Supplementary Information (SI)

Endohedral Boron-doped Scandium Clusters $B_mSc_{n-m}^{+/0}$ (m = 2 – 3, n = 3-13): Triangular - Linear Rearrangement of the B_3 Dopant

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Content

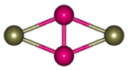
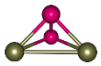
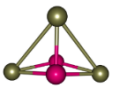
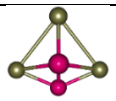
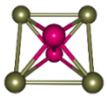
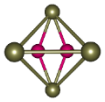
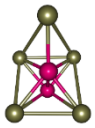
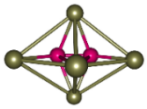
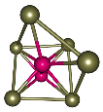
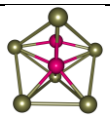
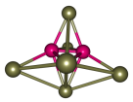
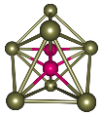
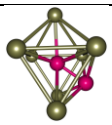
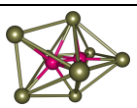
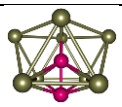
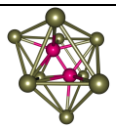
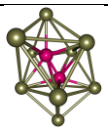
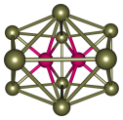
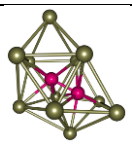
Isomer	*(M) - rE*	*Isomer*	*(M) - rE*	*Isomer*	*(M) - rE*
 **c.1.C.1**	(3) 0.0	 **c.1.C.2**	(1) 1.4 (3) 14.8		
 **c.2.C.1.**	(2) 0.0 (4) 20.3	 **c.2.C.2**	(2) 5.8 (4) 20.8		
 **c.3.C.1**	(1) 0.0 (3) 3.2	 **c.3.C.2**	(5) 13.1	 **c.3.C.3**	(1) 17.8
 **c.4.C.1**	(2) 0.0 (4) 3.7 (6) 9.9	 **c.4.C.2**	(2) 3.5 (4) 6.9		
 **c.5.C.1**	(1) 0.0 (3) 2.3	 **c.5.C.2**	(3) 1.2 (5) 2.1	 **c.5.C.3**	(5) 5.3 (3) 5.5
 **c.6.C.1**	(2) 0.0 (4) 1.6 (6) 3.2	 **c.6.C.2**	(2) 2.5	 **c.6.C.3**	(4) 3.0
 **c.7.C.1**	(5) 0.0 (3) 1.8 (7) 3.7	 **c.7.C.2**	(5) 2.8 (3) 4.4		
 **c.8.C.1**	(6) 0.0 (4) 2.8 (8) 3.5	 **c.8.C.2**	(6) 0.5 (2) 0.9 (4) 1.2		
 **c.9.C.1**	(3) 0.0 (5) 2.1 (7) 2.4 (1) 2.4				
 **c.10.C.1**	(2) 0.0 (4) 0.7 (6) 1.2 (8) 1.4	 **c.10.C.2**	(8) 0.2 (6) 0.7 (10) 1.4		
 **c.11.C.1**	(7) 0.0 (9) 0.7 (5) 1.4 (3) 2.3				

Figure S1: The Structures, Multiplicities (M, in bracket) and Relative Energies (rE, kcal.mol^{-1}) of the lowest-lying cationic $B_2Sc_{n-2}^+$ (n = 3-13) clusters calculated at the PBE/ Def2-TZVP theory method.

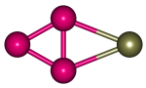
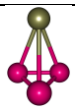
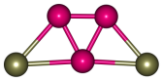
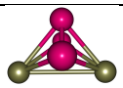
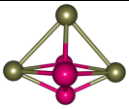
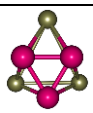
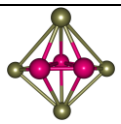
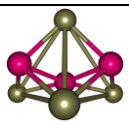
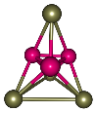
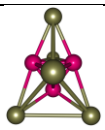
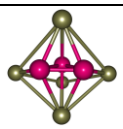
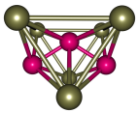
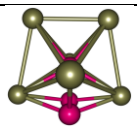
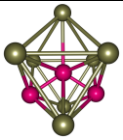
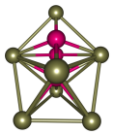
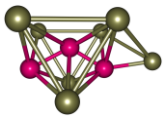
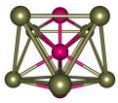
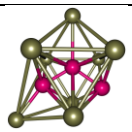
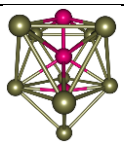
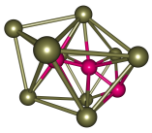
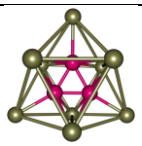
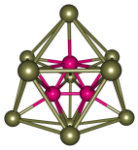
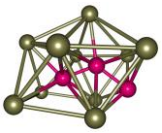
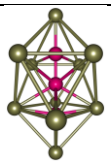
Isomer	*(M) - rE*	*Isomer*	*(M) - rE*	*Isomer*	*(M) - rE*
 **c.1.D.1**	(2) 0.0 (4) 12.0	 **c.1.D.2**	(2) 0.0 (4) 23.5		
 **c.2.D.1**	(1) 0.0 (3) 15.9	 **c.2.D.2**	(1) 0.7 (3) 9.5		
 **c.3.D.1**	(2) 0.0 (4) 7.8	 **c.3.D.2**	(2) 0.2 (4) 4.6		
 **c.4.D.1**	(1) 0.0 (3) 7.4	 **c.4.D.2**	(1) 6.5	 **c.4.D.3**	(1) 6.9
 **c.5.D.1**	(2) 0.0 (4) 6.9	 **c.5.D.2**	(4) 0.5 (2) 0.9		
 **c.6.D.1**	(3) 0.0 (1) 4.4 (5) 4.6	 **c.6.D.2**	(7) 8.5 (5) 9.2 (3) 10.6		
 **c.7.D.1**	(2) 0.0 (4) 1.8 (6) 5.3	 **c.7.D.2**	(4) 7.6 (2) 9.9	 **c.7.D.3**	(2) 11.3
 **c.8.D.1**	(1) 0.0 (3) 3.2 (5) 4.4	 **c.8.D.2**	(5) 0.1 (3) 1.1 (7) 2.3 (1) 5.5		
 **c.9.D.1**	(6) 0.0 (4) 0.2 (2) 0.5	 **c.9.D.2**	(6) 0.5 (4) 0.9 (2) 1.1	 **c.9.D.3**	(8) 3.2 (6) 3.9
 **c.10.D.1**	(5) 0.0 (3) 0.7 (7) 1.4 (9) 2.3	 **c.10.D.2**	(9) 0.7 (7) 1.4 (5) 1.8	 **c.10.D.3**	(7) 0.9 (3) 1.8 (5) 1.8 (9) 6.0

Figure S2: The Structures, Multiplicities (M, in bracket) and Relative Energies (rE, kcal.mol^{-1}) of the lowest-lying cationic $B_3Sc_{n-3}^+$ (n = 4-13) clusters calculated at the PBE/ Def2-TZVP theory method.

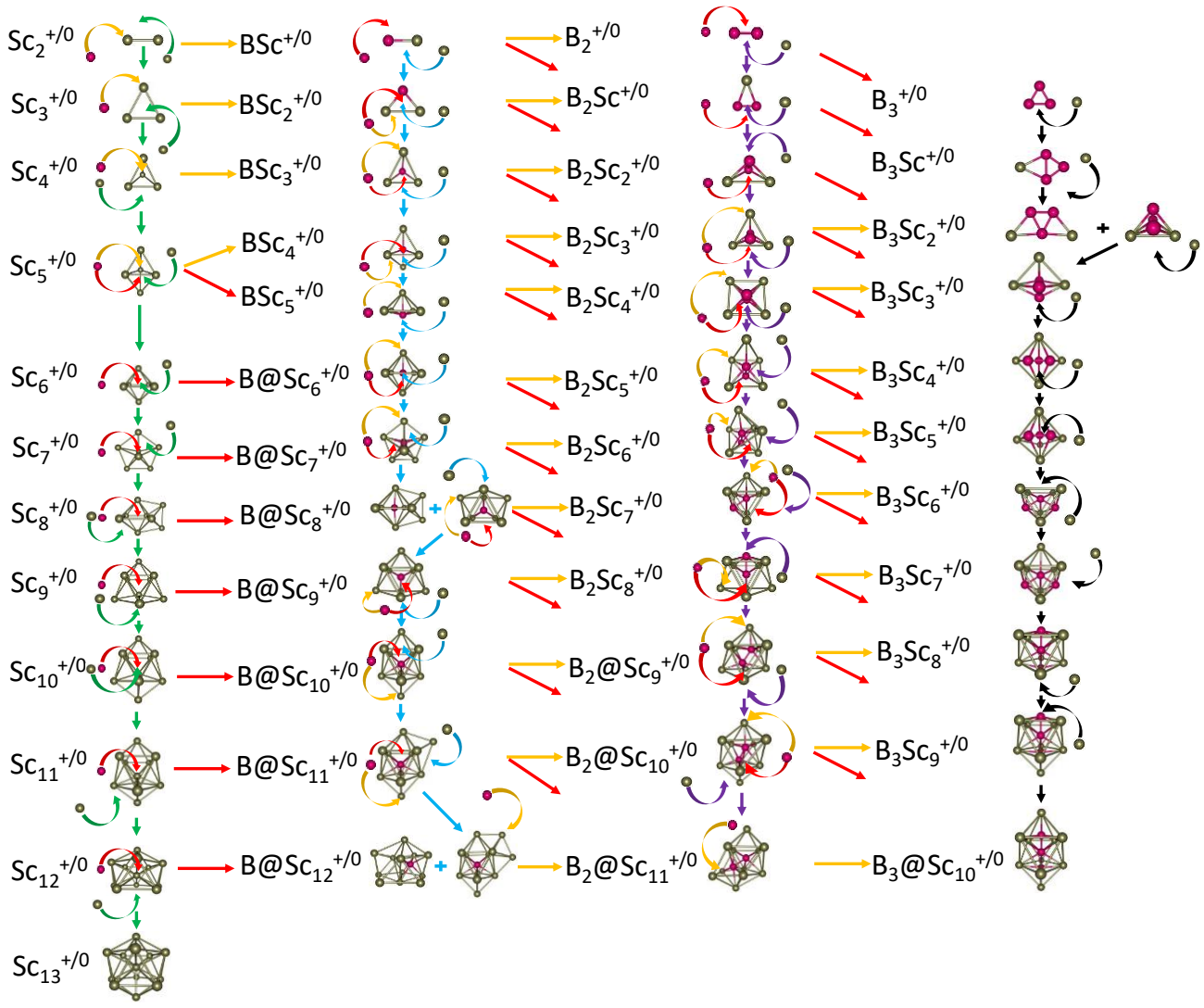


Figure S3: Structural evolution of the $B_mSc_{n-m}^{+/0}$ clusters (m = 0 - 3; n = 3-13). Green, blue, violet and black arrows illustrate the stepwise structural changes by adding one Sc atom to the $B_mSc_{n-m}^{+/0}$ clusters with m = 0, 1, 2 and 3, respectively. The $B@Sc_n^{+/0}$ cluster are referenced from Ref.1. Yellow and red arrows present trends in substitution and addition of B atom into the clusters, respectively.

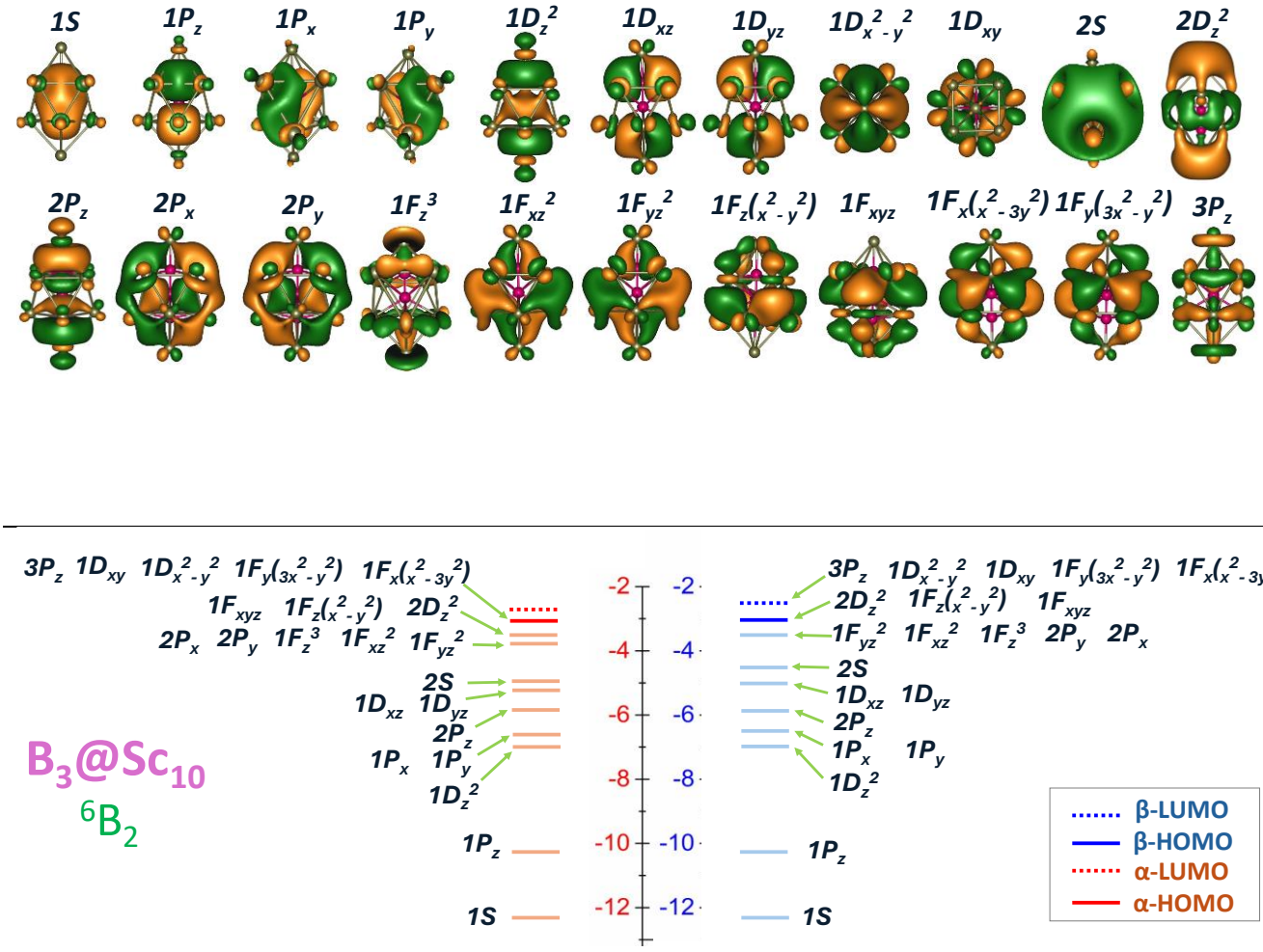


Figure S4: Energy levels of molecular orbitals (MOs) of **n.10.D.1** in its $^{6}B_2$ electronic ground state (PBE/Def2-TZVP).

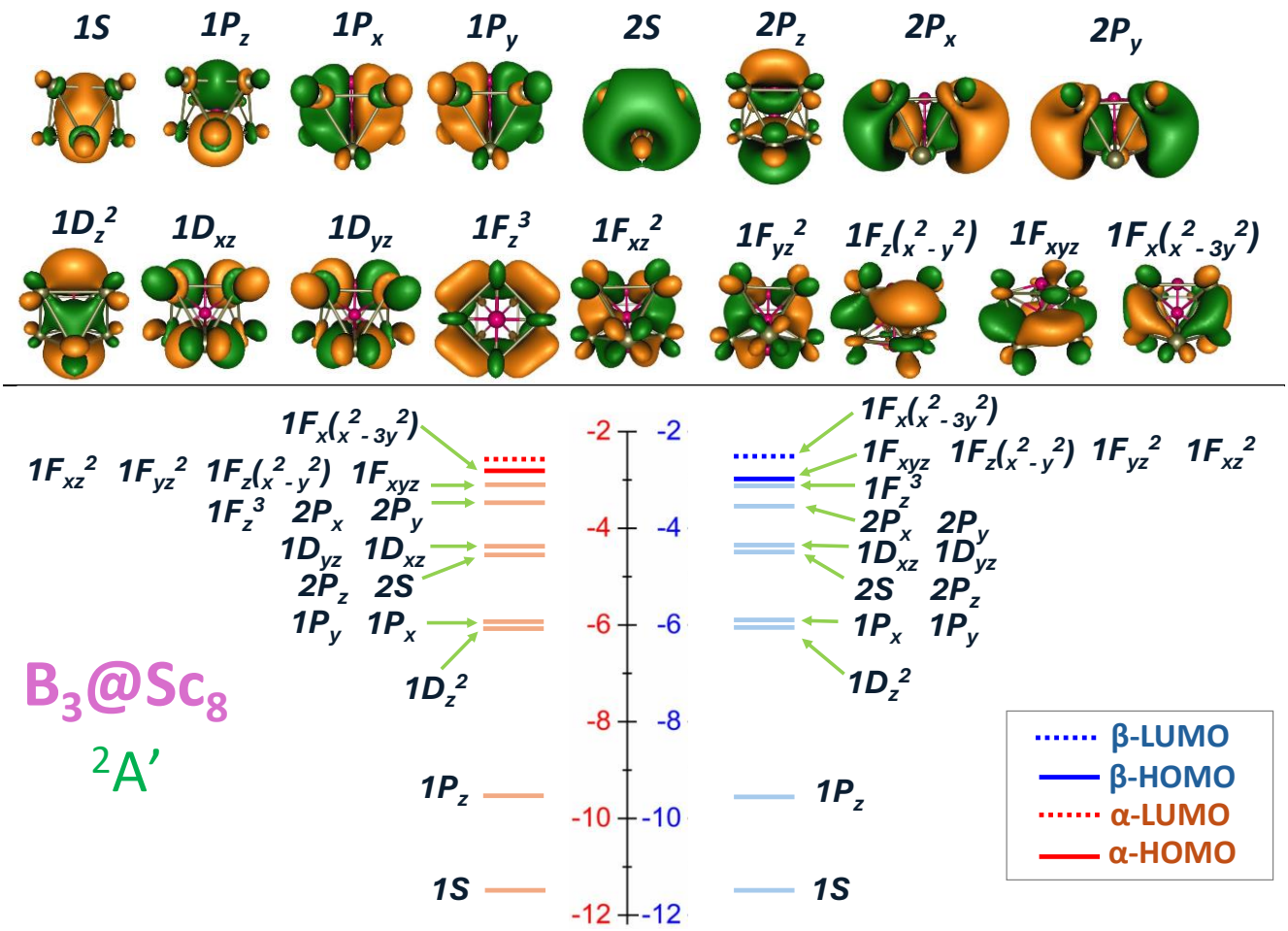


Figure S5: Energy levels of molecular orbitals (MOs) of **n.8.D.1** in its ^{2}A' electronic ground state, PBE/ Def2-TZVP.

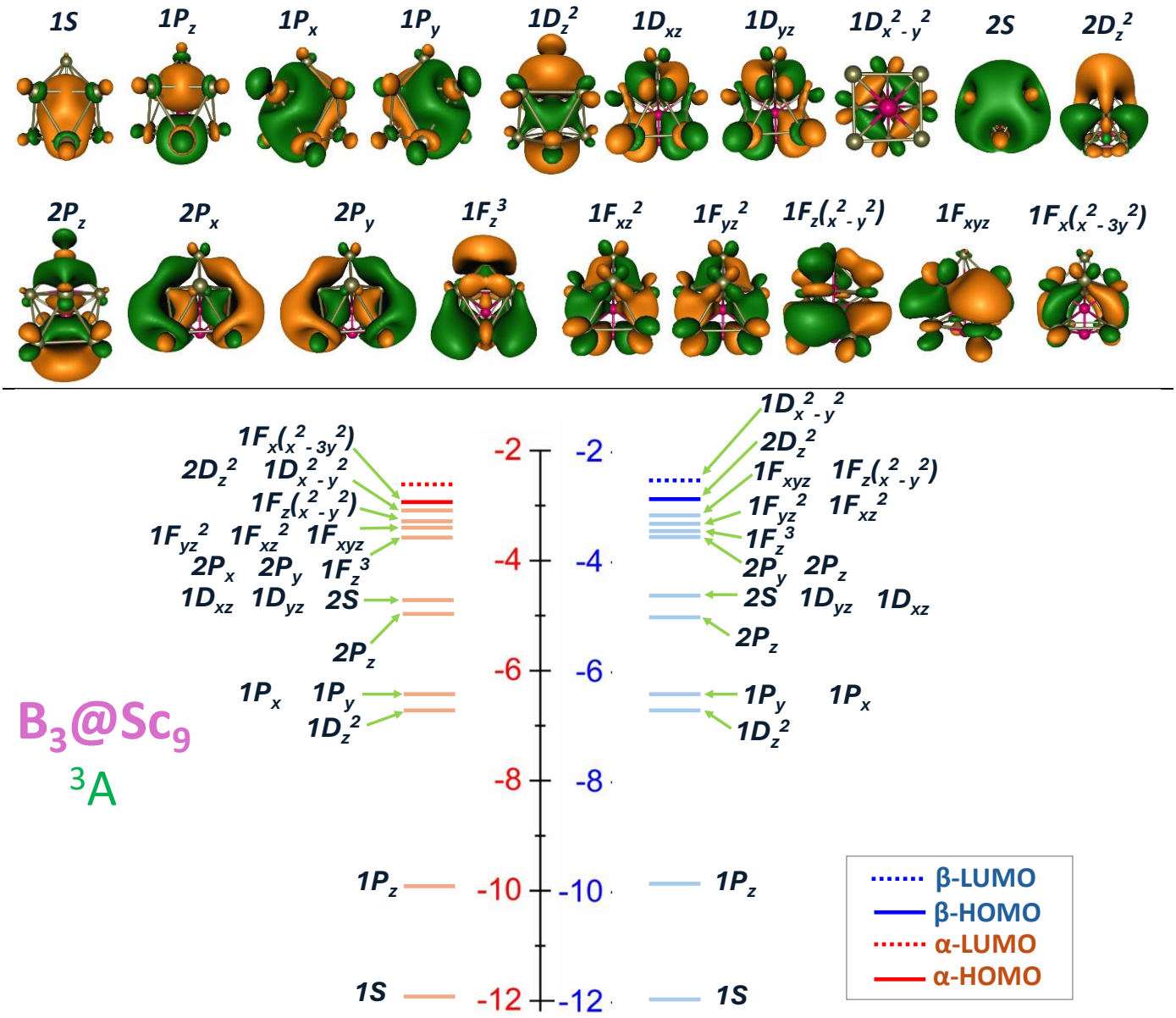


Figure S6: Energy levels of molecular orbitals (MOs) of **n.9.D.2** in its ^{3}A electronic ground state, PBE/ Def2-TZVP.

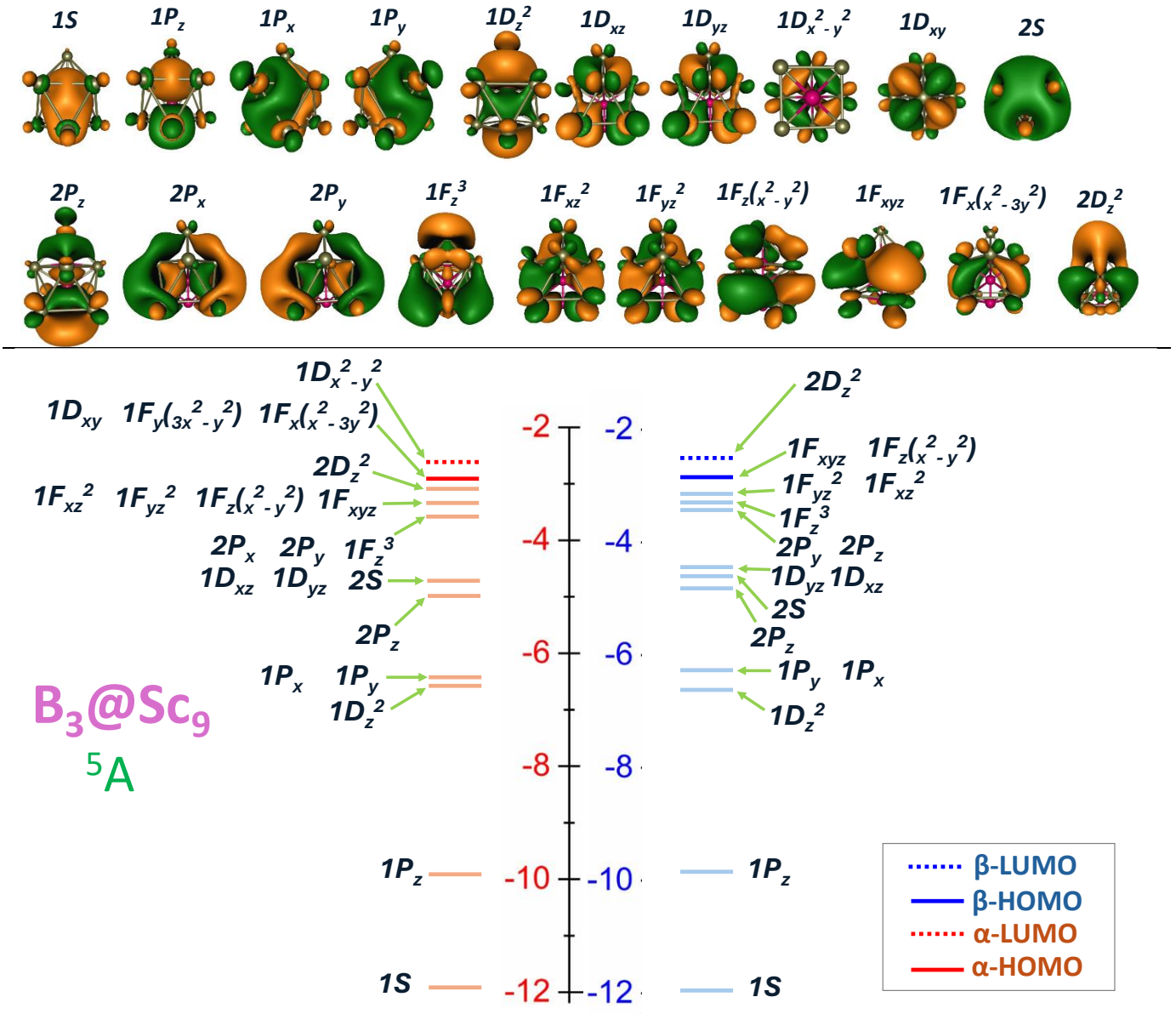


Figure S7: Energy levels of molecular orbitals (MOs) of **n.9.D.2** in its ^{5}A electronic ground state, PBE/ Def2-TZVP.

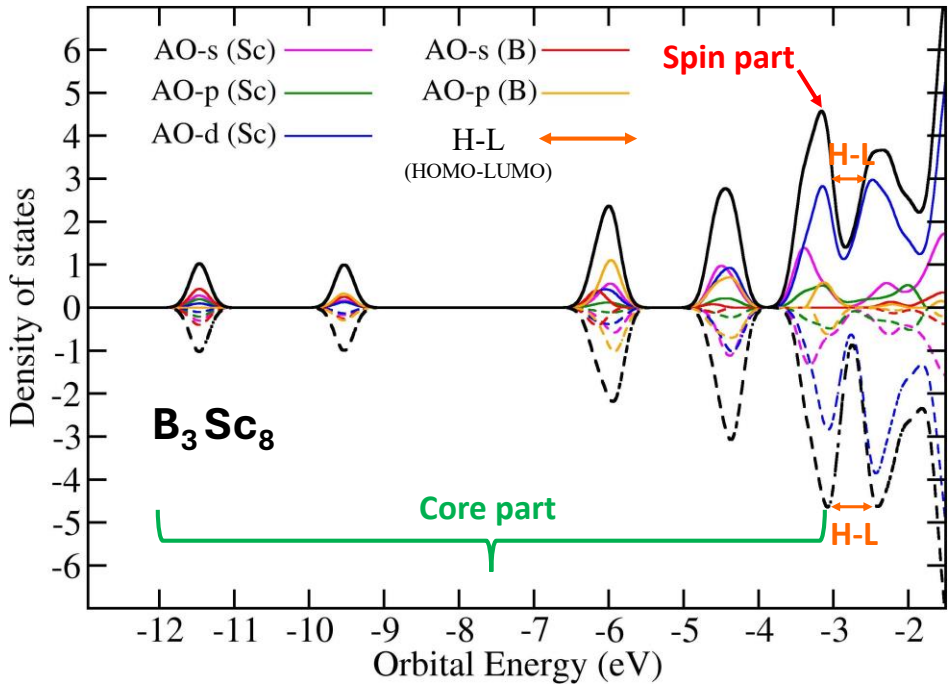


Figure S8. Calculated density of states (DOS) for the **n.8.D.1** isomer at ^{2}A' electronic state. Positive and negative DOS represent spin-up and spin-down electrons, respectively.

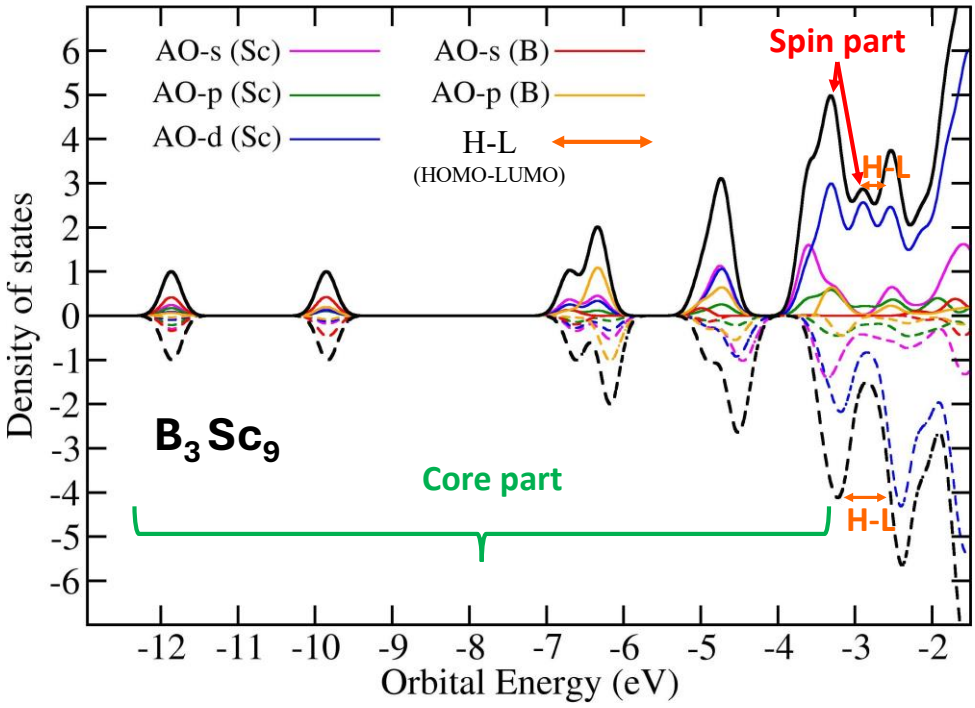


Figure S9. Calculated density of states (DOS) for the **n.9.D.2** isomer at ^{3}A electronic state. Positive and negative DOS represent spin-up and spin-down electrons, respectively.

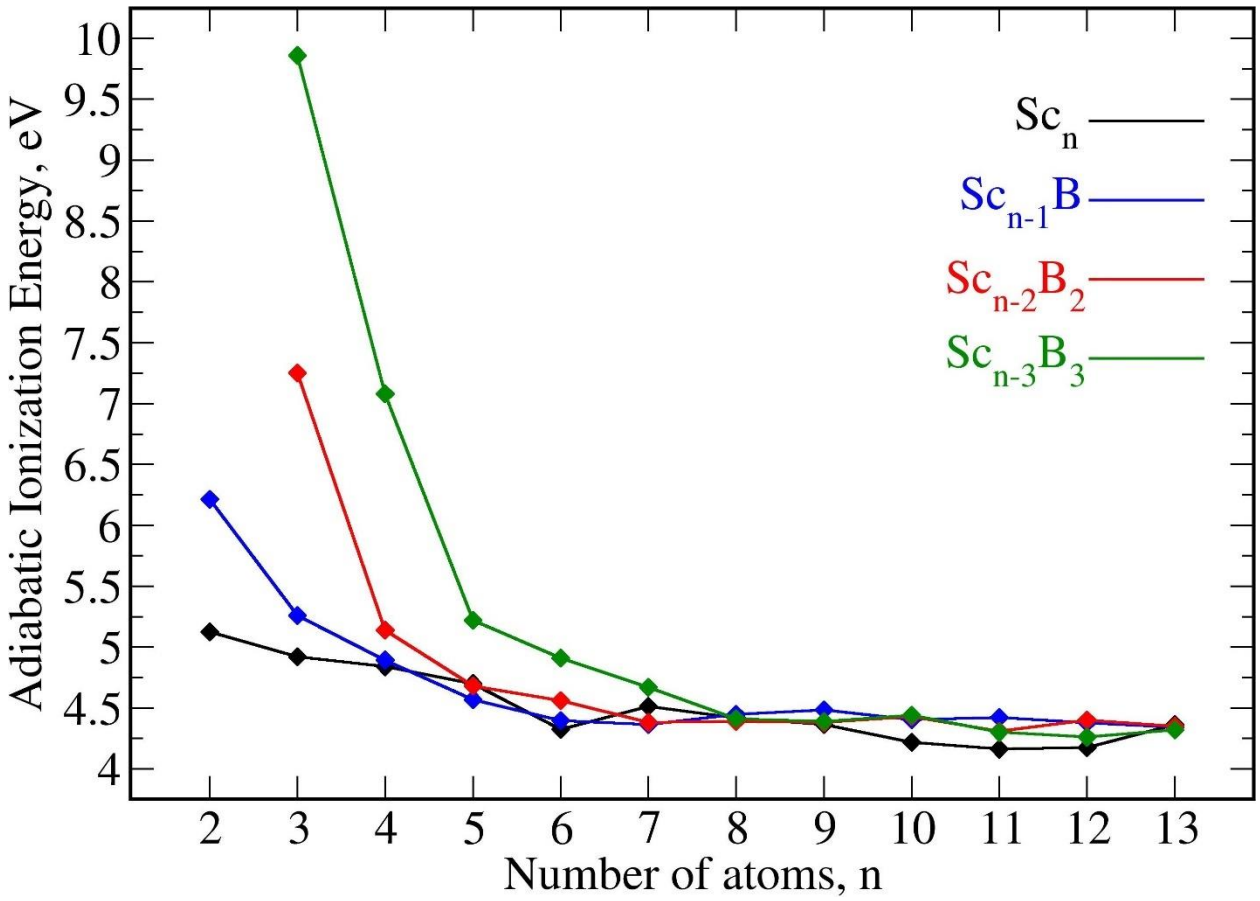


Figure S10: Adiabatic ionization energy of the $B_mSc_{n-m}^{+/0}$ (m = 0–3, n = 3-13). Values given in eV from PBE/Def2-TZPV + ZPE computations.

Table S1: Natural Electron Configuration (NEC) and Natural Charge of **n.8.D.1**, **n.9.D.2** and **n.10.D.1** isomers at their most stable spin state.

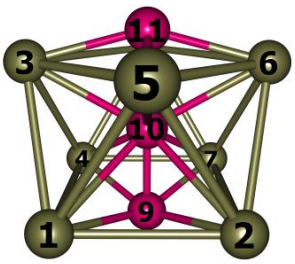
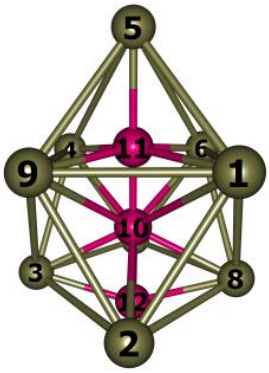
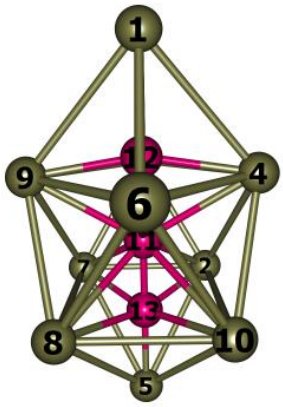
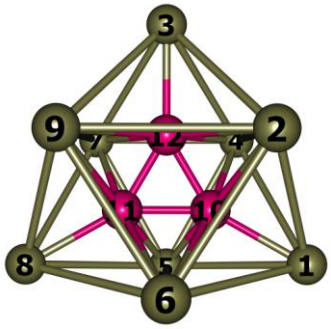
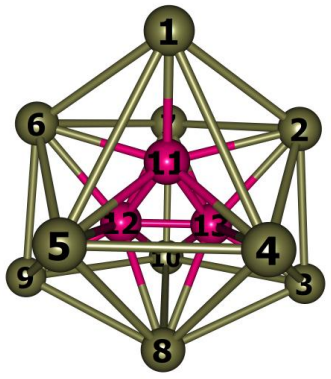
Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **n.8.D.1** doublet	1	Sc	0.4	4S(0.64) 3d(1.66) 4p(0.32)
	2	Sc	0.4	4S(0.64) 3d(1.66) 4p(0.32)
	3	Sc	0.3	4S(0.63) 3d(1.73) 4p(0.32)
	4	Sc	0.4	4S(0.64) 3d(1.66) 4p(0.32)
	5	Sc	0.4	4S(0.65) 3d(1.60) 4p(0.32)
	6	Sc	0.3	4S(0.63) 3d(1.73) 4p(0.32)
	7	Sc	0.4	4S(0.64) 3d(1.66) 4p(0.32)
	8	Sc	0.4	4S(0.65) 3d(1.60) 4p(0.32)
	9	B	-1.4	2S(1.05) 2p(3.25)
	10	B	-0.4	2S(0.68) 2p(2.57)
	11	B	-1.4	2S(1.05) 2p(3.25)
 **n.9.D.2** triplet	1	Sc	0.3	4S(0.62) 3d(1.79) 4p(0.32)
	2	Sc	0.5	4S(0.60) 3d(1.62) 4p(0.30)
	3	Sc	0.4	4S(0.58) 3d(1.68) 4p(0.33)
	4	Sc	0.2	4S(0.62) 3d(1.80) 4p(0.33)
	5	Sc	0.4	4S(0.91) 3d(1.54) 4p(0.15)
	6	Sc	0.2	4S(0.62) 3d(1.80) 4p(0.33)
	7	Sc	0.5	4S(0.59) 3d(1.63) 4p(0.30)
	8	Sc	0.4	4S(0.58) 3d(1.68) 4p(0.33)
	9	Sc	0.3	4S(0.62) 3d(1.79) 4p(0.32)
	10	B	-0.6	2S(0.65) 2p(2.85)
	11	B	-1.5	2S(0.80) 2p(3.50)
	12	B	-1.3	2S(1.06) 2p(3.19)
 **n.10.D.1** sextet	1	Sc	0.5	4S(0.92) 3d(1.51) 4p(0.14)
	2	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	3	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	4	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	5	Sc	0.5	4S(0.92) 3d(1.51) 4p(0.14)
	6	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	7	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	8	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	9	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	10	Sc	0.3	4S(0.60) 3d(1.75) 4p(0.32)
	11	B	-0.6	2S(0.58) 2p(3.01)
	12	B	-1.4	2S(0.80) 2p(3.55)
	13	B	-1.4	2S(0.80) 2p(3.55)

Table S2: Natural Electron Configuration (NEC) and Natural Charge of **n.9.D.3** and **n.10.D.2** isomers at their most stable spin state.

Isomers	Atom's number		Natural Charge	Natural Electron Configuration
 **n.9.D.3** nonet	1	Sc	0.5	4S(0.71) 3d(1.58) 4p(0.23)
	2	Sc	0.3	4S(0.58) 3d(1.78) 4p(0.32)
	3	Sc	0.4	4S(0.74) 3d(1.61) 4p 0.22)
	4	Sc	0.3	4S(0.59) 3d(1.78) 4p(0.34)
	5	Sc	0.3	4S(0.57) 3d(1.79) 4p(0.33)
	6	Sc	0.4	4S(0.58) 3d(1.74) 4p(0.31)
	7	Sc	0.3	4S(0.59) 3d(1.78) 4p(0.34)
	8	Sc	0.5	4S(0.71) 3d(1.58) 4p(0.23)
	9	Sc	0.3	4S(0.58) 3d(1.78) 4p(0.32)
	10	B	-1.1	2S(0.72) 2p(3.34)
	11	B	-1.1	2S(0.72) 2p(3.34)
	12	B	-1.1	2S(0.73) 2p(3.31)
 **n.10.D.2** sextet	1	Sc	0.5	4S(0.60) 3d(1.70) 4p(0.19)
	2	Sc	0.2	4S(0.61) 3d(1.93) 4p(0.31)
	3	Sc	0.5	4S(0.67) 3d(1.60) 4p(0.22)
	4	Sc	0.2	4S(0.61) 3d(1.88) 4p(0.29)
	5	Sc	0.2	4S(0.61) 3d(1.88) 4p(0.29)
	6	Sc	0.2	4S(0.61) 3d(1.93) 4p(0.31)
	7	Sc	0.2	4S(0.62) 3d(1.86) 4p(0.28)
	8	Sc	0.0	4S(0.58) 3d(2.04) 4p(0.35)
	9	Sc	0.5	4S(0.67) 3d(1.60) 4p(0.22)
	10	Sc	0.3	4S(0.60) 3d(1.80) 4p(0.25)
	11	B	-1.0	2S(0.72) 2p(3.26)
	12	B	-1.0	2S(0.73) 2p(3.20)
	13	B	-1.0	2S(0.73) 2p(3.20)

Coordinates of the lowest-lying $B_2Sc_{n-2}^{+/0}$ clusters with n = 3 - 13

Isomer	Spin state		Coordinate		
c.1.C.1	triplet	21	0.000000000	0.000000000	0.629363000
		5	0.000000000	0.790507000	-1.321662000
		5	0.000000000	-0.790507000	-1.321662000
n.1.C.1	doublet	21	0.000000000	0.000000000	0.641103000
		5	0.000000000	0.771613000	-1.346317000
		5	0.000000000	-0.771613000	-1.346317000

Isomer	Spin state		Coordinate		
c.2.C.1	doublet	21	0.000000000	1.994506000	0.000000000
		21	0.000000000	-1.994506000	0.000000000
		5	0.000000000	0.000000000	0.796407000
		5	0.000000000	0.000000000	-0.796405000
n.2.C.1	triplet	21	-0.129960000	-0.204950000	1.568562000
		21	-0.129960000	-0.204950000	-1.568562000
		5	1.221622000	0.432304000	0.000000000
		5	-0.129960000	1.289280000	0.000000000

Isomer	Spin state		Coordinate		
c.3.C.1	singlet	21	0.000000000	1.870734000	0.000000000
		21	1.620104000	-0.935367000	0.000000000
		21	-1.620104000	-0.935367000	0.000000000
		5	0.000000000	0.000000000	1.018043000
		5	0.000000000	0.000000000	-1.018043000
n.3.C.1	doublet	21	0.000000000	1.817443000	0.000000000
		21	1.573952000	-0.908722000	0.000000000
		21	-1.573952000	-0.908722000	0.000000000
		5	0.000000000	0.000000000	1.160991000
		5	0.000000000	0.000000000	-1.160991000

Isomer	Spin state		Coordinate		
c.4.C.1	doublet	21	0.000004000	-2.027284000	0.000000000
		21	2.027285000	-0.000002000	0.000000000
		21	-0.000003000	2.027292000	0.000000000
		21	-2.027286000	-0.000008000	0.000000000
		5	-0.000003000	0.000004000	-1.026424000
		5	-0.000003000	0.000004000	1.026424000
n.4.C.1	triplet	21	0.026405000	-2.023598000	0.000000000
		21	-0.051756000	2.036770000	0.000000000
		21	-2.022785000	0.063868000	0.000000000
		21	2.035562000	-0.089330000	0.000000000
		5	0.026405000	0.025807000	-1.003744000
		5	0.026405000	0.025807000	1.003744000

Isomer	Spin state	Coordinate			
		21	1.751837000	0.000135000	-1.477152000
		21	1.578579000	-0.000096000	1.353991000
		21	-0.292396000	-2.021609000	0.158620000
c.5.C.1	singlet	21	-0.292407000	2.021554000	0.158797000
		21	-2.492732000	0.000036000	-0.265898000
		5	-0.720553000	-0.000060000	1.054776000
		5	-0.341549000	-0.000025000	-0.753875000
		21	-0.885358000	1.530564000	-0.951485000
		21	-0.885438000	-1.530502000	-0.951497000
		21	1.763694000	-1.465633000	0.339216000
n.5.C.1	quartet	21	1.763745000	1.465563000	0.339252000
		21	-1.972284000	0.000009000	1.354581000
		5	0.846333000	-0.000004000	-1.079030000
		5	0.059355000	-0.000004000	0.532746000

Isomer	Spin state	Coordinate			
		21	-0.644949000	1.248359000	1.317501000
		21	1.566857000	-1.592298000	-0.972219000
		21	-2.404659000	0.496618000	-0.951224000
		21	0.645187000	1.248425000	-1.317459000
c.6.C.1	doublet	21	2.404721000	0.496349000	0.951292000
		21	-1.567154000	-1.592187000	0.972095000
		5	-0.507123000	-0.640945000	-0.710228000
		5	0.507105000	-0.641171000	0.710287000
		21	1.889439000	1.226154000	-0.847906000
		21	-1.042017000	1.747600000	-0.921107000
		21	0.372758000	0.805412000	1.772143000
		21	1.889679000	-1.472771000	0.399751000
n.6.C.1	triplet	21	-2.298044000	-0.230968000	0.741583000
		21	-0.781046000	-1.752873000	-1.280307000
		5	0.158586000	-0.052290000	-0.286164000
		5	-0.287818000	-1.302437000	0.856710000

Isomer	Spin state	Coordinate			
		21	0.065998000	0.793783000	2.112359000
		21	0.065998000	0.793783000	-2.112359000
		21	0.065998000	-2.092533000	1.471335000
		21	0.065998000	-2.092533000	-1.471335000
c.7.C.1	quintet	21	-0.885445000	2.793823000	0.000000000
		21	2.388607000	-0.328896000	0.000000000
		21	-1.998902000	-0.076222000	0.000000000
		5	0.743538000	1.256370000	0.000000000
		5	0.229807000	-0.379432000	0.000000000
		21	1.114052000	1.670402000	1.499746000
		21	1.114052000	-1.254381000	1.584346000
		21	-1.548069000	0.418856000	-1.635983000
		21	1.114052000	1.670402000	-1.499746000
n.7.C.1	quartet	21	1.114052000	-1.254381000	-1.584346000
		21	-1.548069000	0.418856000	1.635983000
		21	-1.227798000	-2.086479000	0.000000000
		5	-0.601886000	1.683457000	0.000000000
		5	0.046351000	0.066782000	0.000000000

Isomer	Spin state	Coordinate			
c.8.C.1	sextet	21	0.445815000	1.872601000	-1.111426000
		21	2.481830000	-0.758139000	-1.277101000
		21	2.482478000	0.757260000	1.276819000
		21	-2.481647000	1.277528000	-0.757880000
		21	0.444361000	-1.873331000	1.111680000
		21	-0.445512000	-1.111326000	-1.872843000
		21	-2.482671000	-1.276493000	0.757658000
		21	-0.444632000	1.112011000	1.872928000
		5	0.818260000	-0.000531000	0.000316000
		5	-0.818356000	0.000069000	0.000376000
n.8.C.1	quintet	21	1.205988000	-1.492012000	1.566772000
		21	1.205988000	1.491596000	1.566337000
		21	-1.166901000	-2.540050000	0.000000000
		21	1.205988000	-1.492012000	-1.566772000
		21	-1.499497000	0.000213000	1.592454000
		21	-1.167008000	2.540698000	0.000000000
		21	1.205988000	1.491596000	-1.566337000
		21	-1.499497000	0.000213000	-1.592454000
		5	1.950943000	-0.000386000	0.000000000
		5	0.186653000	-0.000628000	0.000000000

Isomer	Spin state	Coordinate			
c.9.C.1	triplet	21	1.260467000	2.052693000	0.000000000
		21	-0.857370000	1.533406000	-2.094556000
		21	1.755815000	-0.072125000	-2.094317000
		21	1.755815000	-0.072125000	2.094317000
		21	-0.857370000	1.533406000	2.094556000
		21	-0.857370000	-1.395359000	-1.469642000
		21	-0.857370000	-1.395359000	1.469642000
		21	1.520038000	-2.473144000	0.000000000
		21	-2.893080000	0.239272000	0.000000000
		5	0.785574000	-0.339678000	0.000000000
		5	-0.657799000	0.546882000	0.000000000
n.9.C.1	doublet	21	-2.071346000	1.574844000	1.206108000
		21	0.148267000	2.368940000	-0.788458000
		21	-2.688747000	-0.708230000	-0.860692000
		21	0.000053000	0.000340000	-2.457160000
		21	2.688908000	0.708051000	-0.860501000
		21	2.071120000	-1.574989000	1.206212000
		21	0.925554000	1.138787000	1.708052000
		21	-0.925808000	-1.139124000	1.707648000
		21	-0.148000000	-2.368663000	-0.788975000
		5	-0.791317000	0.250911000	-0.151711000
		5	0.791312000	-0.250729000	-0.151675000

Isomer	Spin state	Coordinate			
		21	-3.074437000	-0.660105000	-0.617610000
		21	-1.915770000	2.047195000	-0.284911000
		21	-1.787089000	-0.421146000	2.104755000
		21	-0.589990000	-0.111741000	-2.203756000
		21	1.178540000	-1.234518000	1.766740000
		21	-0.633422000	-2.282512000	-0.263335000
c.10.C.1	doublet	21	0.441133000	1.610648000	1.602701000
		21	2.186928000	-1.663677000	-1.270071000
		21	1.042236000	2.128735000	-1.188429000
		21	3.098838000	0.590267000	0.374967000
		5	-0.695926000	0.088377000	0.171316000
		5	0.918660000	-0.101594000	-0.259736000
		21	-0.557769000	-1.752926000	1.433749000
		21	-0.558178000	-1.749745000	-1.437780000
		21	2.196390000	-2.073823000	-0.002194000
		21	-1.919325000	1.260218000	1.610242000
		21	-1.920163000	1.264442000	-1.606627000
		21	-3.065865000	-0.971496000	-0.000791000
n.10.C.1	triplet	21	1.142102000	0.483220000	-2.202639000
		21	0.408483000	2.269663000	0.002755000
		21	1.143404000	0.477630000	2.203211000
		21	3.092616000	0.816723000	0.000206000
		5	-0.732313000	0.157185000	0.000041000
		5	0.893195000	-0.257595000	-0.000596000

Isomer	Spin state	Coordinate			
		21	-2.655531000	-1.339370000	0.000083000
		21	0.376936000	-2.736347000	0.000131000
		21	-2.609975000	1.286091000	1.500221000
		21	2.318164000	-0.826938000	1.511517000
		21	-2.609963000	1.285901000	-1.500396000
		21	2.318181000	-0.827108000	-1.511416000
c.11.C.1	septet	21	-0.638155000	-0.907440000	-2.110388000
		21	3.218871000	1.644637000	-0.000075000
		21	0.518671000	1.648845000	-1.496375000
		21	0.518645000	1.649009000	1.496199000
		21	-0.638173000	-0.907197000	2.110501000
		5	0.521861000	-0.300663000	0.000017000
		5	-1.016082000	0.426322000	-0.000026000
		21	2.679015000	1.417092000	-0.000538000
		21	0.603517000	0.908249000	-2.088705000
		21	-2.375085000	0.804476000	-1.535667000
		21	0.603021000	0.910550000	2.087779000
		21	-2.375554000	0.806926000	1.534331000
		21	-0.500676000	2.655295000	-0.001571000
n.11.C.1	octet	21	-3.066044000	-1.657023000	0.000765000
		21	-0.428215000	-1.717487000	1.515856000
		21	2.610007000	-1.184108000	1.483884000
		21	2.610638000	-1.185198000	-1.481951000
		21	-0.427318000	-1.719522000	-1.514212000
		5	-0.680166000	0.166409000	-0.000176000
		5	0.960284000	-0.331259000	0.000299000

Coordinates of the lowest-lying $B_3Sc_{n-3}^{+/0}$ clusters with n = 4 - 13

Isomer	Spin state		Coordinate		
c.1.D.1	doublet	21	1.023971000	-0.006918000	-0.000054000
		5	-0.915986000	0.820967000	0.000302000
		5	-2.309392000	0.056556000	-0.000346000
		5	-1.075302000	-0.848466000	0.000271000
c.1.D.2	doublet	21	0.886353000	-0.000073000	-0.041573000
		5	-1.089917000	0.819181000	0.468952000
		5	-1.090587000	-0.818741000	0.469343000
		5	-1.542179000	-0.000132000	-0.763687000
n.1.D.1	singlet	21	-0.966938000	-0.000003000	0.000031000
		5	0.940401000	-0.911439000	-0.000164000
		5	0.940293000	0.911387000	-0.000164000
		5	2.180446000	0.000063000	0.000198000

Isomer	Spin state		Coordinate		
c.2.D.1	singlet	21	2.175850000	-0.292061000	0.000000000
		21	-2.175851000	-0.292051000	0.000000000
		5	0.791913000	1.316201000	0.000000000
		5	0.000000000	-0.179139000	0.000000000
		5	-0.791909000	1.316209000	0.000000000
n.2.D.1	doublet	21	1.544076000	-0.319121000	-0.000004000
		21	-1.544074000	-0.319123000	-0.000004000
		5	-0.000006000	1.507227000	0.000020000
		5	0.000002000	0.586681000	1.276217000
		5	-0.000001000	0.586719000	-1.276203000

Isomer	Spin state		Coordinate		
c.3.D.1	doublet	21	-1.995880000	0.528928000	0.000000000
		21	2.011737000	0.512501000	-0.000001000
		21	-0.020395000	-1.570814000	-0.000003000
		5	0.026418000	0.366363000	1.165419000
		5	0.026412000	0.366396000	-1.165418000
		5	-0.033771000	1.490659000	0.000014000
n.3.D.1	singlet	21	-0.000043000	-1.569490000	-0.000001000
		21	1.972464000	0.518271000	0.000004000
		21	-1.972442000	0.518318000	0.000003000
		5	0.000029000	0.366682000	1.194088000
		5	0.000033000	0.366673000	-1.194088000
		5	0.000027000	1.504828000	-0.000022000

Isomer	Spin state	Coordinate			
		21	0.788865000	-1.820807000	0.455506000
		21	-0.788946000	1.820822000	0.455465000
		21	-2.140250000	-0.642859000	-0.627611000
c.4.D.1	singlet	21	2.140316000	0.642813000	-0.627592000
		5	-0.783232000	-0.324894000	1.033891000
		5	0.000018000	0.000009000	-0.621991000
		5	0.783270000	0.325012000	1.033874000
		21	-2.277390000	0.215641000	-0.539967000
		21	2.184978000	-0.336204000	-0.568727000
		21	-0.269993000	-1.915198000	0.409375000
n.4.D.1	doublet	21	0.386444000	1.983226000	0.338889000
		5	-0.040356000	0.046516000	-0.633682000
		5	-0.861869000	0.228728000	1.068907000
		5	0.801257000	-0.054600000	1.078580000

Isomer	Spin state	Coordinate			
		21	-0.683611000	1.738333000	-0.000409000
		21	1.753044000	-1.691114000	0.000333000
		21	-1.750866000	-0.443749000	-1.595969000
		21	-1.750836000	-0.442752000	1.596216000
c.5.D.1	doublet	21	2.273910000	1.097552000	-0.000211000
		5	0.544920000	-0.009764000	0.934306000
		5	-0.424609000	-1.064853000	0.000215000
		5	0.544790000	-0.010112000	-0.934356000
		21	0.098670000	-2.273263000	-0.156030000
		21	0.987703000	-0.004497000	1.643823000
		21	-2.428098000	0.010953000	-0.486030000
		21	0.119212000	2.272294000	-0.155995000
n.5.D.1	triplet	21	1.795024000	-0.008091000	-1.257006000
		5	-1.080207000	0.859748000	1.031035000
		5	-0.236421000	0.001145000	-0.334860000
		5	-1.087917000	-0.849960000	1.031026000

Isomer	Spin state	Coordinate			
		21	1.580503000	0.000010000	1.573252000
		21	1.538724000	-1.621733000	-0.862848000
		21	-1.580503000	-0.000010000	1.573252000
		21	-1.538724000	1.621733000	-0.862848000
c.6.D.1	triplet	21	-1.538696000	-1.621785000	-0.862816000
		21	1.538696000	1.621785000	-0.862816000
		5	0.000000000	-1.499362000	0.740747000
		5	0.000000000	1.499362000	0.740747000
		5	0.000000000	0.000000000	-0.201233000
		21	-1.505820000	1.580383000	0.900491000
		21	-1.505894000	-1.580280000	0.900664000
		21	-1.537526000	-0.000063000	-1.636758000
		21	1.537498000	-0.000150000	-1.636767000
n.6.D.1	quartet	21	1.505889000	-1.580316000	0.900625000
		21	1.505859000	1.580443000	0.900483000
		5	0.000023000	0.000025000	0.126016000
		5	0.000016000	1.518799000	-0.753464000
		5	-0.000062000	-1.518894000	-0.753253000

Isomer	Spin state	Coordinate			
		21	-1.103722000	-1.331245000	1.515663000
		21	-1.103722000	1.715340000	1.509935000
		21	-1.103722000	1.715340000	-1.509935000
		21	1.668968000	0.452862000	1.515580000
c.7.D.1	doublet	21	-1.103722000	-1.331245000	-1.515663000
		21	1.668968000	0.452862000	-1.515580000
		21	1.393732000	-2.166285000	0.000000000
		5	0.634030000	1.771727000	0.000000000
		5	-1.875069000	0.157169000	0.000000000
		5	-0.089427000	0.139061000	0.000000000
		21	1.482261000	0.676940000	-1.597739000
		21	-0.781994000	-1.429591000	-1.597721000
		21	1.771943000	-1.904536000	0.000000000
		21	-0.267615000	2.527020000	0.000000000
		21	-2.501236000	0.448972000	0.000000000
n.7.D.1	triplet	21	-0.781994000	-1.429591000	1.597721000
		21	1.482261000	0.676940000	1.597739000
		5	-0.131241000	0.140954000	0.000000000
		5	-0.781994000	0.840604000	1.502502000
		5	-0.781994000	0.840604000	-1.502502000

Isomer	Spin state	Coordinate			
		21	-1.300742000	1.546487000	1.546496000
		21	-1.300742000	-1.546490000	1.546494000
		21	1.300749000	2.187079000	0.000000000
		21	-1.300742000	1.546487000	-1.546496000
		21	1.300750000	0.000002000	2.187077000
c.8.D.1	singlet	21	1.300748000	-2.187076000	0.000000000
		21	-1.300742000	-1.546490000	-1.546494000
		21	1.300750000	0.000002000	-2.187077000
		5	-1.784248000	0.000001000	0.000000000
		5	-0.000071000	-0.000004000	0.000000000
		5	1.784190000	0.000001000	0.000000000
		21	-2.006081000	-0.289377000	1.528432000
		21	0.679064000	-1.909750000	1.528462000
		21	-1.225148000	2.202571000	0.000000000
		21	-2.006081000	-0.289377000	-1.528432000
		21	0.679064000	1.125344000	2.186142000
n.8.D.1	doublet	21	2.519732000	-0.057204000	0.000000000
		21	0.679064000	-1.909750000	-1.528462000
		21	0.679064000	1.125344000	-2.186142000
		5	-0.930571000	-1.542248000	0.000000000
		5	0.001100000	0.002005000	0.000000000
		5	0.935023000	1.549476000	0.000000000
		21	-0.073641000	-1.629286000	1.556276000
		21	1.368230000	-1.492734000	-1.185092000
		21	-1.710468000	-1.534517000	-1.172407000
		21	1.368203000	1.492910000	-1.184944000
		21	-2.648722000	-0.000100000	1.214278000
n.8.D.2	quartet	21	-0.073699000	1.629114000	1.556474000
		21	3.315846000	-0.000045000	0.720661000
		21	-1.710499000	1.534624000	-1.172233000
		5	-0.192394000	0.000118000	-1.940909000
		5	-0.304716000	0.000019000	-0.128856000
		5	1.189058000	0.000009000	0.671111000

Isomer	Spin state	Coordinate			
c.9.D.1	sextet	21	3.266452000	0.001348000	0.002756000
		21	0.935745000	-0.290064000	2.221204000
		21	0.942484000	-2.217799000	-0.288878000
		21	0.938239000	2.218981000	0.292804000
		21	-1.665384000	1.322553000	1.719771000
		21	-1.658878000	1.721774000	-1.326492000
		21	0.944791000	0.291673000	-2.215276000
		21	-1.661803000	-1.724049000	1.320183000
		21	-1.655572000	-1.324304000	-1.725823000
		5	1.159885000	0.000802000	0.003294000
		5	-0.502414000	0.000260000	0.000044000
		5	-2.278981000	-0.001528000	-0.004379000
c.9.D.2	sextet	21	0.969006000	2.210867000	-0.004863000
		21	-1.653678000	1.559744000	-1.537232000
		21	-1.686102000	-1.529961000	-1.535494000
		21	0.904143000	-2.262589000	0.004607000
		21	3.272100000	-0.015237000	-0.001119000
		21	0.957883000	0.003966000	2.233562000
		21	-1.685764000	-1.523475000	1.541712000
		21	-1.653371000	1.566202000	1.530433000
		21	0.957714000	-0.005622000	-2.231849000
		5	-0.496583000	0.003504000	-0.000513000
		5	1.160938000	-0.042344000	0.001476000
		5	-2.268468000	0.022478000	0.000059000
n.9.D.1	triplet	21	-1.620631000	-1.920254000	-1.077044000
		21	1.484484000	-2.286267000	-0.480014000
		21	2.377729000	-0.095691000	1.587339000
		21	1.802124000	2.069852000	-0.552310000
		21	-1.343927000	2.044244000	-1.145445000
		21	-2.942840000	0.190902000	0.846190000
		21	-0.298835000	1.528820000	1.635537000
		21	-0.472748000	-1.430110000	1.668562000
		21	0.544253000	-0.074605000	-2.286434000
		5	0.695694000	-0.001303000	0.070726000
		5	-0.961167000	0.039886000	-0.166649000
		5	2.241114000	-0.151528000	-0.728882000
n.9.D.2	triplet	21	0.916121000	-1.610854000	1.568611000
		21	-1.702378000	-0.002603000	2.159633000
		21	-1.633529000	2.183075000	-0.011170000
		21	0.958048000	1.594494000	-1.549654000
		21	3.269677000	-0.000386000	0.022768000
		21	0.957874000	-1.590710000	-1.553386000
		21	-1.654340000	0.002909000	-2.193317000
		21	-1.633900000	-2.182950000	-0.016688000
		21	0.916619000	1.607054000	1.572256000
		5	-0.513139000	-0.000114000	-0.001100000
		5	1.151513000	-0.000247000	0.030583000
		5	-2.293980000	0.000238000	-0.025510000

Isomer	Spin state	Coordinate			
		21	0.001102000	1.023979000	-2.131832000
		21	-0.002231000	-2.011099000	-1.797326000
		21	-0.002705000	-2.314315000	1.041934000
		21	1.536777000	0.237801000	1.958926000
		21	-2.415134000	1.442191000	-0.455410000
		21	-1.536682000	0.240973000	1.958853000
c.10.D.1	quintet	21	-2.739693000	-1.603677000	-0.147193000
		21	2.736087000	-1.609681000	-0.146985000
		21	2.418534000	1.436556000	-0.455328000
		21	0.003966000	3.132976000	0.245529000
		5	0.000960000	0.959849000	0.242941000
		5	0.859069000	-0.429894000	-0.270899000
		5	-0.860120000	-0.427911000	-0.270952000
		21	0.000000000	0.000000000	3.747262000
		21	1.574625000	1.574625000	-1.309184000
		21	0.000000000	2.226856000	1.309184000
		5	0.000000000	0.000000000	1.650032000
		21	2.226856000	0.000000000	1.309184000
		21	0.000000000	0.000000000	-3.747262000
n.10.D.1	sextet	21	0.000000000	-2.226856000	1.309184000
		21	-1.574625000	1.574625000	-1.309184000
		5	0.000000000	0.000000000	-1.650032000
		21	-1.574625000	-1.574625000	-1.309184000
		21	-2.226856000	0.000000000	1.309184000
		21	1.574625000	-1.574625000	-1.309184000
		5	0.000000000	0.000000000	0.000000000
		21	0.000395000	3.120711000	-0.293406000
		21	-2.384653000	1.423058000	0.442743000
		21	-2.744124000	-1.605201000	0.180420000
		21	-1.512616000	0.204400000	-1.982609000
		21	1.513599000	0.200152000	-1.983191000
		21	2.386233000	1.422054000	0.439617000
n.10.D.2	sextet	21	0.002471000	1.092514000	2.144667000
		21	-0.000924000	-2.306050000	-1.042661000
		21	2.741756000	-1.607984000	0.183224000
		21	-0.002064000	-1.964816000	1.827568000
		5	0.000213000	0.955797000	-0.222446000
		5	0.861870000	-0.433490000	0.286834000
		5	-0.862383000	-0.433421000	0.286844000
		21	0.152134000	-2.176828000	0.847509000
		21	2.640219000	-1.432171000	-0.647915000
		21	-0.213648000	-1.479707000	-1.952585000
		21	-2.679441000	-1.543755000	-0.119930000
		21	-0.213679000	1.479796000	-1.952531000
		21	-1.292244000	-0.000047000	2.245490000
n.10.D.3	dectet	21	1.968669000	-0.000025000	1.960412000
		21	2.640193000	1.432210000	-0.647884000
		21	-2.679461000	1.543729000	-0.119872000
		21	0.152117000	2.176792000	0.847590000
		5	-1.919019000	0.000019000	-1.610942000
		5	-0.885274000	0.000004000	-0.135757000
		5	0.809878000	-0.000002000	-0.186490000

References

1. Nguyen-Ha, B.-N.; Tam, N. M.; Pham-Ho, M. P.; Nguyen, M. T., Boron-doped scandium clusters $B@Sc_{n-1}^{-/0/+}$ with n = 2–13: uncovering the smallest endohedrally doped cages. *RSC Adv.* **2024,** *14* (47), 34718-34732.