Supplementary Information File

The Boron-doped Scandium Clusters $B@Sc_n^{-/0/+}$ with n = 2-13: Uncovering the Smallest Endohedrally Doped Cages

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Content

Table S1. Electronic structure and HOMO-LUMO gap (eV) of the Sc_3 trimer at $^2A_1$' state computed using the PBE, B3PW91, PB86, TPSSh and M05 functionals with the def2-TZVP basis set.

Functional	**Electronic structure**	**HOMO-LUMO gap (eV)**	
		Alpha	**Beta**
PBE	$1S^2 1P^6 2S^1$	0.66	0.42
B3PW91	$1S^2 1P^6 2S^1$	2.07	1.81
BP86	$1S^2 1P^6 2S^1$	0.68	0.43
TPSSh	$1S^2 1P^6 2S^1$	1.52	1.19
M05	$1S^2 1P^6 2S^1$	2.50	1.89

n	Cation				Neutral				Anion			
	Structure	*(M) - rE*	*Structure*	*(M) - rE*	*Structure*	*(M) - rE*	*Structure*	*(M) - rE*	*Structure*	*(M) - rE*	*Structure*	*(M) - rE*
2	 **c.2.A.1**	(4) 0.00 (2) 6.17 (6) 10.15			 **n.2.A.1**	(5) 0.00 (3) 3.86 (1) 8.95			 **a.2.A.1**	(4) 0.00 (6) 3.75 (2) 6.87		
3	 **c.3.A.1**	(3) 0.00 (7) 0.85 (5) 1.02			 **n.3.A.1**	(2) 0.00 (4) 5.34 (6) 6.37			 **a.3.A.1**	(1) 0.00 (3) 5.00 (5) 5.38		
4	 **c.4.A.1**	(2) 0.00 (4) 4.71 (6) 5.79			 **n.4.A. 1**	(3) 0.00 (1) 5.76 (5) 6.22			 **a.4.A. 1**	(4) 0.00 (2) 2.40 (6) 8.25		
5	 **c.5.A.1**	(5) 0.00 (3) 1.29 (1) 3.04 (7) 3.94			 **n.5.A.1**	(6) 0.00 (4) 0.10 (2) 0.12 (8) 0.27			 **a.5.A.1**	(7) 0.00 (5) 1.35 (3) 2.38 (1) 5.74	 **a.5.A.2**	(7) 11.18 (5) 14.42
6	 **c.6.A.1**	(6) 0.00 (4) 2.81 (8) 2.95 (2) 4.53	 **c.6.A.2**	(6) 9.07 (4) 9.35	 **n.6.A.1**	(7) 0.00 (5) 0.11 (3) 1.95 (9) 2.04	 **n.6.A.2**	(5) 10.28	 **a.6.A.1**	(6) 0.00 (8) 0.02 (4) 0.91 (2) 3.03	 **a.6.A.2**	(6) 2.58 (4) 2.68
7	 **c.7.A.1**	(7) 0.00 (5) 0.96 (3) 1.29 (9) 1.65	 **c.7.A.2**	(5) 9.47	 **n.7.A.1**	(2) 0.00 (4) 1.89 (6) 2.05 (8) 2.13	 **n.7.A.2**	(4) 0.45	 **a.7.A.1**	(3) 0.00 (5) 1.04 (7) 1.98 (1)5.72	 **a.7.A.2**	(3) 11.41
8	 **c.8.A.1**	(4) 0.00 (2) 0.03 (6) 0.76 (8) 1.44	 **c.8.A.2**	(2) 8.20 (4) 8.28	 **n.8.A.1**	(5) 0.00 (3) 1.05 (7) 2.00 (1) 7.12	 **n.8.A.2**	(3) 8.90 (5) 9.76	 **a.8.A.1**	(2) 0.00 (6) 0.68 (4) 0.81 (8) 2.71		
9	 **c.9.A.1**	(3) 0.00 (5) 0.55	 **c.9.A.2**	(11) 0.81 (9) 0.88 (5) 0.88 (7) 1.45	 **n.9.A.1**	(2) 0.00 (4) 0.53 (6) 0.77	 **n.9.A.2**	(10) 0.36 (4) 1.61 (6) 1.83 (8) 1.96	 **a.9.A.1**	(3) 0.00 (7) 0.35 (5) 0.48 (9) 2.36	 **a.9.A.2**	(9) 0.96 (7) 2.41 (5) 2.53 (3) 2.98
10	 **c.10.A.1**	(8) 0.00 (10) 0.80 (6) 1.82	 **c.10.A.2**	(2) 1.94 (4) 2.26 (6) 2.64	 **n.10.A.1**	(5) 0.00 (3) 0.92 (7) 1.43	 **n.10.A.2**	(13) 0.11 (11) 0.49 (9) 2.80	**a.10.A.1**	(14) 0.00 (12) 1.68 (10) 2.40	**a.10.A.2**	(4) 0.40 (2) 0.89 (6) 1.88
11	**c.11.A.1**	(3) 0.00 (11) 0.37 (13) 0.56 (5) 1.34	**c.11.A.2**	(13) 1.13 (11) 2.98 (7) 6.42	**n.11.A.1**	(2) 0.00 (4) 0.27 (6) 0.49 (8) 1.45	**n.11.A.2**	(12) 1.95 (10) 2.69	**a.11.A.1**	(3) 0.00 (5) 0.01 (1) 2.30 (7) 3.29	**a.11.A.2**	(11) 1.90 (9) 4.17
12	**c.12.A.1**	(14) 0.00 (16) 0.34 (12) 1.45 (10) 1.47	**c.12.A.2**	(8) 1.45 (6) 0.09 (10) 4.38	**n.12.A.1**	(13) 0.00 (17) 0.36 (15) 0.51 (7) 1.21	**n.12.A.2**	(7) 2.41 (9) 2.45	**a.12.A.1**	(12) 0.00 (14) 0.29 (16) 1.82 (6) 2.77	**a.12.A.2**	(8) 2.62 (10) 0.67
13	**c.13.A.1**	(19) 0.00 (17) 4.44 (21) 10.16			**n.13.A.1**	(20) 0.00 (18) 5.33 (16) 9.48 (22) 20.80			**a.13.A.1**	(19) 0.00 (21) 4.29 (17) 4.00 (23) 23.66		

Figure S2: The Structures, Multiplicities (M, in bracket) and Relative Energies (rE, kcal.mol^{-1}) of the lowest-lying $Sc_n^{+/0/-}$ (n = 2-13) clusters calculated at the PBE/ Def2-TZVP theory method.

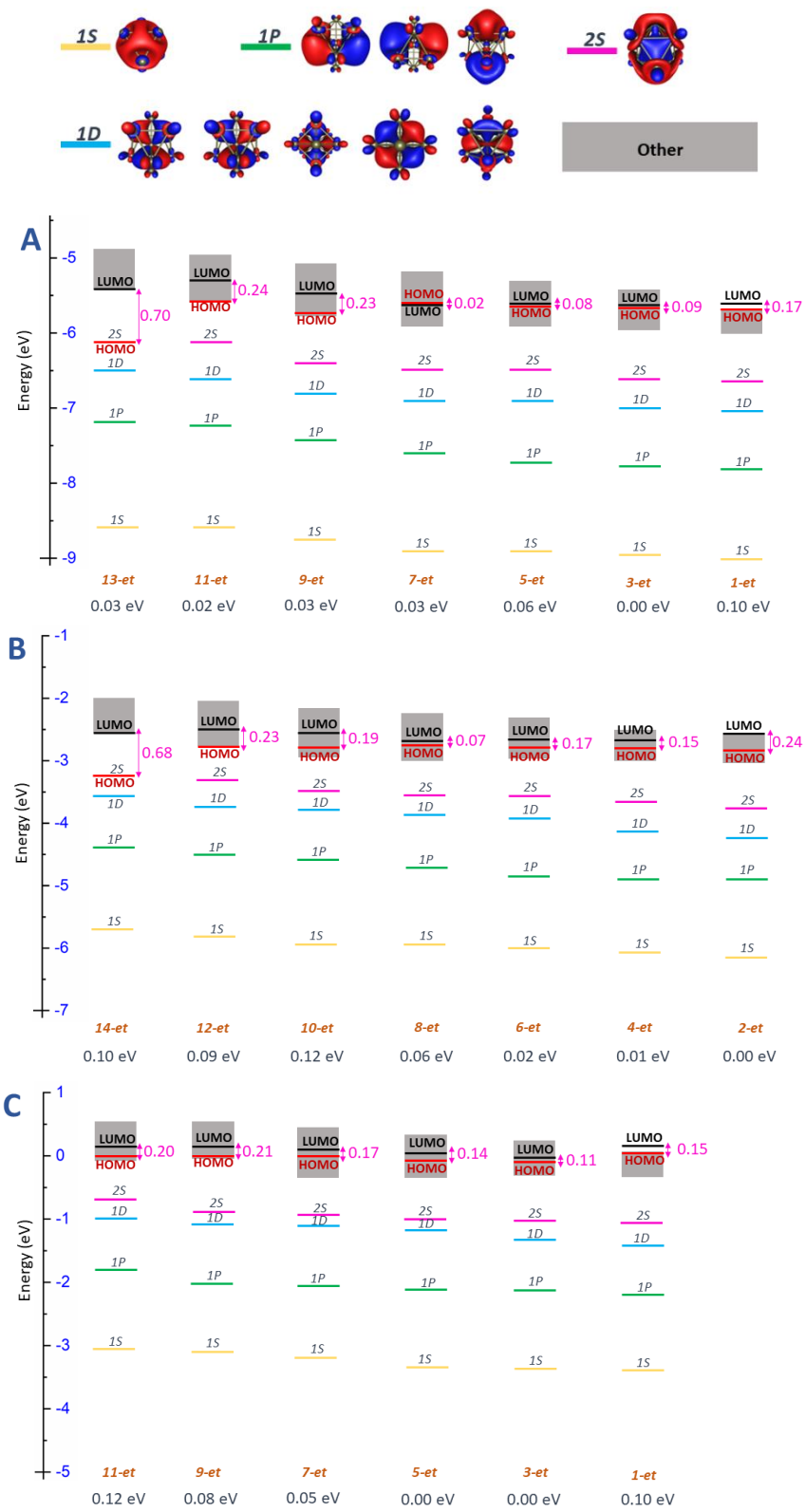

Figure S2: The molecular orbital (MO) diagram illustrates the beta side (excluding the singlet state) of the cationic (A), neutral (B), and anionic (C) Sc_{11} clusters across different spin states. This analysis was calculated using the PBE/Def2-TZVP method.

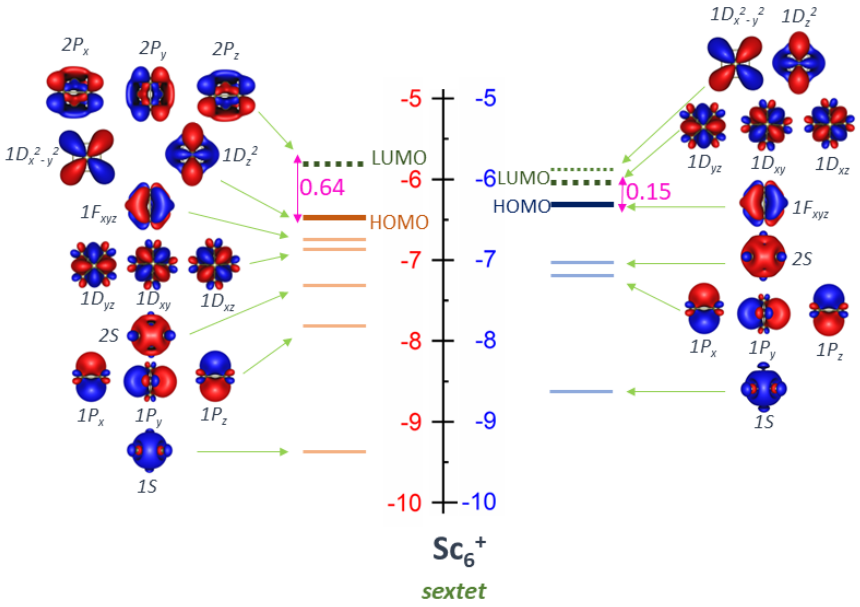

Figure S3: Molecular orbital (MO) diagram of cationic Sc_6^+ cluster at sextet spin state, using the PBE/ Def2-TZVP theory method. Left and right sides denote alpha and beta, respectively.

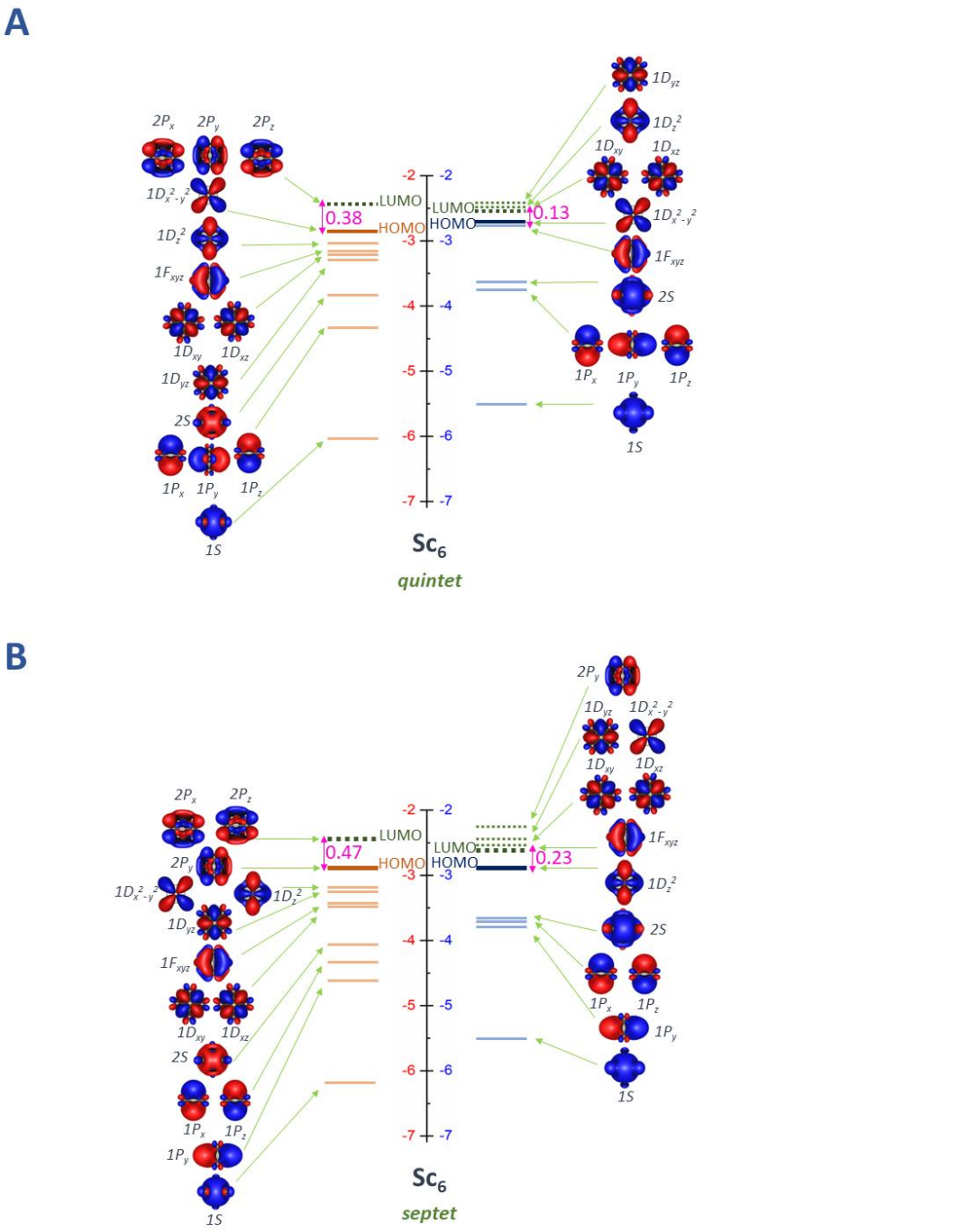

Figure S4: Molecular orbital (MO) diagram of neutral Sc_6 cluster at (A) quintet spin state and (B) septet spin state, using the PBE/ Def2-TZVP theory method. Left and right sides denote alpha and beta, respectively.

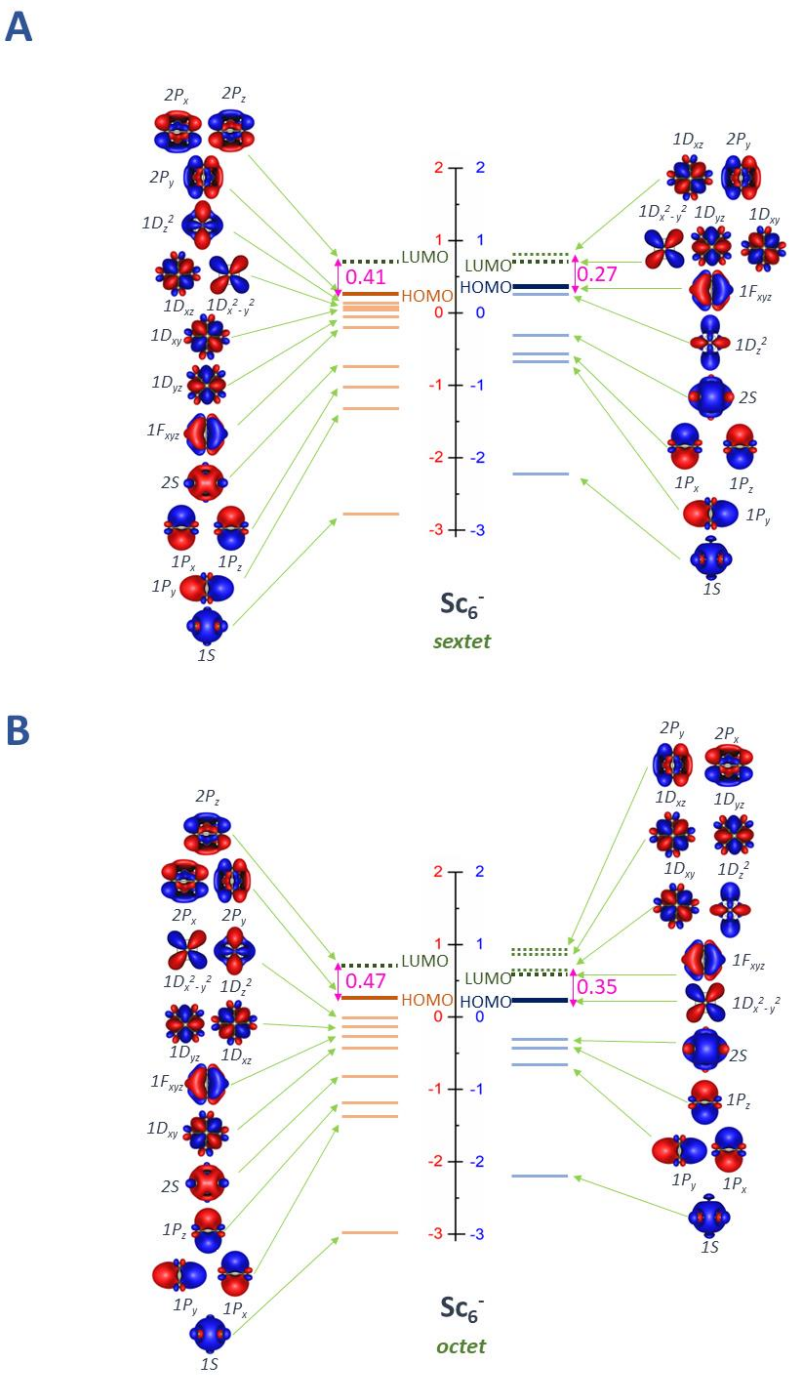

Figure S5: Molecular orbital (MO) diagram of anionic Sc_6^- cluster at (A) sextet spin state and (B) octet spin state, using the PBE/ Def2-TZVP theory method. Left and right sides denote alpha and beta, respectively.

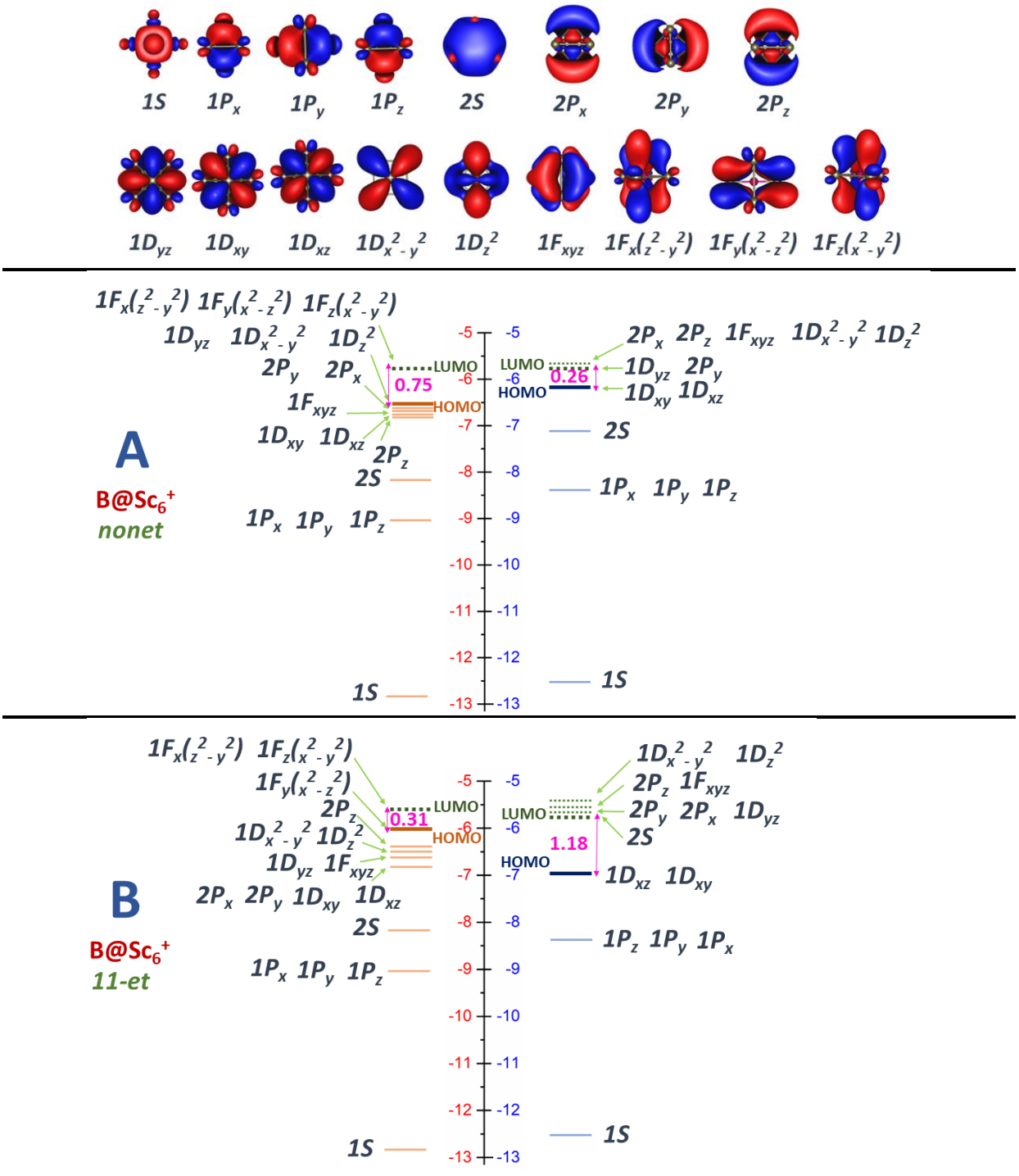

Figure S6: Molecular orbital (MO) diagram of cationic $B@Sc_6^+$ cluster at **A**: a nonet spin state and **B**: a 11-et spin state, using the PBE/ Def2-TZVP method. Left and right sides denote alpha and beta electrons, respectively.

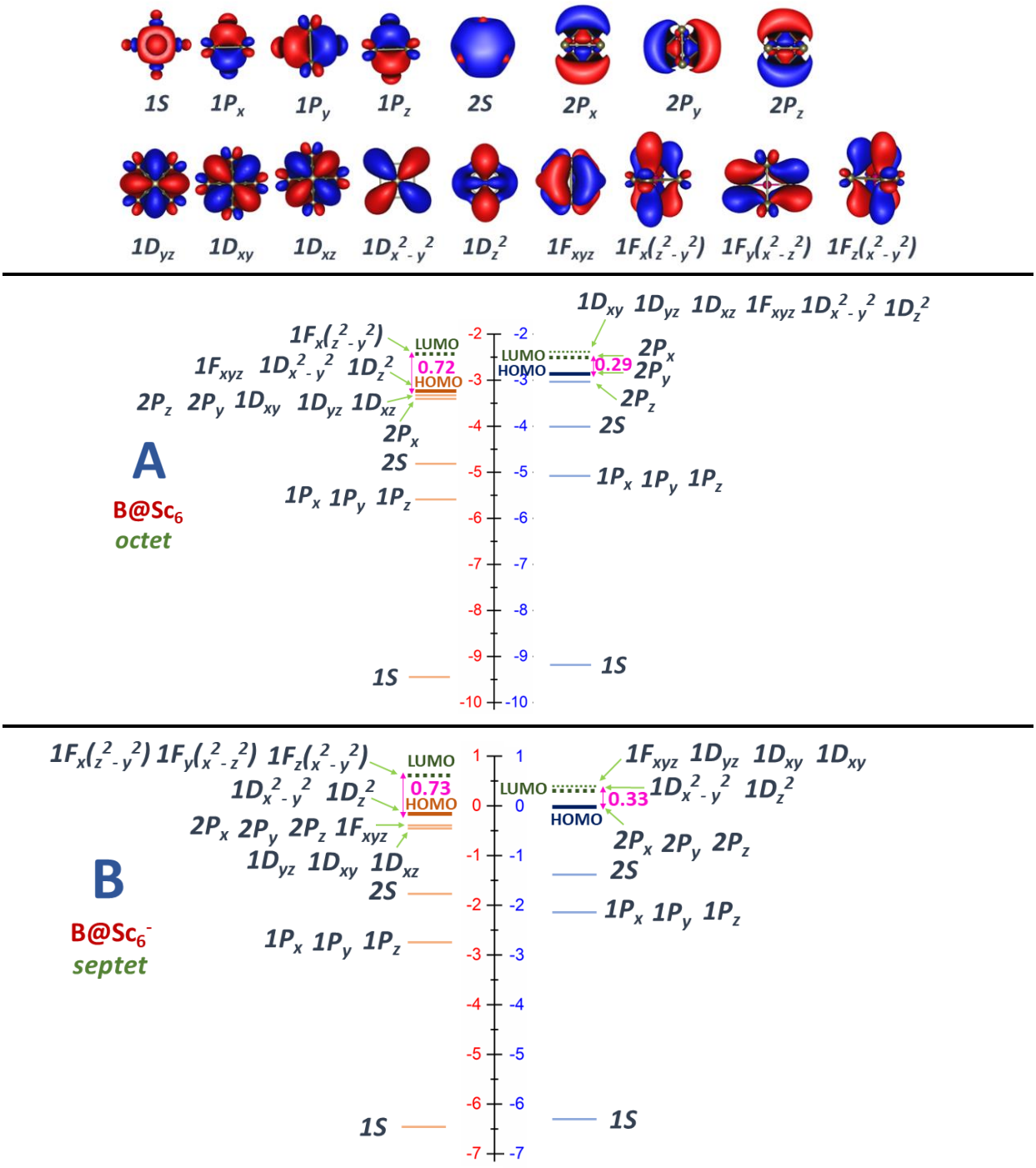

Figure S7: Molecular orbital (MO) diagram of **A**: neutral $B@Sc_6$ cluster at an octet spin state, and **B**: an anionic $B@Sc_6^+$ at septet spin state, using the PBE/ Def2-TZVP method. Left and right sides denote alpha and beta electrons, respectively.

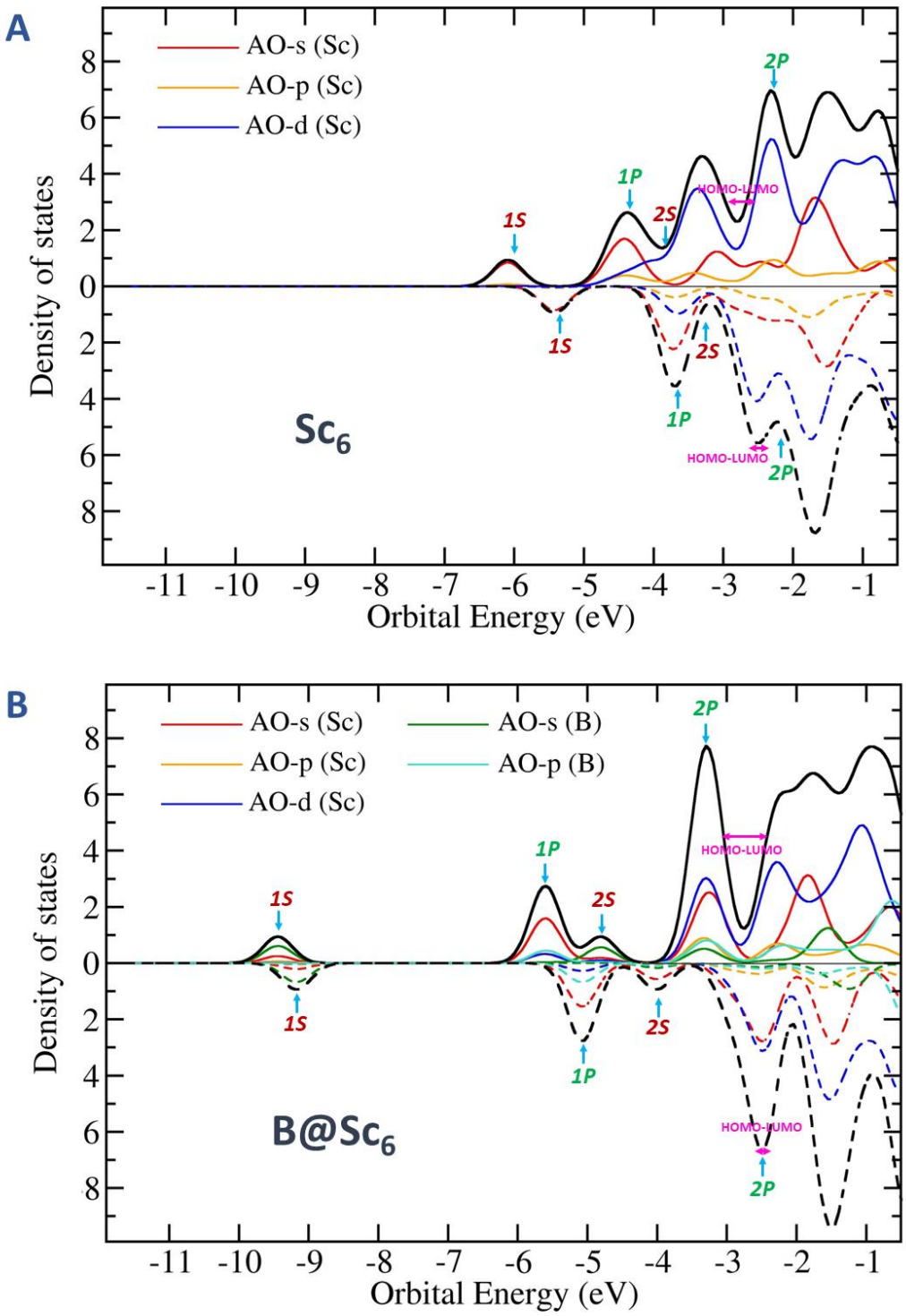

Figure S8. Calculated density of states (DOS) for the lowest-lying neutral clusters of (A) Sc_6, and (B) $B@Sc_6$. Positive and negative DOS represent spin-up and spin-down electrons, respectively.

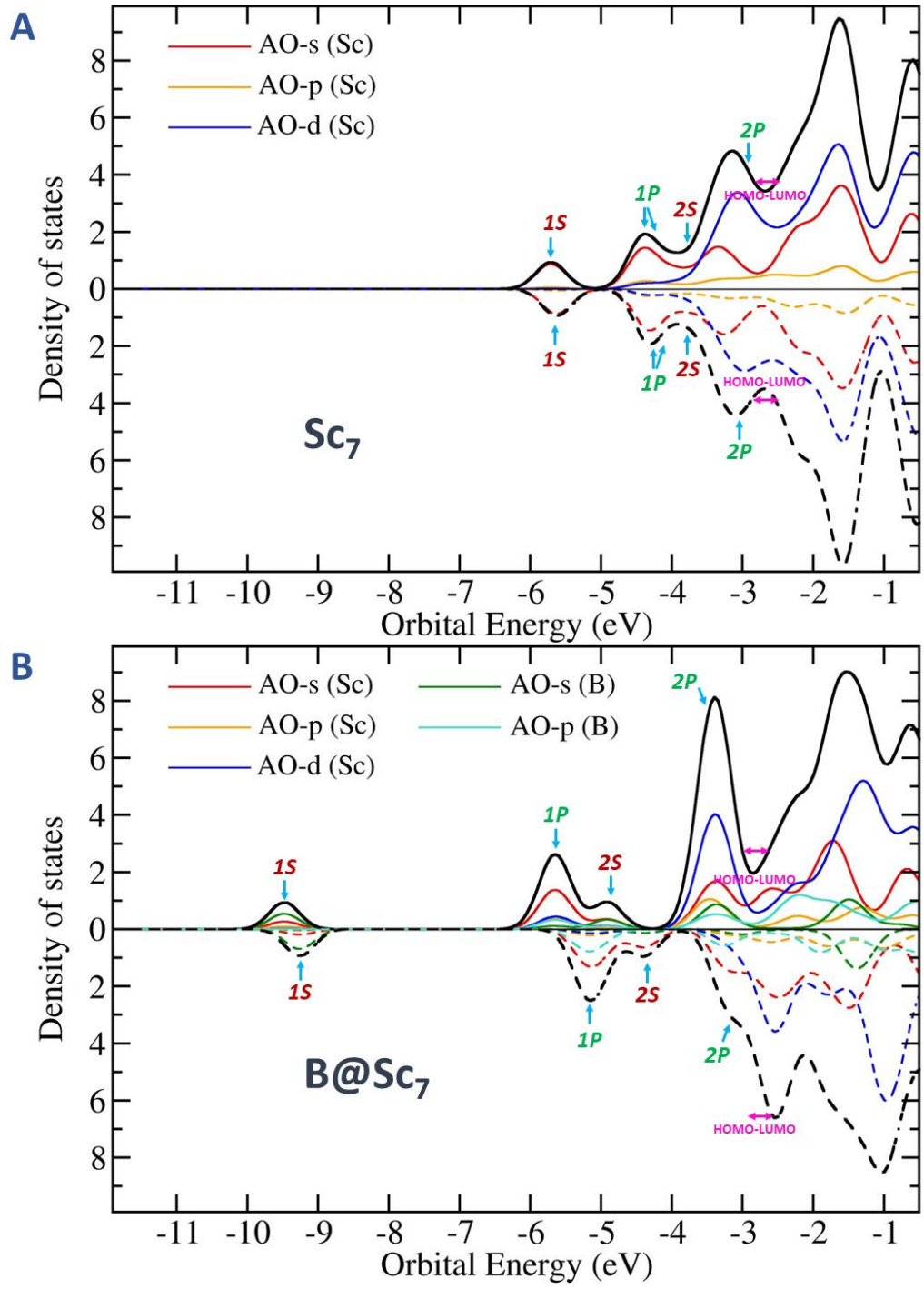

Figure S9. Calculated density of states (DOS) for the lowest-lying neutral clusters of (A) Sc_7, and (B) $B@Sc_7$. Positive and negative DOS represent spin-up and spin-down electrons, respectively.

Coordinates of the lowest-lying $Sc_n^{+/0/-}$ clusters.

Isomer	Spin state		Coordinate		
c.2.A.1	quartet	21	0.000000000	0.000000000	1.280819000
		21	0.000000000	0.000000000	-1.280819000
n.2.A.1	quintet	21	0.000000000	0.000000000	1.309529000
		21	0.000000000	0.000000000	-1.309529000
a.2.A.1	quartet	21	0.000000000	0.000000000	1.354342000
		21	0.000000000	0.000000000	-1.354342000

Isomer	Spin state		Coordinate		
c.3.A.1	triplet	21	1.410456000	0.888705000	0.000000000
		21	-1.410456000	0.674886000	0.000000000
		21	0.000000000	-1.563591000	0.000000000
n.3.A.1	doublet	21	0.000000000	1.635733000	0.000000000
		21	1.416586000	-0.817866000	0.000000000
		21	-1.416586000	-0.817866000	0.000000000
a.3.A.1	singlet	21	0.000000000	-1.386889000	-0.800785000
		21	0.000000000	0.000000000	1.601569000
		21	0.000000000	1.386889000	-0.800785000

Isomer	Spin state		Coordinate		
c.4.A.1	doublet	21	-0.057253000	-1.441045000	1.045581000
		21	-1.490573000	0.020313000	-1.001783000
		21	0.054736000	1.511107000	0.951069000
		21	1.493090000	-0.090375000	-0.994867000
n.4.A.1	triplet	21	-0.894903000	1.203244000	-0.954750000
		21	-1.203033000	-0.894969000	0.954919000
		21	1.203181000	0.894677000	0.954990000
		21	0.894756000	-1.202953000	-0.955160000
a.4.A.1	quartet	21	-1.280137000	-0.487786000	1.146058000
		21	-0.699579000	1.054650000	-1.260314000
		21	1.277846000	0.887612000	0.877168000
		21	0.701870000	-1.454475000	-0.762912000

Isomer	Spin state		Coordinate		
c.5.A.1	quintet	21	-0.075095000	-1.500133000	-0.843198000
		21	0.147886000	0.005500000	1.729327000
		21	-0.075387000	1.494754000	-0.852614000
		21	2.390101000	-0.000224000	-0.096985000
		21	-2.387506000	0.000103000	0.063470000
n.5.A.1	sextet	21	-0.000007000	0.870284000	1.507355000
		21	2.327919000	0.000051000	0.000000000
		21	-0.000007000	-1.740660000	0.000000000
		21	-0.000007000	0.870284000	-1.507355000
		21	-2.327899000	0.000041000	0.000000000
a.5.A.1	septet	21	0.000000000	1.498123000	-0.865011000
		21	0.000000000	0.000000000	1.729959000
		21	-2.388117000	0.000000000	0.000032000
		21	2.388117000	0.000000000	0.000032000
		21	0.000000000	-1.498123000	-0.865011000

Isomer	Spin state	Coordinate			
c.6.A.1	sextet	21	-0.017946000	-0.000016000	2.129820000
		21	-0.017946000	-0.000016000	-2.129820000
		21	-0.017946000	2.129866000	0.000000000
		21	2.118795000	0.000012000	0.000000000
		21	-0.017925000	-2.129783000	0.000000000
		21	-2.047031000	-0.000063000	0.000000000
n.6.A.1	septet	21	-0.000043000	-2.006274000	-0.321191000
		21	0.000058000	-0.321016000	2.005706000
		21	0.000853000	2.006239000	0.320759000
		21	-0.000624000	0.321052000	-2.006070000
		21	2.289598000	-0.000346000	0.000036000
		21	-2.289842000	0.000344000	0.000759000
a.6.A.1	octet	21	-2.213433000	0.177547000	-0.000537000
		21	-0.177675000	-2.213095000	-0.000515000
		21	2.213387000	-0.177690000	0.000363000
		21	0.000616000	0.000482000	-1.915090000
		21	0.177606000	2.213176000	0.000337000
		21	-0.000502000	-0.000419000	1.915442000

Isomer	Spin state	Coordinate			
c.7.A.1	septet	21	0.000018000	-0.001250000	1.487865000
		21	2.516477000	0.781278000	0.000000000
		21	-2.516097000	0.783307000	0.000000000
		21	1.583411000	-2.069166000	0.000000000
		21	0.000018000	2.575290000	0.000000000
		21	0.000018000	-0.001250000	-1.487865000
		21	-1.583846000	-2.068210000	0.000000000
n.7.A.1	doublet	21	-0.000025000	-0.014502000	1.392309000
		21	1.561150000	2.090945000	0.000000000
		21	-2.514819000	-0.780583000	0.000000000
		21	-0.000025000	-2.591365000	0.000000000
		21	-1.560806000	2.091232000	0.000000000
		21	-0.000025000	-0.014502000	-1.392309000
		21	2.514551000	-0.781225000	0.000000000
a.7.A.1	triplet	21	0.000112000	0.039048000	-1.415564000
		21	0.004576000	2.590815000	0.000023000
		21	1.531525000	-2.104570000	-0.000004000
		21	-1.538923000	-2.099317000	0.000000000
		21	2.515648000	0.763260000	0.000003000
		21	0.000088000	0.039006000	1.415553000
		21	-2.513026000	0.771757000	-0.000012000

Isomer	Spin state	Coordinate			
c.8.A.1	quartet	21	2.528274000	1.493759000	-0.000017000
		21	-0.685474000	2.039759000	-0.000008000
		21	0.591024000	-0.001777000	-1.672276000
		21	-2.416960000	0.013070000	-1.489378000
		21	0.591030000	-0.001757000	1.672277000
		21	-2.416953000	0.013098000	1.489384000
		21	2.519846000	-1.498394000	0.000014000
		21	-0.710787000	-2.057758000	0.000005000
n.8.A.1	quintet	21	-1.581348000	-0.616825000	0.000000000
		21	-1.496533000	2.413975000	0.000000000
		21	0.000008000	-2.514580000	1.551717000
		21	0.000008000	0.717449000	2.063203000
		21	0.000008000	-2.514580000	-1.551717000
		21	0.000008000	0.717449000	-2.063203000
		21	1.581317000	-0.616783000	0.000000000
		21	1.496533000	2.413895000	0.000000000
a.8.A.1	doublet	21	2.496787000	1.566063000	0.000050000
		21	0.568339000	0.000184000	-1.589558000
		21	0.568690000	-0.000181000	1.589680000
		21	-0.660414000	-2.106979000	-0.000028000
		21	-0.660350000	2.106985000	0.000181000
		21	-2.405049000	0.000216000	-1.492402000
		21	-2.404690000	-0.000162000	1.492479000
		21	2.496686000	-1.566128000	-0.000401000

Isomer	Spin state	Coordinate			
c.9.A.1	triplet	21	1.515035000	-2.705705000	-0.575512000
		21	0.752084000	0.001558000	-1.284881000
		21	2.559737000	0.003841000	0.901869000
		21	-0.143022000	-1.472674000	1.394796000
		21	-1.621305000	-1.661374000	-1.157780000
		21	-2.794387000	-0.004762000	1.058579000
		21	-1.626768000	1.656783000	-1.157010000
		21	-0.147593000	1.471512000	1.394977000
		21	1.506220000	2.710822000	-0.575037000
n.9.A.1	doublet	21	-0.184509000	-1.459243000	1.376172000
		21	-1.633581000	1.617014000	-1.193074000
		21	1.583581000	2.664874000	-0.573533000
		21	0.742232000	-0.000142000	-1.251427000
		21	1.582261000	-2.665565000	-0.573625000
		21	-1.634216000	-1.616320000	-1.192972000
		21	-2.817752000	0.000641000	1.085261000
		21	-0.183857000	1.459271000	1.376132000
		21	2.545841000	-0.000530000	0.947065000
a.9.A.1	triplet	21	2.424736000	0.828098000	0.963863000
		21	-1.982163000	1.076217000	-1.216597000
		21	0.764614000	0.198144000	-1.272680000
		21	2.319109000	-2.122910000	-0.511488000
		21	0.296128000	-1.389434000	1.367280000
		21	-0.683533000	1.352942000	1.403406000
		21	0.594237000	2.988988000	-0.614526000
		21	-2.713284000	-0.866233000	1.057825000
		21	-1.019842000	-2.065813000	-1.177083000

Isomer	Spin state	Coordinate			
c.10.A.1	octet	21	-0.940898000	-2.236776000	-1.078973000
		21	-2.935491000	-0.006788000	-0.001649000
		21	-0.952974000	2.231691000	1.078478000
		21	1.673938000	0.742368000	2.116749000
		21	1.671797000	2.120493000	-0.737203000
		21	-0.945491000	-1.081171000	2.233620000
		21	1.680296000	-0.733982000	-2.115114000
		21	1.681866000	-2.112336000	0.738631000
		21	-0.948990000	1.076652000	-2.234453000
		21	0.015948000	-0.000151000	-0.000086000
n.10.A.1	quintet	21	-3.389667000	0.000012000	0.591587000
		21	-1.838716000	1.623001000	-1.413497000
		21	-1.838883000	-1.622812000	-1.413680000
		21	-0.862528000	-1.504509000	1.392145000
		21	1.536467000	-2.500009000	-0.208099000
		21	1.816459000	0.000005000	1.666747000
		21	3.411057000	-0.000009000	-0.786129000
		21	1.536411000	2.500004000	-0.208107000
		21	-0.862442000	1.504322000	1.392293000
		21	0.491843000	-0.000004000	-1.013259000
a.10.A.1	14-et	21	-0.076133000	2.894901000	-0.171740000
		21	2.616799000	1.603741000	-1.122779000
		21	-2.697444000	1.464028000	-1.122779000
		21	-1.593428000	0.865020000	1.589578000
		21	-2.468939000	-1.513433000	-0.171495000
		21	0.047702000	-1.812301000	1.589616000
		21	0.080645000	-3.068027000	-1.122784000
		21	2.545064000	-1.381566000	-0.171498000
		21	1.545707000	0.947581000	1.589602000
		21	0.000027000	0.000055000	-0.885722000

Isomer	Spin state	Coordinate			
		21	-0.373102000	-0.014519000	-0.000128000
		21	-1.364468000	1.803081000	-1.715520000
		21	1.397979000	-2.181426000	-0.000124000
		21	1.402575000	2.169584000	0.000270000
		21	-1.389194000	-1.796198000	-1.725720000
c.11.A.1	triplet	21	1.400074000	0.005274000	-2.174251000
		21	-3.292289000	0.013648000	-0.000248000
		21	-1.364766000	1.802240000	1.715837000
		21	3.572511000	-0.010754000	0.000016000
		21	-1.389343000	-1.795780000	1.725600000
		21	1.400022000	0.004851000	2.174267000
		21	-1.378955000	-1.772319000	1.727219000
		21	1.395131000	-2.175679000	-0.001346000
		21	3.560977000	0.002624000	-0.000136000
		21	1.413146000	2.187182000	0.001335000
		21	1.404658000	-0.006292000	-2.176376000
n.11.A.1	doublet	21	-3.243785000	-0.009133000	0.000180000
		21	-1.399434000	1.768494000	1.727668000
		21	1.404843000	-0.009083000	2.176197000
		21	-1.379367000	-1.770176000	-1.729286000
		21	-1.399719000	1.770658000	-1.725403000
		21	-0.377495000	0.013722000	-0.000053000
		21	-3.540724000	-0.006209000	0.000056000
		21	-1.389931000	0.003979000	-2.191213000
		21	-1.378950000	-2.222356000	0.000024000
		21	-1.372934000	2.206633000	0.000074000
		21	-1.389846000	0.003920000	2.191175000
a.11.A.1	triplet	21	1.343955000	1.903676000	1.642776000
		21	1.371360000	-1.898783000	1.622348000
		21	3.251378000	0.015063000	-0.000237000
		21	1.371174000	-1.899265000	-1.622303000
		21	1.343795000	1.904343000	-1.642557000
		21	0.390723000	-0.011002000	-0.000142000

Isomer	Spin state	Coordinate			
		21	2.402262000	-1.297230000	-1.525029000
		21	0.488648000	2.667836000	1.029666000
		21	-1.180841000	2.460989000	-1.525816000
		21	-2.385957000	1.289381000	1.030124000
		21	-0.491802000	-2.684779000	-1.525905000
		21	-0.000051000	0.000095000	2.704633000
c.12.A.1	14-et	21	1.172319000	-2.445584000	1.029880000
		21	-2.706229000	-0.362082000	-1.524866000
		21	-1.963067000	-1.871226000	1.030022000
		21	2.687999000	0.359599000	1.030318000
		21	1.976778000	1.882812000	-1.525378000
		21	-0.000059000	0.000190000	-0.227649000
		21	1.272639000	-2.436068000	-1.515501000
		21	0.005036000	0.010475000	2.698981000
		21	-0.397577000	-2.650191000	1.038074000
		21	2.408031000	-1.206759000	1.027431000
		21	1.896301000	1.928625000	1.020066000
		21	2.694422000	0.457834000	-1.517808000
n.12.A.1	13-et	21	0.404151000	2.693875000	-1.523564000
		21	-1.251253000	2.393866000	1.022351000
		21	-2.451708000	1.227375000	-1.514223000
		21	-1.928457000	-1.961847000	-1.518061000
		21	-2.648234000	-0.450865000	1.033456000
		21	-0.003350000	-0.006320000	-0.251201000
		21	-1.029703000	-0.829062000	2.551214000
		21	-1.029549000	2.170280000	-1.576823000
		21	1.515049000	2.758782000	0.000000000
		21	1.514909000	0.852496000	2.623817000
		21	-1.029549000	2.170280000	1.576823000
		21	1.514909000	0.852496000	-2.623817000
a.12.A.1	12-et	21	1.514909000	-2.231978000	1.621526000
		21	1.514909000	-2.231978000	-1.621526000
		21	-1.029703000	-0.829062000	-2.551214000
		21	0.272575000	0.000108000	0.000000000
		21	-1.029768000	-2.682518000	0.000000000
		21	-2.698987000	0.000155000	0.000000000

Isomer	Spin state	Coordinate			
		21	1.871993000	-0.040463000	-2.387092000
		21	1.542510000	2.533698000	-0.592352000
		21	2.946655000	-0.074110000	0.557131000
		21	1.416050000	-2.605131000	-0.603831000
		21	-0.002049000	0.000128000	-0.054649000
		21	-1.007146000	-1.611074000	-2.366858000
c.13.A.1	19-et	21	0.904593000	-1.626999000	2.381823000
		21	-1.826123000	0.039946000	2.407473000
		21	-2.973215000	0.074794000	-0.560114000
		21	-1.403185000	2.582393000	0.601350000
		21	0.984017000	1.570505000	2.388131000
		21	-1.528947000	-2.512454000	0.590218000
		21	-0.925153000	1.668767000	-2.361231000
		21	1.438503000	-2.433381000	-1.035241000
		21	1.262555000	-1.795633000	2.060055000
		21	-1.336479000	-2.655976000	0.471240000
		21	-1.199459000	-1.349735000	-2.408535000
		21	0.000081000	-0.000002000	0.000143000
		21	1.484145000	0.317818000	-2.599592000
n.13.A.1	20-et	21	-3.005902000	-0.042311000	-0.162167000
		21	-1.438551000	2.433396000	1.035154000
		21	1.336448000	2.655987000	-0.471309000
		21	1.199465000	1.349803000	2.408583000
		21	-1.484215000	-0.317822000	2.599595000
		21	-1.262536000	1.795543000	-2.060041000
		21	3.005944000	0.042312000	0.162117000
		21	-1.587558862	2.555177126	0.000000000
		21	-2.559630523	0.000000000	1.569746322
		21	0.000000000	-1.589153903	2.566961464
		21	0.000000000	1.589153903	-2.566961464
		21	1.587558862	-2.555177126	0.000000000
		21	0.000000000	1.589153903	2.566961464
a.13.A.1	19-et	21	2.559630523	0.000000000	1.569746322
		21	1.587558862	2.555177126	0.000000000
		21	2.559630523	0.000000000	-1.569746322
		21	-2.559630523	0.000000000	-1.569746322
		21	-1.587558862	-2.555177126	0.000000000
		21	0.000000000	-1.589153903	-2.566961464
		21	0.000000000	0.000000000	0.000000000

Coordinates of the lowest-lying $Sc_{n-1}B^{+/0/-}$ clusters.

Isomer	Spin state		Coordinate		
c.1.B.1	quartet	21	0.000000000	0.000000000	0.405933000
		5	0.000000000	0.000000000	-1.704920000
n.1.B.1	quintet	21	0.000000000	0.000000000	0.403846000
		5	0.000000000	0.000000000	-1.696154000
a.1.B.1	quartet	21	0.000000000	0.000000000	0.417786000
		5	0.000000000	0.000000000	-1.754701000

Isomer	Spin state		Coordinate		
c.2.B.1	singlet	21	0.000000000	0.000000000	2.002332000
		21	0.000000000	0.000000000	-2.002332000
		5	0.000000000	0.000000000	0.000000000
n.2.B.1	doublet	21	0.000000000	1.375316000	0.000000000
		21	-0.330463000	-1.335026000	0.000000000
		5	1.387943000	-0.169220000	0.000000000
a.2.B.1	singlet	21	-1.436770000	-0.159603000	0.000000000
		21	1.436770000	-0.159603000	0.000000000
		5	0.000000000	1.340664000	0.000000000

Isomer	Spin state		Coordinate		
c.3.B.1	doublet	21	-1.568768000	-0.832588000	0.091938000
		21	-0.000628000	1.687595000	0.075548000
		21	1.569374000	-0.831590000	0.091947000
		5	0.000088000	-0.098349000	-1.089616000
n.3.B.1	triplet	21	-1.154549000	1.261025000	-0.095068000
		21	-0.514851000	-1.630341000	-0.095068000
		21	1.669394000	0.369315000	-0.095073000
		5	0.000024000	0.000004000	1.197877000
a.3.B.1	quartet	21	0.000000000	1.693674000	-0.099691000
		21	-1.466765000	-0.846837000	-0.099691000
		21	1.466765000	-0.846837000	-0.099691000
		5	0.000000000	0.000000000	1.256102000

Isomer	Spin state		Coordinate		
c.4.B.1	quintet	21	-0.594201000	2.187054000	0.000000000
		21	-0.594201000	-0.348185000	1.573249000
		21	1.617627000	-1.587355000	0.000000000
		21	-0.594201000	-0.348185000	-1.573249000
		5	0.692901000	0.406017000	0.000000000
n.4.B.1	sextet	21	-0.000067000	1.496838000	-0.706904000
		21	2.192014000	-0.000118000	0.597182000
		21	-2.192004000	-0.000222000	0.597168000
		21	0.000084000	-1.496541000	-0.707155000
		5	-0.000116000	0.000177000	0.922778000
a.4.B.1	quintet	21	0.588825045	-2.210078157	0.000000000
		21	0.588825045	0.319339023	1.501812108
		21	-1.573431115	1.674884120	0.000000000
		21	0.588825045	0.319339023	-1.501812108
		5	-0.810783060	-0.434631031	0.000000000

Isomer	Spin state	Coordinate			
c.5.B.1	octet	21	-1.695179000	-1.423486000	-0.451309000
		21	-1.540827000	1.552168000	-0.282387000
		21	1.695100000	-1.423565000	-0.451360000
		21	1.540937000	1.552066000	-0.282301000
		21	-0.000030000	-0.251659000	1.639107000
		5	-0.000004000	-0.023206000	-0.721347000
n.5.B.1	singlet	21	2.056130000	-0.373037000	0.000000000
		21	0.000000000	-0.373022000	2.056131000
		21	-2.056130000	-0.373028000	0.000000000
		21	0.000000000	-0.373022000	-2.056131000
		21	0.000000000	1.802414000	0.000000000
		5	-0.000002000	-1.303279000	0.000000000
a.5.B.1	octet	21	1.616509000	1.496268000	0.375491000
		21	-1.617367000	1.495552000	0.375307000
		21	-1.616533000	-1.496211000	0.375155000
		21	1.616982000	-1.495718000	0.375521000
		21	0.000433000	0.000092000	-1.660735000
		5	-0.000103000	0.000074000	0.668896000

Isomer	Spin state	Coordinate			
c.6.B.1	nonet	21	1.332383000	-0.430791000	-1.694224000
		21	1.330788000	-1.251408000	1.222179000
		21	-1.325301000	1.279866000	-1.249493000
		21	1.329365000	1.684446000	0.474487000
		21	-1.324058000	-1.722766000	-0.485254000
		21	-1.326704000	0.440753000	1.732363000
		5	-0.069189000	-0.000420000	-0.000243000
n.6.B.1	octet	21	-0.000005000	0.056264000	2.202944000
		21	-1.467466000	1.623413000	0.000000000
		21	1.485321000	-1.669130000	0.000000000
		21	1.466782000	1.624032000	0.000000000
		21	-1.484625000	-1.669761000	0.000000000
		21	-0.000005000	0.056264000	-2.202944000
		5	-0.000005000	-0.088549000	0.000000000
a.6.B.1	septet	21	1.266439000	1.807870000	-0.094884000
		21	1.280353000	-0.801352000	1.612389000
		21	1.294553000	-0.976035000	-1.501111000
		21	-1.295702000	1.078329000	1.428398000
		21	-1.267148000	-1.796433000	0.220714000
		21	-1.278533000	0.687637000	-1.665550000
		5	0.000158000	-0.000064000	0.000189000

Isomer	Spin state		Coordinate		
c.7.B.1	octet	21	0.379907000	2.367838000	-0.000057000
		21	-0.000866000	0.000204000	-2.174364000
		21	-1.699166000	-1.692631000	0.000263000
		21	0.000508000	-0.000275000	2.174277000
		21	1.084721000	-2.138943000	-0.000482000
		21	2.369685000	0.370651000	-0.000270000
		21	-2.134830000	1.093196000	0.000634000
		5	0.000172000	-0.000167000	-0.000007000
n.7.B.1	septet	21	-0.053574000	-0.000309000	2.173796000
		21	-1.941919000	1.369181000	0.000052000
		21	-1.919679000	-1.398846000	-0.000028000
		21	-0.053605000	-0.000203000	-2.173814000
		21	0.779941000	-2.250631000	-0.000023000
		21	0.744386000	2.261999000	0.000030000
		21	2.414633000	0.018641000	-0.000011000
		5	0.125230000	0.000705000	-0.000010000
a.7.B.1	octet	21	-2.049346000	1.229534000	0.000004000
		21	-1.862038000	-1.491997000	0.000131000
		21	0.832162000	-2.214723000	0.000109000
		21	0.101971000	-0.004378000	-2.194100000
		21	2.386632000	0.175253000	-0.000118000
		21	0.505313000	2.309892000	-0.000141000
		21	0.102205000	-0.004023000	2.194105000
		5	-0.070974000	0.001856000	0.000040000

Isomer	Spin state		Coordinate		
c.8.B.1	triplet	21	-1.505645000	-1.604669000	-1.193381000
		21	1.505864000	-1.604751000	-1.193197000
		21	1.501422000	1.603913000	-1.192520000
		21	2.582965000	-0.019447000	0.999123000
		21	-1.501209000	1.603806000	-1.192727000
		21	-0.000124000	1.570147000	1.428107000
		21	-0.000131000	-1.530441000	1.442267000
		21	-2.583180000	-0.019433000	0.998920000
		5	0.000158000	0.003673000	-0.405683000
n.8.B.1	doublet	21	-2.086245000	0.666459000	0.000000000
		21	-0.000005000	2.195777000	1.519259000
		21	1.436120000	-2.184237000	0.000000000
		21	-1.436092000	-2.184265000	0.000000000
		21	-0.000005000	2.195777000	-1.519259000
		21	-0.000005000	-0.654299000	-2.227716000
		21	-0.000005000	-0.654299000	2.227716000
		21	2.086239000	0.666473000	0.000000000
		5	0.000000000	-0.199019000	0.000000000
a.8.B.1	triplet	21	-2.147441000	-0.086657000	1.479189000
		21	0.672051000	-0.006876000	-2.178326000
		21	2.045300000	1.576192000	0.000813000
		21	0.672530000	-0.009560000	2.178235000
		21	-0.556055000	-2.200927000	-0.001316000
		21	-2.147909000	-0.084972000	-1.478845000
		21	2.256623000	-1.365808000	-0.001029000
		21	-0.791061000	2.178155000	0.001278000
		5	-0.016965000	0.001903000	0.000008000

Isomer	Spin state	Coordinate			
c.9.B.1	doublet	21	-0.001064000	-1.759164000	-1.558603000
		21	-2.562464000	-1.421405000	-0.017611000
		21	-1.528424000	0.889771000	-1.595000000
		21	1.529456000	0.888004000	-1.595092000
		21	0.001753000	2.889722000	0.023959000
		21	2.560729000	-1.424376000	-0.017645000
		21	1.530486000	0.857951000	1.603153000
		21	-1.529448000	0.859768000	1.603085000
		21	-0.001048000	-1.788996000	1.553564000
		5	0.000106000	0.036646000	0.000796000
n.9.B.1	triplet	21	1.590123000	2.626289000	0.000000000
		21	-0.807676000	1.537555000	1.496177000
		21	1.750742000	-0.022736000	1.504189000
		21	1.750742000	-0.022736000	-1.504189000
		21	-0.807676000	1.537555000	-1.496177000
		21	-0.807676000	-1.305411000	-2.258427000
		21	0.692413000	-2.466290000	0.000000000
		21	-0.807676000	-1.305411000	2.258427000
		21	-2.515813000	-0.517775000	0.000000000
		5	-0.157503000	-0.256366000	0.000000000
a.9.B.1	quartet	21	0.881103000	-0.052292000	-2.105217000
		21	0.881096000	0.052601000	2.105210000
		21	-1.633407000	1.526246000	1.452181000
		21	-1.632465000	-1.452457000	1.526589000
		21	-1.632454000	-1.526712000	-1.452358000
		21	0.881234000	-2.105566000	0.052463000
		21	3.100002000	0.000684000	-0.000015000
		21	0.880734000	2.105521000	-0.052454000
		21	-1.633407000	1.451995000	-1.526399000
		5	-0.388233000	-0.000084000	0.000001000

Isomer	Spin state	Coordinate			
		21	-1.281929000	1.489121000	1.487616000
		21	-1.281938000	1.487626000	-1.489114000
		21	1.281925000	-0.001021000	-2.104894000
		21	-1.281940000	-1.489098000	-1.487638000
		21	3.491863000	0.000024000	-0.000012000
c.10.B.1	septet	21	-1.281929000	-1.487628000	1.489110000
		21	1.281931000	0.000994000	2.104899000
		21	1.281944000	-2.104934000	0.001013000
		21	1.281940000	2.104920000	-0.000999000
		21	-3.491880000	0.000000000	0.000017000
		5	0.000054000	-0.000014000	0.000004000
		21	1.279337000	1.482069000	1.455573000
		21	3.523437000	-0.000127000	0.021985000
		21	-1.302741000	0.001460000	-2.098241000
		21	-1.259698000	-2.081919000	0.012029000
		21	-1.326422000	-0.001411000	2.101397000
n.10.B.1	doublet	21	1.279316000	-1.484182000	1.453482000
		21	-3.520770000	0.000007000	-0.025349000
		21	-1.259697000	2.081831000	0.014954000
		21	1.295094000	-1.490654000	-1.468320000
		21	1.295164000	1.492937000	-1.466134000
		5	-0.012688000	-0.000041000	-0.005778000
		21	-1.275265000	-1.519548000	1.438629000
		21	-3.534487000	0.000035000	-0.000005000
		21	-1.275243000	1.519548000	-1.438603000
		21	-1.275276000	-1.438622000	-1.519539000
		21	1.275256000	0.057113000	-2.091676000
a.10.B.1	quintet	21	1.275234000	-2.091711000	-0.057138000
		21	-1.275239000	1.438616000	1.519552000
		21	1.275274000	-0.057141000	2.091663000
		21	1.275251000	2.091698000	0.057113000
		21	3.534524000	0.000014000	0.000005000
		5	-0.000125000	-0.000004000	-0.000003000

Isomer	Spin state	Coordinate			
c.11.B.1	sextet	21	1.497614000	-0.351821000	2.073920000
		21	-0.162913000	2.112840000	1.490569000
		21	-1.422621000	-0.530377000	1.609954000
		21	-3.312117000	-1.893422000	-0.003359000
		21	0.399635000	-2.236058000	0.006683000
		21	-2.890823000	1.447900000	0.006798000
		21	-1.418964000	-0.526078000	-1.613131000
		21	3.457700000	-1.357678000	0.009327000
		21	2.434588000	1.540328000	-0.006436000
		21	-0.160657000	2.110297000	-1.498723000
		21	1.500296000	-0.370994000	-2.074928000
		5	0.328700000	0.231265000	-0.002835000
n.11.B.1	triplet	21	-1.501870000	-0.354248000	2.082680000
		21	-1.497629000	-0.358536000	-2.080960000
		21	0.179535000	2.104566000	-1.454542000
		21	1.399102000	-0.551457000	-1.602387000
		21	0.169284000	2.112852000	1.442318000
		21	3.363602000	-1.843155000	0.001309000
		21	-0.452205000	-2.235040000	0.006446000
		21	2.920541000	1.386818000	0.000594000
		21	1.392687000	-0.534674000	1.612045000
		21	-3.475730000	-1.329342000	-0.003890000
		21	-2.416091000	1.553529000	-0.003490000
		5	-0.341158000	0.204486000	-0.000519000
a.11.B.1	quartet	21	-1.423125000	-0.507235000	1.676808000
		21	-1.423129000	-0.507231000	-1.676809000
		21	-0.111692000	2.121533000	-1.505220000
		21	1.495614000	-0.367101000	-2.055988000
		21	-0.111694000	2.121528000	1.505226000
		21	3.429735000	-1.413485000	0.000006000
		21	0.341699000	-2.231877000	-0.000005000
		21	2.452412000	1.516138000	-0.000005000
		21	1.495615000	-0.367099000	2.055985000
		21	-3.330825000	-1.767629000	0.000002000
		21	-2.883492000	1.346698000	0.000001000
		5	0.289308000	0.234187000	-0.000002000

Isomer	Spin state	Coordinate			
		21	-3.989552000	-0.274172000	-0.039838000
		21	-1.334410000	-0.253887000	-1.525369000
		21	-2.316435000	2.284651000	0.012308000
		21	-1.359064000	-0.268549000	1.487447000
		21	-2.467635000	-2.677647000	0.030490000
		21	0.618650000	-2.145693000	-0.049756000
c.12.B.1	triplet	21	1.702331000	-0.475738000	2.106776000
		21	1.751972000	-0.375154000	-2.116959000
		21	3.614690000	-1.614161000	-0.005218000
		21	0.385406000	2.195504000	1.478735000
		21	2.842755000	1.315444000	0.034467000
		21	0.399874000	2.224461000	-1.413532000
		5	0.635967000	0.272752000	0.001894000
		21	3.974150000	-0.193743000	0.000595000
		21	2.309986000	2.289225000	-0.000023000
		21	2.551041000	-2.646297000	-0.000223000
		21	1.329356000	-0.267765000	-1.505639000
		21	1.328821000	-0.267126000	1.505900000
		21	-1.734539000	-0.429367000	-2.090136000
n.12.B.1	doublet	21	-3.595432000	-1.632389000	0.000279000
		21	-0.409929000	2.189124000	1.436034000
		21	-2.876237000	1.336028000	-0.000688000
		21	-0.409396000	2.188284000	-1.437155000
		21	-1.735115000	-0.427936000	2.090325000
		21	-0.574517000	-2.195294000	0.000731000
		5	-0.664394000	0.240474000	-0.000003000
		21	2.751255000	-1.249512000	-1.340262000
		21	2.751529000	1.785248000	-0.411923000
		21	2.751061000	-0.535558000	1.751996000
		21	0.538619000	0.561781000	-1.836170000
		21	-0.727085000	2.852529000	-0.658503000
		21	-0.726397000	-1.995995000	-2.141061000
a.12.B.1	triplet	21	-2.483390000	0.518123000	-1.694688000
		21	-2.482449000	-1.727686000	0.398783000
		21	-2.482606000	1.208494000	1.296603000
		21	-0.725996000	-0.856058000	2.799326000
		21	0.538789000	-1.871319000	0.431652000
		21	0.538319000	1.310006000	1.404284000
		5	-1.014924000	-0.000218000	-0.000150000