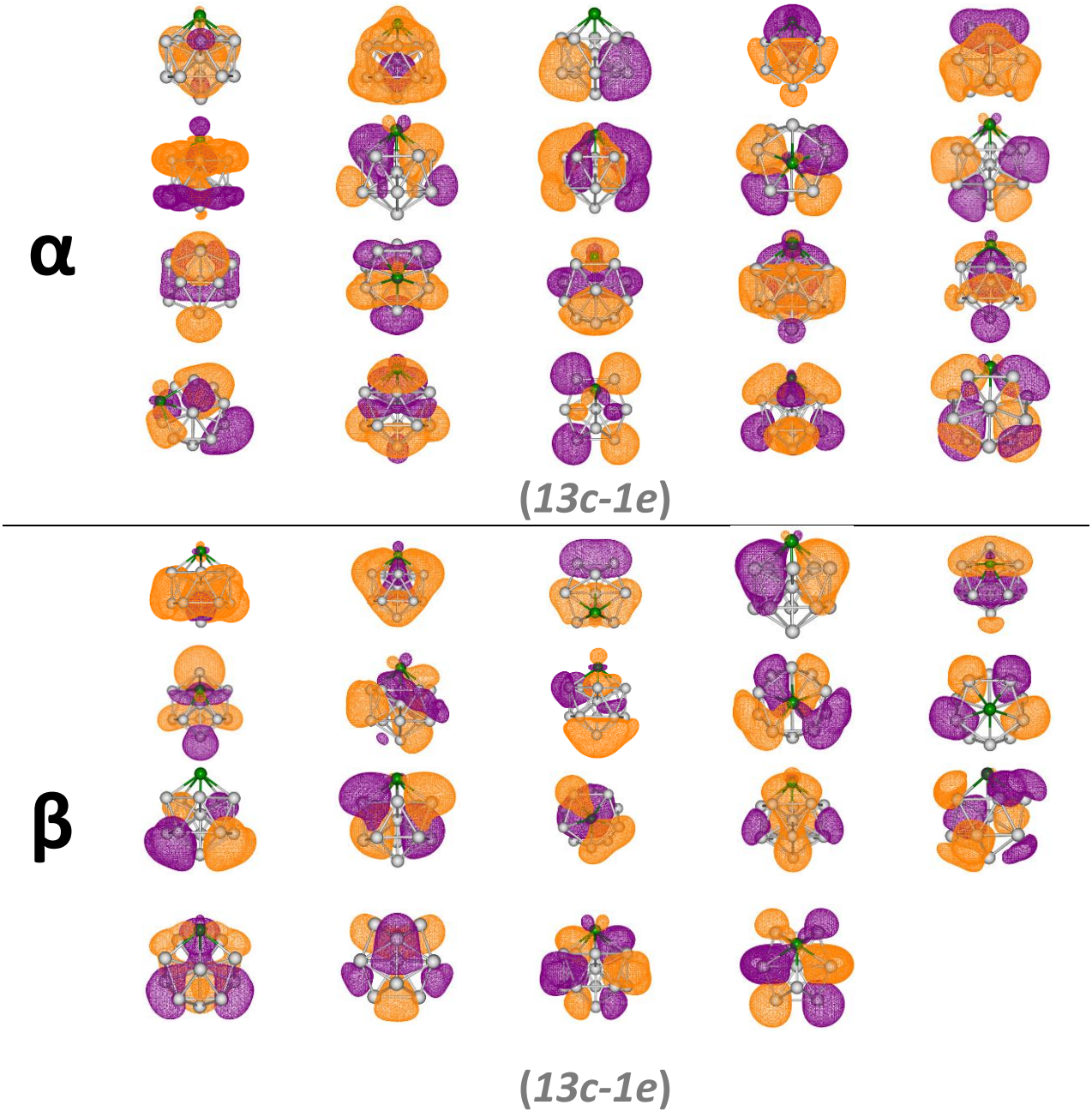


Figure S30: The metallic aromaticity arising from *(13c-1e)* delocalized bonds in the neutral icosahedral **n.13.B.1** isomer via AdNDP analysis.

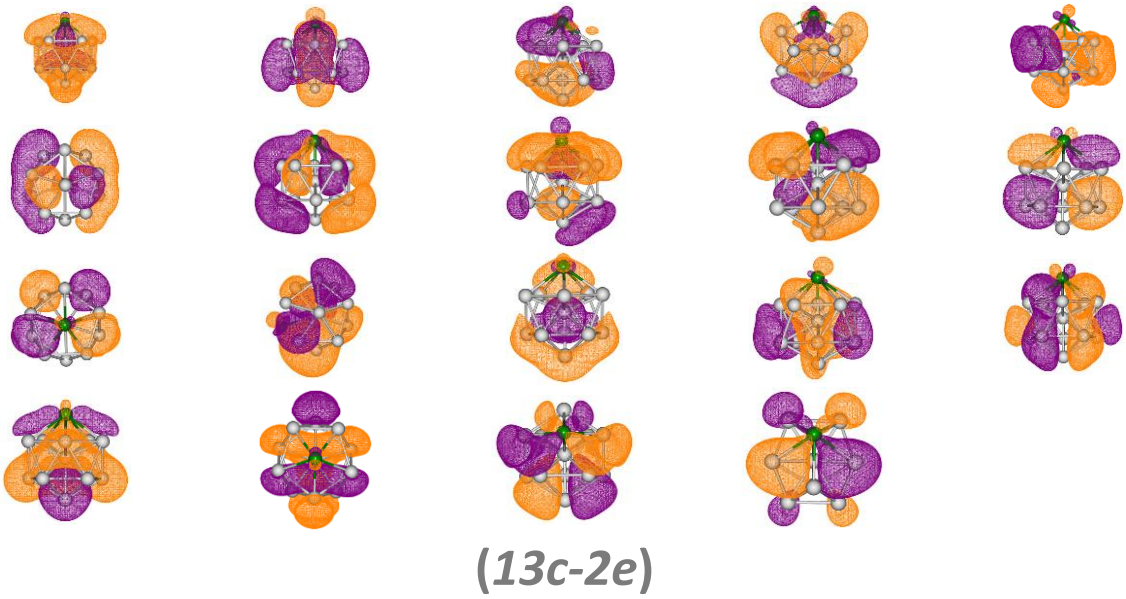


Figure S31: The metallic aromaticity arising from *(13c-2e)* delocalized bonds in the cationic icosahedral **c.13.B.1** isomer via AdNDP analysis.

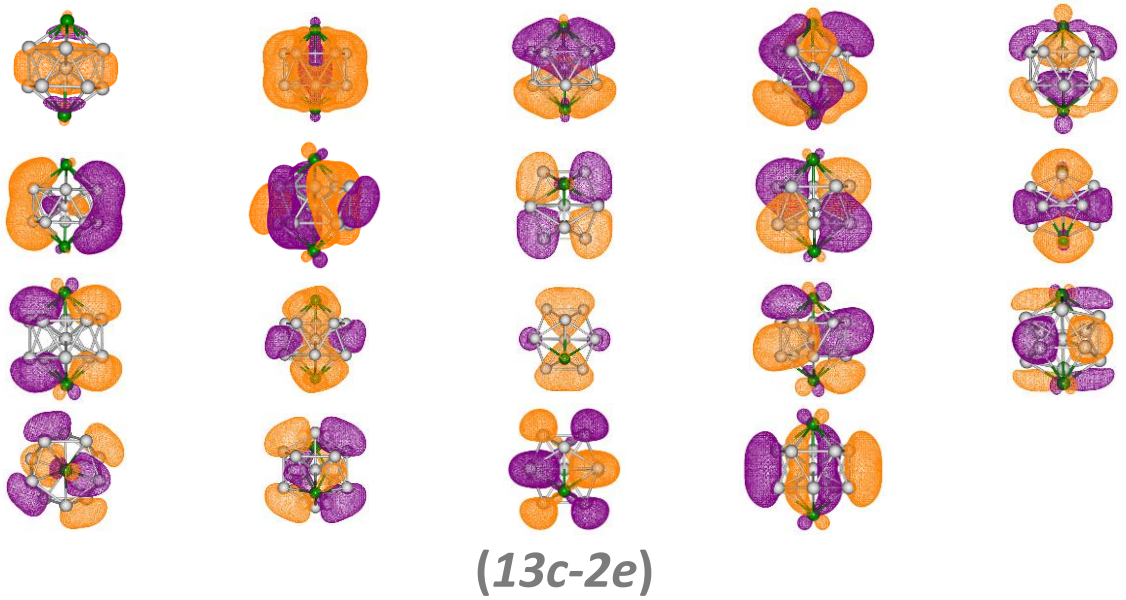


Figure S32: The metallic aromaticity arising from *(13c-2e)* delocalized bonds in the cationic icosahedral **c.13.C.1** isomer via AdNDP analysis.

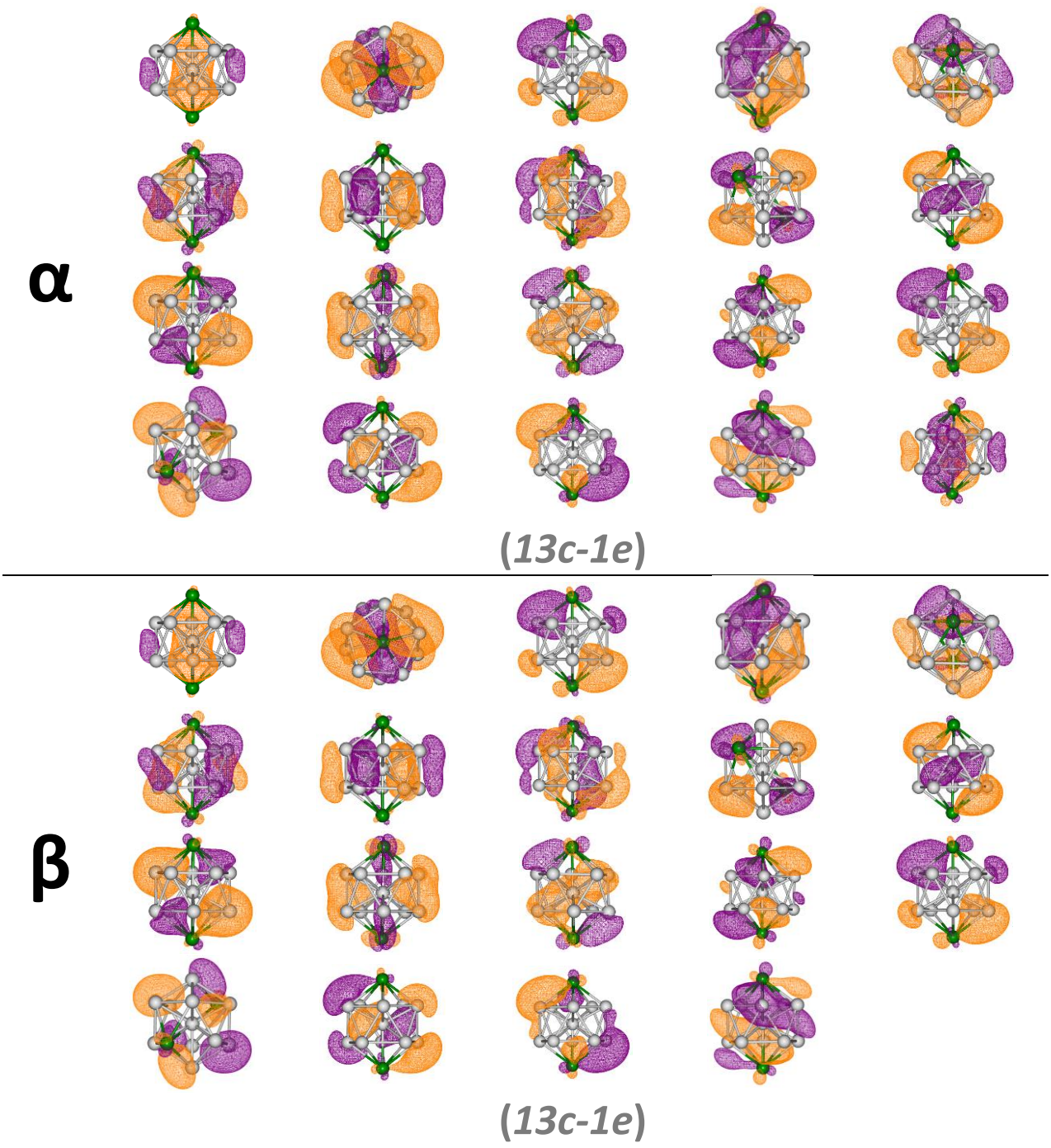


Figure S33: The metallic aromaticity arising from *(13c-1e)* delocalized bonds in the neutral icosahedral **n.13.C.1** isomer via AdNDP analysis.

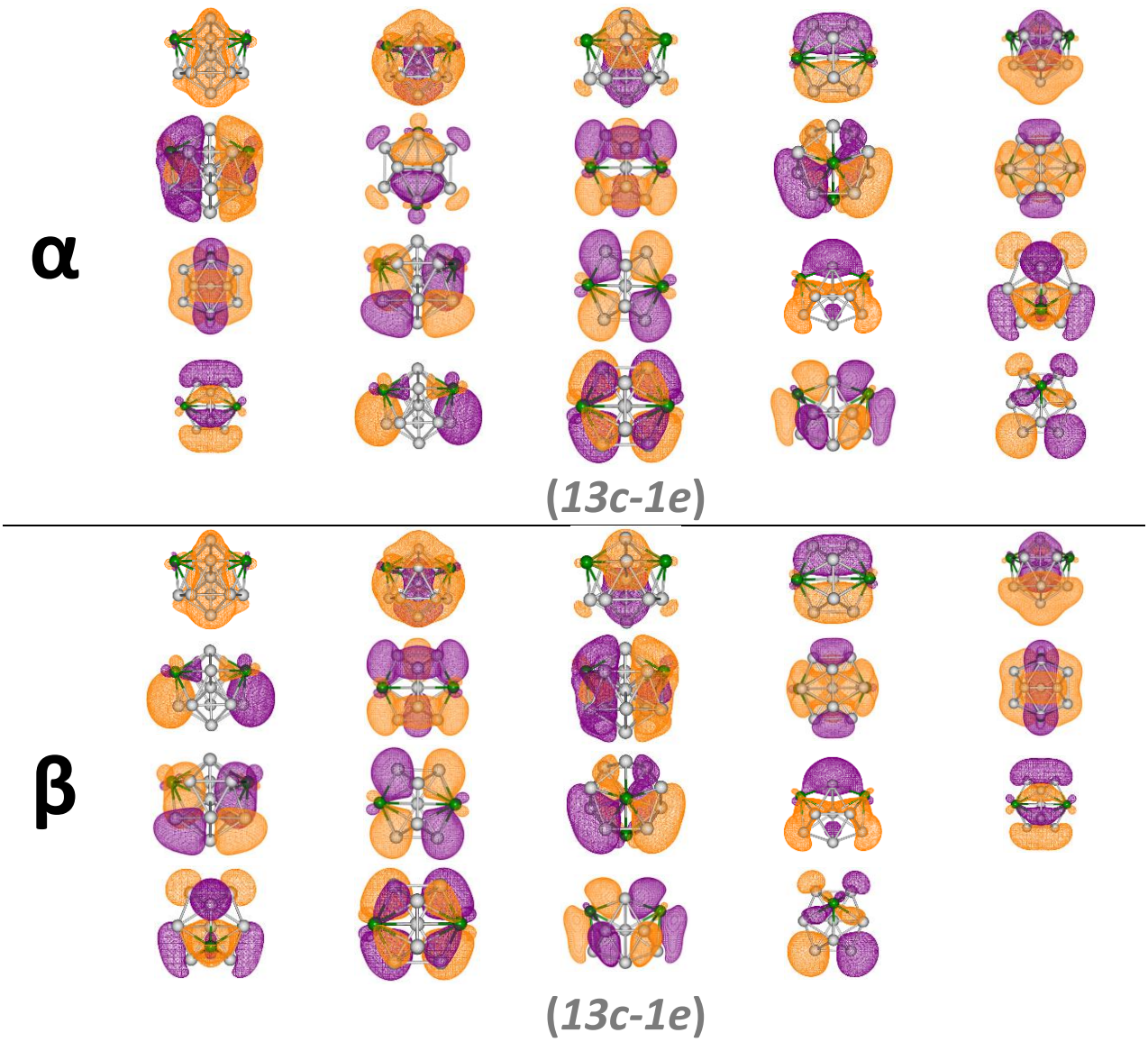


Figure S34: The metallic aromaticity arising from *(13c-1e)* delocalized bonds in the neutral icosahedral **n.13.C.2** isomer via AdNDP analysis.

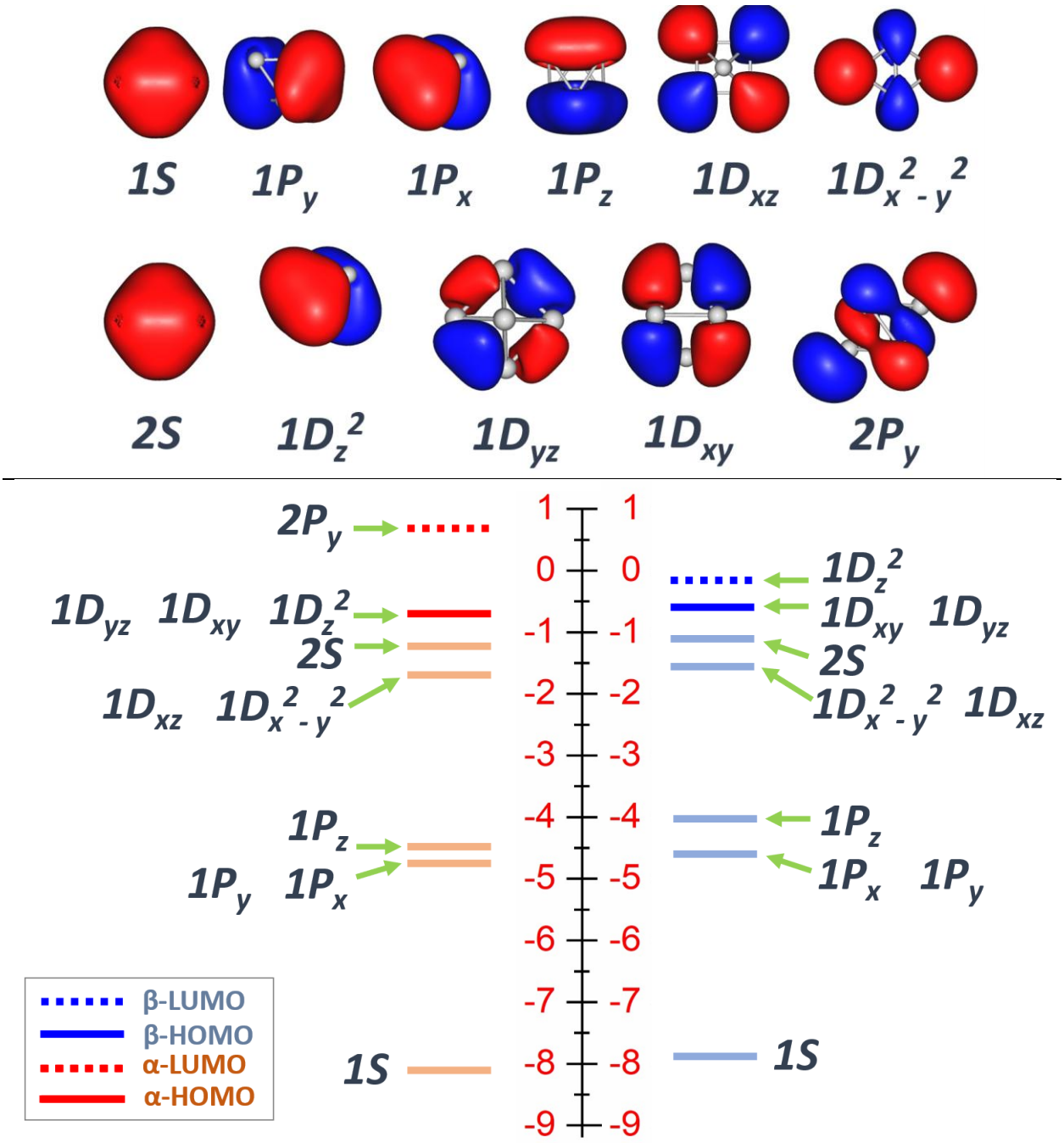


Figure S35: Energy levels of molecular orbitals (MOs) of the **a.6.A.1** at doublet state, PBE/ Def2-TZVP.

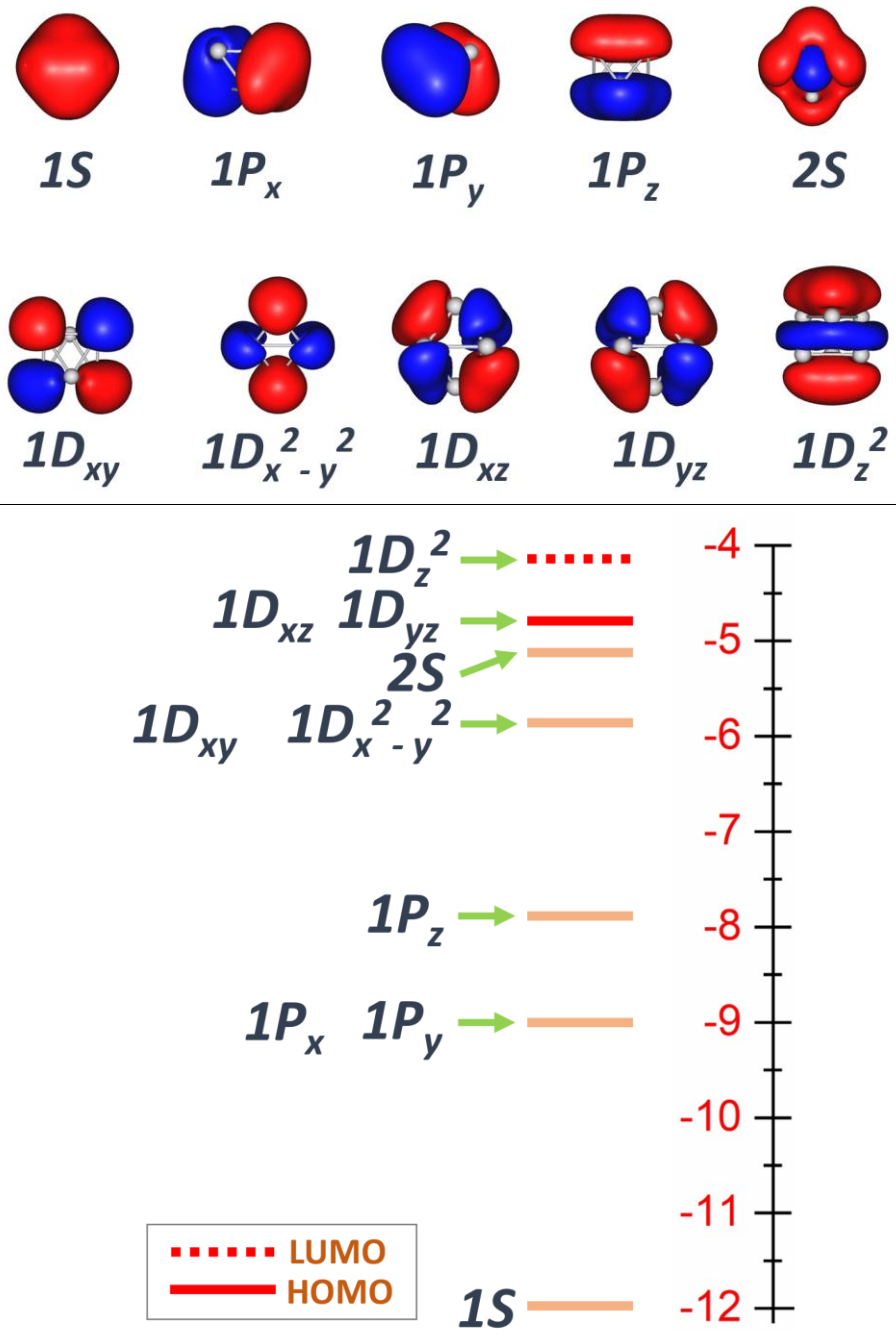


Figure S36: Energy levels of molecular orbitals (MOs) of the **n.6.A.1** at singlet state, PBE/ Def2-TZVP.

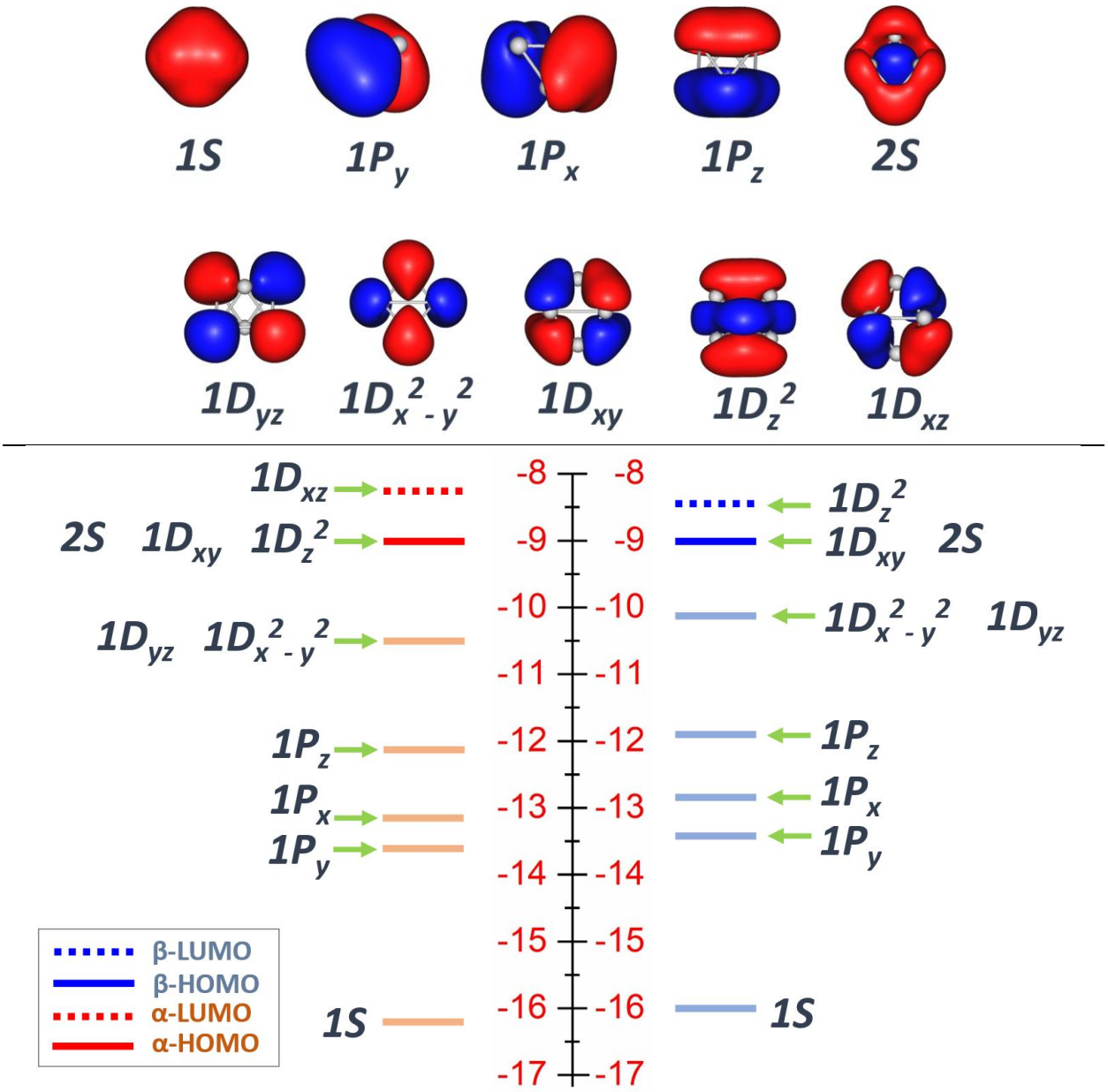


Figure S37: Energy levels of molecular orbitals (MOs) of the **c.6.A.1** at doublet state, PBE/ Def2-TZVP.

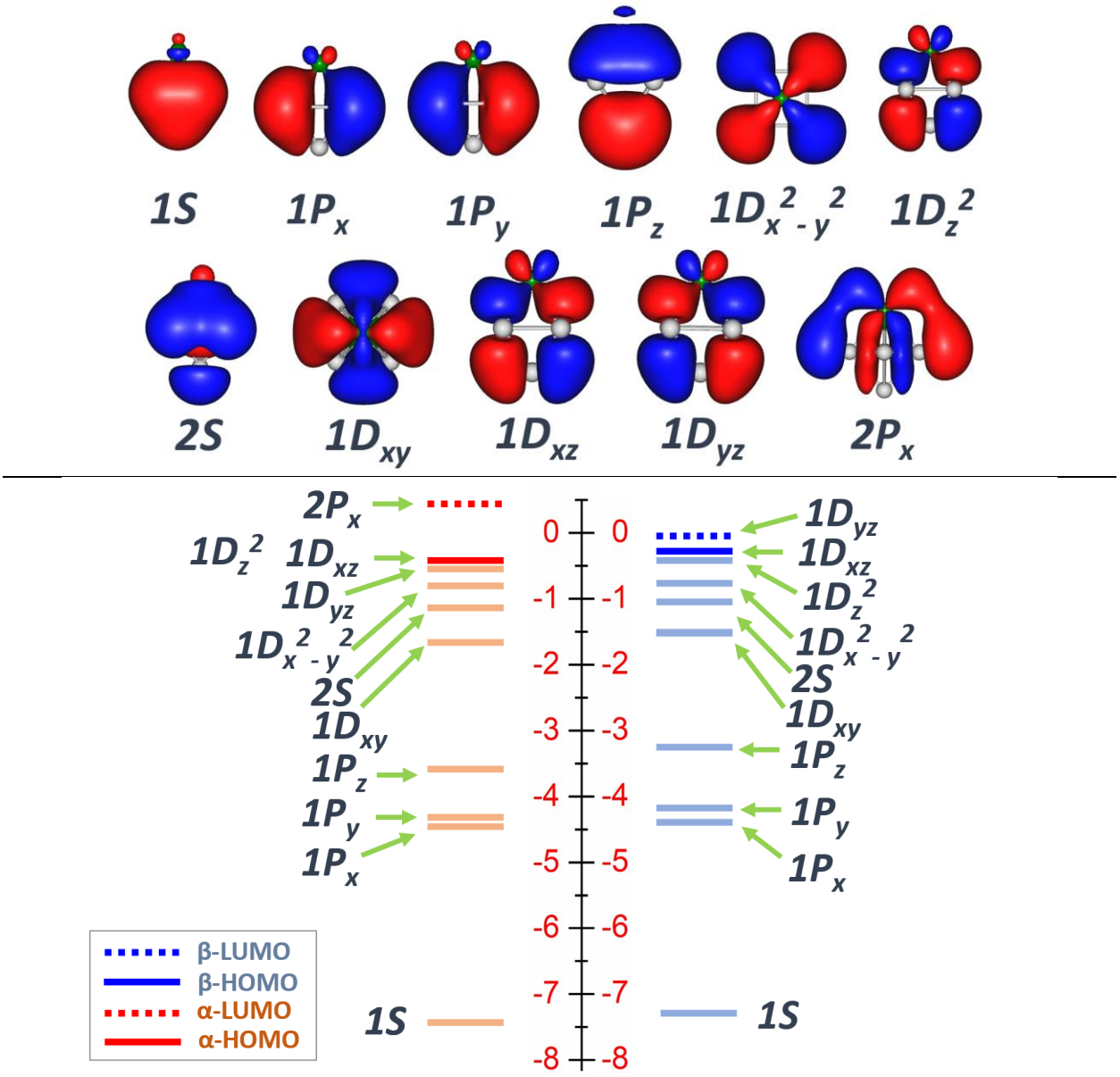


Figure S38: Energy levels of molecular orbitals (MOs) of the **a.6.B.1** at doublet state, PBE/ Def2-TZVP.

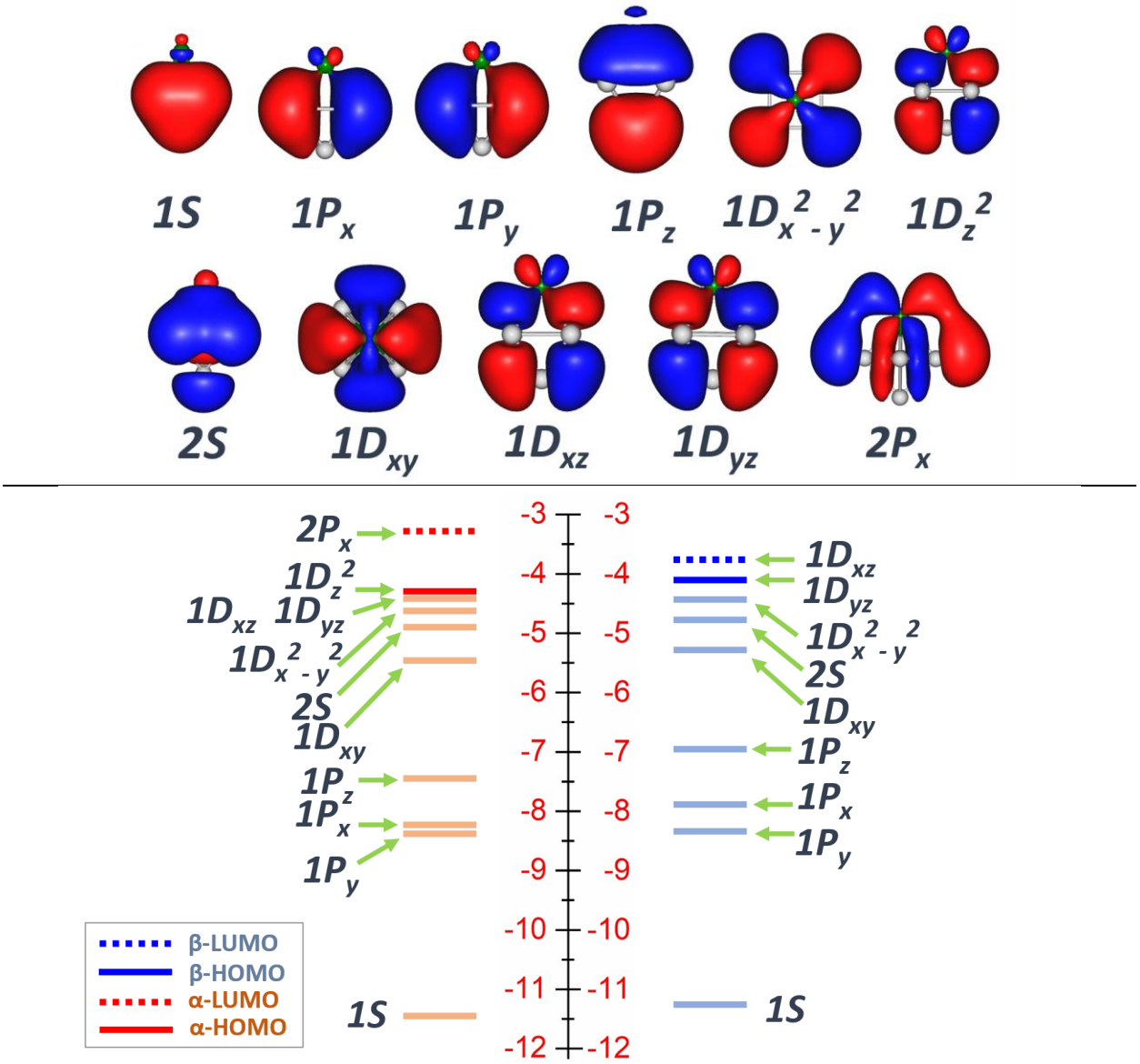


Figure S39: Energy levels of molecular orbitals (MOs) of the **n.6.B.1** at triplet state, PBE/ Def2-TZVP.

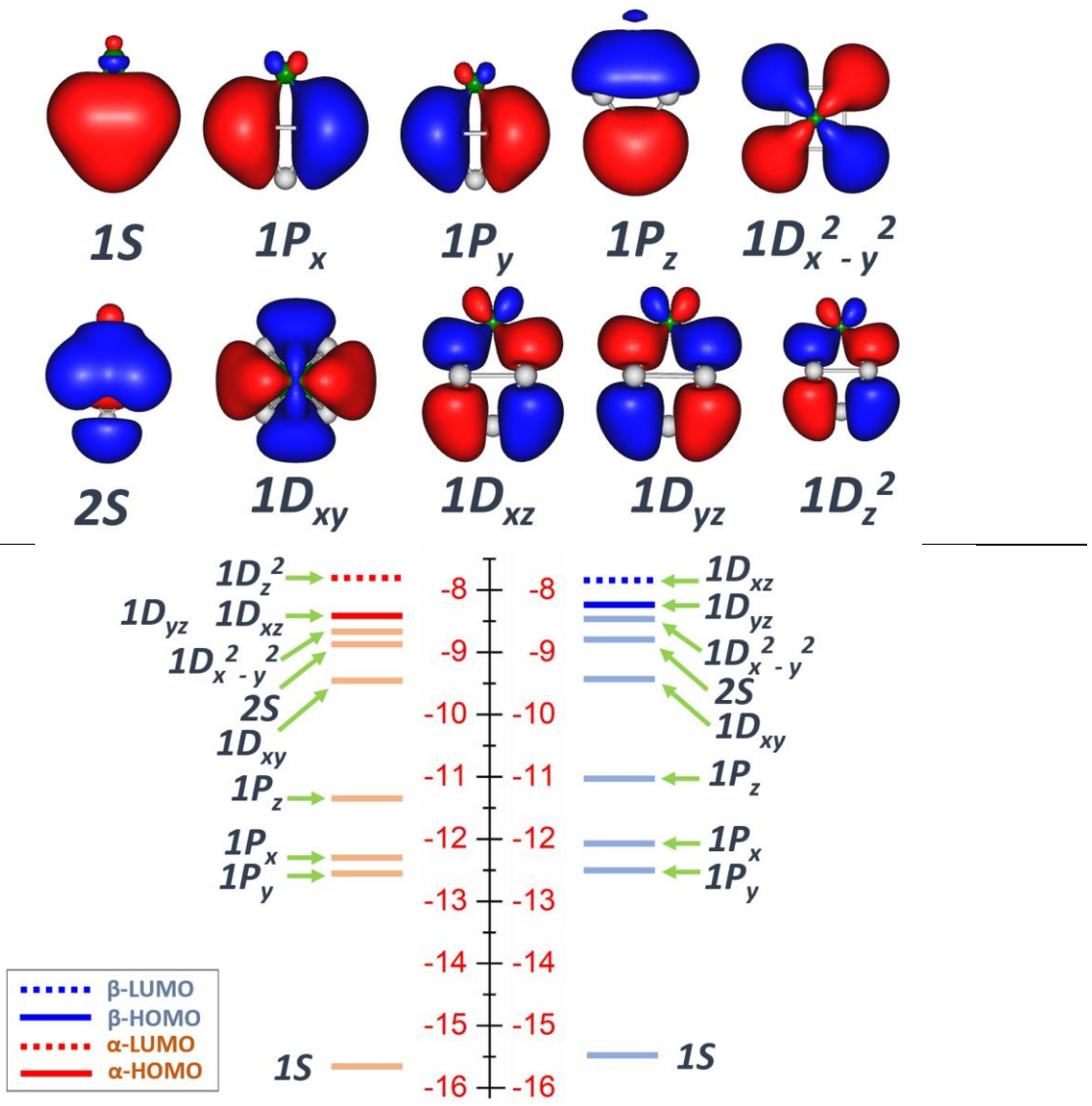


Figure S40: Energy levels of molecular orbitals (MOs) of the **c.6.B.2** at doublet state, PBE/ Def2-TZVP.

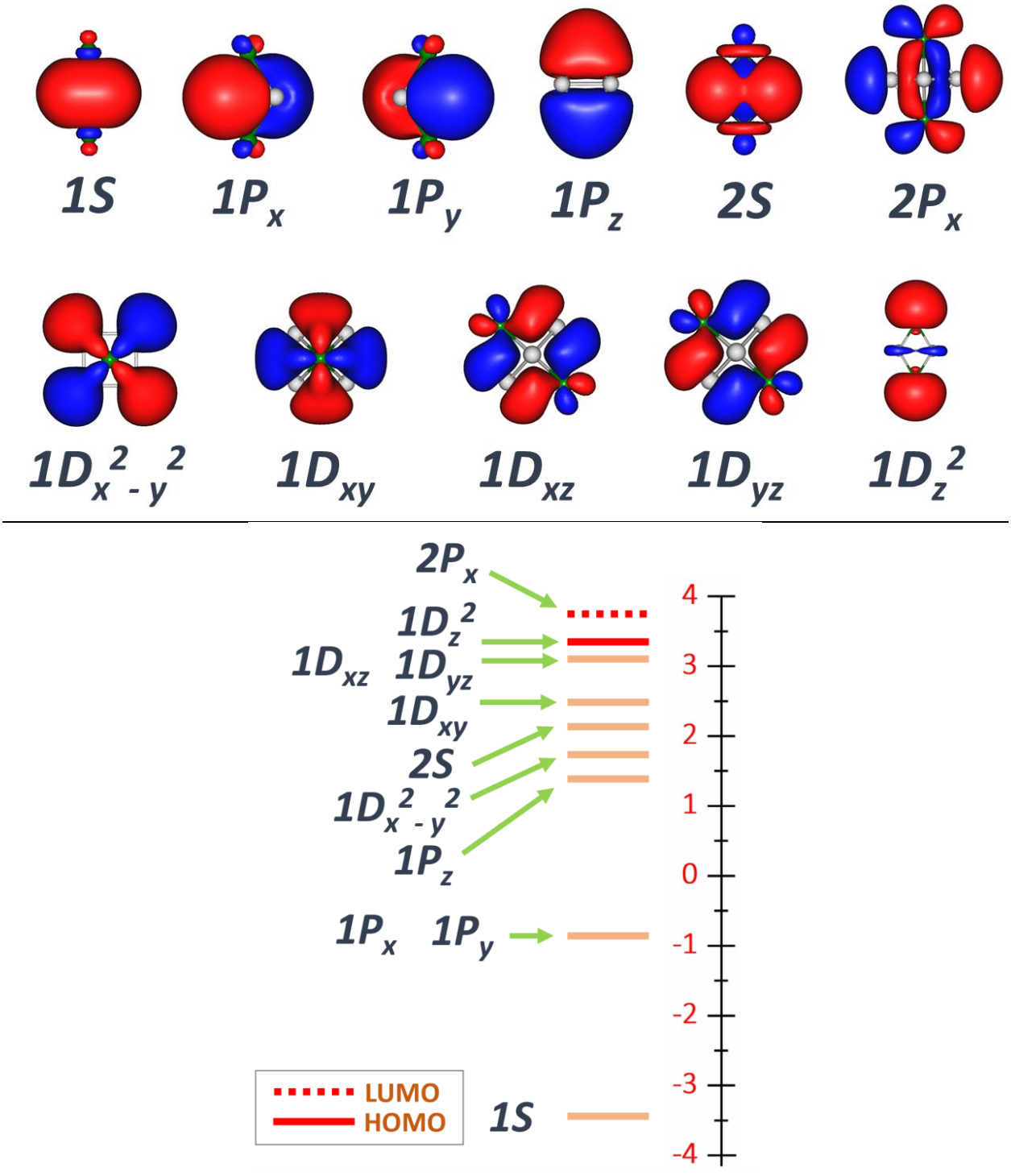


Figure S41: Energy levels of molecular orbitals (MOs) of the **da.6.C.2** at singlet state, PBE/ Def2-TZVP.

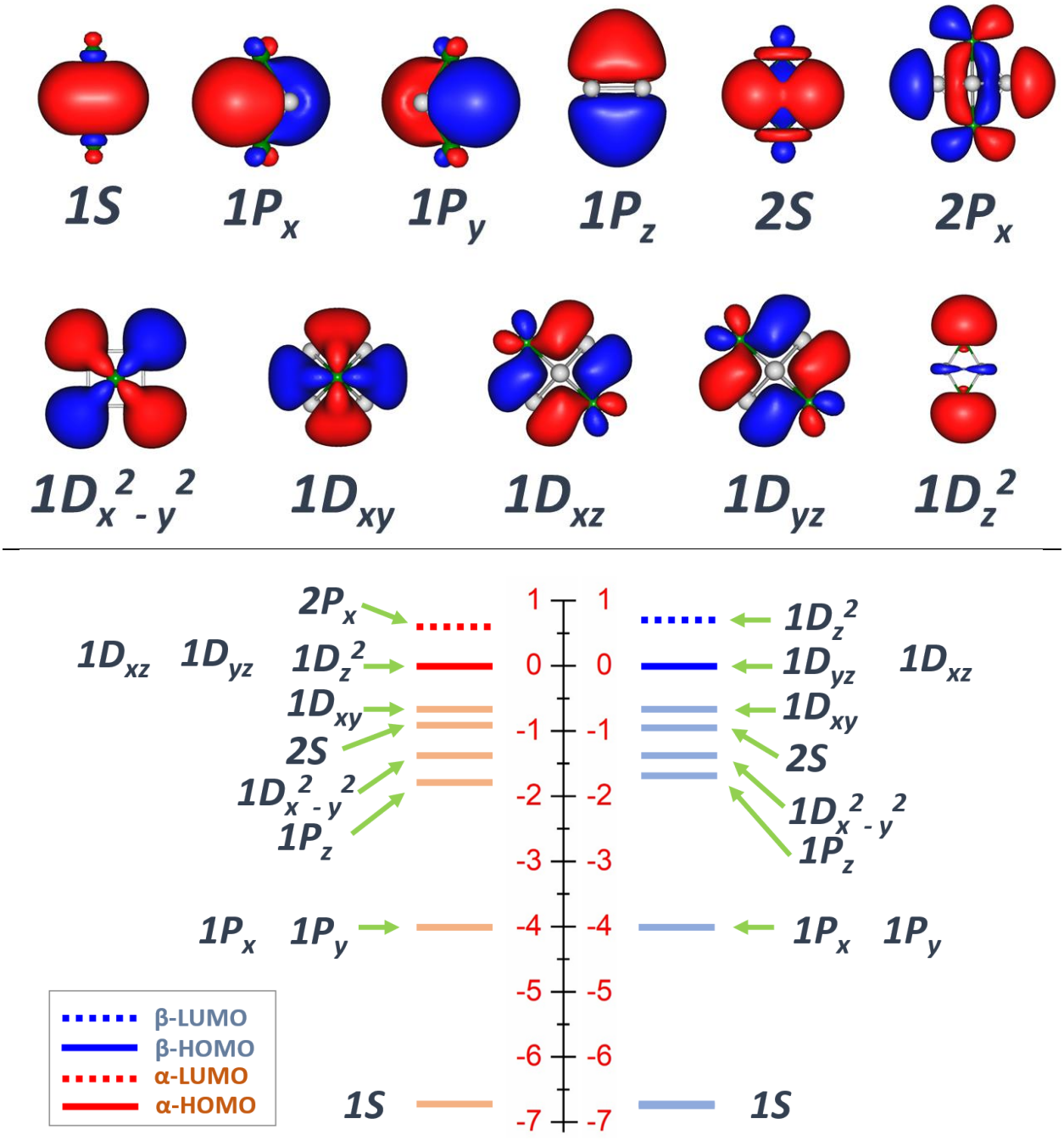


Figure S42: Energy levels of molecular orbitals (MOs) of the **a.6.C.1** at doublet state, PBE/ Def2-TZVP.

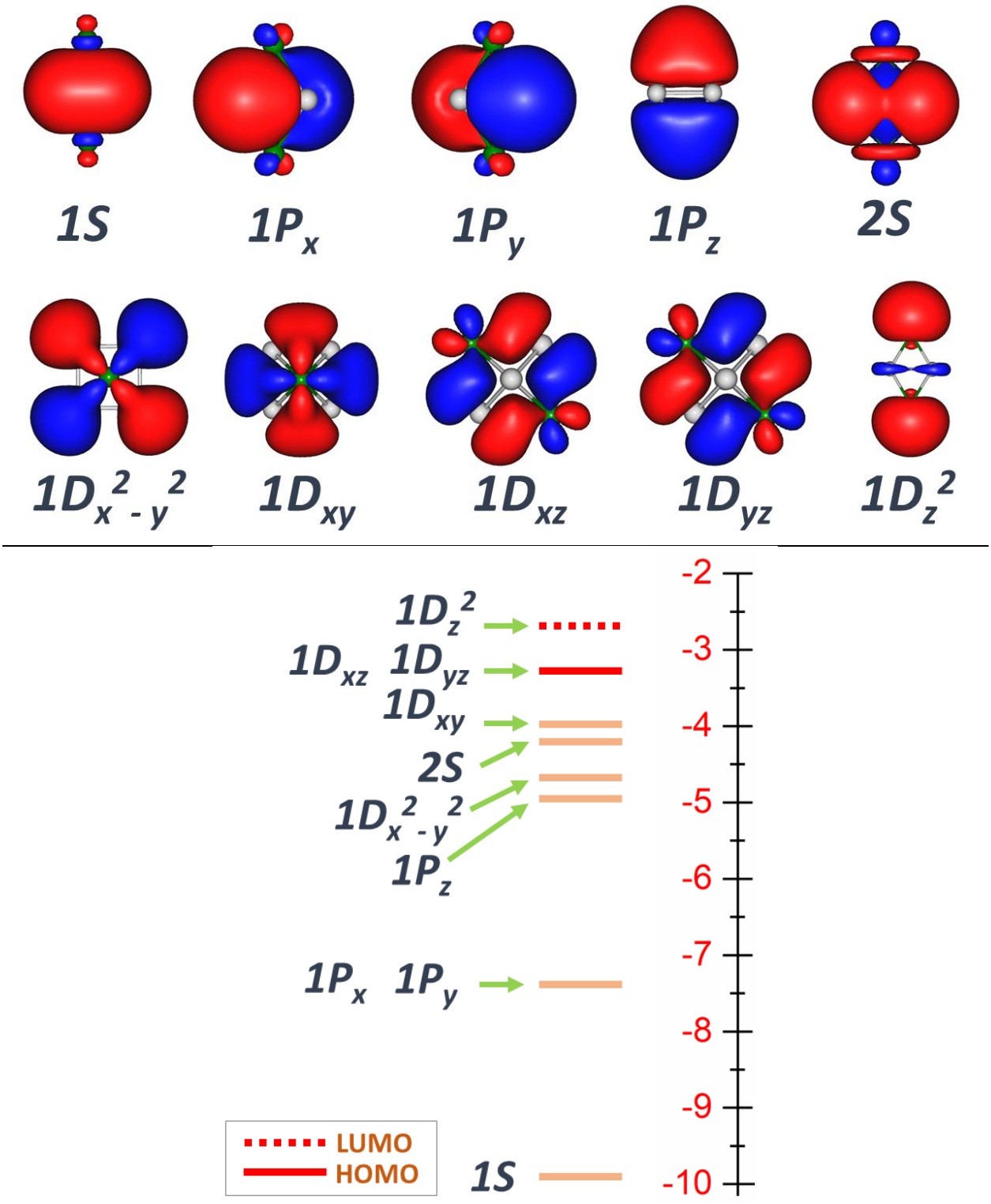


Figure S43: Energy levels of molecular orbitals (MOs) of the **n.6.C.1** at singlet state, PBE/ Def2-TZVP.

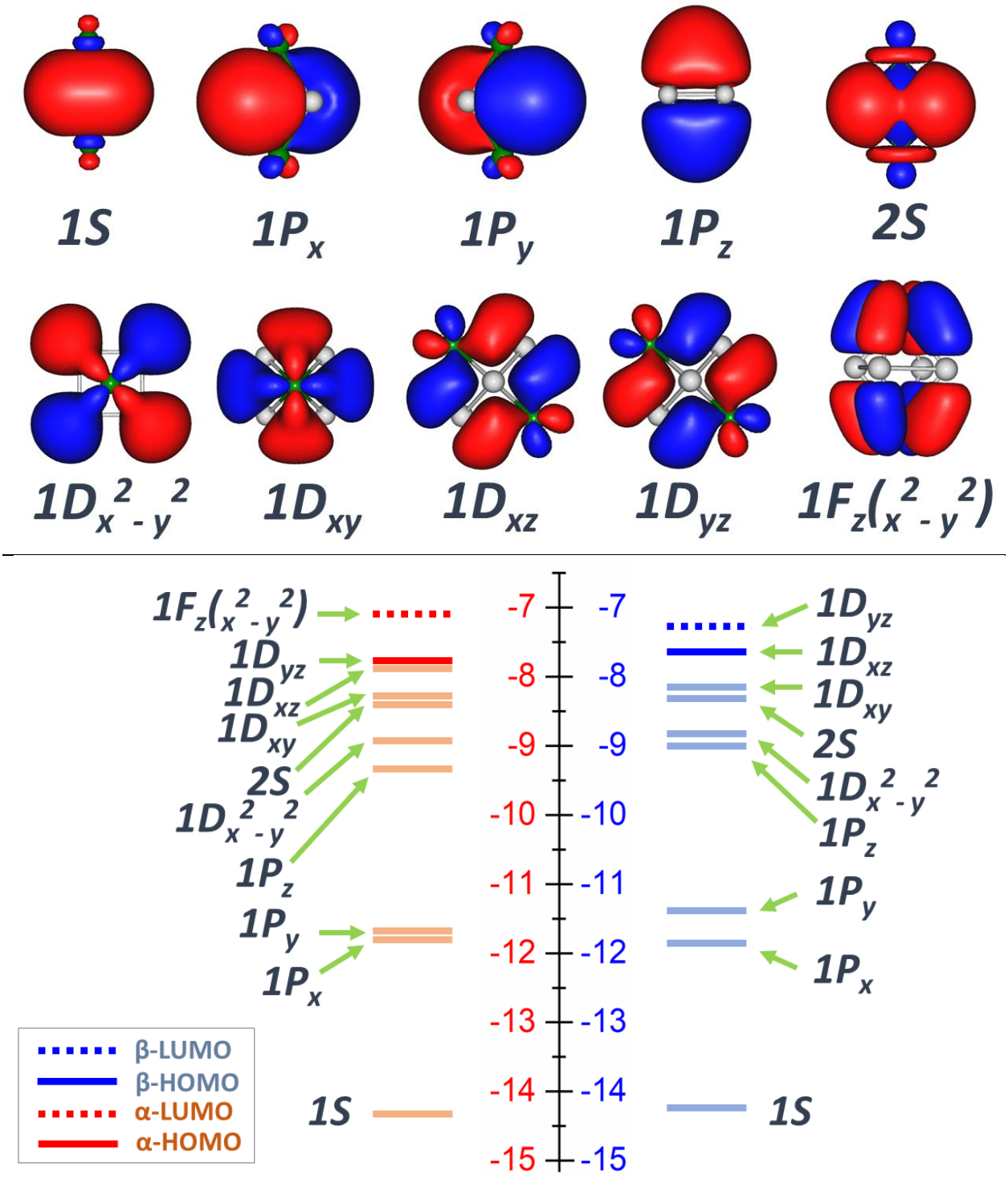
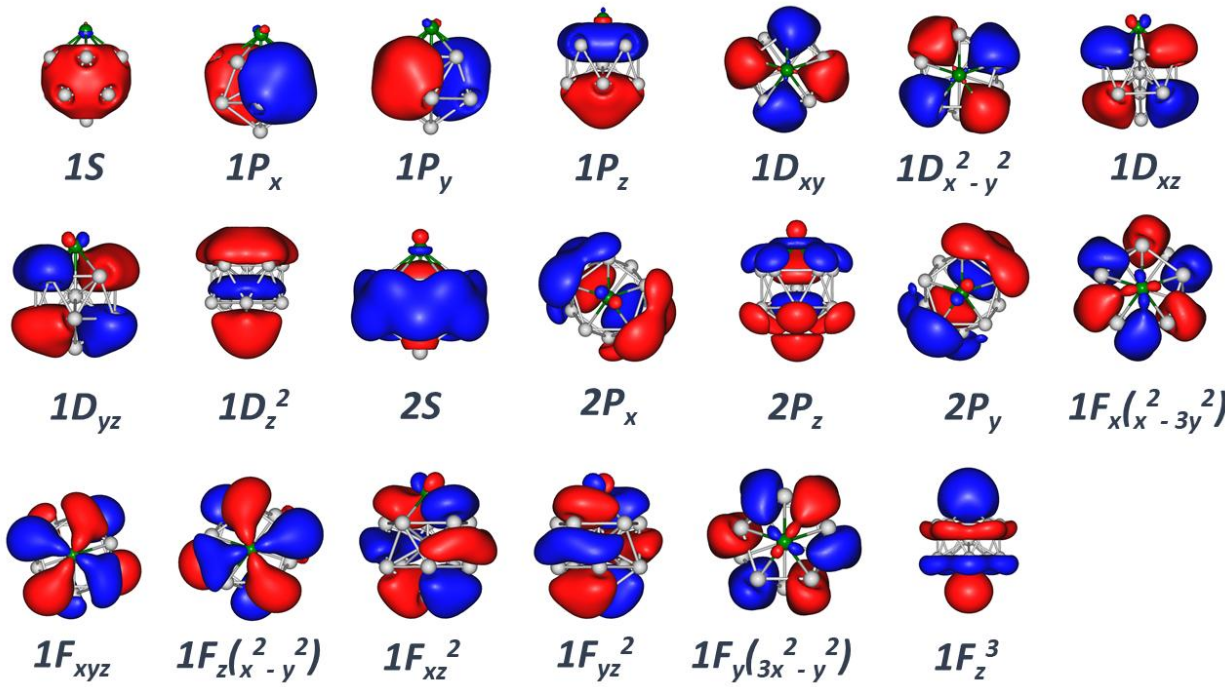


Figure S44: Energy levels of molecular orbitals (MOs) of the **c.6.C.1** at singlet state, PBE/ Def2-TZVP.



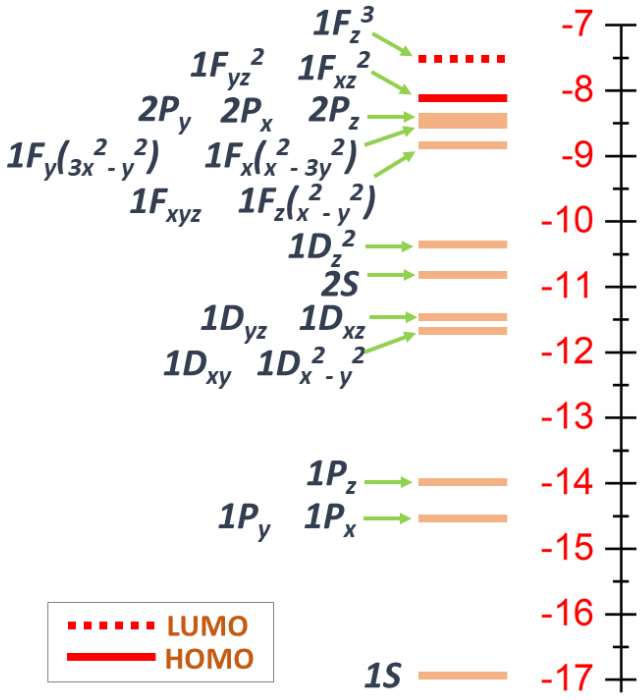


Figure S45: Energy levels of molecular orbitals (MOs) of the **c.13.B.1** at singlet state, PBE/ Def2-TZVP.

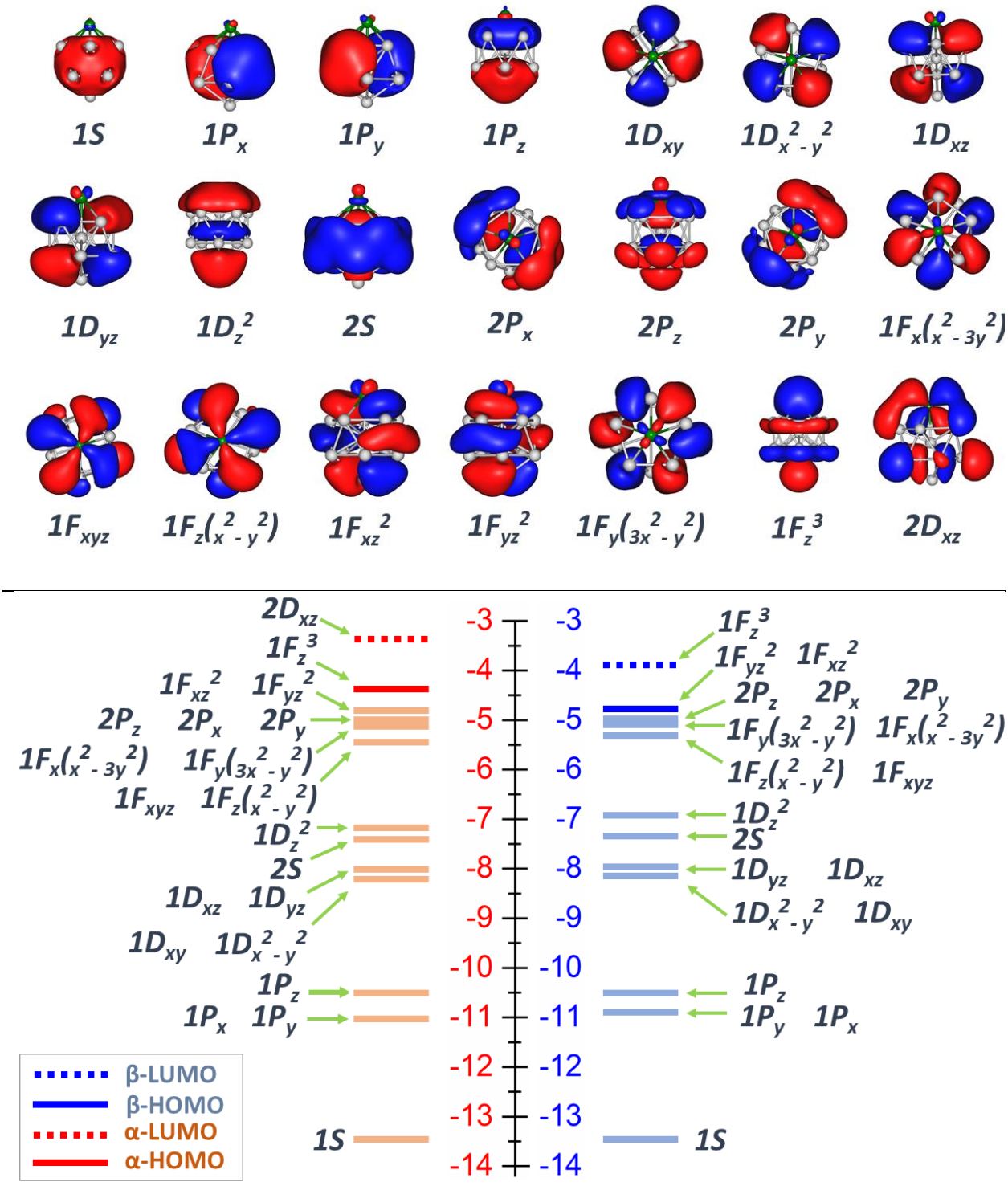


Figure S46: Energy levels of molecular orbitals (MOs) of the **n.13.B.1** at doublet state, PBE/ Def2-TZVP.

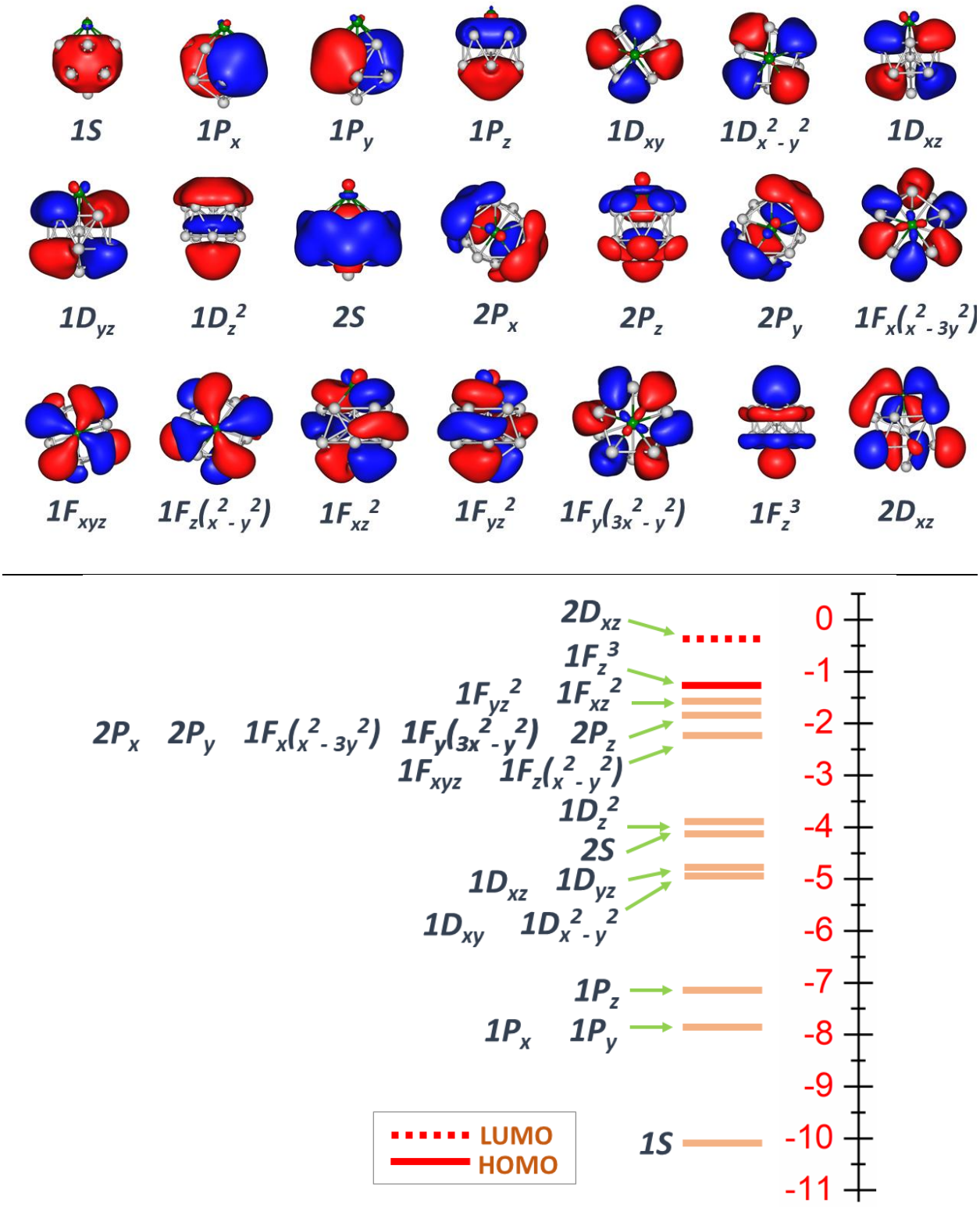


Figure S47: Energy levels of molecular orbitals (MOs) of the **a.13.B.1** at singlet state, PBE/ Def2-TZVP.

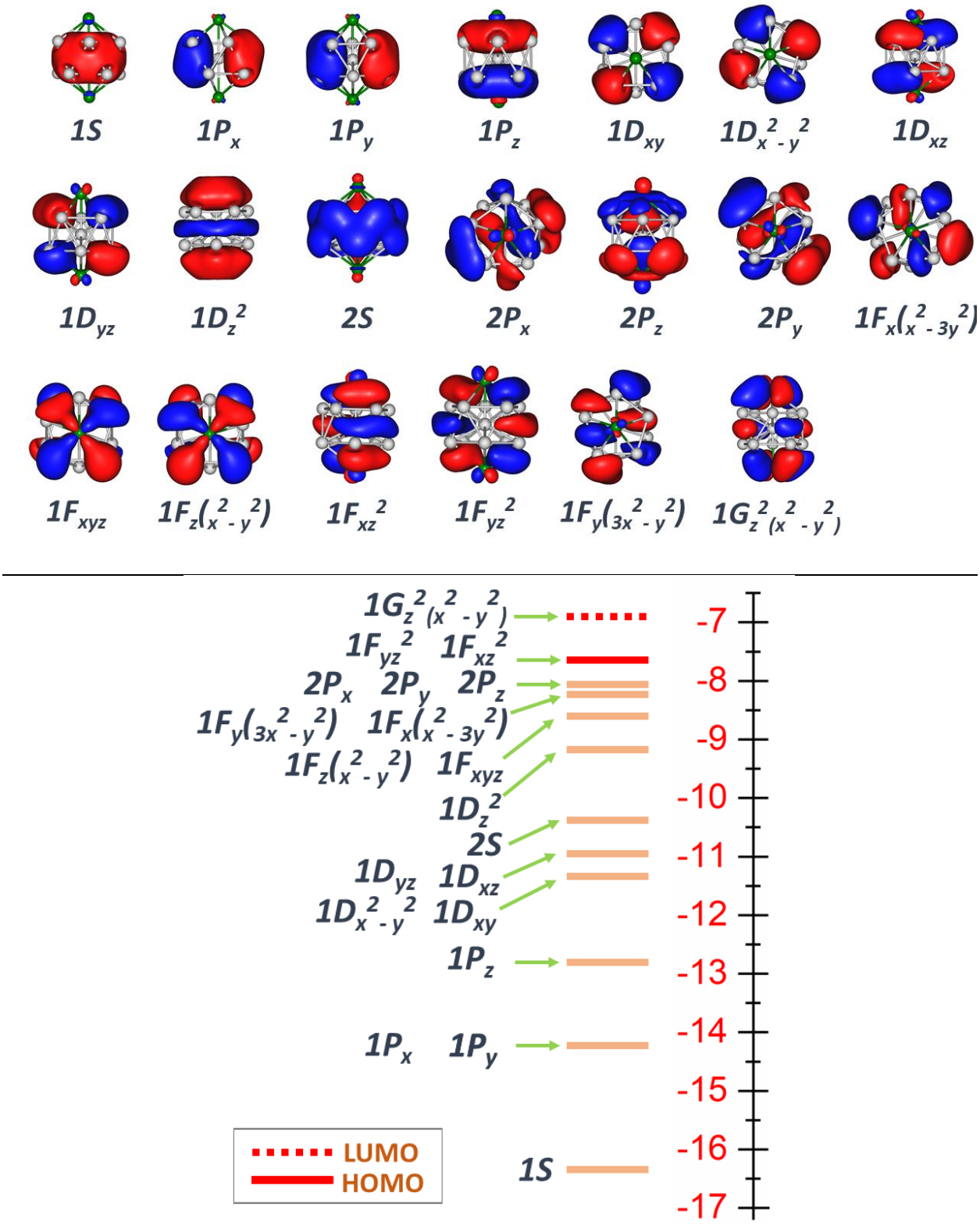


Figure S48: Energy levels of molecular orbitals (MOs) of the **c.13.C.1** at singlet state, PBE/ Def2-TZVP.

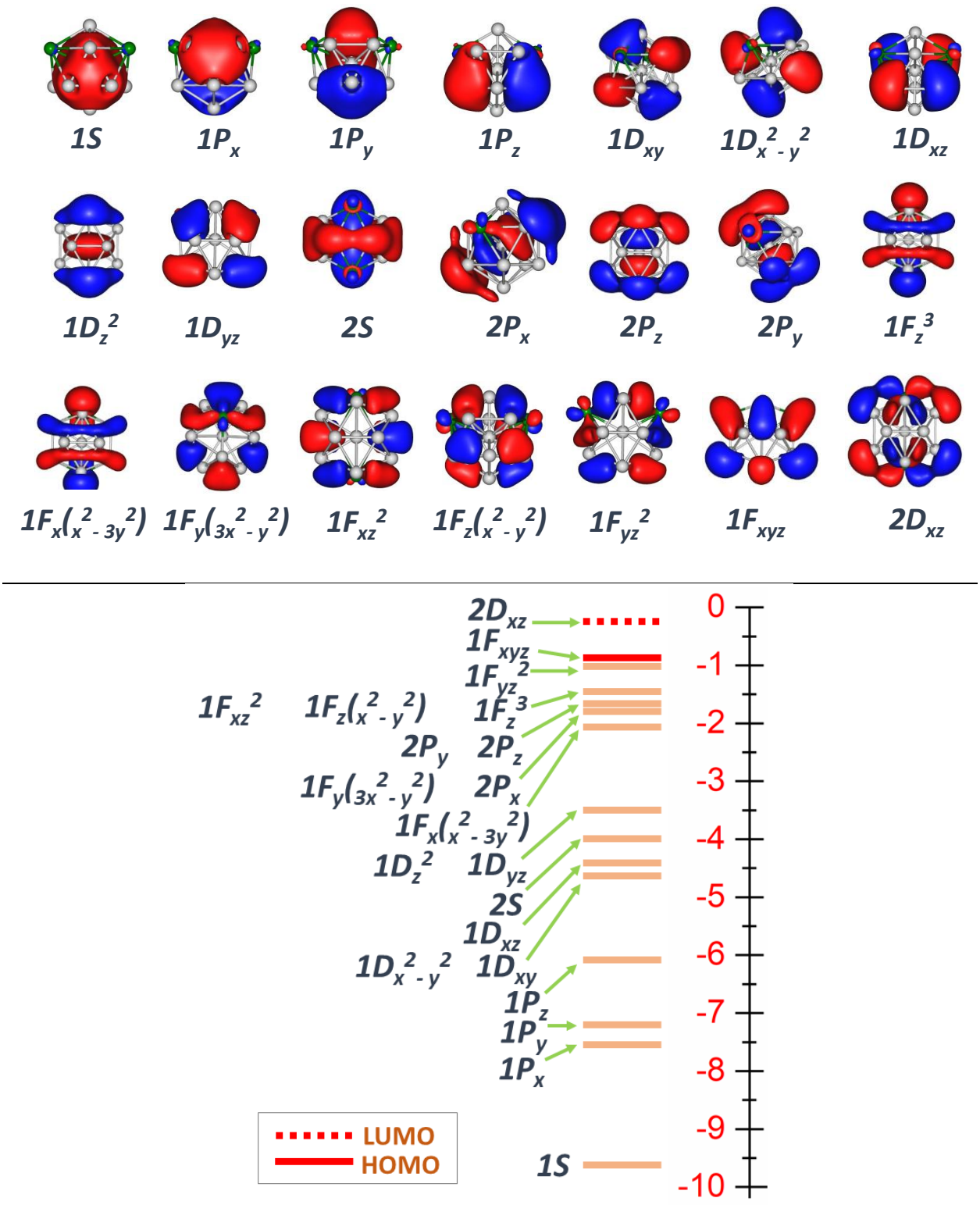


Figure S49: Energy levels of molecular orbitals (MOs) of the **a.13.C.1** at singlet state, PBE/ Def2-TZVP.

Coordinates of the lowest-lying $ScAl_{n-1}^{+/0/-}$ clusters with n = 3 - 15

Isomer	Spin state		Coordinate		
c.3.B.1	triplet	13	1.285189000	-1.127385000	-0.000000000
		13	-1.285189000	-1.127385000	0.000000000
		21	0.000000000	1.395811000	0.000000000
n.3.B.1	doublet	13	0.000000000	1.236675000	-1.058706000
		13	-0.000000000	-1.236675000	-1.058706000
		21	-0.000000000	-0.000000000	1.310779000
a.3.B.1	singlet	13	0.000000000	1.258634000	-1.033006000
		13	-0.000000000	-1.258634000	-1.033006000
		21	0.000000000	0.000000000	1.278960000

Isomer	Spin state		Coordinate		
c.4.B.1	doublet	13	0.785886000	1.354658000	0.753172000
		13	0.786553000	-1.354483000	0.753066000
		13	0.905640000	0.000204000	-1.432509000
		21	-1.534048000	-0.000234000	-0.045642000
n.4.B.1	triplet	13	-1.706246000	-0.243079000	0.000000000
		13	0.471940000	-0.990143000	1.329292000
		13	0.471940000	-0.990143000	-1.329292000
		21	0.471940000	1.376368000	0.000000000
a.4.B.1	doublet	13	-1.657815000	-0.254939000	-0.000000000
		13	0.458545000	-0.941848000	1.459738000
		13	0.458545000	-0.941848000	-1.459738000
		21	0.458545000	1.323916000	0.000000000

Isomer	Spin state		Coordinate		
c.5.B.1	singlet	13	1.797108000	-0.508549000	0.580162000
		13	0.507534000	1.796559000	0.582088000
		13	-1.798077000	0.506741000	0.579552000
		13	-0.508001000	-1.797753000	0.578548000
		21	0.000889000	0.001858000	-1.436407000
n.5.B.1	doublet	13	1.951964000	-0.011363000	-0.559868000
		13	-0.012634000	-1.753082000	-0.614478000
		13	0.012689000	1.753101000	-0.614427000
		13	-1.951919000	0.011381000	-0.560019000
		21	-0.000062000	-0.000024000	1.454014000
a.5.B.1	triplet	13	0.000000000	1.868768000	-0.589313000
		13	-0.000000000	-1.868768000	-0.589313000
		13	-1.868769000	0.000000000	-0.589308000
		13	1.868769000	-0.000000000	-0.589308000
		21	0.000000000	0.000000000	1.459246000

Isomer	Spin state	Coordinate			
c.6.B.1	doublet	13	-0.790333000	-1.385486000	0.449245000
		13	-2.985531000	0.000030000	-0.250364000
		13	1.106881000	-1.288859000	-1.298943000
		13	-0.790343000	1.385374000	0.449598000
		13	1.106949000	1.289412000	-1.298280000
		21	1.456234000	-0.000291000	1.206365000
n.6.B.1	triplet	13	-0.000000000	1.865071000	-0.215716000
		13	-0.000000000	0.000000000	-2.157205000
		13	1.861233000	-0.120034000	-0.215638000
		13	-1.861233000	0.120034000	-0.215638000
		13	0.000000000	-1.865071000	-0.215716000
		21	0.000000000	-0.000000000	1.869470000
a.6.B.1	doublet	13	-0.206587000	-1.251968000	1.360868000
		13	-2.312175000	-0.121449000	-0.000000000
		13	-0.206587000	-1.251968000	-1.360868000
		13	-0.206587000	1.296156000	-1.330396000
		13	-0.206587000	1.296156000	1.330396000
		21	1.942894000	0.020474000	0.000000000

Isomer	Spin state	Coordinate			
c.7.B.1	singlet	13	1.887749000	-1.278058000	0.000712000
		13	-0.485227000	-2.263953000	-0.000102000
		13	1.888214000	1.277397000	-0.000711000
		13	-0.484420000	2.264113000	0.000123000
		13	0.180160000	0.000372000	1.640950000
		13	0.180161000	-0.000426000	-1.640965000
		21	-1.960299000	0.000343000	-0.000005000
n.7.B.1	doublet	13	-1.946055000	-1.234222000	-0.138254000
		13	-1.945909000	1.234656000	0.138200000
		13	-0.138583000	-0.026193000	1.698722000
		13	0.424626000	-2.143324000	0.058806000
		13	-0.138760000	0.026119000	-1.698384000
		13	0.425367000	2.143443000	-0.058957000
		21	2.054814000	-0.000296000	-0.000082000
a.7.B.1	singlet	13	-0.152172000	-1.279090000	1.363197000
		13	-0.152011000	1.279738000	1.362568000
		13	2.111354000	1.259525000	-0.000076000
		13	-0.151896000	1.279218000	-1.363048000
		13	-0.152291000	-1.279621000	-1.362690000
		13	2.110775000	-1.259974000	0.000061000
		21	-2.237090000	0.000126000	-0.000008000

Isomer	Spin state	Coordinate			
		13	-1.577045000	1.776361000	-0.124891000
		13	2.520627000	-0.313385000	-1.179603000
		13	-0.434908000	0.124354000	1.715621000
c.8.B.1	doublet	13	0.267300000	-1.775906000	0.053910000
		13	-0.073365000	0.069545000	-1.696474000
		13	1.026640000	1.713622000	0.077891000
		13	2.131491000	-0.319609000	1.340412000
		21	-2.389982000	-0.789274000	-0.115679000
		13	0.435104000	0.085251000	1.634500000
		13	-2.116313000	-0.193365000	1.309880000
		13	0.053659000	0.034169000	-1.567817000
n.8.B.1	triplet	13	-0.849880000	1.822948000	0.101094000
		13	1.831707000	1.799600000	-0.124206000
		13	-2.536112000	-0.125620000	-1.198428000
		13	-0.434466000	-1.926254000	0.087466000
		21	2.238663000	-0.926547000	-0.150113000
		13	-1.744009000	0.696085000	0.000000000
		13	0.064595000	-0.308153000	1.651580000
		13	0.064595000	2.343995000	1.315621000
a.8.B.1	quartet	13	0.064595000	-0.308153000	-1.651580000
		13	0.064595000	2.343995000	-1.315621000
		13	1.572570000	-2.048500000	0.000000000
		13	1.827028000	0.693892000	0.000000000
		21	-1.184839000	-2.112910000	0.000000000

Isomer	Spin state	Coordinate			
		13	-0.878752000	-1.854542000	0.112274000
		13	0.648539000	0.000363000	1.700974000
		13	-0.879646000	1.854524000	0.111682000
		13	3.164959000	0.000223000	-0.770060000
c.9.B.1	singlet	13	1.817404000	1.914590000	0.199305000
		13	1.817933000	-1.914467000	0.199071000
		13	0.318589000	-0.000043000	-1.368488000
		13	-1.996251000	-0.000219000	1.606809000
		21	-2.484099000	-0.000266000	-1.109065000
		13	0.860719000	-1.980085000	0.147442000
		13	-0.794956000	0.000000000	1.447648000
		13	-2.955807000	0.000001000	-0.590814000
		13	0.860722000	1.980084000	0.147442000
n.9.B.1	doublet	13	-1.751955000	2.149330000	0.056515000
		13	1.795306000	0.000000000	1.626866000
		13	-0.258141000	0.000001000	-1.310859000
		13	-1.751958000	-2.149329000	0.056516000
		21	2.473759000	-0.000002000	-0.978564000
		13	2.880747000	-0.000005000	-0.548425000
		13	1.709479000	-2.253139000	0.010906000
		13	-0.860391000	2.080958000	0.155196000
		13	-1.710935000	0.000004000	1.614240000
a.9.B.1	singlet	13	0.832349000	-0.000006000	1.366510000
		13	0.245956000	0.000007000	-1.234531000
		13	1.709487000	2.253134000	0.010912000
		13	-0.860398000	-2.080954000	0.155199000
		21	-2.442943000	-0.000000000	-0.947148000

Isomer	Spin state	Coordinate			
		13	-1.098304000	0.139547000	1.392458000
		13	-2.381109000	-1.710136000	-0.591804000
		13	-0.369053000	-2.389343000	0.779176000
		13	1.435153000	-0.461761000	1.477429000
c.10.B.1	doublet	13	1.657655000	-1.967974000	-0.697065000
		13	0.973262000	2.046865000	0.882551000
		13	-2.981639000	0.741730000	-0.596773000
		13	-0.133575000	0.047125000	-1.061637000
		13	-1.251940000	2.559518000	-0.191737000
		21	2.568769000	0.615599000	-0.862084000
		13	-1.486739000	-2.363155000	-0.299243000
		13	-3.090913000	-0.437326000	-0.573486000
		13	-2.185763000	1.921577000	-0.522583000
		13	0.703254000	-2.152555000	0.944609000
n.10.B.1	singlet	13	-0.037017000	2.359172000	0.763697000
		13	2.093633000	1.830733000	-0.646842000
		13	-1.153408000	-0.093820000	1.341888000
		13	-0.114399000	0.070361000	-1.104205000
		13	1.413165000	0.293406000	1.486584000
		21	2.388401000	-0.884243000	-0.860736000
		13	-0.848753000	1.277821000	1.444027000
		13	-2.676531000	0.005571000	-0.220367000
		13	-0.142476000	0.000445000	-0.954037000
		13	2.577198000	-0.004723000	-1.266112000
a.10.B.1	doublet	13	1.132353000	-2.299125000	-0.436713000
		13	-0.853782000	-1.274421000	1.443393000
		13	-1.477113000	2.408172000	-0.849602000
		13	1.143065000	2.293720000	-0.436811000
		13	-1.488125000	-2.400955000	-0.850648000
		21	1.630673000	-0.004026000	1.316634000

Isomer	Spin state	Coordinate			
		13	2.919716000	-1.249798000	-0.600380000
		13	0.840021000	-2.570985000	0.106079000
		13	-0.895724000	-1.261541000	1.529927000
		13	-1.498392000	-2.420235000	-1.007101000
		13	0.069375000	0.000018000	-0.951223000
c.11.B.1	singlet	13	1.482035000	-0.000088000	1.326801000
		13	2.919688000	1.250118000	-0.599687000
		13	0.839672000	2.571207000	0.105821000
		13	-1.498807000	2.420122000	-1.007046000
		13	-0.895745000	1.261457000	1.529854000
		21	-2.650662000	-0.000170000	-0.268076000
		13	2.828280000	-1.254564000	-0.647227000
		13	0.887112000	-2.592487000	0.284089000
		13	-0.981641000	-1.293217000	1.513004000
		13	-1.352698000	-2.414509000	-1.048935000
		13	0.110745000	-0.000015000	-0.981231000
n.11.B.1	doublet	13	1.348615000	0.000052000	1.371713000
		13	2.827939000	1.255119000	-0.647031000
		13	0.886552000	2.592818000	0.283955000
		13	-1.353322000	2.414350000	-1.048776000
		13	-0.981874000	1.292934000	1.512989000
		21	-2.612201000	-0.000299000	-0.366817000
		13	2.095560000	-1.249520000	-1.307456000
		13	-0.147899000	-1.474052000	2.658025000
		13	2.095560000	-1.249520000	1.307456000
		13	-0.147899000	1.163182000	2.345417000
		13	-2.272710000	-0.004273000	1.349580000
a.11.B.1	singlet	13	-0.147899000	1.163182000	-2.345417000
		13	-1.183101000	2.082697000	-0.000000000
		13	-2.272710000	-0.004273000	-1.349580000
		13	-0.147899000	-1.474052000	-2.658025000
		13	-0.199109000	-1.028047000	0.000000000
		21	1.441208000	1.284323000	-0.000000000

Isomer	Spin state	Coordinate			
		13	-1.096808000	2.261969000	1.369027000
		13	-1.096808000	-0.401511000	2.223820000
		13	-2.429036000	0.229832000	-0.000000000
		13	-1.096808000	-0.401511000	-2.223820000
		13	-1.096808000	2.261969000	-1.369027000
		13	1.134104000	1.164261000	-2.385918000
c.12.B.1	doublet	13	1.380111000	-1.459213000	-1.739902000
		13	1.134104000	1.164261000	2.385918000
		13	1.380111000	-1.459213000	1.739902000
		13	2.880275000	-0.144606000	0.000000000
		13	0.250367000	0.343277000	0.000000000
		21	-0.831260000	-2.203509000	-0.000000000
		13	-0.000324000	1.879781000	1.528787000
		13	-2.377861000	0.022096000	-1.688873000
		13	1.390262000	2.305184000	-0.900095000
		13	2.377702000	0.023125000	-1.688843000
		13	2.209757000	0.499847000	1.054028000
		13	1.808651000	-1.933861000	0.110861000
n.12.B.1	singlet	13	-1.807702000	-1.934731000	0.110636000
		13	-0.000090000	0.042132000	-0.413403000
		13	0.000786000	-2.214311000	-1.818031000
		13	-1.391427000	2.304567000	-0.899974000
		13	-2.210016000	0.498773000	1.054097000
		21	0.000162000	-0.923991000	2.198120000
		13	-1.519549000	1.783077000	0.870383000
		13	-1.365266000	-1.907170000	-1.595898000
		13	-0.131685000	2.403277000	-1.472653000
		13	2.241420000	0.855087000	-1.556826000
		13	1.334698000	1.928986000	0.861128000
a.12.B.1	doublet	13	2.280685000	-0.612482000	0.824254000
		13	0.124743000	-2.387734000	0.724063000
		13	-0.000832000	0.007794000	-0.340494000
		13	1.554192000	-1.760544000	-1.598479000
		13	-2.316186000	0.637012000	-1.555543000
		13	-2.211122000	-0.831239000	0.823650000
		21	0.005510000	-0.071850000	2.486352000

Isomer	Spin state	Coordinate			
		13	0.994376000	-2.403644000	0.196579000
		13	0.993772000	1.829064000	-1.572048000
		13	0.994166000	-0.929695000	-2.225285000
		13	-1.320004000	0.544429000	-2.299132000
		13	-1.319589000	-2.018441000	-1.228573000
		13	-2.634370000	-0.000375000	0.000219000
c.13.B.1	singlet	13	-1.320220000	2.354797000	-0.192704000
		13	-1.319541000	-1.792359000	1.539921000
		13	-1.319969000	0.910756000	2.180214000
		13	0.993989000	-0.555625000	2.346938000
		13	0.993632000	2.060512000	1.253670000
		13	-0.034305000	-0.000056000	0.000027000
		21	2.660706000	0.000394000	0.000108000
		13	0.000000000	2.387620000	1.021278000
		13	2.270762000	0.737815000	1.021278000
		13	2.243320000	-0.728899000	-1.325134000
		13	1.403408000	-1.931625000	1.021278000
		13	1.386448000	1.908282000	-1.325134000
		13	0.000000000	0.000000000	-2.778386000
n.13.B.1	doublet	13	-1.386448000	1.908282000	-1.325134000
		13	-2.270762000	0.737815000	1.021278000
		13	-2.243320000	-0.728899000	-1.325134000
		13	-0.000000000	-2.358766000	-1.325134000
		13	0.000000000	0.000000000	-0.058254000
		13	-1.403408000	-1.931625000	1.021278000
		21	0.000000000	0.000000000	2.696522000
		13	-0.000000000	2.372878000	1.054769000
		13	2.256741000	0.733260000	1.054769000
		13	2.236173000	-0.726577000	-1.333656000
		13	1.394743000	-1.919699000	1.054769000
		13	1.382031000	1.902203000	-1.333656000
		13	0.000000000	0.000000000	-2.976302000
a.13.B.1	singlet	13	-1.382031000	1.902203000	-1.333656000
		13	-2.256741000	0.733260000	1.054769000
		13	-2.236173000	-0.726577000	-1.333656000
		13	-0.000000000	-2.351252000	-1.333656000
		13	0.000000000	0.000000000	-0.076045000
		13	-1.394743000	-1.919699000	1.054769000
		21	0.000000000	0.000000000	2.752769000

Isomer	Spin state	Coordinate			
		13	-1.159259000	-0.861833000	-2.243015000
		13	1.213883000	0.811727000	-2.271107000
		13	1.002960000	2.375372000	-0.000576000
		13	-1.084531000	1.936879000	-1.754291000
		13	-1.084467000	1.937551000	1.753553000
		13	-2.845520000	1.180661000	-0.000215000
c.14.B.1	doublet	13	-1.159268000	-0.860903000	2.243506000
		13	-2.781834000	-1.333052000	0.000247000
		13	-0.117936000	0.016323000	0.000023000
		13	-0.610701000	-2.732136000	0.000542000
		13	1.355216000	-1.732825000	1.467575000
		13	1.214060000	0.812879000	2.270681000
		13	1.355191000	-1.733534000	-1.466835000
		21	2.910889000	0.113218000	-0.000055000
		13	-1.731438000	-1.894588000	-0.000049000
		13	0.548886000	-2.151768000	-1.400843000
		13	1.346786000	0.251847000	-2.368719000
		13	2.269209000	1.756317000	0.000045000
		13	-1.397796000	-0.139309000	-2.089677000
		13	-0.053650000	2.323917000	1.401030000
		13	-2.206860000	1.475049000	-0.000016000
n.14.B.1	singlet	13	-0.053617000	2.323957000	-1.400977000
		13	-3.964323000	-0.448029000	0.000018000
		13	0.231524000	0.066069000	-0.000002000
		13	-1.397843000	-0.139359000	2.089628000
		13	1.346741000	0.251785000	2.368742000
		13	0.548853000	-2.151801000	1.400795000
		21	2.794089000	-0.943482000	0.000016000
		13	1.792454000	-1.056115000	-1.404136000
		13	-2.120823000	1.236890000	1.456566000
		13	-0.828482000	-1.145410000	2.236711000
		13	1.792542000	-1.056891000	1.403468000
		13	0.536080000	1.281370000	2.245247000
		13	2.201783000	1.444021000	0.000184000
		13	-0.256873000	2.721155000	0.000646000
a.14.B.1	doublet	13	0.535766000	1.282473000	-2.244722000
		13	-2.121052000	1.237567000	-1.455744000
		13	4.093352000	-0.494430000	-0.000096000
		13	-0.238224000	0.077607000	0.000011000
		13	-0.131790000	-2.563223000	-0.000645000
		13	-0.828667000	-1.144311000	-2.237224000
		21	-2.739946000	-1.127103000	-0.000165000

Isomer	Spin state	Coordinate			
		13	0.263028000	-1.410515000	2.291429000
		13	2.601649000	-0.000026000	1.692009000
		13	1.760737000	2.322417000	0.125964000
		13	0.546099000	-1.370732000	-2.169289000
		13	-1.720515000	0.000015000	-1.553622000
		13	0.546106000	1.370785000	-2.169258000
		13	-1.021706000	2.234308000	-0.025888000
c.14.B.1	singlet	13	0.263032000	1.410475000	2.291455000
		13	-1.901309000	-0.000011000	1.442400000
		13	-3.678038000	-1.364109000	-0.190904000
		13	-3.678035000	1.364111000	-0.190872000
		13	0.474326000	-0.000001000	0.072129000
		13	1.760725000	-2.322423000	0.125929000
		13	-1.021707000	-2.234303000	-0.025931000
		21	2.974899000	0.000006000	-1.062009000
		13	-0.358865000	1.313354000	2.365849000
		13	-2.559566000	-0.247774000	1.688654000
		13	-1.496093000	-2.402216000	0.077770000
		13	-0.681289000	1.458135000	-2.105178000
		13	1.649795000	0.169070000	-1.641932000
		13	-0.535574000	-1.294988000	-2.242671000
		13	1.205538000	-2.129506000	-0.151718000
n.14.B.1	doublet	13	-0.146070000	-1.491271000	2.261534000
		13	1.897354000	0.044245000	1.478241000
		13	3.506456000	1.417648000	-0.162647000
		13	3.802811000	-1.208830000	-0.252934000
		13	-0.454776000	-0.003146000	0.071452000
		13	-1.897571000	2.218584000	0.257174000
		13	0.866205000	2.285951000	0.062584000
		21	-2.970410000	-0.080015000	-1.056207000
		13	0.263028000	-1.410515000	2.291429000
		13	2.601649000	-0.000026000	1.692009000
		13	1.760737000	2.322417000	0.125964000
		13	0.546099000	-1.370732000	-2.169289000
		13	-1.720515000	0.000015000	-1.553622000
		13	0.546106000	1.370785000	-2.169258000
		13	-1.021706000	2.234308000	-0.025888000
a.14.B.1	singlet	13	0.263032000	1.410475000	2.291455000
		13	-1.901309000	-0.000011000	1.442400000
		13	-3.678038000	-1.364109000	-0.190904000
		13	-3.678035000	1.364111000	-0.190872000
		13	0.474326000	-0.000001000	0.072129000
		13	1.760725000	-2.322423000	0.125929000
		13	-1.021707000	-2.234303000	-0.025931000
		21	2.974899000	0.000006000	-1.062009000

Coordinates of the lowest-lying $Sc_2Al_{n-2}^{+/0/-}$ clusters with n = 3 - 15

Isomer	Spin state		Coordinate		
c.3.C.1	triplet	21	1.013494000	1.122408000	-0.000000000
		21	0.000000000	-1.512215000	0.000000000
		13	-1.637182000	0.629687000	-0.000000000
n.3.C.1	doublet	13	1.575420000	0.562361000	0.000000000
		21	-0.975260000	1.191949000	0.000000000
		21	-0.000000000	-1.540077000	-0.000000000
a.3.C.1	singlet	13	1.602140000	0.614544000	0.000000000
		21	-0.000000000	-1.483045000	0.000000000
		21	-0.991801000	1.102613000	0.000000000

Isomer	Spin state		Coordinate		
c.4.C.1	doublet	13	0.000098000	-1.183107000	1.254010000
		13	-0.000234000	-1.187057000	-1.251432000
		21	1.503159000	0.733568000	-0.000884000
		21	-1.503074000	0.733676000	-0.000712000
n.4.C.1	triplet	13	-0.000023000	1.225966000	-1.286822000
		13	0.000014000	1.225921000	1.286854000
		21	1.398206000	-0.758913000	-0.000028000
		21	-1.398199000	-0.758922000	0.000008000
a.4.C.1	quartet	13	-1.321457000	-0.000004000	1.289077000
		13	-1.321466000	-0.000002000	-1.289066000
		21	0.818045000	1.308554000	-0.000006000
		21	0.818051000	-1.308550000	-0.000001000

Isomer	Spin state		Coordinate		
c.5.C.1	triplet	13	-0.251208000	0.379069000	1.911027000
		13	-1.859660000	0.737199000	0.000000000
		13	-0.251208000	0.379069000	-1.911027000
		21	-0.251208000	-1.602716000	-0.000000000
		21	1.713446000	0.677032000	-0.000000000
n.5.C.1	quartet	13	2.167390000	-0.000023000	0.245082000
		13	-2.167394000	-0.000021000	0.245053000
		13	-0.000012000	-0.000157000	1.699436000
		21	0.000006000	1.465883000	-0.677590000
		21	0.000004000	-1.465758000	-0.677858000
a.5.C.1	singlet	13	0.000003000	-0.226757000	2.289566000
		13	0.000003000	-1.752900000	-0.000000000
		13	0.000003000	-0.226757000	-2.289566000
		21	1.337723000	0.682947000	0.000000000
		21	-1.337729000	0.682928000	-0.000000000

Isomer	Spin state	Coordinate			
c.6.C.1	doublet	13	-0.000000000	-1.866417000	-0.000000000
		13	-1.866415000	0.000003000	0.000000000
		13	0.000000000	1.866417000	-0.000000000
		13	1.866415000	-0.000003000	0.000000000
		21	-0.000000000	0.000000000	2.090183000
		21	-0.000000000	0.000000000	-2.090183000
n.6.C.1	singlet	13	0.000000000	1.809539000	-0.000000000
		13	-0.000000000	-1.809539000	-0.000000000
		13	-1.809539000	0.000000000	-0.000000000
		13	1.809539000	-0.000000000	-0.000000000
		21	0.000000000	0.000000000	2.135843000
		21	0.000000000	0.000000000	-2.135843000
a.6.C.1	doublet	13	0.000000000	1.812515000	-0.000000000
		13	-0.000000000	-1.812515000	-0.000000000
		13	-1.812515000	0.000000000	-0.000000000
		13	1.812515000	-0.000000000	-0.000000000
		21	0.000000000	0.000000000	2.198305000
		21	0.000000000	0.000000000	-2.198305000

Isomer	Spin state	Coordinate			
c.7.C.1	singlet	13	1.168298000	1.277402000	1.302270000
		13	-1.100605000	1.666323000	0.000093000
		13	1.168482000	1.277694000	-1.301905000
		13	-0.234031000	-0.898191000	1.320287000
		13	-0.234030000	-0.897705000	-1.320513000
		21	-2.692387000	-0.479856000	-0.000048000
		21	2.216888000	-1.021659000	-0.000097000
n.7.C.1	doublet	13	1.922294000	0.463771000	0.000000000
		13	-0.074917000	-0.013307000	1.642836000
		13	-2.197857000	0.808195000	0.000000000
		13	-0.074917000	-0.013307000	-1.642836000
		13	-1.419548000	-1.637659000	0.000000000
		21	1.217026000	-2.142568000	0.000000000
		21	-0.074917000	2.385424000	0.000000000
a.7.C.1	triplet	13	0.000000000	1.308798000	-1.930104000
		13	-0.000000000	-1.308798000	-1.930104000
		13	-1.560204000	0.000000000	-0.086016000
		13	1.560204000	-0.000000000	-0.086016000
		13	0.000000000	-0.000000000	2.140649000
		21	0.000000000	-2.284990000	0.585492000
		21	0.000000000	2.284990000	0.585492000

Isomer	Spin state	Coordinate			
c.8.C.1	doublet	13	-0.214832000	-1.092968000	-1.268158000
		13	-0.792159000	1.332280000	1.106320000
		13	1.847105000	1.082878000	1.332360000
		13	0.214643000	-1.094642000	1.266953000
		13	-1.846947000	1.084473000	-1.331097000
		13	0.792395000	1.333561000	-1.104838000
		21	2.510072000	-0.818694000	-0.458203000
		21	-2.510199000	-0.819047000	0.457250000
n.8.C.1	triplet	13	0.311665000	-1.104720000	-1.271912000
		13	-0.722750000	1.303619000	-1.122556000
		13	-1.943763000	1.124339000	1.278223000
		13	-0.311662000	-1.104866000	1.271797000
		13	0.722741000	1.303495000	1.122687000
		13	1.943767000	1.124474000	-1.278105000
		21	2.458133000	-0.819132000	0.521127000
		21	-2.458131000	-0.819080000	-0.521210000
a.8.C.1	doublet	13	1.443403000	-1.315349000	0.992281000
		13	-0.873074000	-2.271467000	0.195737000
		13	0.086073000	-0.221789000	-1.266351000
		13	2.772616000	-0.583664000	-1.193422000
		13	-0.708459000	0.166453000	1.558676000
		13	-1.090839000	2.208333000	-0.281100000
		21	-2.527802000	-0.155305000	-0.453264000
		21	1.518928000	1.404223000	0.449660000

Isomer	Spin state	Coordinate			
c.9.C.1	singlet	13	0.000000000	0.110609000	-1.060236000
		13	1.280657000	0.168010000	1.483974000
		13	-0.000017000	2.456420000	0.233761000
		13	2.361364000	1.575924000	-0.529750000
		13	-1.280642000	0.168020000	1.483970000
		13	-2.361387000	1.575900000	-0.529755000
		13	0.000010000	-2.092998000	0.706962000
		21	-2.349997000	-1.226306000	-0.553709000
		21	2.350006000	-1.226289000	-0.553721000
n.9.C.1	doublet	13	-0.000012000	0.089613000	-1.080788000
		13	1.269931000	0.223574000	1.505031000
		13	-0.001521000	2.351360000	0.367563000
		13	2.344551000	1.558265000	-0.643440000
		13	-1.269198000	0.221649000	1.505331000
		13	-2.345196000	1.557811000	-0.643529000
		13	0.000687000	-2.071783000	0.773346000
		21	-2.319198000	-1.217014000	-0.551919000
		21	2.319667000	-1.216146000	-0.552162000
a.9.C.1	singlet	13	0.000000000	1.308798000	-1.930104000
		13	-0.000000000	-1.308798000	-1.930104000
		13	-1.560204000	0.000000000	-0.086016000
		13	1.560204000	-0.000000000	-0.086016000
		13	0.000000000	-0.000000000	2.140649000
		21	0.000000000	-2.284990000	0.585492000
		21	0.000000000	2.284990000	0.585492000

Isomer	Spin state	Coordinate			
		13	1.091338000	2.797821000	0.727694000
		13	-2.155472000	0.570572000	-1.106876000
		13	0.487828000	-1.697148000	1.148994000
		13	-0.560628000	-1.611914000	-1.273309000
c.10.C.1	doublet	13	0.646710000	0.700562000	-1.147306000
		13	2.166277000	0.485383000	1.128721000
		13	-1.058060000	2.858004000	-0.689290000
		13	-0.678893000	0.676069000	1.191494000
		21	-2.342338000	-1.501502000	0.802946000
		21	2.380038000	-1.457143000	-0.790640000
		13	-2.012273000	-0.742848000	1.148068000
		13	-1.691632000	-1.861655000	-1.138843000
		13	-2.012267000	0.742831000	-1.148075000
		13	-1.691660000	1.861642000	1.138839000
n.10.C.1	singlet	13	2.580440000	-1.228231000	0.208170000
		13	0.142086000	-2.419955000	0.590316000
		13	2.580428000	1.228256000	-0.208160000
		13	0.142060000	2.419952000	-0.590315000
		21	0.607545000	-0.163200000	-1.581446000
		21	0.607533000	0.163205000	1.581447000
		13	0.213785000	2.396863000	-0.714602000
		13	-1.989476000	0.673331000	-1.196674000
		13	2.512116000	1.263153000	-0.199873000
		13	-1.989429000	-0.672645000	1.197139000
a.10.C.1	doublet	13	-1.704257000	1.966946000	1.012499000
		13	-1.705596000	-1.966089000	-1.012397000
		13	2.511683000	-1.264068000	0.199590000
		13	0.212903000	-2.396921000	0.714150000
		21	0.600159000	0.304063000	1.585461000
		21	0.599723000	-0.304416000	-1.585357000

Isomer	Spin state	Coordinate			
		13	1.320222000	-1.227333000	-1.479152000
		13	1.882896000	1.493656000	-1.035709000
		13	0.767768000	-1.819070000	1.084387000
		13	0.724255000	0.863616000	1.306139000
		13	-0.638523000	0.414424000	-1.050162000
c.11.C.1	singlet	13	-3.247188000	0.040449000	-0.414676000
		13	-0.001020000	3.166161000	-0.484312000
		13	-1.907445000	2.020751000	0.781739000
		13	-1.519952000	-0.563841000	1.504318000
		21	3.117748000	-0.481903000	0.478463000
		21	-1.496470000	-2.234981000	-0.610055000
		13	0.003019000	-0.045025000	-0.811754000
		13	2.281420000	-1.332370000	-1.603278000
		13	0.142446000	-2.679150000	-0.358986000
		13	-0.515322000	-1.142215000	1.714840000
		13	2.008053000	-1.251017000	1.014000000
n.11.C.1	doublet	13	2.371580000	1.253308000	-0.993487000
		13	-0.008549000	2.636603000	-0.681580000
		13	-2.199663000	1.375264000	-1.458758000
		13	-1.789196000	1.044764000	1.173400000
		21	-2.476507000	-1.251368000	-0.294509000
		21	1.056543000	1.337933000	1.536074000
		13	-2.915775000	-0.620414000	0.738691000
		13	1.745017000	-1.171243000	1.516861000
		13	0.794509000	-2.080235000	-1.027292000
		13	-1.745017000	-1.171243000	-1.516861000
		13	-2.059653000	1.442119000	-0.729173000
a.11.C.1	singlet	13	0.000000000	2.871724000	-0.000000000
		13	2.059653000	1.442119000	0.729173000
		13	2.915775000	-0.620414000	-0.738691000
		13	-0.794509000	-2.080235000	1.027292000
		21	0.450172000	0.615278000	-1.620931000
		21	-0.450172000	0.615278000	1.620931000

Isomer	Spin state	Coordinate			
c.12.C.1	doublet	13	0.939927000	-2.260832000	0.903006000
		13	-1.562157000	-1.352061000	1.424453000
		13	-1.562351000	1.351329000	1.424439000
		13	-1.077769000	2.382920000	-0.973129000
		13	1.478882000	1.897884000	-1.676494000
		13	-0.033168000	-0.000792000	-0.517560000
		13	-1.075624000	-2.384479000	-0.972691000
		13	0.623766000	0.000111000	2.161645000
		13	0.937960000	2.261622000	0.902874000
		13	1.481133000	-1.896871000	-1.676507000
		21	2.694888000	0.001377000	0.165826000
		21	-2.788115000	-0.000653000	-0.784895000
n.12.C.1	singlet	13	-0.628743000	2.381614000	-1.604219000
		13	0.653777000	2.202238000	0.887176000
		13	0.654653000	-2.201888000	0.887441000
		13	-0.154347000	-0.000112000	-0.441361000
		13	1.804557000	-1.427097000	-1.633016000
		13	-2.825537000	-0.000594000	-1.188362000
		13	-1.944623000	1.761018000	0.614988000
		13	1.803853000	1.427799000	-1.633118000
		13	-0.627532000	-2.381992000	-1.604241000
		13	-1.943886000	-1.761840000	0.614990000
		21	2.366157000	0.000545000	0.816303000
		21	-0.380360000	-0.000016000	2.340667000
a.12.C.1	doublet	13	2.647660000	-0.005812000	-0.429307000
		13	1.016402000	-1.413679000	-2.276559000
		13	1.142789000	2.267758000	0.398459000
		13	1.031961000	1.399200000	-2.279564000
		13	-0.055522000	0.000628000	-0.289332000
		13	-1.122545000	-1.358577000	1.680022000
		13	-1.126761000	1.368001000	1.671953000
		13	-1.235011000	2.315578000	-0.939599000
		13	-1.239482000	-2.319260000	-0.923359000
		13	1.141827000	-2.265679000	0.407693000
		21	-2.822752000	0.001741000	-0.286287000
		21	1.460032000	0.005589000	2.130798000

Isomer	Spin state	Coordinate			
		13	2.362361000	-1.158755000	0.000000000
		13	0.729283000	-1.158599000	2.246769000
		13	-1.911425000	-1.157827000	1.388199000
		13	-1.911425000	-1.157827000	-1.388199000
		13	-0.729607000	1.158430000	-2.246491000
		13	0.729283000	-1.158599000	-2.246769000
c.13.C.1	singlet	13	-0.000165000	-0.000025000	-0.000000000
		13	1.911155000	1.157972000	1.388717000
		13	-0.729607000	1.158430000	2.246491000
		13	1.911155000	1.157972000	-1.388717000
		13	-2.361906000	1.158976000	-0.000000000
		21	-0.000018000	-2.875132000	0.000000000
		21	0.000575000	2.875040000	-0.000000000
		13	1.232213000	1.217623000	1.989809000
		13	-1.166767000	-0.027729000	2.360399000
		13	1.064605000	-2.256801000	-0.829910000
		13	-1.270887000	-2.227313000	0.636540000
		13	1.105338000	-1.547839000	1.816861000
		13	-1.232146000	-1.218088000	-1.989324000
n.13.C.1	doublet	13	1.166636000	0.028488000	-2.360226000
		13	-1.064591000	2.256863000	0.829449000
		13	-0.000005000	0.000004000	0.000016000
		13	-1.105365000	1.547660000	-1.817028000
		13	1.270949000	2.227541000	-0.635958000
		21	-2.874050000	0.053908000	0.002862000
		21	2.874063000	-0.054160000	-0.003251000
		13	-0.000000000	2.310444000	1.615055000
		13	-2.264010000	1.366638000	0.053838000
		13	-2.264010000	-1.366638000	0.053838000
		13	1.398764000	-0.000000000	2.360613000
		13	-0.000000000	-2.310444000	1.615055000
		13	-1.398764000	0.000000000	2.360613000
a.13.C.1	singlet	13	2.264010000	-1.366638000	0.053838000
		13	2.264010000	1.366638000	0.053838000
		13	-1.353403000	0.000000000	-2.141940000
		13	-0.000000000	-0.000000000	0.080084000
		13	1.353403000	-0.000000000	-2.141940000
		21	0.000000000	-2.536568000	-1.226609000
		21	0.000000000	2.536568000	-1.226609000

Isomer	Spin state	Coordinate			
c.14.C.1	doublet	13	-2.208494000	-0.620556000	1.290436000
		13	0.367996000	-1.513411000	2.193656000
		13	-0.609401000	0.966455000	2.526372000
		13	1.013675000	2.509052000	1.263839000
		13	0.367996000	-1.513411000	-2.193656000
		13	-0.609401000	0.966455000	-2.526372000
		13	-2.208494000	-0.620556000	-1.290436000
		13	2.348456000	0.229270000	-1.445159000
		13	2.348456000	0.229270000	1.445159000
		13	0.076979000	0.051689000	0.000000000
		13	2.046454000	-2.063723000	0.000000000
		13	1.013675000	2.509052000	-1.263839000
		21	-0.754019000	-2.845798000	0.000000000
		21	-1.689916000	2.146530000	0.000000000
n.14.C.1	singlet	13	0.969098000	-0.637558000	2.441914000
		13	0.195296000	1.907398000	1.673993000
		13	-1.595991000	-0.141474000	1.822940000
		13	-3.977110000	-0.334100000	0.488755000
		13	2.179523000	0.125971000	-1.860798000
		13	0.465835000	-2.082748000	-1.788192000
		13	2.259325000	-1.883527000	0.219698000
		13	-0.431407000	0.487955000	-2.536796000
		13	0.287020000	-0.053688000	-0.046135000
		13	-1.973244000	-1.241010000	-0.963402000
		13	-0.373240000	-2.510053000	0.863289000
		13	0.779230000	2.336279000	-0.944403000
		21	2.796555000	0.881402000	0.756332000
		21	-2.044000000	1.611228000	-0.366866000
a.14.C.1	doublet	13	0.979086000	0.909985000	-2.349837000
		13	0.065649000	-1.663818000	-1.911128000
		13	-1.612570000	0.514359000	-1.754872000
		13	-3.964572000	0.469500000	-0.486870000
		13	2.168365000	-0.501225000	1.838473000
		13	0.560498000	1.777355000	2.072043000
		13	2.411617000	1.798674000	0.048163000
		13	-0.488705000	-0.826037000	2.426285000
		13	0.296063000	0.046652000	0.058774000
		13	-1.944610000	1.187436000	1.093633000
		13	-0.202176000	2.634644000	-0.478575000
		13	0.711304000	-2.468672000	0.598060000
		21	2.768829000	-0.813625000	-0.920069000
		21	-2.137368000	-1.587570000	0.205597000

Isomer	Spin state	Coordinate			
		13	0.601838000	-1.353603000	-2.203560000
		13	0.870858000	1.395450000	-2.149103000
		13	2.114931000	2.182701000	0.318569000
		13	0.503641000	1.356596000	2.381900000
		13	-3.224219000	1.907567000	-0.136053000
		13	0.476517000	-0.007297000	0.064270000
		13	-1.829809000	0.219678000	1.435815000
c.15.C.1	singlet	13	-0.603804000	2.423157000	0.046659000
		13	2.506720000	-0.359086000	1.698308000
		13	0.075424000	-1.407441000	2.312581000
		13	-1.502791000	0.253292000	-1.683446000
		13	1.383640000	-2.420157000	0.191196000
		13	-3.866416000	-0.557283000	-0.355188000
		21	3.030911000	-0.069134000	-1.088875000
		21	-1.487334000	-2.180220000	-0.100901000
		13	0.583478000	-1.349433000	-2.181693000
		13	0.756304000	1.390339000	-2.159934000
		13	1.979824000	2.284840000	0.250184000
		13	0.418696000	1.392867000	2.339886000
		13	-3.355294000	1.863261000	-0.136519000
		13	0.486333000	-0.009320000	0.065804000
		13	-1.828364000	0.145791000	1.392766000
n.15.C.1	doublet	13	-0.757725000	2.410202000	0.024644000
		13	2.563739000	-0.187529000	1.696539000
		13	0.188531000	-1.407702000	2.286491000
		13	-1.571023000	0.185743000	-1.599250000
		13	1.588110000	-2.361947000	0.133099000
		13	-3.779711000	-0.704066000	-0.289378000
		21	3.023859000	0.032215000	-1.068681000
		21	-1.335653000	-2.293624000	-0.059619000
		13	-0.545722000	1.360647000	-2.162528000
		13	-0.658050000	-1.368609000	-2.180786000
		13	-1.861630000	-2.370341000	0.165718000
		13	-0.354812000	-1.416867000	2.307186000
		13	3.443195000	-1.816661000	-0.130076000
		13	-0.500218000	0.019626000	0.065362000
		13	1.821618000	-0.087856000	1.378233000
a.15.C.1	singlet	13	0.882647000	-2.413555000	0.011754000
		13	-2.612836000	0.028400000	1.708289000
		13	-0.298732000	1.411039000	2.266568000
		13	1.631982000	-0.136710000	-1.530613000
		13	-1.767340000	2.322719000	0.062910000
		13	3.743312000	0.824076000	-0.234581000
		21	-3.026608000	-0.114733000	-1.050552000
		21	1.216876000	2.370599000	-0.018815000