

Quantum rules for planar boron nanoclusters

Athanasios G. Arvanitidis,^a Truong Ba Tai,^a Minh Tho Nguyen,^a and Arnout Ceulemans^a

SUPPLEMENTARY INFORMATION

Part.1

Table of Contents

1. Examples for the planar B ₁₈ (-), B ₂₀ (-) and elongated B ₁₆ (0) cluster.....	2
2. Tables with the correlation of DFT σ - and π - orbital energies and particle-on-a-disk spectrum.....	6
2. Diagrams of the correlation of DFT σ - and π -orbital energies and particle-on-a-disk spectrum.....	20
I. Correlation.....	20
II. Sloped diagrams.....	24
3. XYZ Coordinates of boron clusters.....	29

Part.2

Orbital plots.....	39-78
--------------------	-------

^aDepartment of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium,
Fax: (+32)16-327992) E-mail: arnout.ceulemans@chem.kuleuven.be

1. Examples for the planar B₁₈(-), B₂₀(-) and elongated B₁₆(0) cluster.

1.1 B₁₈(-):

The anionic B₁₈ cluster consists of an inner 6-atom triangulation, surrounded by an outer ring of thirteen atoms. The energy correlation diagrams (in Hartree), relative to the ground root are given in Tables 1 and 2 for σ and π orbitals respectively. As indicated in the Table 7, some σ -levels have a mixed label, due to strong orbital hybridization.

Table 1. Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B ₁₈ (-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
46	HOMO	2 ϕ	0.5836	3 π	0.5723
42	HOMO-4	2 ϕ	0.5154	1 ι	0.4795
41	HOMO-5	2 γ , 3 π	0.5064	1 ι	0.4795
40	HOMO-6	3 π	0.5064	2 ϕ	0.4391
39	HOMO-7	1 η	0.4716	2 ϕ	0.4391
38	HOMO-8	1 π , 1 η	0.4716	1 η	0.3491
35	HOMO-11	1 ι	0.4526	1 η	0.3491
34	HOMO-12	3 σ	0.4394	3 σ	0.3390
33	HOMO-13	2 δ	0.4268	2 δ	0.3192
32	HOMO-14	2 δ	0.4268	2 δ	0.3192
30	HOMO-16	1 γ	0.3664	1 γ	0.2541
29	HOMO-17	1 γ	0.3664	1 γ	0.2541
28	HOMO-18	1 ϕ	0.2613	2 π	0.2131
27	HOMO-19	2 π	0.2539	2 π	0.2131
26	HOMO-20	2 π	0.2539	1 ϕ	0.1713
25	HOMO-21	1 ϕ	0.2419	1 ϕ	0.1713
24	HOMO-22	1 δ	0.1472	2 σ	0.1211
23	HOMO-23	1 δ	0.1472	1 δ	0.1010
22	HOMO-24	2 σ	0.1409	1 δ	0.1010
21	HOMO-25	1 π	0.0640	1 π	0.0436
20	HOMO-26	1 π	0.0640	1 π	0.0436
19	HOMO-27	1 σ	0.0000	1 σ	0.0000

Table 2. Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B ₁₈ (-)	MO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
45	HOMO-1	1 δ	0.5601	2 σ	0.5695
44	HOMO-2	1 δ	0.5601	1 δ	0.5386
43	HOMO-3	2 σ	0.5399	1 δ	0.5386
37	HOMO-9	1 π	0.4553	1 π	0.4505
36	HOMO-10	1 π	0.4553	1 π	0.4505
31	HOMO-15	1 σ	0.3833	1 σ	0.3833

In Figure 1 we plot the correlation diagram, again noting the bimodal aspects of the slopes, related to the basic orbital composition of the in-plane orbitals. Figure 2(original paper) shows the orbitals with maximum number of radial and angular nodes. There are at maximum two radial nodes (3 σ), exactly as in the case of the B₁₃ cluster. The existence of an outer ring with twelve atoms gives rise to a wave with twelve sign changes, based on 2p-orbitals on the twelve outer

atoms, forming a ring with six angular nodes. The $m=6$ angular quantum number is represented by the Greek character ι (iota).

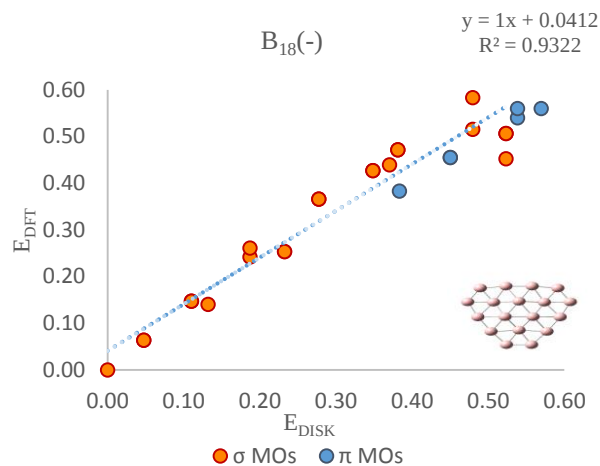


Figure 1. $B_{18}(-)$: correlation between DFT orbital energies and particle-on-a-disk spectrum

1.2 $B_{20}(-)$:

The anionic B_{20} cluster consists of a triple arrangement, with one central atom, surrounded by a hexagon, and an outer ring of 13 atoms. The energy correlations (in Hartree), relative to the ground root are given in Tables 3 and 4 for σ and π orbitals respectively.

Table 3. Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum

B ₂₀ (-)	MO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
51	HOMO	2 γ	0.5687	2 γ	0.5545
50	HOMO-1	2 γ	0.5599	2 γ	0.5545
47	HOMO-4	2 ϕ	0.5392	3 π	0.5004
45	HOMO-6	3 π	0.4667	3 π	0.5004
44	HOMO-7	3 π	0.4599	1 ι	0.4192
41	HOMO-10	3 σ	0.4553	1 ι	0.4192
40	HOMO-11	2 ϕ	0.4480	2 ϕ	0.3839
39	HOMO-12	2 δ	0.4418	2 ϕ	0.3839
38	HOMO-13	2 δ	0.4308	1 η	0.3053
37	HOMO-14	1 ι	0.4207	1 η	0.3053
36	HOMO-15	1 ι	0.4146	3 σ	0.2964
34	HOMO-17	1 η	0.3971	2 δ	0.2791
33	HOMO-18	1 η	0.3813	2 δ	0.2791
32	HOMO-19	1 γ	0.3658	1 γ	0.2222
31	HOMO-20	1 γ	0.2982	1 γ	0.2222
30	HOMO-21	2 π	0.2367	2 π	0.1863
29	HOMO-22	2 π	0.2334	2 π	0.1863
28	HOMO-23	1 ϕ	0.2238	1 ϕ	0.1498
27	HOMO-24	1 ϕ	0.2026	1 ϕ	0.1498
26	HOMO-25	2 σ	0.1399	2 σ	0.1059
25	HOMO-26	1 δ	0.1351	1 δ	0.0883
24	HOMO-27	1 δ	0.1312	1 δ	0.0883
23	HOMO-28	1 π	0.0647	1 π	0.0381
22	HOMO-29	1 π	0.0617	1 π	0.0381
21	HOMO-30	1 σ	0.0000	1 σ	0.0000

Table 4. Correlation of DFT σ -orbital energies and spectrum of a particle-on-a-disk.

B ₂₀ (-)	MO	DFT		Particle in a circular box	
		Label	E(Ha)	Label	E(Ha)
49	HOMO-2	2 σ	0.5497	2 σ	0.5578
48	HOMO-3	1 δ	0.5413	1 δ	0.5313
46	HOMO-5	1 δ	0.5375	1 δ	0.5313
43	HOMO-8	1 π	0.4586	1 π	0.4553
42	HOMO-9	1 π	0.4561	1 π	0.4553
35	HOMO-16	1 σ	0.3975	1 σ	0.3975

Figure 3 shows the correlation plot with the characteristic change of slope. Figure 2(original paper) represents the 3 σ -orbital with the two radial nodes. The orbital with the highest number of angular nodes is again a 1 ι -orbital with twelve sign changes. How does this fit in with the 13 atoms on the outer ring? This is explained by group theory. A wave with m angular nodes will change $2m$ times when going around a ring. So for a ring with $2m$ atoms this maximal sign change can be achieved by a function which transforms as $\cos(m\phi)$. As a result this function will transform irreducibly in the ideal point group C_{2m} and attain the highest ring quantum number allowed by that point group. For a ring with an odd number $2m+1$ of atoms, the irreducible representation with the highest ring quantum number in the point group would require a half-integral quantum number $m+1/2$, which is however a spinor representation instead of a real orbital representation. As a result the highest orbital quantum number in C_{2m+1} is also equal to m . Note however that this irrep will be twofold degenerate. This is confirmed by the observation of two 1 ι orbitals in Table 3.

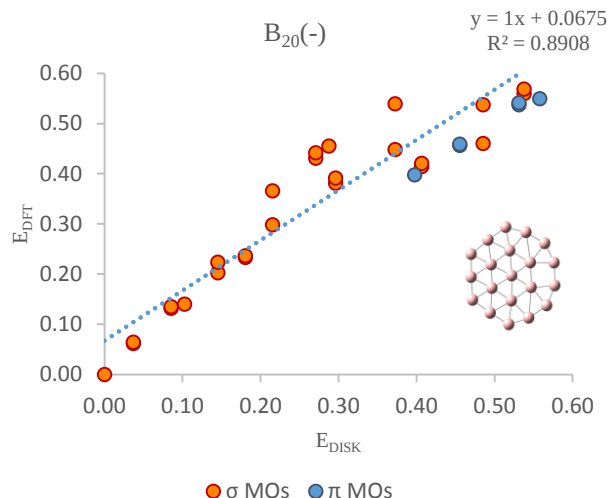


Figure 3. B₂₀(-): correlation between DFT orbital energies and particle-on-a-disk spectrum

1.3 Elongated B₁₆(0):

In Table 5 we list the orbital energies for B₁₆(0) with the corresponding rectangular quantum numbers. In spite of the crude model applied, the rectangular box provides a very accurate description of the spectrum. Both the principal series ($n_x, 1$) and ($1, n_y$) are present, as well as several combination modes. The highest longitudinal quantum number is equal to 6, while the transversal quantum number cannot exceed 4. The HOMO-4 and HOMO-6 have pronounced densities on the capping atoms and cannot be assigned with the rectangular quantum numbers.

Table 5. Orbital energies (Hartree), and rectangular quantum numbers for B₁₆(0)

B ₁₆ (0)					
σ	Label	E(Ha)	π	Label	E(Ha)
HOMO	3,4	0.62960	HOMO-1	2,2	0.59605
HOMO-4	?	0.47813	HOMO-2	1,2	0.53741
HOMO-5	2,4	0.46178	HOMO-3	3,1	0.51494
HOMO-6	?	0.41262	HOMO-9	2,1	0.28552
HOMO-7	6,2	0.38252	HOMO-13	1,1	0.22848
HOMO-8	1,4	0.32318			
HOMO-10	5,2	0.26436			
HOMO-11	3,3	0.25477			
HOMO-12	6,1	0.23823			
HOMO-14	4,3	0.21297			
HOMO-15	1,3	0.20976			
HOMO-16	4,2	0.19787			
HOMO-17	5,1	0.19573			
HOMO-18	3,2	0.15964			
HOMO-19	4,1	0.15589			
HOMO-20	2,2	0.14998			
HOMO-21	1,2	0.13143			
HOMO-22	3,1	0.12590			
HOMO-23	2,1	0.08278			

2. Correlation of DFT σ - and π - orbital energies and particle-on-a-disk spectrum.

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₇(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
17	HOMO-1	2 π	0.4806	2 π	0,4334
16	HOMO-2	2 π	0.4806	1 φ	0,3485
15	HOMO-3	1 φ	0.4410	1 φ	0,3485
14	HOMO-4	2 σ	0.4209	2 σ	0,2164
12	HOMO-6	1 δ	0.3733	1 δ	0,2054
11	HOMO-7	1 δ	0.3517	1 δ	0,2054
10	HOMO-8	1 π	0.1790	1 π	0,0769
9	HOMO-9	1 π	0.1501	1 π	0,0769
8	HOMO-10	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₇(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
18	HOMO	1 π	0.5357	1 π	0.4750
13	HOMO-5	1 σ	0.3837	1 σ	0,3837

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₇(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
12	HOMO	2 π	0.4901	2 π	0,7019
17	HOMO-1	2 π	0.4901	1 φ	0,5644
15	HOMO-2	1 φ	0.4385	1 φ	0,5644
14	HOMO-3	2 σ	0.4265	2 σ	0,3505
12	HOMO-5	1 δ	0.3532	1 δ	0,3327
11	HOMO-6	1 δ	0.3531	1 δ	0,3327
10	HOMO-7	1 π	0.1623	1 π	0,1245
9	HOMO-8	1 π	0.1623	1 π	0,1245
8	HOMO-9	1 σ	0,0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₇(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
13	HOMO-4	1 σ	0.3837	1 σ	0,3837

+

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₈(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
19	HOMO-2	2π	0.4539	2π	0.4413
18	HOMO-3	2π	0.4539	2π	0.4413
17	HOMO-4	1φ	0.3891	1φ	0.3548
16	HOMO-5	1φ	0.3891	1φ	0.3548
15	HOMO-6	2σ	0.3834	2σ	0.2508
13	HOMO-8	1δ	0.2910	1δ	0.2092
12	HOMO-9	1δ	0.2910	1δ	0.2092
11	HOMO-10	1π	0.1154	1π	0.0904
10	HOMO-11	1π	0.1154	1π	0.0904
9	HOMO-12	1σ	0.0000	1σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₈(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
21	HOMO	1π	0.4958	1π	0.4958
20	HOMO-1	1π	0.4958	1π	0.4958
14	HOMO-7	1σ	0.3742	1σ	0,3742

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₈(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
19	HOMO-1	2π	0.4462	2π	0,4089
18	HOMO-2	2π	0.4426	2π	0,4089
17	HOMO-3	2σ	0.3954	1φ	0,3288
16	HOMO-4	1φ	0.3713	1φ	0,3288
15	HOMO-5	1φ	0.3711	2σ	0,2042
13	HOMO-7	1δ	0.2789	1δ	0,1938
12	HOMO-8	1δ	0.2761	1δ	0,1938
11	HOMO-9	1π	0.1256	1π	0,0725
10	HOMO-10	1π	0.1176	1π	0,0725
9	HOMO-11	1σ	0.0000	1σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₈(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
20	HOMO	1π	0.4937	1π	0,4938
14	HOMO-6	1σ	0.3565	1σ	0.3565

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₈(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
19	HOMO-2	2 π	0,4447	2 π	0.4292
18	HOMO-3	2 π	0,4372	2 π	0.4292
17	HOMO-4	1 φ	0,3881	1 φ	0.3451
16	HOMO-5	1 φ	0,3880	1 φ	0.3451
14	HOMO-7	2 σ	0,3724	2 σ	0.2439
13	HOMO-8	1 δ	0,2911	1 δ	0.2034
12	HOMO-9	1 δ	0,2909	1 δ	0.2034
11	HOMO-10	1 π	0,1214	1 π	0.0879
10	HOMO-11	1 π	0,1120	1 π	0.0879
9	HOMO-12	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₈(-)	HOMO	DFT		Particle in circular box	
	O	Label	E(Ha)	Label	E(Ha)
21	HOMO	1 π	0,5042	1 π	0.4961
20	HOMO-1	1 π	0,4880	1 π	0.4961
15	HOMO-6	1 σ	0,3734	1 σ	0,3734

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₉(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
23	HOMO	!	0.5580	2 δ	0,5516
22	HOMO-1	2 π	0.5288	1 γ	0,4392
21	HOMO-2	2 π	0.5288	1 γ	0,4392
18	HOMO-5	2 σ	0.4564	1 φ	0,3682
17	HOMO-6	1 φ	0.4564	1 φ	0,3682
16	HOMO-7	1 φ	0.4166	2 σ	0,2961
14	HOMO-9	1 δ	0.3607	1 δ	0,1745
13	HOMO-10	1 δ	0.3606	1 δ	0,1745
12	HOMO-11	1 π	0.1764	1 π	0,0653
11	HOMO-12	1 π	0.1764	1 π	0,0653
10	HOMO-13	1 σ	0,0000	1 σ	0,0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₉(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
20	HOMO-3	1 π	0.4993	1 π	0.4993
19	HOMO-4	1 π	0.4993	1 π	0.4993
15	HOMO-10	1 σ	0.3577	1 σ	0.3577

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₉(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
21	HOMO-2	2 π	0,3993	1 γ	0,4016
20	HOMO-3	2 π	0,3993	2 π	0,3367
19	HOMO-4	1 γ	0,3630	2 π	0,3367
17	HOMO-6	2 σ	0,3225	1 ϕ	0,2707
16	HOMO-7	1 ϕ	0,3223	1 ϕ	0,2707
15	HOMO-8	1 ϕ	0,3223	2 σ	0,1914
14	HOMO-9	1 δ	0,2306	1 δ	0,1596
13	HOMO-10	1 δ	0,2306	1 δ	0,1596
12	HOMO-11	1 π	0,0951	1 π	0,0689
11	HOMO-12	1 π	0,0951	1 π	0,0689
10	HOMO-13	1 σ	0,0000	1 σ	0,0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₉(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
23	HOMO	1 π	0,4587	1 π	0,5692
22	HOMO-1	1 π	0,4587	1 π	0,5692
18	HOMO-5	1 σ	0,3630	1 σ	0,3630

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₂(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
30	HOMO	1 γ ,2 δ	0,5236	3 σ	0,5123
29	HOMO-1	1 γ ,2 δ	0,5236	2 δ	0,4823
26	HOMO-4	3 σ	0,4700	2 δ	0,4823
25	HOMO-5	2 π ,1 γ	0,4397	1 γ	0,3840
24	HOMO-6	2 π	0,4397	1 γ	0,3840
23	HOMO-7	2 π	0,4212	2 π	0,3220
22	HOMO-8	1 γ	0,4212	2 π	0,3220
20	HOMO-10	1 ϕ	0,3758	1 ϕ	0,2588
19	HOMO-11	1 ϕ	0,3288	1 ϕ	0,2588
18	HOMO-12	2 σ	0,2086	2 σ	0,1608
17	HOMO-13	1 δ	0,2052	1 δ	0,1523
16	HOMO-14	1 δ	0,2052	1 δ	0,1523
15	HOMO-15	1 π	0,0865	1 π	0,0571
14	HOMO-16	1 π	0,0865	1 π	0,0571
13	HOMO-17	1 σ	0,0000	1 σ	0,0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₂(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)

28	HOMO-2	1π	0,4942	1π	0.4961
27	HOMO-3	1π	0,4942	1π	0.4961
21	HOMO-9	1σ	0,3958	1σ	0,3958

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₂(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
30	HOMO	$1\gamma, 2\delta$	0.5210	3σ	0,5054
29	HOMO-1	$1\gamma, 2\delta$	0.5197	2δ	0,4759
26	HOMO-4	3σ	0.4677	2δ	0,4759
25	HOMO-5	$2\pi, 1\gamma$	0.4380	1γ	0,3788
24	HOMO-6	2π	0.4375	1γ	0,3788
23	HOMO-7	1γ	0.4168	2π	0,3176
22	HOMO-8	2π	0.4146	2π	0,3176
20	HOMO-10	1φ	0.3753	1φ	0,2554
19	HOMO-11	1φ	0.3293	1φ	0,2554
18	HOMO-12	2σ	0.2131	2σ	0,1586
17	HOMO-13	1δ	0.2088	1δ	0,1506
16	HOMO-14	1δ	0.2050	1δ	0,1506
15	HOMO-15	1π	0.0920	1π	0,0563
14	HOMO-16	1π	0.0870	1π	0,0563
13	HOMO-17	1σ	0.0000	1σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₂(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
28	HOMO-2	1π	0.5049	1π	0.5031
27	HOMO-3	1π	0.5012	1π	0.5031
21	HOMO-9	1σ	0.4026	1σ	0.4026

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₂(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
29	HOMO-1	$1\gamma, 2\delta$	0,5096	3σ	0,4321
28	HOMO-2	$1\gamma, 2\delta$	0,5028	2δ	0,4068
25	HOMO-5	3σ	0,3830	2δ	0,4068
24	HOMO-6	$2\pi, 1\gamma$	0,2649	1γ	0,3239
23	HOMO-7	2π	0,2238	1γ	0,3239
22	HOMO-8	1γ	0,2065	2π	0,2716
21	HOMO-9	2π	0,1753	2π	0,2716
19	HOMO-11	1φ	0,1585	1φ	0,2184
18	HOMO-12	1φ	0,1567	1φ	0,2184
17	HOMO-13	2σ	0,1319	2σ	0,1543
16	HOMO-14	1δ	0,1110	1δ	0,1287

15	HOMO-15	1 δ	0,1109	1 δ	0,1287
14	HOMO-16	1 π	0,0821	1 π	0,0556
13	HOMO-17	1 π	0,0764	1 π	0,0556
12	HOMO-18	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₂(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
30	HOMO	1 δ	0,5956	1 δ	0.5910
27	HOMO-3	1 π	0,3946	1 π	0.3548
26	HOMO-4	1 π	0,3872	1 π	0.3548
20	HOMO-10	1 σ	0,1750	1 σ	0,1750

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₃(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
32	HOMO	2 δ	0.5033	1 η	0,5248
31	HOMO-1	2 δ	0.4850	3 σ	0,4049
28	HOMO-4	3 σ	0.4490	2 δ	0,3812
27	HOMO-5	1 η	0.4193	2 δ	0,3812
26	HOMO-6	2 π	0.4074	1 γ	0,3035
25	HOMO-7	2 π	0.4070	1 γ	0,3035
23	HOMO-9	1 γ	0.3810	2 π	0,2545
22	HOMO-10	1 γ	0.3804	2 π	0,2545
21	HOMO-11	1 ϕ	0.3194	1 ϕ	0,2046
20	HOMO-12	1 ϕ	0.2842	1 ϕ	0,2046
19	HOMO-13	2 σ	0.1861	2 σ	0,1271
18	HOMO-14	1 δ	0.1754	1 δ	0,1260
17	HOMO-15	1 δ	0.1744	1 δ	0,1206
16	HOMO-16	1 π	0.0779	1 π	0,0452
15	HOMO-17	1 π	0.0677	1 π	0,0452
14	HOMO-18	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₃(+)	HOMO	DFT		Particle in circular box	
	O	Label	E(Ha)	Label	E(Ha)
30	HOMO-2	1 π	0.4749	1 π	0.4726
29	HOMO-3	1 π	0.4703	1 π	0.4726
24	HOMO-8	1 σ	0.3848	1 σ	0.3848

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₄(0) 2nd stable	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
34	HOMO-1	2 δ	0.5298	1 η	0,4918
33	HOMO-2	3 π ,1 η	0.5188	1 η	0,4918
30	HOMO-4	1 γ ,2 δ	0.4758	3 σ	0,4776
29	HOMO-6	3 σ	0.4586	2 δ	0,4497
28	HOMO-7	1 η	0.4473	2 δ	0,4497
27	HOMO-8	2 π	0.4233	1 γ	0,3580
26	HOMO-9	1 γ	0.4225	1 γ	0,3580
25	HOMO-10	1 ϕ ,2 π	0.3931	2 π	0,3002
24	HOMO-12	1 γ	0.3907	2 π	0,3002
22	HOMO-13	1 ϕ	0.2865	1 ϕ	0,2414
21	HOMO-14	1 ϕ	0.2556	1 ϕ	0,2414
20	HOMO-15	2 σ	0.2135	2 σ	0,1706
19	HOMO-16	1 δ	0.1941	1 δ	0,1423
18	HOMO-17	1 δ	0.1457	1 δ	0,1423
17	HOMO-18	1 π	0.0922	1 π	0,0615
16	HOMO-19	1 π	0.0701	1 π	0,0615
15	HOMO-20	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₄(0) O	HOM O	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
35	HOMO	1 δ	0.5620	1 δ	0.5596
32	HOMO-3	1 π	0.4987	1 π	0.4652
30	HOMO-5	1 π	0.4754	1 π	0.4652
24	HOMO-11	1 σ	0.3909	1 σ	0.3909

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₄(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
34	HOMO-1	2 δ	0.5363	1 η	0,4922
33	HOMO-2	3 π ,1 η	0.5220	1 η	0,4922
30	HOMO-5	2 δ	0.4765	3 σ	0,4803
29	HOMO-6	3 σ	0.4637	2 δ	0,4522
28	HOMO-7	1 η	0.4490	2 δ	0,4522
27	HOMO-8	2 π	0.4283	1 γ	0,3600
26	HOMO-9	1 γ	0.4225	1 γ	0,3600
25	HOMO-10	1 γ	0.3961	2 π	0,3019
24	HOMO-11	2 π	0.3959	2 π	0,3019
22	HOMO-13	1 ϕ	0.2950	1 ϕ	0,2427
21	HOMO-14	1 ϕ	0.2569	1 ϕ	0,2427
20	HOMO-15	2 σ	0.2093	2 σ	0,1716
19	HOMO-16	1 δ	0.1993	1 δ	0,1431
18	HOMO-17	1 δ	0.1460	1 δ	0,1431

17	HOMO-18	1π	0.0958	1π	0,0618
16	HOMO-19	1π	0.0702	1π	0,0618
15	HOMO-20	1σ	0.0000	1σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₄(+)	HOMO	DFT		Particle in circular box	
	O				
		Label	E(Ha)	Label	E(Ha)
35	HOMO	1δ	0.5642	1δ	0.5608
32	HOMO-3	1π	0.5067	1π	0.4756
31	HOMO-4	1π	0.4766	1π	0.4518
23	HOMO-12	1σ	0.3935	1σ	0.3935

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₄(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
36	HOMO	$1\eta, 2\phi$	0.5885	2ϕ	0,5937
34	HOMO-2	2δ	0.5234	1η	0,4720
33	HOMO-3	$1\eta, 3\pi$	0.5116	1η	0,4720
30	HOMO-6	2δ	0.4660	3σ	0,4584
29	HOMO-7	3σ	0.4558	2δ	0,4316
28	HOMO-8	1η	0.4490	2δ	0,4316
27	HOMO-9	2π	0.4241	1γ	0,3279
26	HOMO-10	1γ	0.4208	1γ	0,3279
25	HOMO-11	2π	0.3990	2π	0,2881
24	HOMO-12	1γ	0.3929	2π	0,2881
22	HOMO-14	1ϕ	0.2867	1ϕ	0,2317
21	HOMO-15	1ϕ	0.2539	1ϕ	0,2317
20	HOMO-16	2σ	0.2115	2σ	0,1637
19	HOMO-17	1δ	0.1890	1δ	0,1366
18	HOMO-18	1δ	0.1474	1δ	0,1366
17	HOMO-19	1π	0.0892	1π	0,0590
16	HOMO-20	1π	0.0680	1π	0,0590
15	HOMO-21	1σ	0.0000	1σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₄(-)	HOMO	DFT		Particle in circular box	
	O				
		Label	E(Ha)	Label	E(Ha)
35	HOMO-1	1δ	0.5610	1δ	0.5582
32	HOMO-3	1π	0.4926	1π	0.4580
31	HOMO-4	1π	0.4667	1π	0.4580
23	HOMO-13	1σ	0.3821	1σ	0.3821

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₅(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
38	HOMO	1 η ,2 φ	0.5620	2 φ	0,5296
36	HOMO-2	2 φ	0.5011	2 φ	0,5296
35	HOMO-3	2 δ	0.4824	1 η	0,4211
32	HOMO-6	1 π ,2 δ	0.4497	1 η	0,4211
31	HOMO-7	3 σ	0.4375	3 σ	0,4089
30	HOMO-8	1 η	0.4232	2 δ	0,3850
29	HOMO-9	1 η	0.4205	2 δ	0,3850
27	HOMO-10	2 π	0.4065	1 γ	0,3051
26	HOMO-12	1 γ ,2 π	0.3689	1 γ	0,3051
25	HOMO-13	1 γ	0.3610	2 π	0,2570
24	HOMO-14	1 γ	0.3518	2 π	0,2570
23	HOMO-15	1 φ	0.2510	1 φ	0,2066
22	HOMO-16	1 φ	0.2299	1 φ	0,2066
21	HOMO-17	2 σ	0.1904	2 σ	0,1461
20	HOMO-18	1 δ	0.1708	1 δ	0,1218
19	HOMO-19	1 δ	0.1264	1 δ	0,1218
18	HOMO-20	1 π	0.0809	1 π	0,0526
17	HOMO-21	1 π	0.0567	1 π	0,0526
16	HOMO-22	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₅(0)	HOM O	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
37	HOMO-1	1 δ	0.5449	1 δ	0.5363
34	HOMO-4	1 π	0.4623	1 π	0.4784
33	HOMO-5	1 π	0.4409	1 π	0.4511
27	HOMO-11	1 σ	0.3845	1 σ	0.3845

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₅(+)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
36	HOMO-1	2 φ	0.5121	2 φ	0,5407
35	HOMO-2	3 σ ,2 δ	0.4898	1 η	0,4299
32	HOMO-5	2 δ	0.4591	1 η	0,4299
31	HOMO-6	3 σ	0.4444	3 σ	0,4175
30	HOMO-7	1 η	0.4275	2 δ	0,3931
29	HOMO-8	1 η	0.4201	2 δ	0,3931
28	HOMO-9	2 π	0.4122	1 γ	0,3130
26	HOMO-11	1 γ ,2 π	0.3706	1 γ	0,3130
25	HOMO-12	2 π , 1 γ	0.3586	2 π	0,2624
24	HOMO-13	1 γ	0.3573	2 π	0,2624
23	HOMO-14	1 φ	0.2532	1 φ	0,2120
22	HOMO-15	1 φ	0.2286	1 φ	0,2120
21	HOMO-16	2 σ	0.1885	2 σ	0,1491

20	HOMO-17	1 δ	0.1717	1 δ	0,1244
19	HOMO-18	1 δ	0.1284	1 δ	0,1244
18	HOMO-19	1 π	0.0793	1 π	0,0537
17	HOMO-20	1 π	0.0608	1 π	0,0537
16	HOMO-21	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₅(+)	HOMO	DFT		Particle in circular box	
	O				
		Label	E(Ha)	Label	E(Ha)
37	HOMO	1 δ	0.5378	1 δ	0.5409
34	HOMO-3	1 π	0.4625	1 π	0.4835
33	HOMO-4	1 π	0.4387	1 π	0.4604
27	HOMO-10	1 σ	0.3863	1 σ	0.3863

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₅(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
38	HOMO-1	1 η ,2 ϕ	0.5523	2 ϕ	0,5210
36	HOMO-2	2 δ ,2 ϕ	0.4934	2 ϕ	0,5210
35	HOMO-3	1 π ,2 δ	0.4772	1 η	0,4142
32	HOMO-6	1 π ,2 δ	0.4435	1 η	0,4142
31	HOMO-7	3 σ	0.4319	3 σ	0,4023
30	HOMO-8	1 η	0.4195	2 δ	0,3788
29	HOMO-9	1 η	0.4168	2 δ	0,3788
28	HOMO-10	2 π	0.4043	1 γ	0,3015
26	HOMO-12	1 γ ,2 π	0.3663	1 γ	0,3015
25	HOMO-13	1 γ	0.3603	2 π	0,2528
24	HOMO-14	1 γ	0.3477	2 π	0,2528
23	HOMO-15	1 ϕ	0.2508	1 ϕ	0,2033
22	HOMO-16	1 ϕ	0.2290	1 ϕ	0,2033
21	HOMO-17	2 σ	0.1925	2 σ	0,1437
20	HOMO-18	1 δ	0.1726	1 δ	0,1198
19	HOMO-19	1 δ	0.1235	1 δ	0,1198
18	HOMO-20	1 π	0.0810	1 π	0,0518
17	HOMO-21	1 π	0.0544	1 π	0,0518
16	HOMO-22	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₅(-)	HOMO	DFT		Particle in circular box	
	O				
		Label	E(Ha)	Label	E(Ha)
37	HOMO-1	1 δ	0.5300	1 δ	0.5288
34	HOMO-3	1 π	0.4734	1 π	0.4529
33	HOMO-4	1 π	0.4450	1 π	0.4351
27	HOMO-11	1 σ	0.3892	1 σ	0.3892

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₈(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
42	HOMO-3	2 σ ,3 π	0.5288	3 π	0,5429
41	HOMO-4	3 π	0.5288	3 π	0,5429
40	HOMO-5	2 φ	0.5255	2 φ	0,4972
39	HOMO-6	2 φ	0.4902	2 φ	0,4972
38	HOMO-7	1 η ,2 δ	0.4902	1 η	0,3949
35	HOMO-10	3 σ	0.4665	1 η	0,3949
34	HOMO-11	3 σ ,1 η	0.4584	3 σ	0,3835
33	HOMO-12	2 δ	0.4404	2 δ	0,3616
32	HOMO-13	1 η	0.4404	2 δ	0,3616
30	HOMO-15	1 γ	0.3741	1 γ	0,2874
29	HOMO-16	1 γ	0.3741	1 γ	0,2874
28	HOMO-17	2 π	0.2634	2 π	0,2410
27	HOMO-18	2 π	0.2634	2 π	0,2410
26	HOMO-19	1 φ	0.2618	1 φ	0,1938
25	HOMO-20	1 φ	0.2455	1 φ	0,1938
24	HOMO-21	2 σ	0.1494	2 σ	0,1203
23	HOMO-22	1 δ	0.1487	1 δ	0,1142
22	HOMO-23	1 δ	0.1487	1 δ	0,1142
21	HOMO-24	1 π	0.0629	1 π	0,0427
20	HOMO-25	1 π	0.0629	1 π	0,0427
19	HOMO-26	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₈(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
45	HOMO	1 δ	0.5797	2 σ	0.5723
44	HOMO-1	1 δ	0.5797	1 δ	0.5633
43	HOMO-2	2 σ	0.5520	1 δ	0.5633
37	HOMO-8	1 π	0.4670	1 π	0.4574
36	HOMO-9	1 π	0.4670	1 π	0.4574
31	HOMO-14	1 σ	0.3942	1 σ	0.3942

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₉(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
48	HOMO	2 γ	0.5658	2 γ	0.5450
44	HOMO-4	1 η ,2 φ	0.5079	2 γ	0.5450
43	HOMO-5	3 π	0.5010	3 π	0.4566
42	HOMO-6	3 π	0.4834	3 π	0.4566
39	HOMO-9	1 π ,2 φ	0.4497	2 φ	0.4181
38	HOMO-10	2 γ	0.4496	2 φ	0.4181
37	HOMO-11	1 η	0.4343	1 η	0.3325

36	HOMO-12	1 η , 1 ι	0.4338	1 η	0.3325
35	HOMO-13	3 σ	0.4249	3 σ	0.3229
34	HOMO-14	2 δ	0.4154	2 δ	0.3040
32	HOMO-16	2 δ	0.3782	2 δ	0.3040
31	HOMO-17	1 γ	0.3514	1 γ	0.2420
30	HOMO-18	1 γ	0.3314	1 γ	0.2420
29	HOMO-19	2 π	0.2410	2 π	0.2029
28	HOMO-20	2 π	0.2391	2 π	0.2029
27	HOMO-21	1 φ	0.2339	1 φ	0.1632
26	HOMO-22	1 φ	0.2251	1 φ	0.1632
25	HOMO-23	1 δ	0.1423	2 σ	0.1154
24	HOMO-24	1 δ	0.1374	1 δ	0.0962
23	HOMO-25	2 σ	0.1307	1 δ	0.0962
22	HOMO-26	1 π	0.0670	1 π	0.0416
21	HOMO-27	1 π	0.0552	1 π	0.0416
20	HOMO-28	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₉(0)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
47	HOMO-1	1 δ	0.5419	1 δ	0.5542
46	HOMO-2	1 δ	0.5482	1 δ	0.5256
45	HOMO-3	2 σ	0.5330	2 σ	0.5256
40	HOMO-7	1 π	0.4621	1 π	0.4441
39	HOMO-8	1 π	0.4567	1 π	0.4441
33	HOMO-15	1 σ	0.3820	1 σ	0.3820

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

B₁₉(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
48	HOMO-3	2 φ	0.5060	3 π	0,4839
44	HOMO-4	2 φ	0.5019	3 π	0,4839
43	HOMO-6	3 π	0.4444	1 ι	0,4054
42	HOMO-8	3 π	0.4416	1 ι	0,4052
39	HOMO-9	2 δ	0.4187	2 φ	0,3713
38	HOMO-10	2 δ	0.4166	2 φ	0,3713
37	HOMO-11	1 ι	0.4159	1 η	0,2952
36	HOMO-12	1 ι	0.4147	1 η	0,2952
35	HOMO-13	3 σ	0.4136	3 σ	0,2867
34	HOMO-14	1 η	0.3742	2 δ	0,2699
32	HOMO-16	1 η	0.3691	2 δ	0,2699
31	HOMO-17	1 γ	0.3181	1 γ	0,2149
30	HOMO-18	1 γ	0.3083	1 γ	0,2149
29	HOMO-19	2 π	0.2293	2 π	0,1802
28	HOMO-20	2 π	0.2250	2 π	0,1802
27	HOMO-21	1 φ	0.2158	1 φ	0,1448
26	HOMO-22	1 φ	0.2149	1 φ	0,1448

25	HOMO-23	1 δ	0.1293	2 σ	0,1024
24	HOMO-24	1 δ	0.1281	1 δ	0,0854
23	HOMO-25	2 σ	0.1248	1 δ	0,0854
22	HOMO-26	1 π	0.0656	1 π	0,0369
21	HOMO-27	1 π	0.0582	1 π	0,0369
20	HOMO-28	1 σ	0.0000	1 σ	0.0000

Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

B₁₉(-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
47	HOMO	2 σ	0.5232	2 σ	0.5280
46	HOMO-1	1 δ	0.5209	1 δ	0.5015
45	HOMO-2	1 δ	0.5195	1 δ	0.5015
40	HOMO-5	1 π	0.4463	1 π	0.4257
39	HOMO-7	1 π	0.4423	1 π	0.4257
33	HOMO-15	1 σ	0.3730	1 σ	0.3730

Correlation of DFT σ -orbital energies and particle-on-a-disk spectrum.

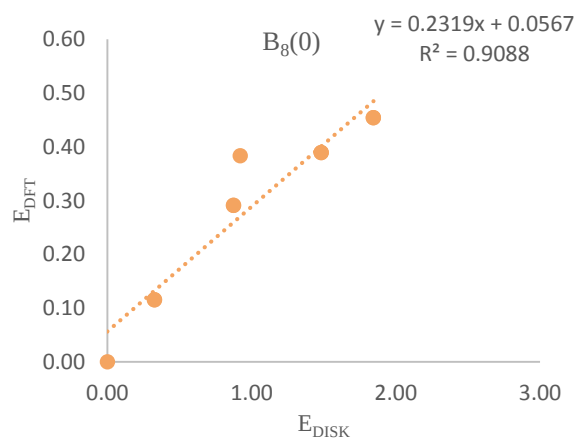
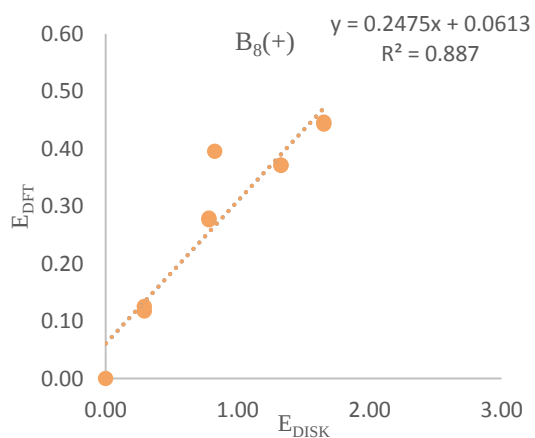
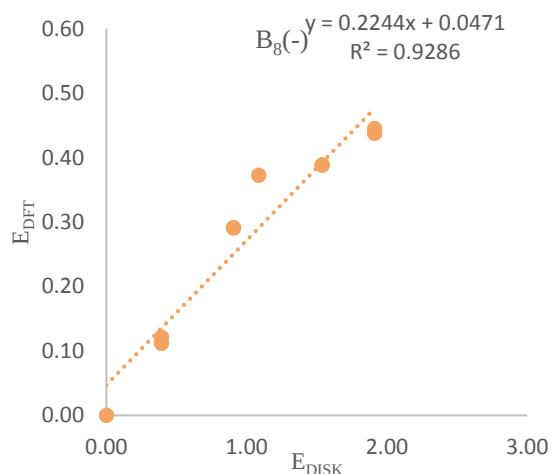
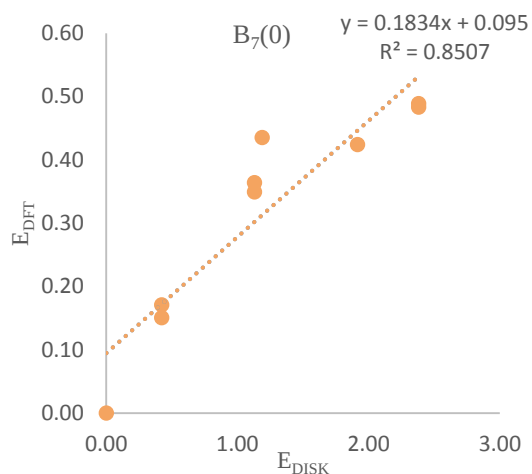
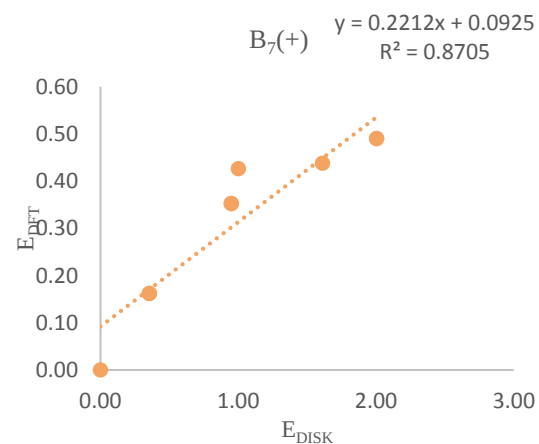
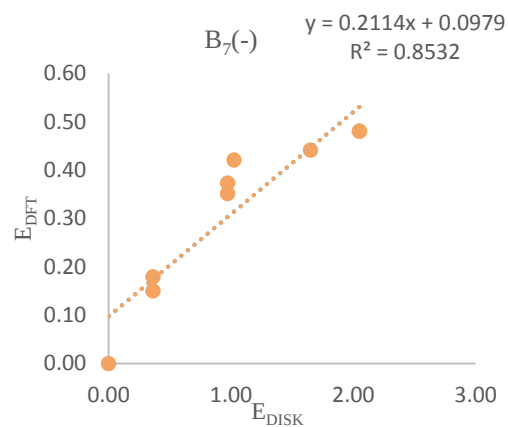
B₂₀(2-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
51	HOMO	3 π ,2 γ	0.5699	2 γ	0,5336
50	HOMO-1	1 ι ,2 γ	0.5658	2 γ	0,5336
46	HOMO-5	2 ϕ	0.5267	3 π	0,4816
45	HOMO-6	3 π	0.4564	3 π	0,4816
44	HOMO-7	3 π	0.4561	1 ι	0,4035
43	HOMO-8	2 ϕ	0.4519	1 ι	0,4035
40	HOMO-11	1 ι	0.4416	2 ϕ	0,3695
39	HOMO-12	1 ι	0.4381	2 ϕ	0,3695
38	HOMO-13	3 σ	0.4254	1 η	0,2938
37	HOMO-14	2 δ	0.4143	1 η	0,2938
36	HOMO-15	2 δ	0.4137	3 σ	0,2853
35	HOMO-16	1 η	0.3906	2 δ	0,2686
34	HOMO-17	1 η	0.3890	2 δ	0,2686
32	HOMO-19	1 γ	0.2935	1 γ	0,2129
31	HOMO-20	1 γ	0.2933	1 γ	0,2129
30	HOMO-21	2 π	0.2317	2 π	0,1793
29	HOMO-22	2 π	0.2314	2 π	0,1793
28	HOMO-23	1 ϕ	0.2189	1 ϕ	0,1442
27	HOMO-24	1 ϕ	0.1989	1 ϕ	0,1442
26	HOMO-25	2 σ	0.1353	2 σ	0,1019
25	HOMO-26	1 δ	0.1293	1 δ	0,0850
24	HOMO-27	1 δ	0.1289	1 δ	0,0850
23	HOMO-28	1 π	0.0633	1 π	0,0367
22	HOMO-29	1 π	0.0583	1 π	0,0367
21	HOMO-30	1 σ	0.0000	1 σ	0.0000

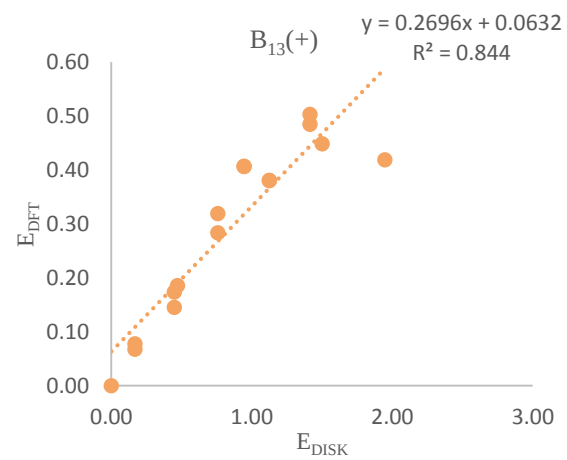
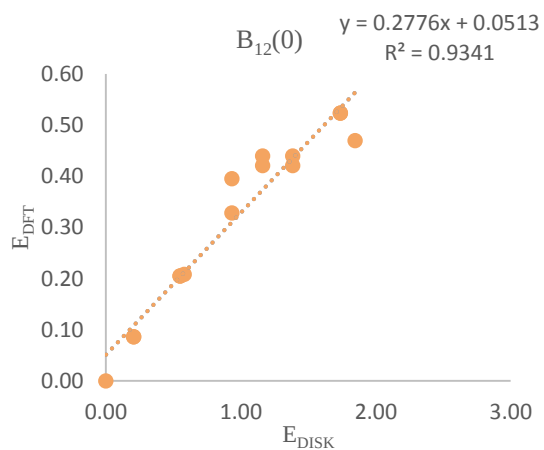
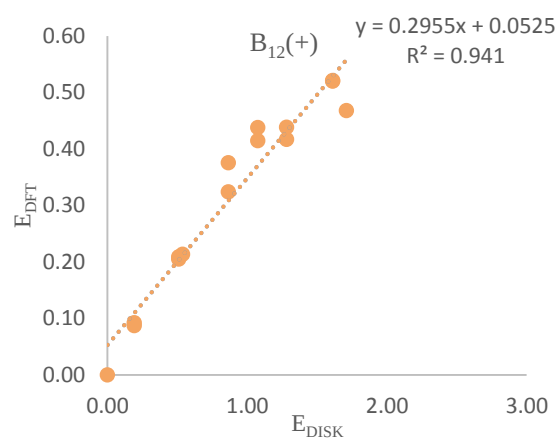
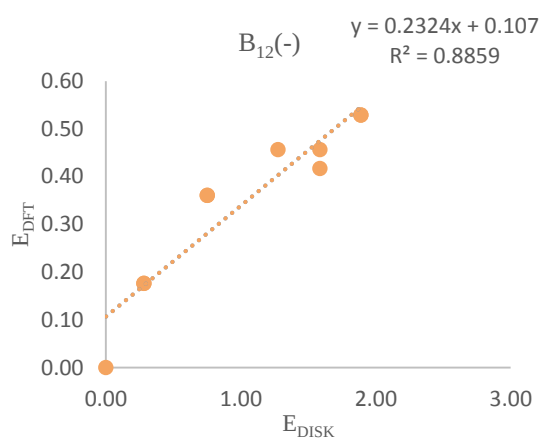
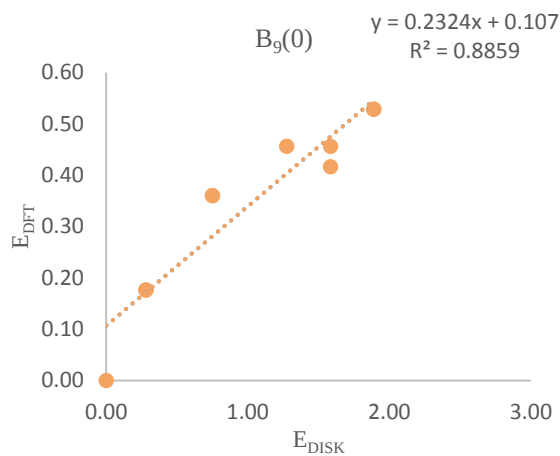
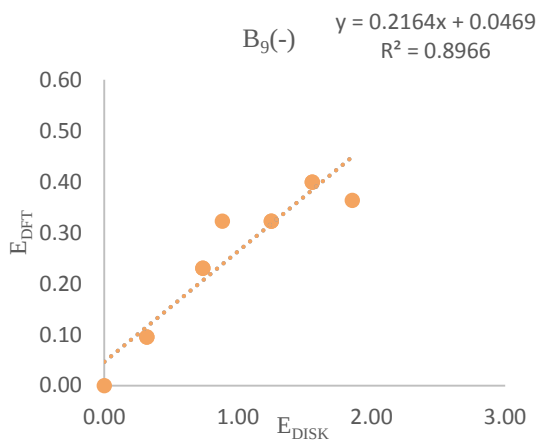
Correlation of DFT π -orbital energies and particle-on-a-disk spectrum.

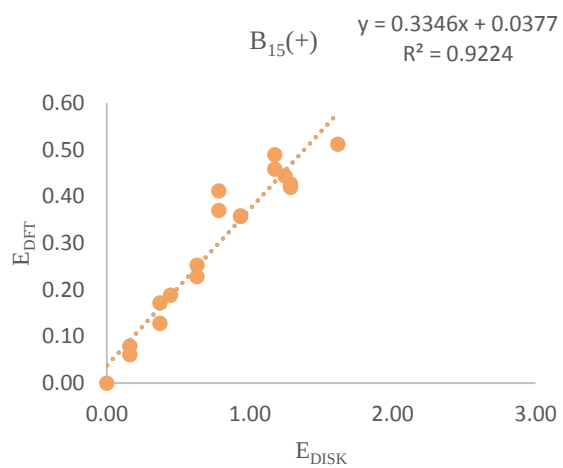
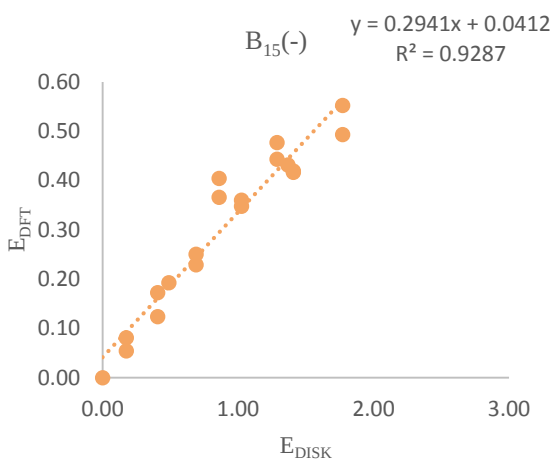
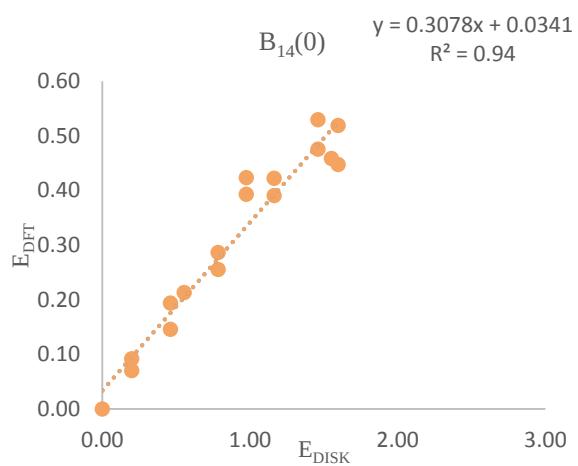
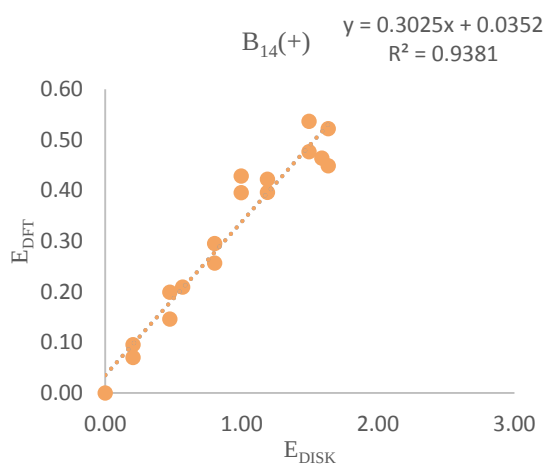
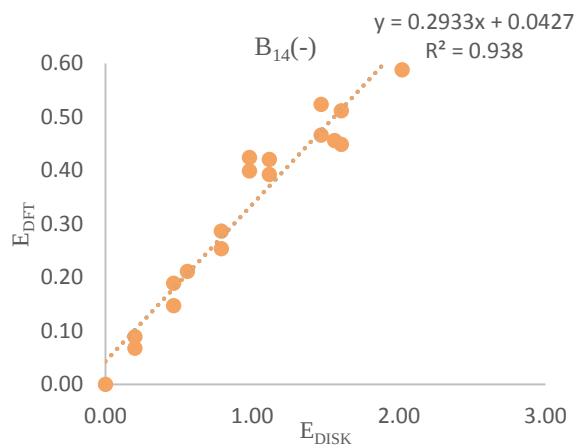
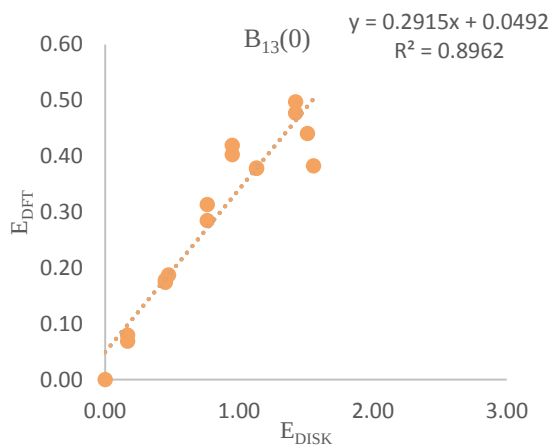
B₂₀(2-)	HOMO	DFT		Particle in circular box	
		Label	E(Ha)	Label	E(Ha)
49	HOMO-2	2 σ	0.5386	2 σ	0.5441
48	HOMO-3	1 δ	0.5303	1 δ	0.4948
47	HOMO-4	1 δ	0.5302	1 δ	0.4750
42	HOMO-9	1 π	0.4489	1 π	0.4186
41	HOMO-10	1 π	0.4459	1 π	0.4186
33	HOMO-18	1 σ	0.3758	1 σ	0.3758

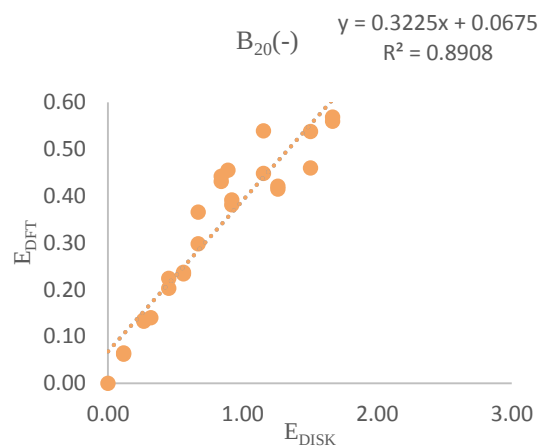
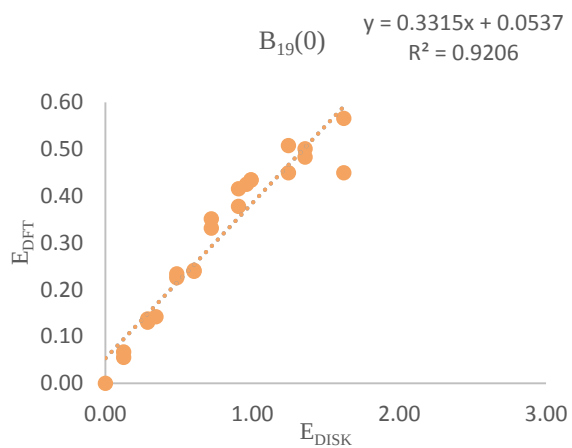
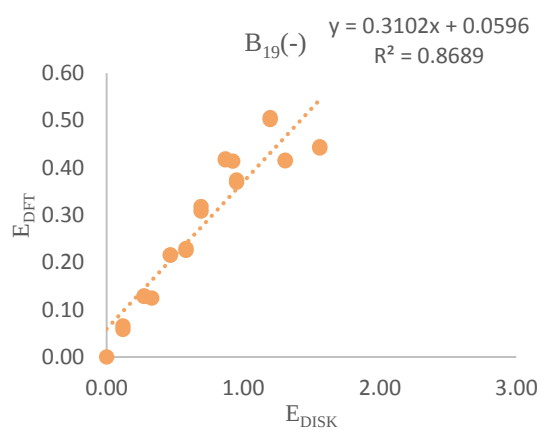
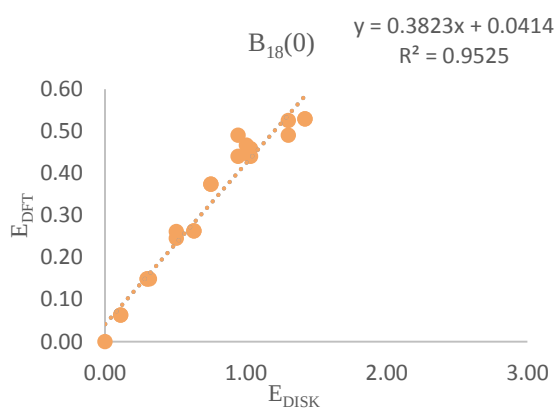
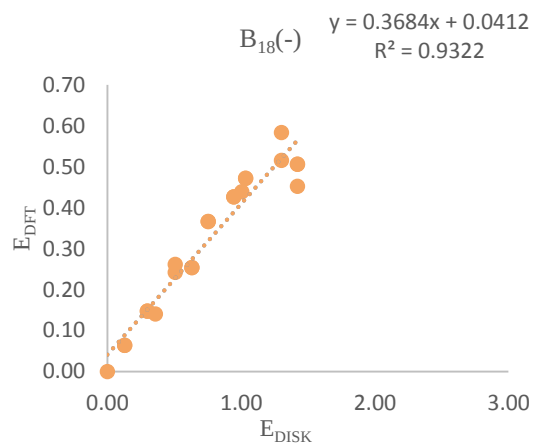
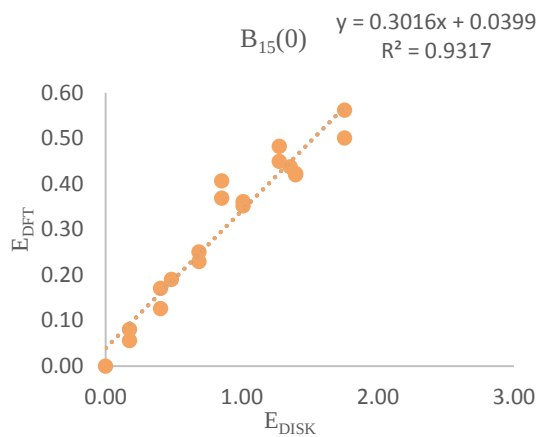
3. Diagrams of the correlation of DFT σ - and π -orbital energies and particle-on-a-disk spectrum.

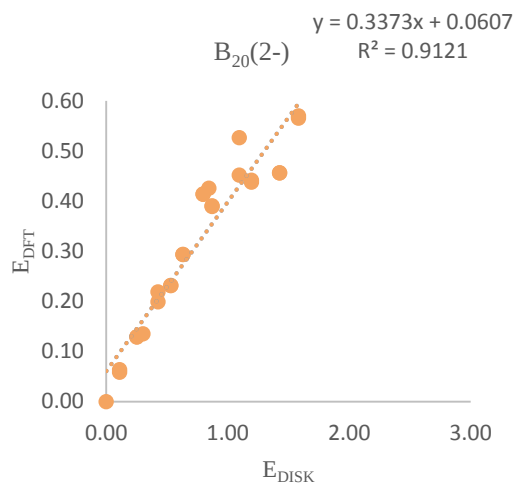
I. Correlated



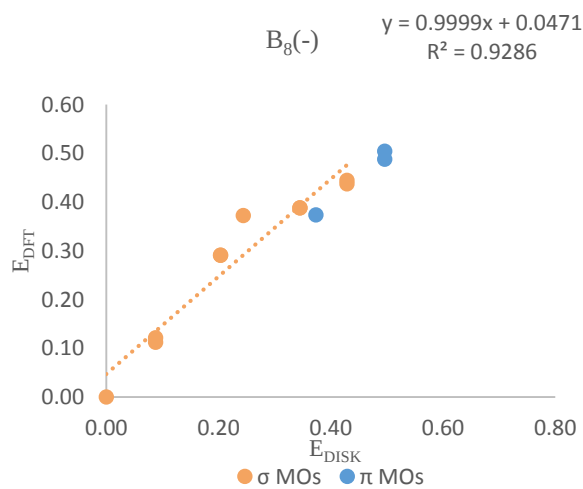
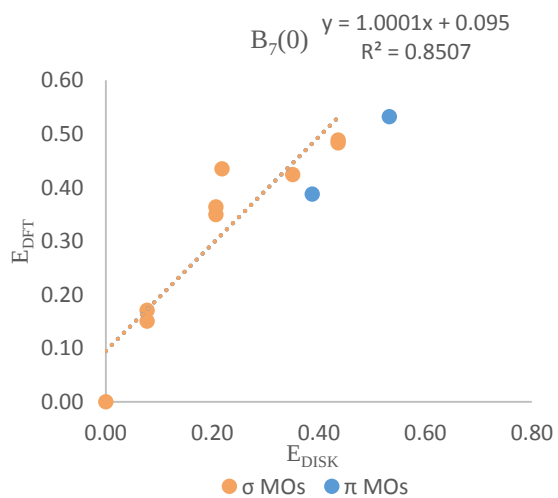
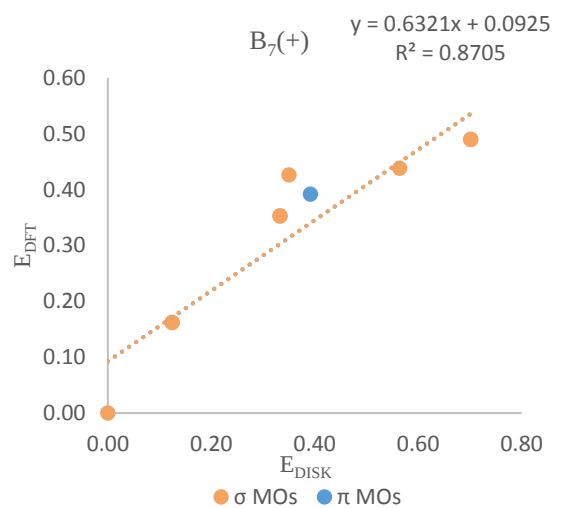
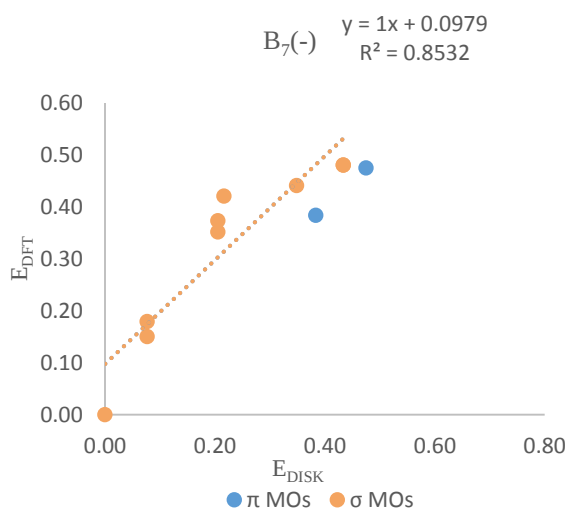


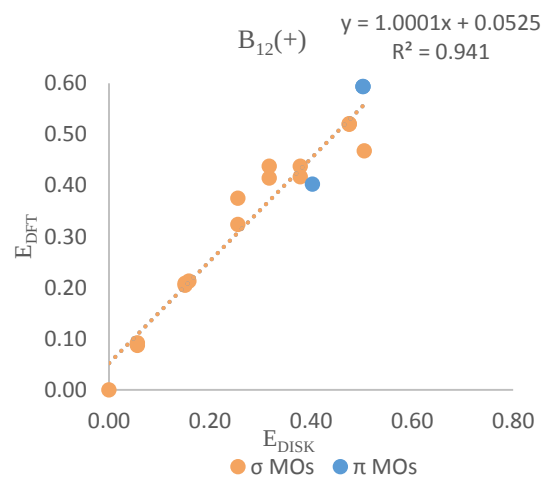
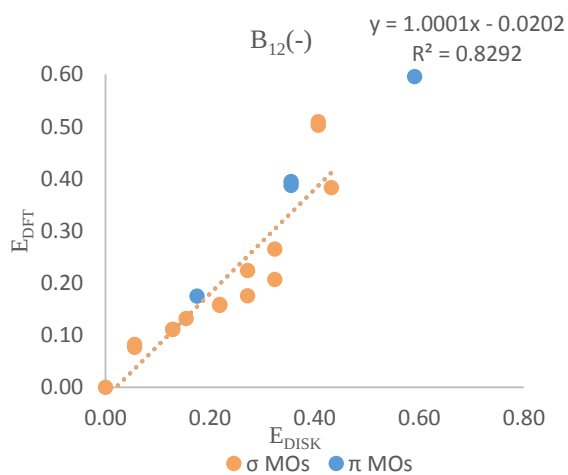
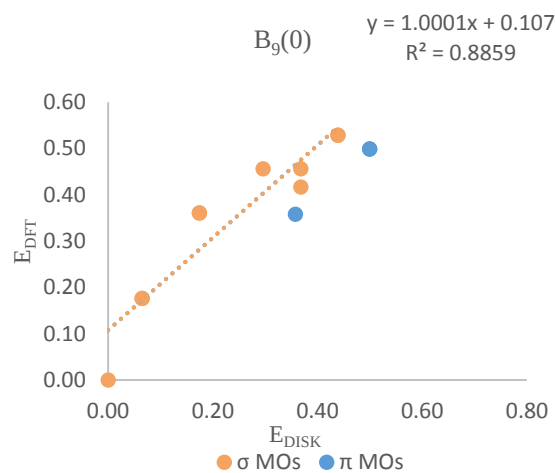
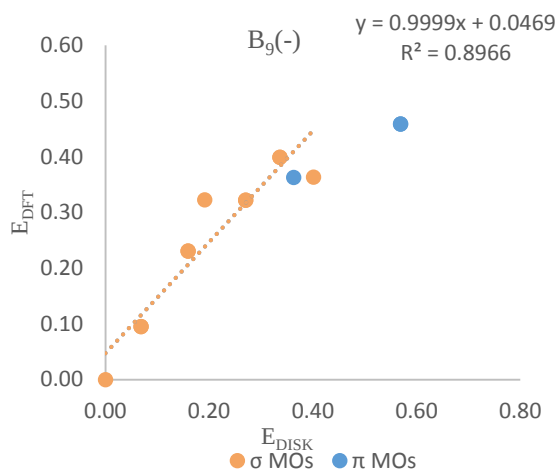
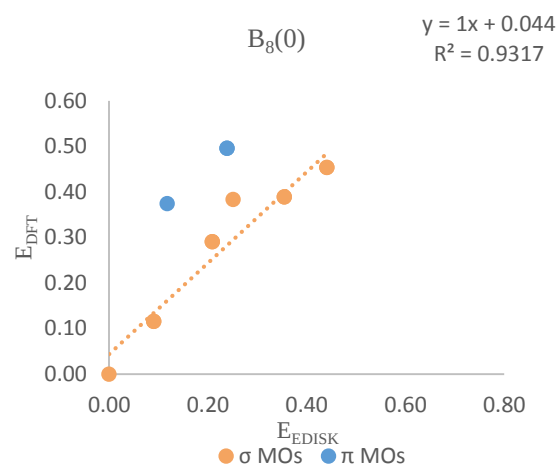
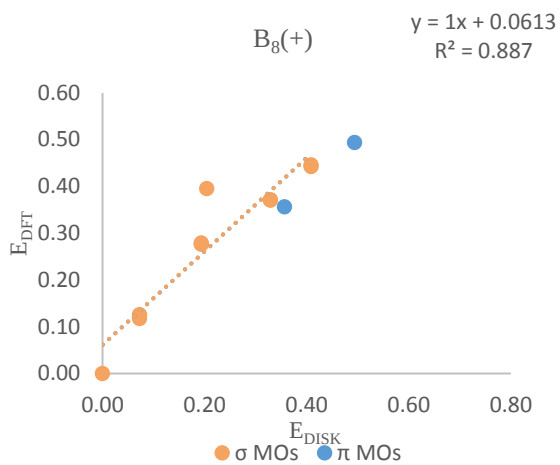


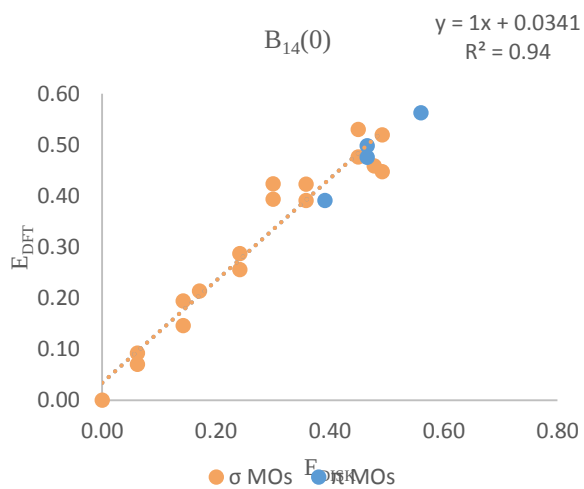
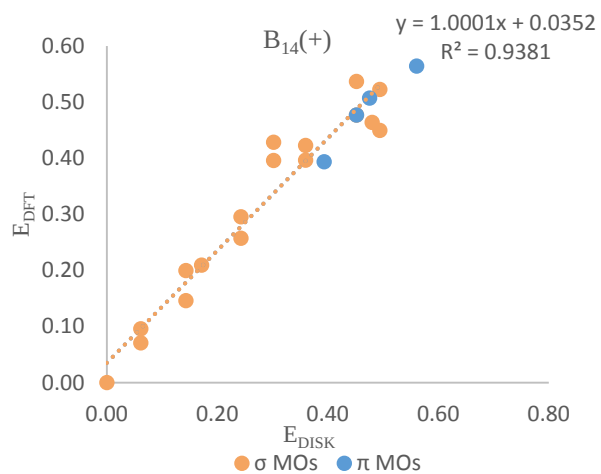
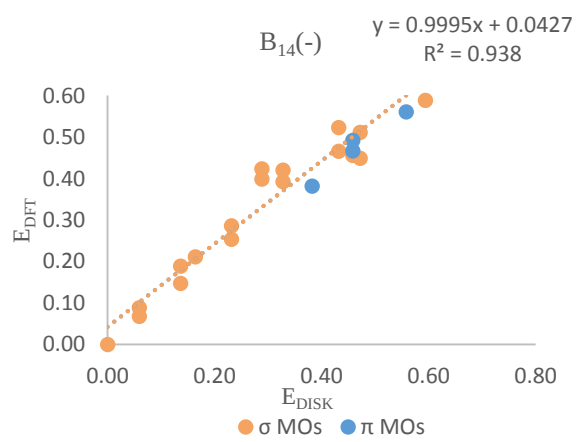
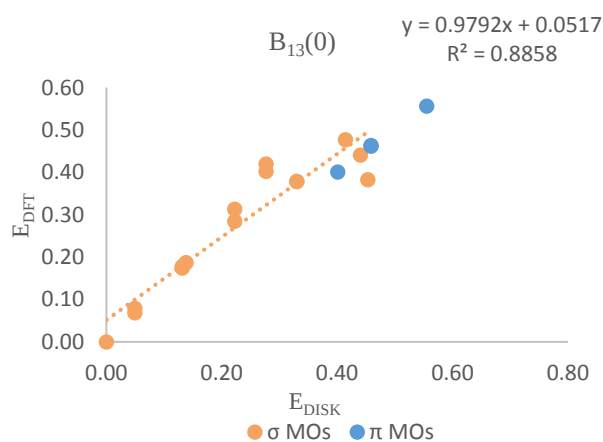
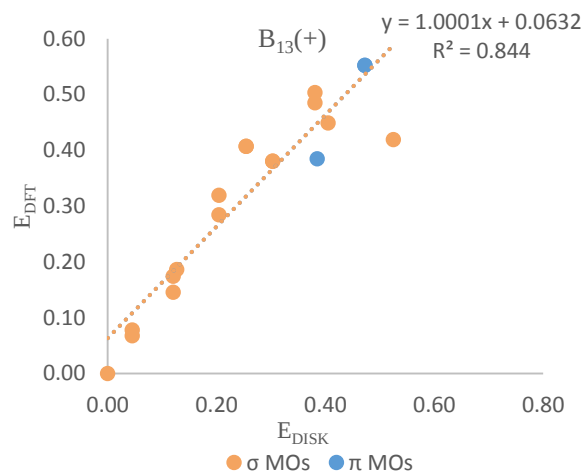
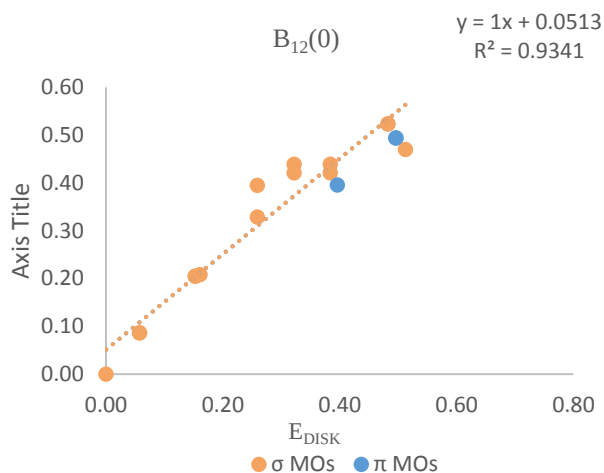


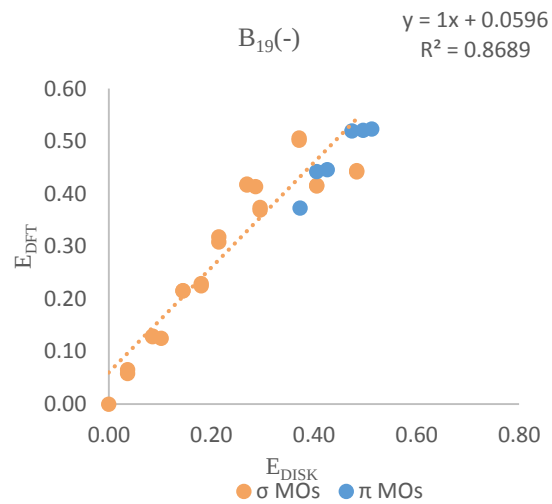
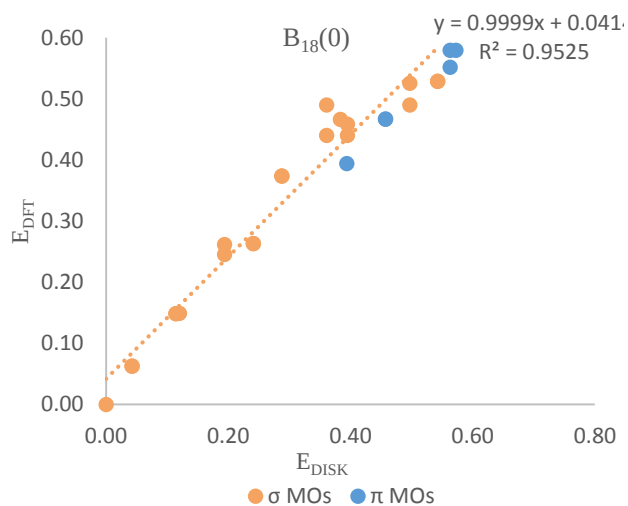
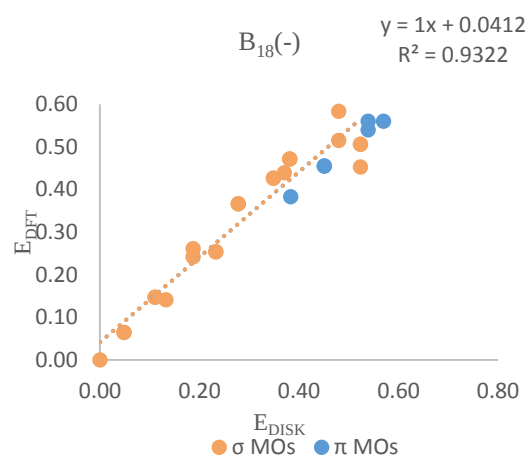
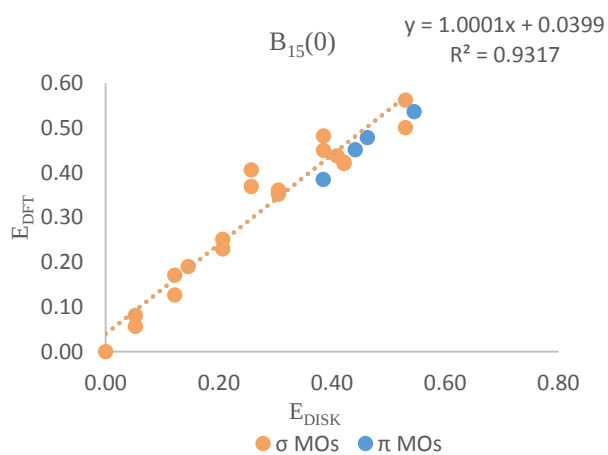
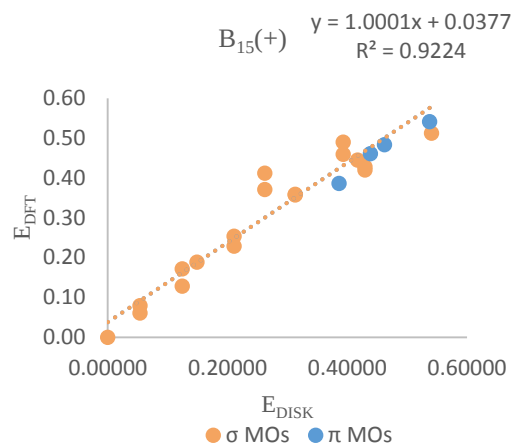
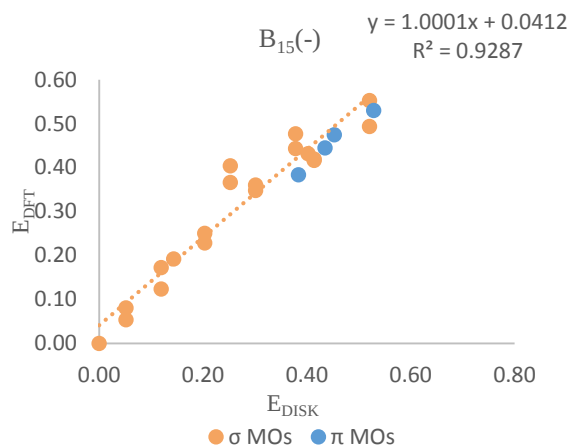


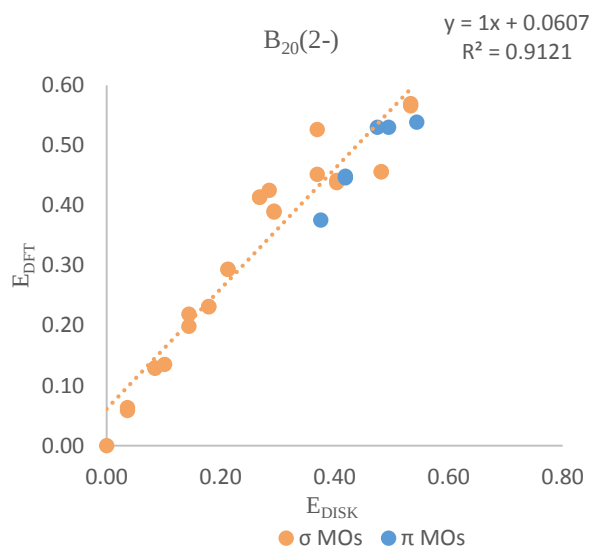
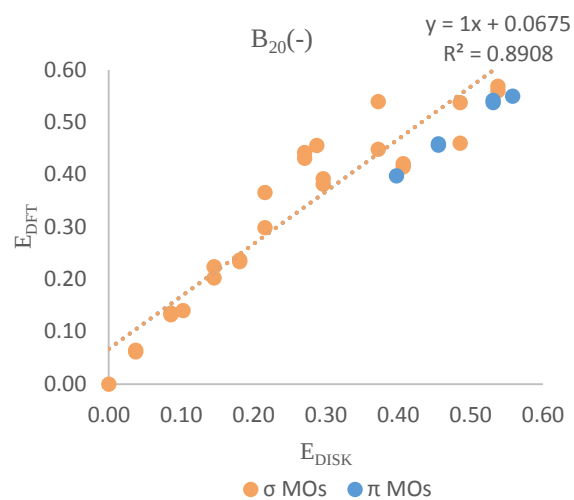
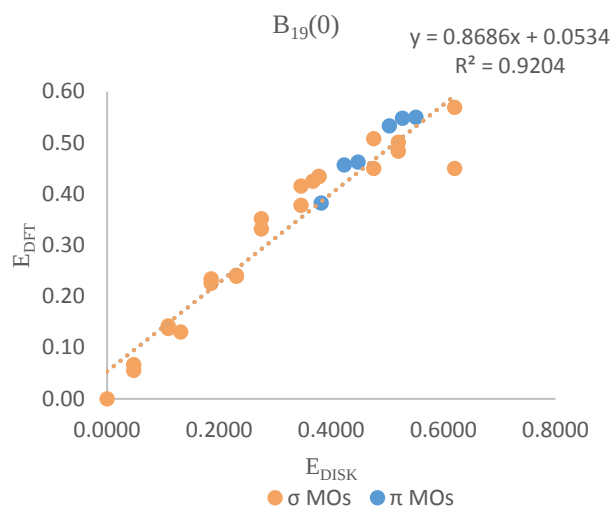
II. Sloped diagrams











4. XYZ Coordinates of boron clusters

B₇(0)

0 2

B	0.00000000	0.00000000	0.56130500
B	0.00000000	1.66989500	0.05365800
B	1.31388000	0.81705300	-0.16715500
B	1.31388000	-0.81705300	-0.16715500
B	-1.31388000	0.81705300	-0.16715500
B	-1.31388000	-0.81705300	-0.16715500
B	0.00000000	-1.66989500	0.05365800

B₇(+)

1 1

B	0.00000000	0.00000000	0.61577400
B	0.00000000	1.58360000	-0.10259700
B	1.37131700	0.79175100	-0.10264500
B	1.37131700	-0.79175100	-0.10264500
B	-1.37131700	0.79175100	-0.10264500
B	-1.37131700	-0.79175100	-0.10264500
B	0.00000000	-1.58360000	-0.10259700

B₇(-)

-1 1

B	0.00000000	0.00000000	0.53313800
B	0.00000000	1.69813100	0.15967800
B	1.23863700	0.83041300	-0.21312300
B	1.23863700	-0.83041300	-0.21312300
B	-1.23863700	0.83041300	-0.21312300
B	-1.23863700	-0.83041300	-0.21312300
B	0.00000000	-1.69813100	0.15967800

B₈(0)

0 3

B	0.00000000	1.79057512	-0.00000000
B	1.39992800	1.11640533	-0.00000000
B	0.77690143	-1.61325244	-0.00000000
B	-0.77690143	-1.61325244	-0.00000000
B	1.74568167	-0.39844045	-0.00000000
B	-1.74568167	-0.39844045	-0.00000000
B	-0.00000000	0.00000000	0.00000000
B	-1.39992800	1.11640533	-0.00000000

B₈(+)

1 2

B	0.00000000	0.00000000	1.80560200
B	0.00000000	1.41165800	1.12576600
B	0.00000000	0.78341700	-1.62678100
B	0.00000000	-0.78341700	-1.62678100
B	0.00000000	1.76030700	-0.40178500
B	0.00000000	-1.76030700	-0.40178500
B	0.00000000	0.00000000	-0.00000100
B	0.00000000	-1.41165800	1.12576600

B₈(-)

-1 2

B	0.00000000	0.00000000	1.79057900
B	0.00000000	1.39992800	1.11640500
B	0.00000000	0.77690200	-1.61325200
B	0.00000000	-0.77690200	-1.61325200
B	0.00000000	1.74566500	-0.39844300
B	0.00000000	-1.74566500	-0.39844300
B	0.00000000	0.00000000	0.00000100
B	0.00000000	-1.39992800	1.11640500

B₉(0)
0 2

B	0.00000000	0.00000000	1.77988500
B	0.00000000	1.39304600	1.11065400
B	0.00000000	-1.39304600	1.11065400
B	0.00000000	1.73682200	-0.39632300
B	0.00000000	-1.73682200	-0.39632300
B	0.00000000	0.77250700	-1.60404400
B	0.00000000	-0.77250700	-1.60404400
B	-0.89394900	0.00000000	-0.00022900
B	0.89394900	0.00000000	-0.00022900

B₉(-)
-1 1

B	0.00000000	1.97579500	0.00000000
B	-0.00000000	-0.00000000	0.00000000
B	0.00000000	-1.97579500	0.00000000
B	1.97579500	0.00000000	0.00000000
B	-1.97579500	-0.00000000	0.00000000
B	-1.39709804	1.39709804	0.00000000
B	1.39709804	1.39709804	0.00000000
B	1.39709804	-1.39709804	0.00000000
B	-1.39709804	-1.39709804	0.00000000

B₁₂(0)
0 1

B	0.00000000	0.97106901	0.39538480
B	-0.77655162	2.29416528	-0.17538208
B	0.77655162	2.29416528	-0.17538208
B	-1.75865919	1.01536236	-0.04528918
B	1.75865919	1.01536236	-0.04528918
B	-2.37508122	-0.47456921	-0.17538208
B	-0.84097043	-0.48553451	0.39538480
B	0.84097043	-0.48553451	0.39538480
B	2.37508122	-0.47456921	-0.17538208
B	-1.59852960	-1.81959607	-0.17538208
B	0.00000000	-2.03072472	-0.04528918
B	1.59852960	-1.81959607	-0.17538208

B₁₂(+)
1 2

B	0.49049117	0.98546220	0.00000000
B	-0.25308371	2.29945427	0.78811100
B	-0.25308371	2.29945427	-0.78811100
B	-0.01164582	1.00839725	1.70842900
B	-0.01164582	1.00839725	-1.70842900
B	-0.20110096	-0.47846673	2.37402800
B	0.46600304	-0.44615979	0.86397600
B	0.46600304	-0.44615979	-0.86397600
B	-0.20110096	-0.47846673	-2.37402800
B	-0.18554908	-1.81349573	1.57387000
B	-0.11973811	-2.12492074	0.00000000
B	-0.18554908	-1.81349573	-1.57387000

B₁₂(-)
-1 2

B	-0.49049100	0.98546200	0.00000000
B	0.25308400	2.29945400	-0.78811100
B	0.25308400	2.29945400	0.78811100
B	0.01164600	1.00839700	-1.70842900
B	0.01164600	1.00839700	1.70842900
B	0.20110100	-0.47846700	-2.37402800
B	-0.46600300	-0.44616000	-0.86397600
B	-0.46600300	-0.44616000	0.86397600
B	0.20110100	-0.47846700	2.37402800
B	0.18554900	-1.81349600	-1.57387000
B	0.11973800	-2.12492100	0.00000000
B	0.18554900	-1.81349600	1.57387000

B₁₃(0)

0 2

B	0.00000000	0.88408600	-0.38805900
B	0.00000000	0.00000000	1.06785300
B	0.00000000	-0.88408600	-0.38805900
B	0.00000000	0.77874800	-2.36859300
B	0.00000000	-0.77874800	-2.36859300
B	0.00000000	2.56971800	-0.07789800
B	0.00000000	-2.56971800	-0.07789800
B	0.00000000	-2.11369300	-1.54806500
B	0.00000000	2.11369300	-1.54806500
B	0.00000000	1.79494000	1.30416600
B	0.00000000	-1.79494000	1.30416600
B	0.00000000	0.76671100	2.54452200
B	0.00000000	-0.76671100	2.54452200

B₁₃(+)

1 1

B	0.00000000	0.88916600	-0.43875700
B	0.00000000	0.00000000	1.01874600
B	0.00000000	-0.88916600	-0.43875700
B	0.00000000	0.79327400	-2.27007200
B	0.00000000	-0.79327400	-2.27007200
B	0.00000000	2.59118800	-0.07159900
B	0.00000000	-2.59118800	-0.07159900
B	0.00000000	-2.15796300	-1.54403700
B	0.00000000	2.15796300	-1.54403700
B	0.00000000	1.80553000	1.30655300
B	0.00000000	-1.80553000	1.30655300
B	0.00000000	0.76867500	2.50853800
B	0.00000000	-0.76867500	2.50853800

B₁₄(0) second structure

0 1

B	0.00000000	2.33783462	0.03394357
B	0.00000000	0.69964327	0.52978421
B	0.00000000	-0.69964327	0.52978421
B	0.00000000	-2.33783462	0.03394357
B	1.40045458	1.71601672	-0.06422763
B	1.37871350	-0.00000000	0.17056108
B	1.40045458	-1.71601672	-0.06422763
B	-1.40045458	1.71601672	-0.06422763
B	-1.37871350	-0.00000000	0.17056108
B	-1.40045458	-1.71601672	-0.06422763
B	2.74318701	0.77803425	-0.31717067
B	2.74318701	-0.77803425	-0.31717067
B	-2.74318701	0.77803425	-0.31717067
B	-2.74318701	-0.77803425	-0.31717067

B₁₄(+)

1 2

B	0.00000000	2.38018300	-0.19148100
B	0.00000000	0.85176800	0.61285100
B	0.00000000	-0.85176800	0.61285100
B	0.00000000	-2.38018300	-0.19148100
B	1.45293200	1.75313300	-0.12403800
B	1.43461500	0.00000000	0.41446000
B	1.45293200	-1.75313300	-0.12403800
B	-1.45293200	1.75313300	-0.12403800
B	-1.43461500	0.00000000	0.41446000
B	-1.45293200	-1.75313300	-0.12403800
B	2.74120600	0.77252800	-0.29387700
B	2.74120600	-0.77252800	-0.29387700
B	-2.74120600	0.77252800	-0.29387700
B	-2.74120600	-0.77252800	-0.29387700

B₁₄(-)
-1 2
B 0.00000000 2.38186000 -0.17101600
B -0.07067959 0.92166293 0.87033115
B -0.07623835 -0.93824103 0.88839669
B 0.00000000 -2.38186000 -0.17101600
B 1.45054100 1.75083000 -0.10699100
B 1.60106676 0.00000000 0.63246863
B 1.45054100 -1.75083000 -0.10699100
B -1.45054100 1.75083000 -0.10699100
B -1.65086774 0.09576009 0.60723392
B -1.45054100 -1.75083000 -0.10699100
B 2.74586300 0.76916900 -0.27054100
B 2.74586300 -0.76916900 -0.27054100
B -2.74586300 0.76916900 -0.27054100
B -2.74586300 -0.76916900 -0.27054100

B₁₅(0)
0 2
B -0.42855630 2.20749460 0.03760588
B 0.00071398 0.71412935 -0.00060452
B 0.00028503 -0.95587056 -0.00097577
B 0.00138300 -2.52587000 -0.00170900
B -1.71393096 1.43491685 0.00701773
B -1.53246500 -0.08789100 -0.17559700
B -1.45157300 -1.90378000 0.00967000
B -3.12546700 0.38735700 0.00954700
B -2.85060400 -1.12026600 0.06329700
B 1.53246800 -0.08781700 0.17632600
B 0.85997771 2.05870172 -0.04923171
B 1.45423600 -1.90314900 -0.00950400
B 2.85224200 -1.11773800 -0.06155000
B 3.12469600 0.39024100 -0.00789700
B 2.22526145 1.39385408 0.01693419

B₁₅(+)
1 1
B -0.55485776 -2.36081511 0.00000000
B -0.15108000 -0.83328000 0.00000000
B 0.00000000 0.84381700 0.00000000
B -0.14075925 2.41753452 0.00000000
B -1.73030880 -1.56582755 0.00000000
B -1.46970780 0.12928911 0.00000000
B -1.45214034 1.85031890 0.00000000
B -2.99336424 -0.51544306 0.00000000
B -2.85437027 1.02317801 0.00000000
B 1.29981702 -0.11181722 0.00000000
B 0.91435152 -1.93143706 0.00000000
B 1.23511406 1.73705095 0.00000000
B 2.45735303 1.10448941 0.00000000
B 3.05310629 -0.26536445 0.00000000
B 2.22930366 -1.51042754 0.00000000

B₁₅(-)
-1 1
B -0.66851800 2.43171700 -0.01747400
B -0.02450593 0.80999074 0.03372018
B -0.02650200 -0.84042900 0.03479100
B -0.07973600 -2.51461700 -0.02493700
B -1.70952495 1.49757953 0.05195637
B -1.57830700 -0.08771400 0.32058400
B -1.52719600 -1.87657300 -0.05631500
B -3.10165800 0.48603200 -0.04720100
B -2.87565300 -1.03828800 -0.17665600
B 1.45069562 -0.04545904 -0.26641571
B 0.85570200 2.32217300 0.01576100
B 1.39160429 -1.82892288 0.04522617
B 2.78377000 -1.18750600 0.16091900
B 3.15284300 0.30223900 -0.02982000
B 2.25238200 1.55264100 -0.0662700

B₁₈(0)
0 1

B	-0.83043700	2.49390900	-0.01500900
B	0.00000000	1.01902100	0.36513100
B	0.88249800	-0.50951100	0.36513100
B	1.74457000	-1.96613400	-0.01500900
B	-1.54579000	0.89246200	-0.25175100
B	-0.88249800	-0.50951100	0.36513100
B	0.00000000	-1.78492500	-0.25175100
B	0.83043700	2.49390900	-0.01500900
B	1.54579000	0.89246200	-0.25175100
B	2.57500700	-0.52777500	-0.01500900
B	-1.74457000	-1.96613400	-0.01500900
B	-2.57500700	-0.52777500	-0.01500900
B	3.20813800	0.93896300	-0.04168100
B	2.41723500	2.30884800	-0.04168100
B	-3.20813800	0.93896300	-0.04168100
B	-2.41723500	2.30884800	-0.04168100
B	-0.79090300	-3.24781100	-0.04168100
B	0.79090300	-3.24781100	-0.04168100

B₁₈(-)
-1 2

B	-2.56486400	0.51888200	-0.01193910
B	-0.88529541	0.51112554	0.33160090
B	0.88529541	0.51112554	0.33160090
B	2.56486400	0.51888200	-0.01193910
B	-1.56553566	-0.90386243	-0.21945199
B	0.00000000	-1.02225109	0.33160090
B	1.56553566	-0.90386243	-0.21945199
B	-1.73179699	1.96179638	-0.01193910
B	0.00000000	1.80772487	-0.21945199
B	1.73179699	1.96179638	-0.01193910
B	0.83306701	-2.48067838	-0.01193910
B	-0.83306701	-2.48067838	-0.01193910
B	0.78772100	3.24843600	-0.04447331
B	-0.78772100	3.24843600	-0.04447331
B	-2.41936760	-2.30640440	-0.04447331
B	-3.20708860	-0.94203160	-0.04447331
B	2.41936760	-2.30640440	-0.04447331
B	3.20708860	-0.94203160	-0.04447331

B₁₉(0)
0 2

B	-0.16217648	1.94372498	0.00000000
B	-0.08212781	3.00032524	-1.38458273
B	0.10862980	1.68193835	2.04016720
B	0.10862980	1.68193835	-2.04016720
B	-0.17176414	3.62642698	0.00000000
B	-0.08212781	3.00032524	1.38458273
B	0.09295356	0.20900437	-2.67941838
B	0.22170537	0.48152845	-0.93948069
B	0.22170537	0.48152845	0.93948069
B	0.09295356	0.20900437	2.67941838
B	0.08242487	-1.29069215	-3.21355365
B	-0.29375360	-1.10206086	-1.57973684
B	0.17774449	-1.10728106	0.00000000
B	-0.29375360	-1.10206086	1.57973684
B	0.08242487	-1.29069215	3.21355365
B	-0.00629229	-2.58795600	-2.36259053
B	-0.04186164	-2.69238578	-0.78728103
B	-0.04186164	-2.69238578	0.78728103
B	-0.00629229	-2.58795600	2.36259053

B₁₉(-)
-1 1

B	0.00000000	0.00000000	1.43987747
B	1.45766575	-0.00000000	0.44496928
B	-1.45766575	-0.00000000	0.44496928

B	1.02970362	-0.00000000	-1.19124763
B	-1.02970362	-0.00000000	-1.19124763
B	0.00000000	0.00000000	-0.04528774
B	1.07087161	-0.00000000	-2.89376274
B	-1.07087161	-0.00000000	-2.89376274
B	2.73595948	-0.00000000	-0.76345240
B	-2.73595948	-0.00000000	-0.76345240
B	2.32231103	-0.00000000	-2.14133610
B	-2.32231103	-0.00000000	-2.14133610
B	3.14499005	-0.00000000	0.65218107
B	-3.14499005	-0.00000000	0.65218107
B	2.32714093	-0.00000000	1.90930033
B	-2.32714093	-0.00000000	1.90930033
B	0.00000000	0.00000000	3.07832059
B	1.16682290	-0.00000000	2.72669785
B	-1.16682290	-0.00000000	2.72669785

B₂₀(-)

-1 2

B	0.00000000	0.85732000	-1.39197600
B	0.00000000	-0.85732000	-1.39197600
B	0.00000000	-1.74735500	0.10492200
B	0.00000000	-0.81885200	1.52234200
B	0.00000000	0.81885200	1.52234200
B	0.00000000	1.74735500	0.10492200
B	0.00000000	0.00000000	0.02542000
B	0.00000000	3.40857600	0.35700300
B	0.00000000	-3.40857600	0.35700300
B	0.00000000	2.57077200	1.71772500
B	0.00000000	-2.57077200	1.71772500
B	0.00000000	0.00000000	3.05357700
B	0.00000000	1.60830300	3.00435500
B	0.00000000	-1.60830300	3.00435500
B	0.00000000	-3.03666900	-1.15456000
B	0.00000000	3.03666900	-1.15456000
B	0.00000000	0.80546000	-3.18726900
B	0.00000000	-0.80546000	-3.18726900
B	0.00000000	2.18081700	-2.51204000
B	0.00000000	-2.18081700	-2.51204000

B₂₀(2-)

-2 1

B	0.00000000	1.46052200	2.75537800
B	0.00000000	0.00000000	1.74848800
B	0.00000000	0.00000000	0.02155900
B	0.00000000	1.49653000	-0.78627200
B	0.00000000	1.46799200	0.92273400
B	0.00000000	-1.46799200	0.92273400
B	0.00000000	-1.49653000	-0.78627200
B	0.00000000	0.00000000	-1.65321100
B	0.00000000	-1.46052200	2.75537800
B	0.00000000	0.00000000	3.43133400
B	0.00000000	2.83397000	1.91165200
B	0.00000000	-2.83397000	1.91165200
B	0.00000000	3.14166500	0.35958100
B	0.00000000	-3.14166500	0.35958100
B	0.00000000	3.14399200	-1.24910400
B	0.00000000	-3.14399200	-1.24910400
B	0.00000000	0.76430600	-3.24069600
B	0.00000000	-0.76430600	-3.24069600
B	0.00000000	2.17207900	-2.44735800
B	0.00000000	-2.17207900	-2.44735800

B₁₀(-)

-1 2

B	0.03375910	1.58723962	-1.38362191
B	-0.16998850	0.01084474	-1.57458630
B	-0.16998850	0.01084474	1.57458630
B	0.03375910	1.58723962	1.38362191
B	0.15368880	2.32148919	0.00000000

B	0.10144238	0.67981061	0.00000000
B	-0.42161723	-0.78723475	0.00000000
B	0.09660366	-1.55938257	1.38628971
B	0.09660366	-1.55938257	-1.38628971
B	0.24539279	-2.28828639	0.00000000

B₁₁(0)

0 2

B	0.00000000	1.57030150	1.58578325
B	0.00000000	0.00000000	1.53595365
B	0.00000000	2.00358066	-1.11630807
B	0.00000000	2.38455658	0.17677156
B	0.00000000	0.77531253	0.01618166
B	0.00000000	-0.77531253	0.01618166
B	0.00000000	-2.00358066	-1.11630807
B	0.00000000	-1.57030150	1.58578325
B	0.00000000	-2.38455658	0.17677156
B	0.00000000	0.75221601	-1.43999350
B	0.00000000	-0.75221601	-1.43999350

B₁₁(+)

1 1

B	-0.00556447	-0.10696932	1.53405604
B	-0.00556447	-0.10696932	-1.53405604
B	0.30503714	0.62634610	0.00000000
B	-0.29744595	-0.92652956	0.00000000
B	0.08235797	-1.83334037	-1.34609570
B	0.08235797	-1.83334037	1.34609570
B	-0.01989537	-2.54217306	0.00000000
B	-0.05496792	1.19815657	-1.37208228
B	-0.05496792	1.19815657	1.37208228
B	-0.02550201	2.12762824	0.57127153
B	-0.02550201	2.12762824	-0.57127153

B₁₁(-)

-1 1

B	0.00000000	1.59330488	1.59900056
B	0.00000000	0.00000000	1.54632786
B	0.00000000	2.00594189	-1.10332276
B	0.00000000	2.38523285	0.19025211
B	0.00000000	0.77619939	0.02756581
B	0.00000000	-0.77619939	0.02756581
B	0.00000000	-2.00594189	-1.10332276
B	0.00000000	-1.59330488	1.59900056
B	0.00000000	-2.38523285	0.19025211
B	0.00000000	0.71411416	-1.42863820
B	0.00000000	-0.71411416	-1.42863820

B₁₃(-)

-1 2

B	0.00000000	1.39509474	2.71695420
B	0.00000000	1.56877015	1.11273012
B	0.00000000	-1.56608585	1.11264139
B	0.00000000	-1.39250126	2.71687530
B	0.00000000	0.00127575	3.45840075
B	0.00000000	0.00132326	1.77990775
B	0.00000000	0.00136881	0.17081875
B	0.00000000	-1.61508023	-0.53243312
B	0.00000000	1.61785765	-0.53234161
B	0.00000000	0.00141643	-1.51173825
B	0.00000000	1.67279350	-2.08756553
B	0.00000000	0.76896836	-3.16978552
B	0.00000000	-0.76604164	-3.16982897
B	0.00000000	-1.68915967	-2.06463527

B₁₄(+) second structure

1 2

B	0.00096000	2.70392400	1.38973500
B	0.00455300	1.10302900	1.52778300
B	-0.01224600	3.45895600	0.00000000
B	0.00096000	2.70392400	-1.38973500
B	0.00455300	1.10302900	-1.52778300
B	0.03188100	0.17639700	0.00000000
B	-0.02039400	1.82394200	0.00000000
B	0.00524791	-0.56263413	1.52283656
B	-0.00681700	-1.55924000	0.00000000
B	0.00524791	-0.56263413	-1.52283656
B	0.00219800	-2.04628500	1.76482100
B	-0.00984300	-3.20357700	0.76628000
B	-0.00984300	-3.20357700	-0.76628000
B	0.00219800	-2.04628500	-1.76482100

B₁₄(-)

- 1 2

B	0.02171100	2.68960800	1.37907800
B	0.05583400	1.09679000	1.53833100
B	-0.09682500	3.43883000	0.00000000
B	0.02171100	2.68960800	-1.37907800
B	0.05583400	1.09679000	-1.53833100
B	0.26398600	0.18195900	0.00000000
B	-0.24792200	1.77677400	0.00000000
B	0.06031300	-0.49083100	1.65971300
B	-0.07765900	-1.53463800	0.00000000
B	0.06031300	-0.49083100	-1.65971300
B	0.02292000	-2.04098900	1.78283300
B	-0.08156800	-3.18604000	0.76979800
B	-0.08156800	-3.18604000	-0.76979800
B	0.02292000	-2.04098900	-1.78283300

B₁₅(0) second structure

0 2

B	-1.40753064	0.12734439	0.72463995
B	1.40906942	-0.01108000	0.72632181
B	0.00128187	-0.11596114	1.53497667
B	0.00194963	0.11663018	0.00000000
B	1.40906942	-0.01108000	-0.72632181
B	-1.40753064	0.12734439	-0.72463995
B	0.00128187	-0.11596114	-1.53497667
B	-1.60891164	0.01064346	-2.22641660
B	-0.60005785	-0.00005786	-3.01336407
B	0.59044765	-0.01088789	-3.01459472
B	1.60095383	-0.01855667	-2.22973471
B	-1.60891164	0.01064346	2.22641660
B	1.60095383	-0.01855667	2.22973471
B	-0.60005785	-0.00005786	3.01336407
B	0.59044765	-0.01088789	3.01459472

B₁₅(+) second structure

1 1

B	-1.46429343	0.00000000	0.72840372
B	1.46429343	0.00000000	0.72840372
B	0.00000000	0.00000000	1.59497018
B	0.00000000	0.00000000	0.00000000
B	1.46429343	0.00000000	-0.72840372
B	-1.46429343	-0.00000000	-0.72840372
B	-0.00000000	0.00000000	-1.59497018
B	-1.70891817	0.00000000	-2.22745837
B	-0.61806540	0.00000000	-3.00395089
B	0.61806540	0.00000000	-3.00395089
B	1.70891817	0.00000000	-2.22745837
B	-1.70891817	0.00000000	2.22745837
B	1.70891817	0.00000000	2.22745837
B	-0.61806540	0.00000000	3.00395089
B	0.61806540	0.00000000	3.00395089

B₁₅(-)
-1 1
B -0.55861700 2.46072700 -0.01181800
B -0.10456600 0.85563000 0.07538000
B -0.05984000 -0.84366800 0.05622000
B -0.16971400 -2.49344600 -0.04190000
B -1.92111400 1.65500200 0.03772800
B -1.60121900 -0.06542300 0.29232600
B -1.60166400 -1.82906300 -0.04858000
B -3.06669200 0.58237500 -0.06991100
B -2.92255900 -0.94818900 -0.15473900
B 1.52375600 -0.08439600 -0.22224200
B 0.95239900 2.23799700 0.00742700
B 1.29795000 -1.94622900 0.05812300
B 2.71888800 -1.25992000 0.13360000
B 3.16656400 0.19568900 -0.06288000
B 2.34642600 1.48291400 -0.04873300

B₁₆(0)
0 1
B -0.10119688 -3.18639594 1.39032294
B 0.03777814 -1.61232094 1.62207293
B -0.05044103 -3.94247894 0.00000000
B -0.10119688 -3.18639594 -1.39032294
B 0.03777814 -1.61232094 -1.62207293
B -0.14776606 -0.77555794 0.00000000
B 0.36552796 -2.32329793 0.00000000
B 0.00000000 0.00000000 1.61799894
B 0.14776606 0.77555794 0.00000000
B 0.00000000 0.00000000 -1.61799894
B -0.03777814 1.61232094 1.62207293
B -0.03777814 1.61232094 -1.62207293
B -0.36552796 2.32329793 0.00000000
B 0.05044103 3.94247894 0.00000000
B 0.10119688 3.18639594 1.39032294
B 0.10119688 3.18639594 -1.39032294

B₁₆(+)
1 2
B 0.00000000 3.22233000 1.40036000
B -0.04656400 1.61092600 1.60554600
B -0.05148900 3.96679700 0.00000000
B 0.00000000 3.22233000 -1.40036000
B -0.04656400 1.61092600 -1.60554600
B 0.17298000 0.76870900 0.00000000
B -0.27009700 2.31179400 0.00000000
B 0.00000000 0.00000000 1.65160600
B -0.17298000 -0.76870900 0.00000000
B 0.00000000 0.00000000 -1.65160600
B 0.04656400 -1.61092600 1.60554600
B 0.04656400 -1.61092600 -1.60554600
B 0.27009700 -2.31179400 0.00000000
B 0.05148900 -3.96679700 0.00000000
B 0.00000000 -3.22233000 1.40036000
B 0.00000000 -3.22233000 -1.40036000

B₁₆(-)
-1 2
B -0.03755147 3.20955073 -1.41140231
B -0.00089542 1.59129810 -1.57642836
B -0.02646442 3.94490696 0.00000000
B -0.03755147 3.20955073 1.41140231
B -0.00089542 1.59129810 1.57642836
B -0.16819501 0.75381686 0.00000000
B 0.20004998 2.33253766 0.00000000
B 0.00000000 0.00000000 -1.59460991
B 0.16819501 -0.75381686 0.00000000
B 0.00000000 0.00000000 1.59460991
B 0.00089542 -1.59129810 -1.57642836
B 0.00089542 -1.59129810 1.57642836

B	-0.20004998	-2.33253766	0.00000000
B	0.02646442	-3.94490696	0.00000000
B	0.03755147	-3.20955073	-1.41140231
B	0.03755147	-3.20955073	1.41140231

B₁₇(0)

0 2

B	2.59706200	-1.92380400	-0.18547300
B	1.02849700	-2.13962600	-0.11355800
B	-0.55952700	-2.15337900	0.22492900
B	-2.13292700	-2.30795900	0.11386000
B	3.40207400	-0.60702800	-0.11486400
B	1.73545300	-0.49533100	-0.06609000
B	0.06937600	-0.53612700	0.30639900
B	-1.53045000	-0.72210300	-0.17546800
B	-3.17385300	-1.19008400	-0.13302000
B	2.90365500	0.89326500	-0.03247200
B	0.88418500	0.87934400	0.52696600
B	-0.79338600	0.97101200	0.02955500
B	-3.13811200	0.35241200	-0.16131800
B	-2.41436500	1.75178900	-0.04103000
B	1.92778300	2.12998600	-0.08452100
B	0.38951600	2.44170400	-0.08967200
B	-1.19498100	2.65592700	-0.00422300

B₁₇(+) second structure

1 1

B	0.10314611	3.54034277	1.36413688
B	0.00505211	1.93382977	1.51413688
B	0.08950911	4.29106877	0.02913688
B	0.10314611	3.54034277	-1.30586312
B	0.00505211	1.93382977	-1.45586312
B	0.04979411	1.09329577	0.02913688
B	-0.22013889	2.66851477	0.02913688
B	0.10314611	0.31909677	1.58913688
B	0.15649811	-0.45510223	0.02913688
B	0.10314611	0.31909677	-1.53086312
B	0.20124011	-1.29563623	1.66413688
B	0.20124011	-1.29563623	-1.60586312
B	0.42643111	-2.03032123	0.02913688
B	-0.06785868	-3.49841884	-0.76049541
B	-0.05480697	-3.59079058	0.65643688
B	-0.00656670	-2.55664730	-1.62603494
B	0.10159969	-2.70421525	1.51454762

B₁₇(-)

-1 1

B	0.00000000	-2.65643200	-1.81641307
B	0.00000000	-1.04734786	-2.03953316
B	-0.00000000	1.04734786	-2.03953316
B	-0.00000000	2.65643200	-1.81641307
B	0.00000000	-3.21562590	-0.65684894
B	0.00000000	-1.65732971	-0.58406726
B	0.00000000	0.00000000	-0.65015398
B	-0.00000000	1.65732971	-0.58406726
B	-0.00000000	3.21562590	-0.65684894
B	0.00000000	-2.55960886	0.78755789
B	0.00000000	-0.79230356	0.83895504
B	-0.00000000	0.79230356	0.83895504
B	-0.00000000	2.55960886	0.78755789
B	0.00000000	2.62062707	1.85672138
B	0.00000000	-2.62062707	1.85672138
B	0.00000000	-0.79481990	2.40517458
B	-0.00000000	0.79481990	2.40517458

B₁₇(-) second structure

-1 1

B	0.04021161	3.42244755	1.32290889
B	-0.07125389	1.81818319	1.48697513
B	0.04407938	4.16070195	0.00000000

B	0.04021161	3.42244755	-1.32290889
B	-0.07125389	1.81818319	-1.48697513
B	-0.01960616	0.96345186	0.00000000
B	-0.27771171	2.54055943	0.00000000
B	0.01406088	0.20354167	1.57788308
B	0.07548251	-0.58562654	0.00000000
B	0.01406088	0.20354167	-1.57788308
B	0.09937565	-1.41109985	1.66879102
B	0.09937565	-1.41109985	-1.66879102
B	0.33358806	-2.16273411	0.00000000
B	-0.16465005	-3.63446729	-0.73754120
B	-0.16465005	-3.63446729	0.73754120
B	-0.08860231	-2.70133408	-1.61122775
B	-0.08860231	-2.70133408	1.61122775

Quantum rules for planar boron nanoclusters

Athanasios G. Arvanitidis,^a Truong Ba Tai,^a Minh Tho Nguyen,^a and Arnout Ceulemans^a

SUPPLEMENTARY INFORMATION

Table of Contents

Orbital Plots

^aDepartment of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium, Fax: (+32)16-327992)

E-mail: arnout.ceulemans@chem.kuleuven.be

B₇(0)



HOMO



HOMO-1



HOMO-2



HOMO-3



HOMO-4



HOMO-5



HOMO-6



HOMO-7



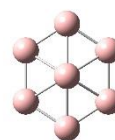
HOMO-8



HOMO-9



HOMO-10



B₇(+)



HOMO



HOMO-1



HOMO-2



HOMO-3



HOMO-4



HOMO-5



HOMO-6



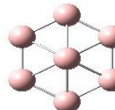
HOMO-7



HOMO-8



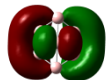
HOMO-9



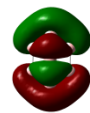
B₇(+)



HOMO



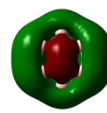
HOMO-1



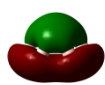
HOMO-2



HOMO-3



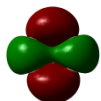
HOMO-4



HOMO-5



HOMO-6



HOMO-7



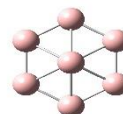
HOMO-8



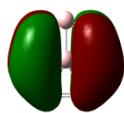
HOMO-9



HOMO-10



B8(0)



HOMO



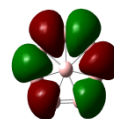
HOMO-1



HOMO-2



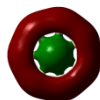
HOMO-3



HOMO-4



HOMO-5



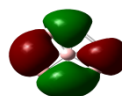
HOMO-6



HOMO-7



HOMO-8



HOMO-9



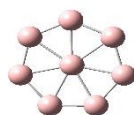
HOMO-10



HOMO-11



HOMO-12



B8(+)



HOMO



HOMO-1



HOMO-2



HOMO-3



HOMO-4



HOMO-5



HOMO-6



HOMO-7



HOMO-8



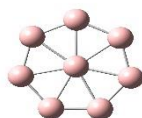
HOMO-9



HOMO-10



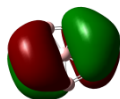
HOMO-11



B8(-)



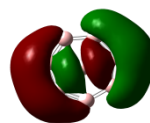
HOMO



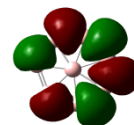
HOMO-1



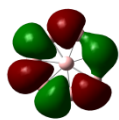
HOMO-2



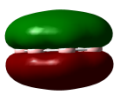
HOMO-3



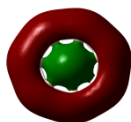
HOMO-4



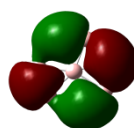
HOMO-5



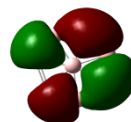
HOMO-6



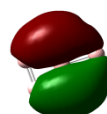
HOMO-7



HOMO-8



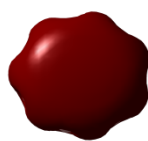
HOMO-9



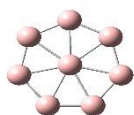
HOMO-10



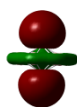
HOMO-11



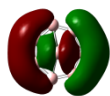
HOMO-12



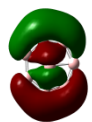
B₉(0)



HOMO



HOMO-1



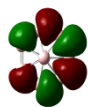
HOMO-2



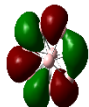
HOMO-3



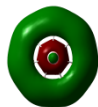
HOMO-4



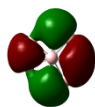
HOMO-5



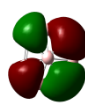
HOMO-6



HOMO-7



HOMO-8



HOMO-9



HOMO-10



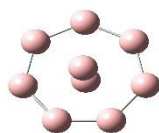
HOMO-11



HOMO-12



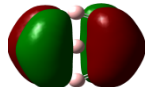
HOMO-13



B₉(-)



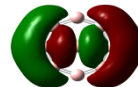
HOMO



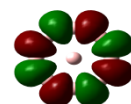
HOMO-1



HOMO-2



HOMO-3



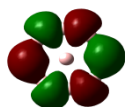
HOMO-4



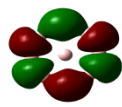
HOMO-5



HOMO-6



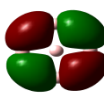
HOMO-7



HOMO-8



HOMO-9



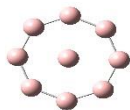
HOMO-10



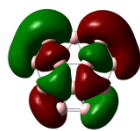
HOMO-11



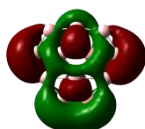
HOMO-12



B₁₂(0)



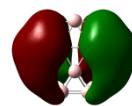
HOMO



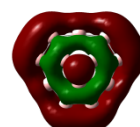
HOMO-1



HOMO-2



HOMO-3



HOMO-4



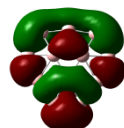
HOMO-5



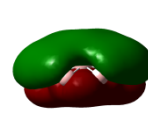
HOMO-6



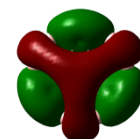
HOMO-7



HOMO-8



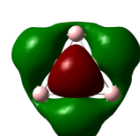
HOMO-9



HOMO-10



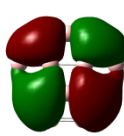
HOMO-11



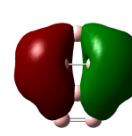
HOMO-12



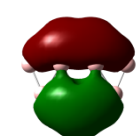
HOMO-13



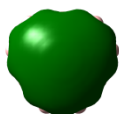
HOMO-14



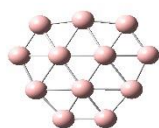
HOMO-15



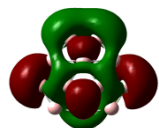
HOMO-16



HOMO-17



B₁₂(+)



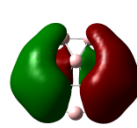
HOMO



HOMO-1



HOMO-2



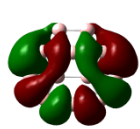
HOMO-3



HOMO-4



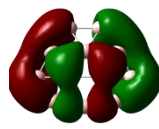
HOMO-5



HOMO-6



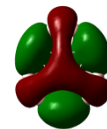
HOMO-7



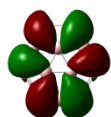
HOMO-8



HOMO-9



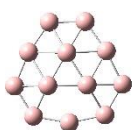
HOMO-10



HOMO-11



HOMO-12



HOMO-13



HOMO-14



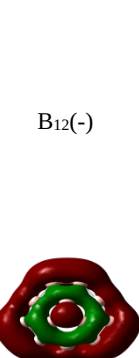
HOMO-15



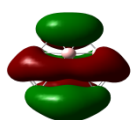
HOMO-16



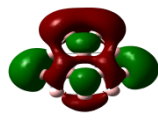
HOMO-17



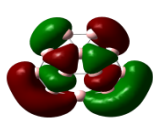
B₁₂(-)



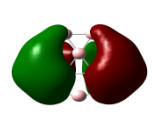
HOMO



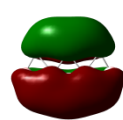
HOMO-1



HOMO-2



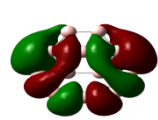
HOMO-3



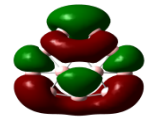
HOMO-4



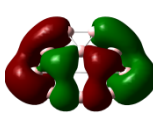
HOMO-5



HOMO-6



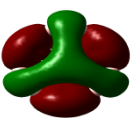
HOMO-7



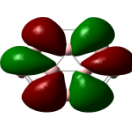
HOMO-8



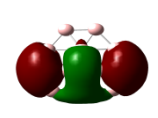
HOMO-9



HOMO-10



HOMO-11



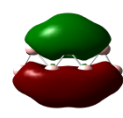
HOMO-12



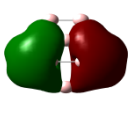
HOMO-13



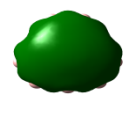
HOMO-14



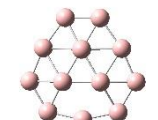
HOMO-15



HOMO-16



HOMO-17



HOMO-18

HOMO-19

HOMO-20

$B_{13}(0)$



HOMO

HOMO-1

HOMO-2

HOMO-3

HOMO-4



HOMO-5

HOMO-6

HOMO-7

HOMO-8

HOMO-9

HOMO-10



HOMO-11

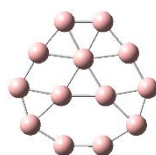
HOMO-12

HOMO-13

HOMO-14

HOMO-15

HOMO-16

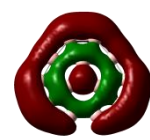
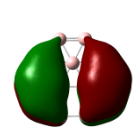
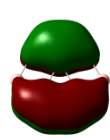
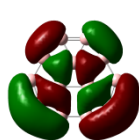
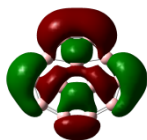


HOMO-17

HOMO-18

HOMO-19

$B_{13}(+)$



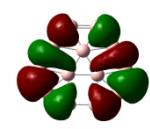
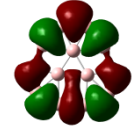
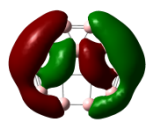
HOMO

HOMO-1

HOMO-2

HOMO-3

HOMO-4



HOMO-5

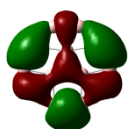
HOMO-6

HOMO-7

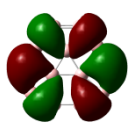
HOMO-8

HOMO-9

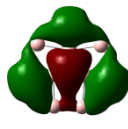
HOMO-10



HOMO-11



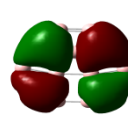
HOMO-12



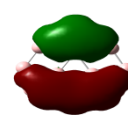
HOMO-13



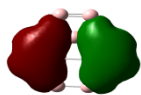
HOMO-14



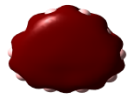
HOMO-15



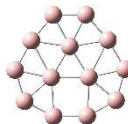
HOMO-16



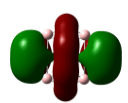
HOMO-17



HOMO-18



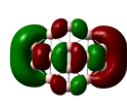
B14(0)
2nd



HOMO



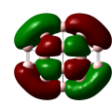
HOMO-1



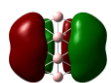
HOMO-2



HOMO-3



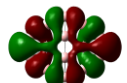
HOMO-4



HOMO-5



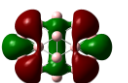
HOMO-6



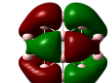
HOMO-7



HOMO-8



HOMO-9



HOMO-10



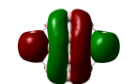
HOMO-11



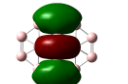
HOMO-12



HOMO-13



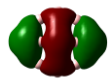
HOMO-14



HOMO-15



HOMO-16



HOMO-17



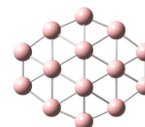
HOMO-18



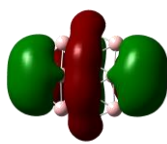
HOMO-19



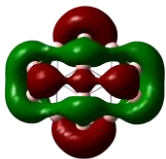
HOMO-20



B₁₄(+)



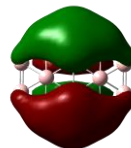
HOMO



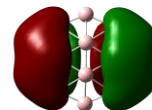
HOMO-1



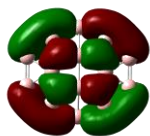
HOMO-2



HOMO-3



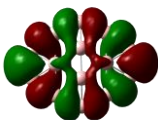
HOMO-4



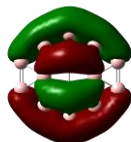
HOMO-5



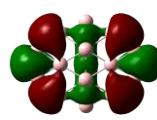
HOMO-6



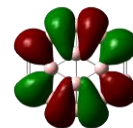
HOMO-7



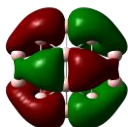
HOMO-8



HOMO-9



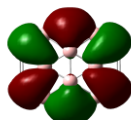
HOMO-10



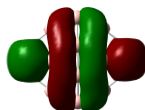
HOMO-11



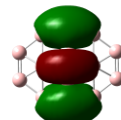
HOMO-12



HOMO-13



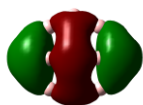
HOMO-14



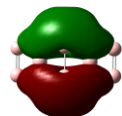
HOMO-15



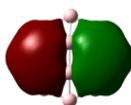
HOMO-16



HOMO-17



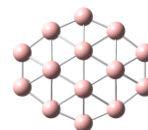
HOMO-18



HOMO-19

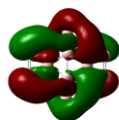


HOMO-20

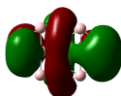


B₁₄(-)

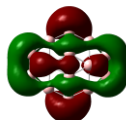
2nd



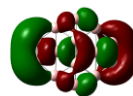
HOMO



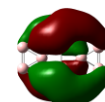
HOMO-1



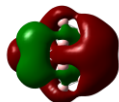
HOMO-2



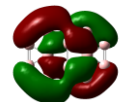
HOMO-3



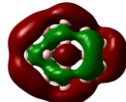
HOMO-4



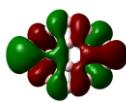
HOMO-5



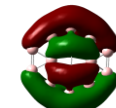
HOMO-6



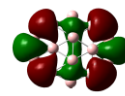
HOMO-7



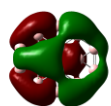
HOMO-8



HOMO-9



HOMO-10



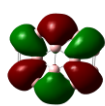
HOMO-11



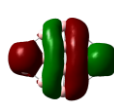
HOMO-12



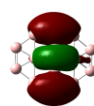
HOMO-13



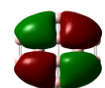
HOMO-14



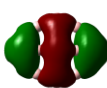
HOMO-15



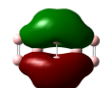
HOMO-16



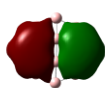
HOMO-17



HOMO-18



HOMO-19



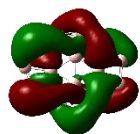
HOMO-20



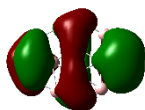
HOMO-21



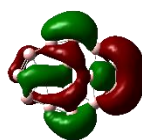
B₁₅(0)



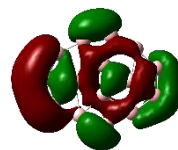
HOMO



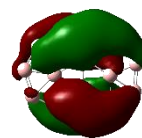
HOMO-1



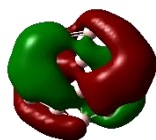
HOMO-2



HOMO-3



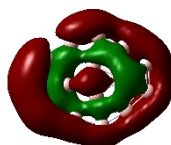
HOMO-4



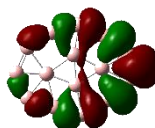
HOMO-5



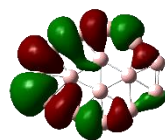
HOMO-6



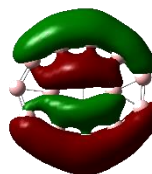
HOMO-7



HOMO-8



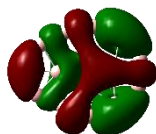
HOMO-9



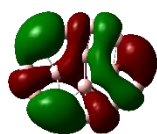
HOMO-10



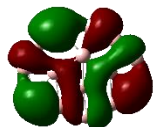
HOMO-11



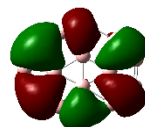
HOMO-12



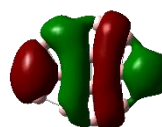
HOMO-13



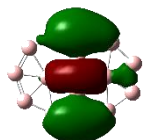
HOMO-14



HOMO-15



HOMO-16



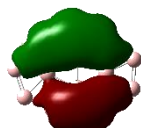
HOMO-17



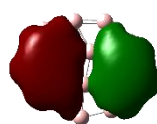
HOMO-18



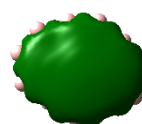
HOMO-19



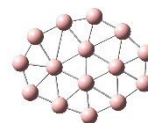
HOMO-20



HOMO-21



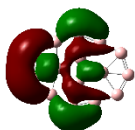
HOMO-22



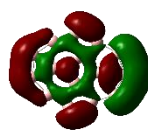
B₁₅(+)



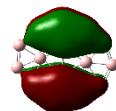
HOMO



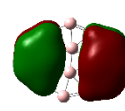
HOMO-1



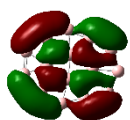
HOMO-2



HOMO-3



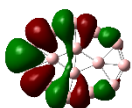
HOMO-4



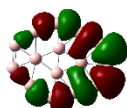
HOMO-5



HOMO-6



HOMO-7



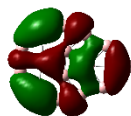
HOMO-8



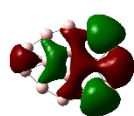
HOMO-9



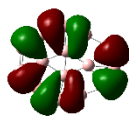
HOMO-10



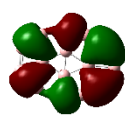
HOMO-11



HOMO-12



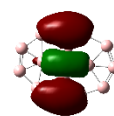
HOMO-13



HOMO-14



HOMO-15



HOMO-16



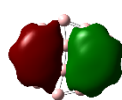
HOMO-17



HOMO-18



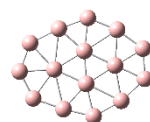
HOMO-19



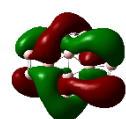
HOMO-20



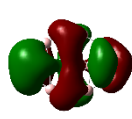
HOMO-21



B₁₅(-)



HOMO



HOMO-1



HOMO-2



HOMO-3



HOMO-4



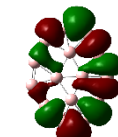
HOMO-5



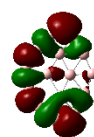
HOMO-6



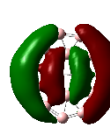
HOMO-7



HOMO-8



HOMO-9



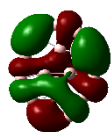
HOMO-10



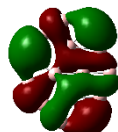
HOMO-11



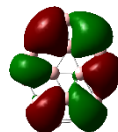
HOMO-12



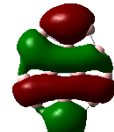
HOMO-13



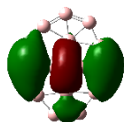
HOMO-14



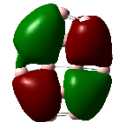
HOMO-15



HOMO-16



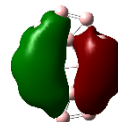
HOMO-17



HOMO-18



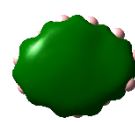
HOMO-19



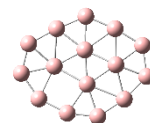
HOMO-20



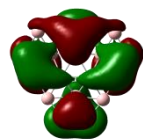
HOMO-21



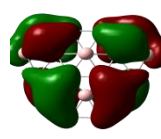
HOMO-22



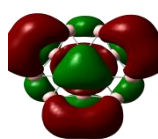
B₁₈(0)



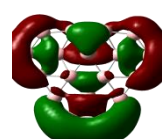
HOMO



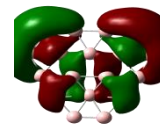
HOMO-1



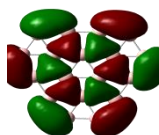
HOMO-2



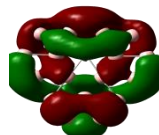
HOMO-3



HOMO-4



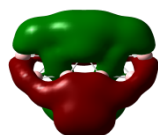
HOMO-5



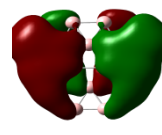
HOMO-6



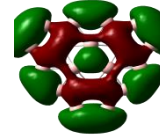
HOMO-7



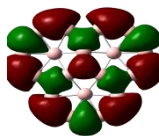
HOMO-8



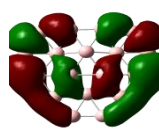
HOMO-9



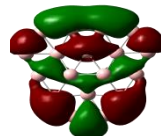
HOMO-10



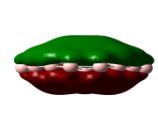
HOMO-11



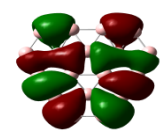
HOMO-12



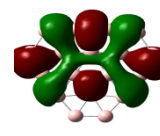
HOMO-13



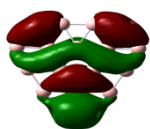
HOMO-14



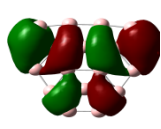
HOMO-15



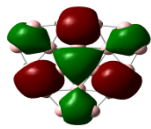
HOMO-16



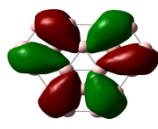
HOMO-17



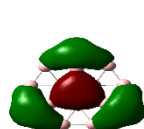
HOMO-18



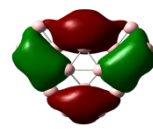
HOMO-19



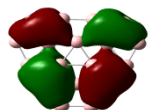
HOMO-20



HOMO-21



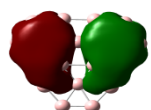
HOMO-22



HOMO-23



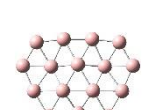
HOMO-24



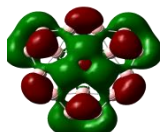
HOMO-25



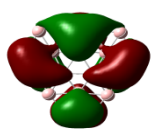
HOMO-26



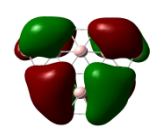
B₁₈(-)



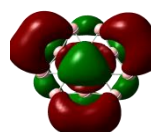
HOMO



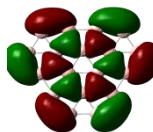
HOMO-1



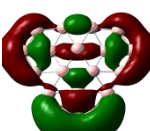
HOMO-2



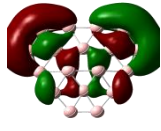
HOMO-3



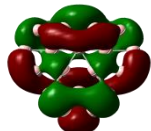
HOMO-4



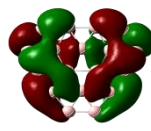
HOMO-5



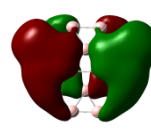
HOMO-6



HOMO-7



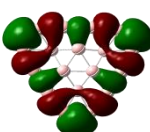
HOMO-8



HOMO-9



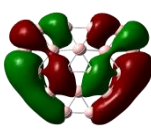
HOMO-10



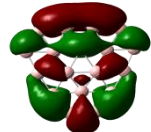
HOMO-11



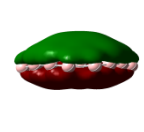
HOMO-12



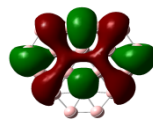
HOMO-13



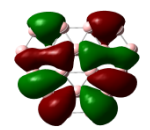
HOMO-14



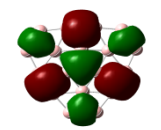
HOMO-15



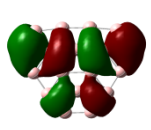
HOMO-16



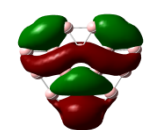
HOMO-17



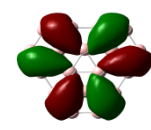
HOMO-18



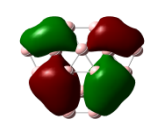
HOMO-19



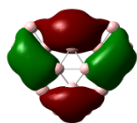
HOMO-20



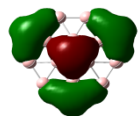
HOMO-21



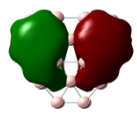
HOMO-22



HOMO-23



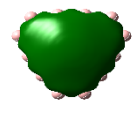
HOMO-24



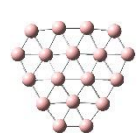
HOMO-25



HOMO-26



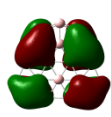
HOMO-27



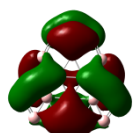
B₁₉(0)



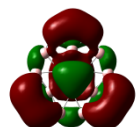
HOMO



HOMO-1



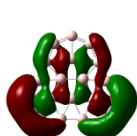
HOMO-2



HOMO-3



HOMO-4



HOMO-5



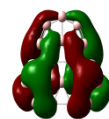
HOMO-6



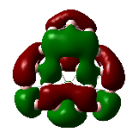
HOMO-7



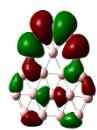
HOMO-8



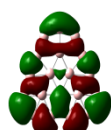
HOMO-9



HOMO-10



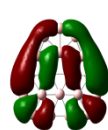
HOMO-11



HOMO-12



HOMO-13



HOMO-14



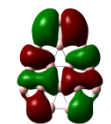
HOMO-15



HOMO-16



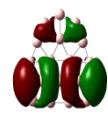
HOMO-17



HOMO-18



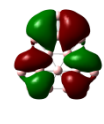
HOMO-19



HOMO-20



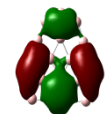
HOMO-21



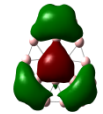
HOMO-22



HOMO-23



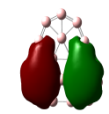
HOMO-24



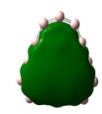
HOMO-25



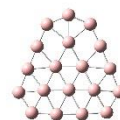
HOMO-26



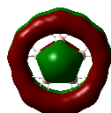
HOMO-27



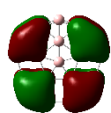
HOMO-28



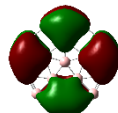
B₁₉(-)



HOMO



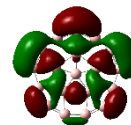
HOMO-1



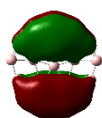
HOMO-2



HOMO-3



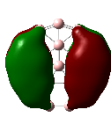
HOMO-4



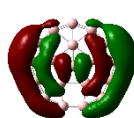
HOMO-5



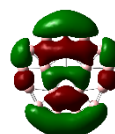
HOMO-6



HOMO-7



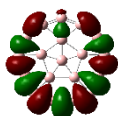
HOMO-8



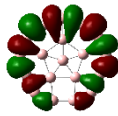
HOMO-9



HOMO-10



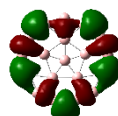
HOMO-11



HOMO-12



HOMO-13



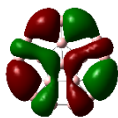
HOMO-14



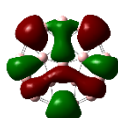
HOMO-15



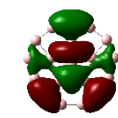
HOMO-16



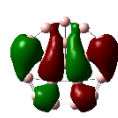
HOMO-17



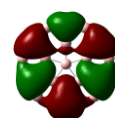
HOMO-18



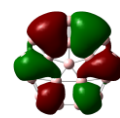
HOMO-19



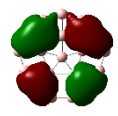
HOMO-20



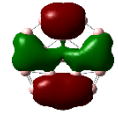
HOMO-21



HOMO-22



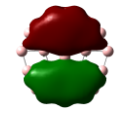
HOMO-23



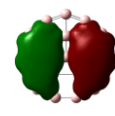
HOMO-24



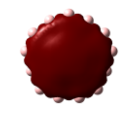
HOMO-25



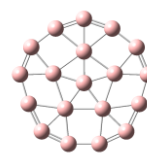
HOMO-26



HOMO-27



HOMO-28



B₂₀(-)

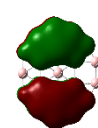
HOMO

HOMO-1

HOMO-2

HOMO-3

HOMO-4



HOMO-5

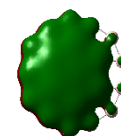
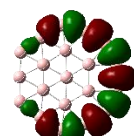
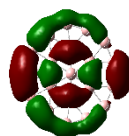
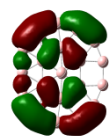
HOMO-6

HOMO-7

HOMO-8

HOMO-9

HOMO-10



HOMO-11

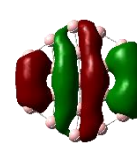
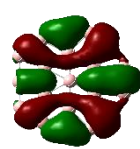
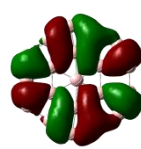
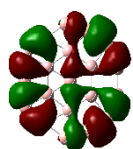
HOMO-12

HOMO-13

HOMO-14

HOMO-15

HOMO-16



HOMO-17

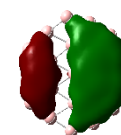
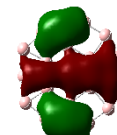
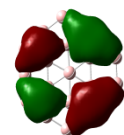
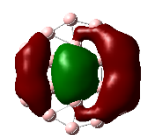
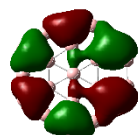
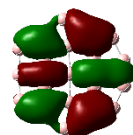
HOMO-18

HOMO-19

HOMO-20

HOMO-21

HOMO-22



HOMO-23

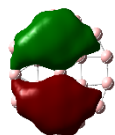
HOMO-24

HOMO-25

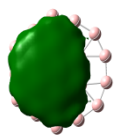
HOMO-26

HOMO-27

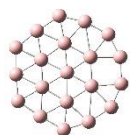
HOMO-28



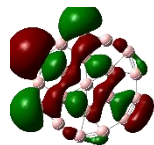
HOMO-29



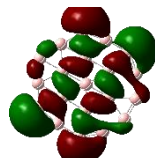
HOMO-30



B₂₀(2-)



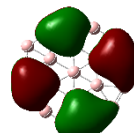
HOMO



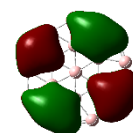
HOMO-1



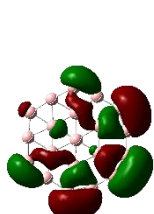
HOMO-2



HOMO-3



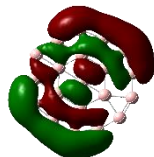
HOMO-4



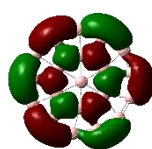
HOMO-5



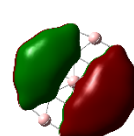
HOMO-6



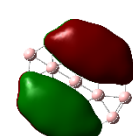
HOMO-7



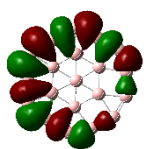
HOMO-8



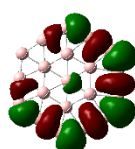
HOMO-9



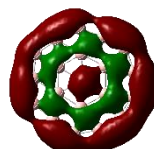
HOMO-10



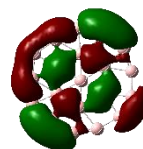
HOMO-11



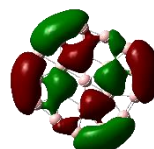
HOMO-12



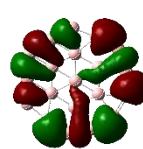
HOMO-13



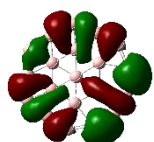
HOMO-14



HOMO-15



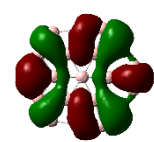
HOMO-16



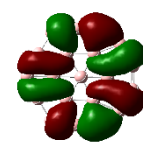
HOMO-17



HOMO-18



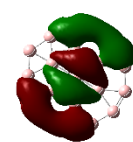
HOMO-19



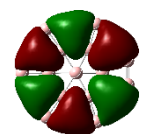
HOMO-20



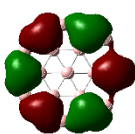
HOMO-21



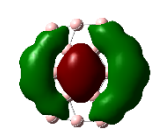
HOMO-22



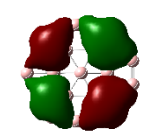
HOMO-23



HOMO-24



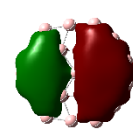
HOMO-25



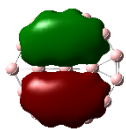
HOMO-26



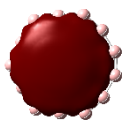
HOMO-27



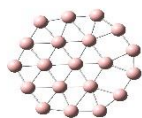
HOMO-28



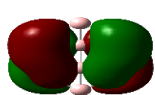
HOMO-29



HOMO-30



B₁₀(0)



HOMO



HOMO-1



HOMO-2



HOMO-3



HOMO-4



HOMO-5



HOMO-6



HOMO-7



HOMO-8



HOMO-9



HOMO-10



HOMO-11



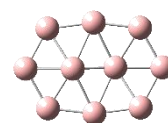
HOMO-12



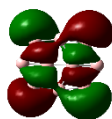
HOMO-13



HOMO-14



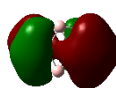
B₁₀(-)



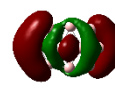
HOMO



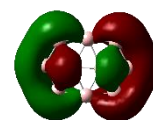
HOMO-1



HOMO-2



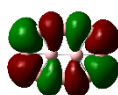
HOMO-3



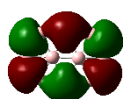
HOMO-4



HOMO-5



HOMO-6



HOMO-7



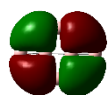
HOMO-8



HOMO-9



HOMO-10



HOMO-11



HOMO-12



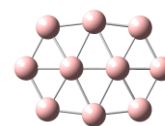
HOMO-13



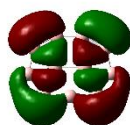
HOMO-14



HOMO-15



B₁₁(-)



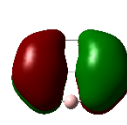
HOMO



HOMO-1



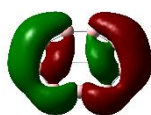
HOMO-2



HOMO-3



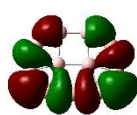
HOMO-4



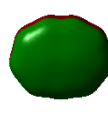
HOMO-5



HOMO-6



HOMO-7



HOMO-8



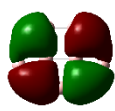
HOMO-9



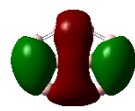
HOMO-10



HOMO-11



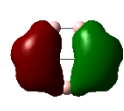
HOMO-12



HOMO-13



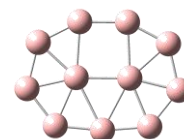
HOMO-14



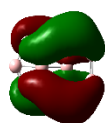
HOMO-15



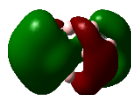
HOMO-16



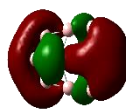
B₁₁(+)



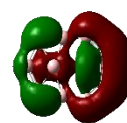
HOMO



HOMO-1



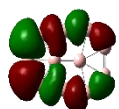
HOMO-2



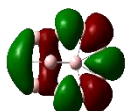
HOMO-3



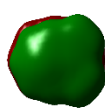
HOMO-4



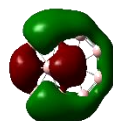
HOMO-5



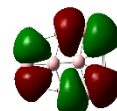
HOMO-6



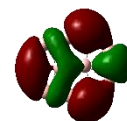
HOMO-7



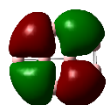
HOMO-8



HOMO-9



HOMO-10



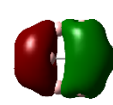
HOMO-11



HOMO-12



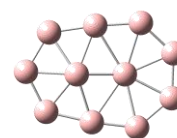
HOMO-13



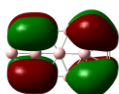
HOMO-14



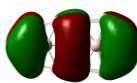
HOMO-15



B₁₃(-)



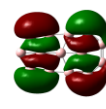
HOMO



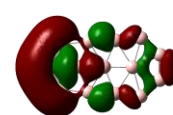
HOMO-1



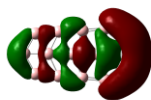
HOMO-2



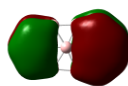
HOMO-3



HOMO-4



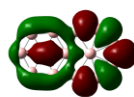
HOMO-5



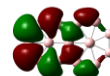
HOMO-6



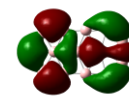
HOMO-7



HOMO-8



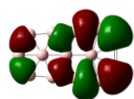
HOMO-9



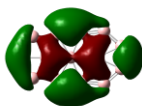
HOMO-10



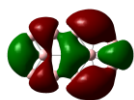
HOMO-11



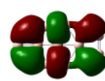
HOMO-12



HOMO-13



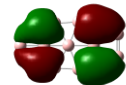
HOMO-14



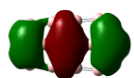
HOMO-15



HOMO-16



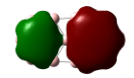
HOMO-17



HOMO-18



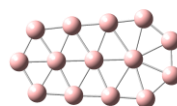
HOMO-19



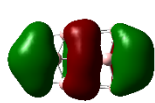
HOMO-20



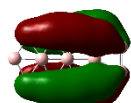
HOMO-21



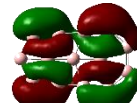
B₁₄(+) second
structure



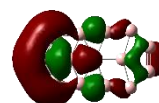
HOMO



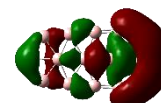
HOMO-1



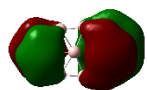
HOMO-2



HOMO-3



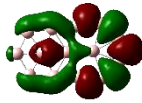
HOMO-4



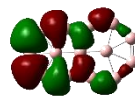
HOMO-5



HOMO-6



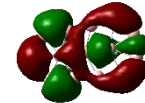
HOMO-7



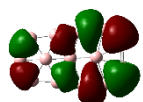
HOMO-8



HOMO-9



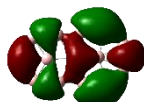
HOMO-10



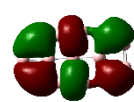
HOMO-11



HOMO-12



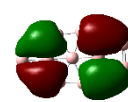
HOMO-13



HOMO-14



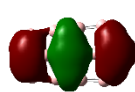
HOMO-15



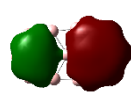
HOMO-16



HOMO-17



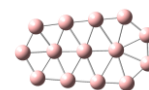
HOMO-18



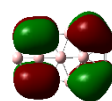
HOMO-19



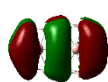
HOMO-20



B₁₄(-)



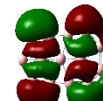
HOMO



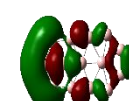
HOMO-1



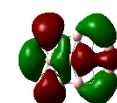
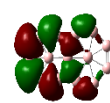
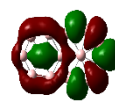
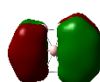
HOMO-2



HOMO-3



HOMO-4



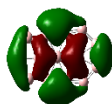
HOMO-5



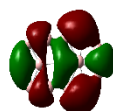
HOMO-6



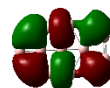
HOMO-7



HOMO-8



HOMO-9



HOMO-10



HOMO-11



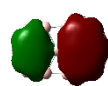
HOMO-12



HOMO-13



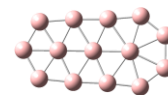
HOMO-14



HOMO-15



HOMO-16



HOMO-17



HOMO-18



HOMO-19



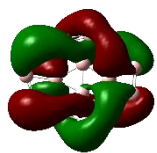
HOMO-20



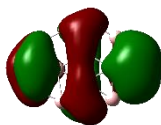
HOMO-21



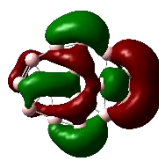
B₁₅(0) second structure



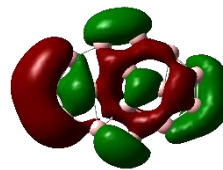
HOMO



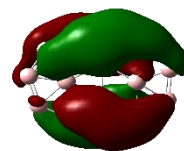
HOMO-1



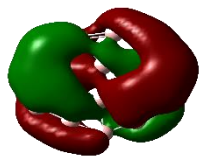
HOMO-2



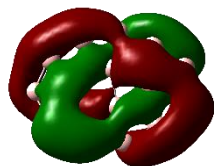
HOMO-3



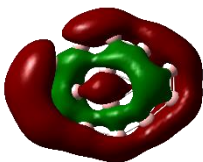
HOMO-4



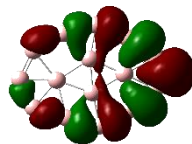
HOMO-5



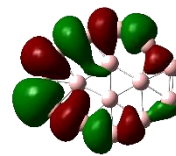
HOMO-6



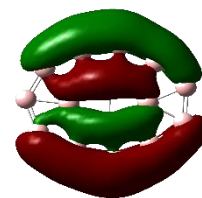
HOMO-7



HOMO-8



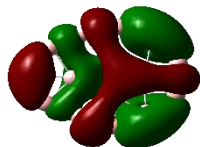
HOMO-9



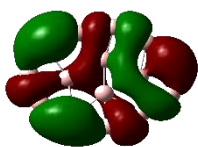
HOMO-10



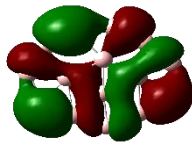
HOMO-11



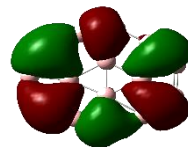
HOMO-12



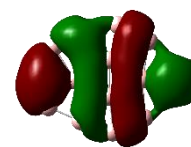
HOMO-13



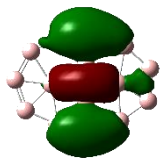
HOMO-14



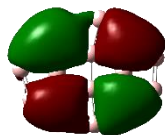
HOMO-15



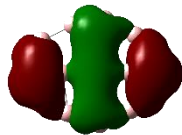
HOMO-16



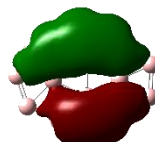
HOMO-17



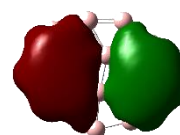
HOMO-18



HOMO-19



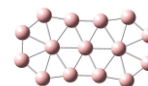
HOMO-20



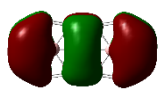
HOMO-21



HOMO-22



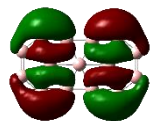
B₁₅(+) second structure



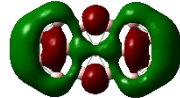
HOMO



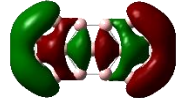
HOMO-1



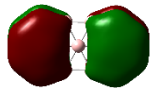
HOMO-2



HOMO-3



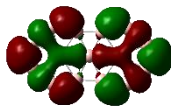
HOMO-4



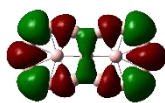
HOMO-5



HOMO-6



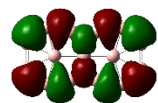
HOMO-7



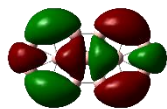
HOMO-8



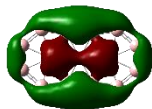
HOMO-9



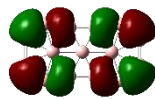
HOMO-10



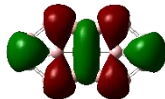
HOMO-11



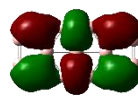
HOMO-12



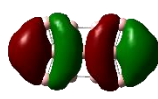
HOMO-13



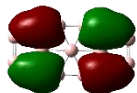
HOMO-14



HOMO-15



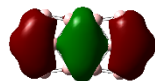
HOMO-16



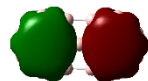
HOMO-17



HOMO-18



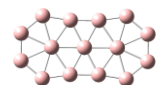
HOMO-19



HOMO-20



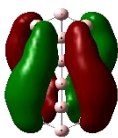
HOMO-21



B₁₆(0)



HOMO



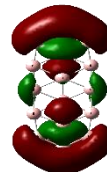
HOMO-1



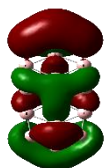
HOMO-2



HOMO-3



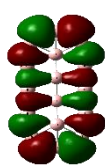
HOMO-4



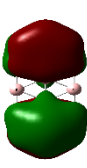
HOMO-5



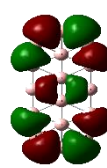
HOMO-6



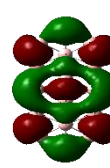
HOMO-7



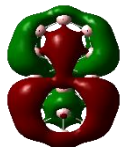
HOMO-8



HOMO-9



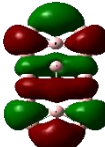
HOMO-10



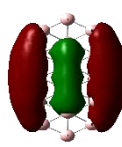
HOMO-11



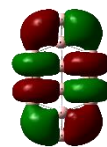
HOMO-12



HOMO-13



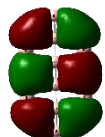
HOMO-14



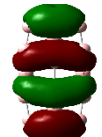
HOMO-15



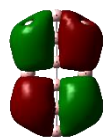
HOMO-16



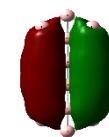
HOMO-17



HOMO-18



HOMO-19



HOMO-20



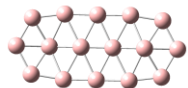
HOMO-21



HOMO-22



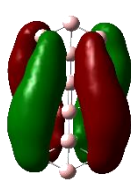
HOMO-23



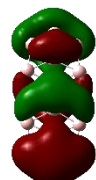
B₁₆(+)



HOMO



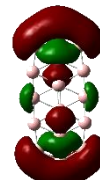
HOMO-1



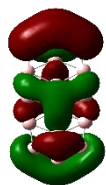
HOMO-2



HOMO-3



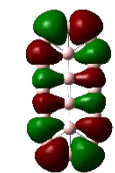
HOMO-4



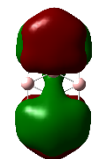
HOMO-5



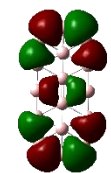
HOMO-6



HOMO-7



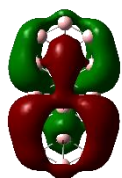
HOMO-8



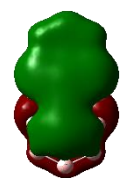
HOMO-9



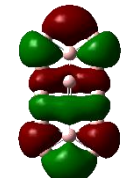
HOMO-10



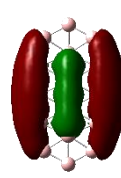
HOMO-11



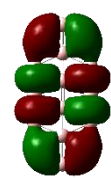
HOMO-12



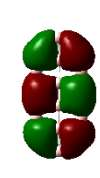
HOMO-13



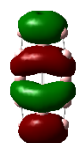
HOMO-14



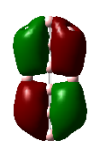
HOMO-15



HOMO-16



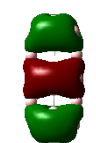
HOMO-17



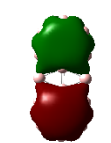
HOMO-18



HOMO-19



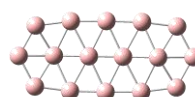
HOMO-20



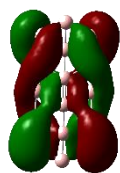
HOMO-21



HOMO-22



B₁₆(-)



HOMO



HOMO-1



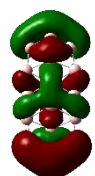
HOMO-2



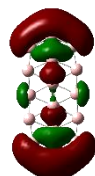
HOMO-3



HOMO-4



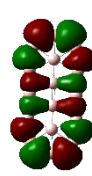
HOMO-5



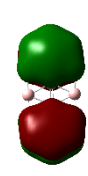
HOMO-6



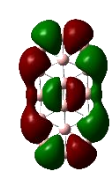
HOMO-7



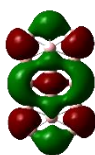
HOMO-8



HOMO-9



HOMO-10



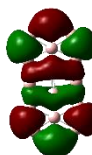
HOMO-11



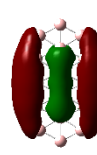
HOMO-12



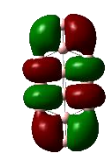
HOMO-13



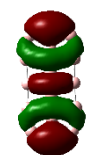
HOMO-14



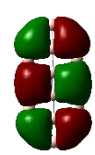
HOMO-15



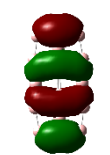
HOMO-16



HOMO-17



HOMO-18



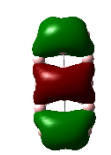
HOMO-19



HOMO-20



HOMO-21



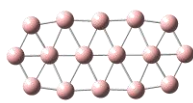
HOMO-22



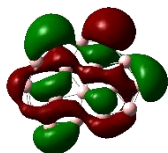
HOMO-23



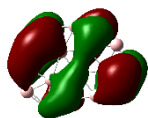
HOMO-24



B₁₇(0)



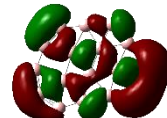
HOMO



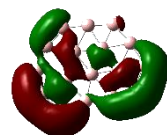
HOMO-1



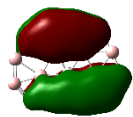
HOMO-2



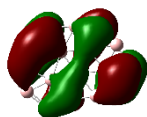
HOMO-3



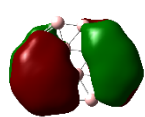
HOMO-4



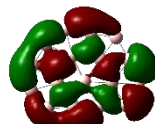
HOMO-5



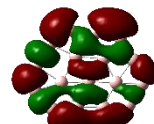
HOMO-6



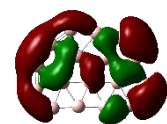
HOMO-7



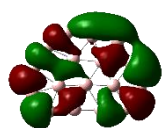
HOMO-8



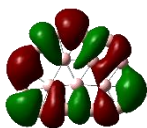
HOMO-9



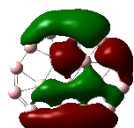
HOMO-10



HOMO-11



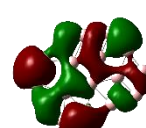
HOMO-12



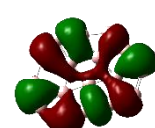
HOMO-13



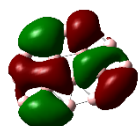
HOMO-14



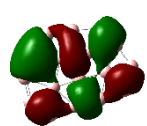
HOMO-15



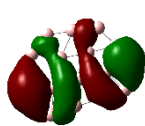
HOMO-16



HOMO-17



HOMO-18



HOMO-19



HOMO-20



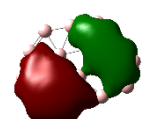
HOMO-21



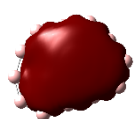
HOMO-22



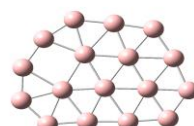
HOMO-23



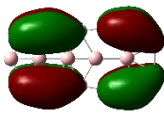
HOMO-24



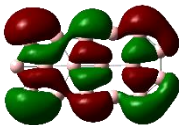
HOMO-25



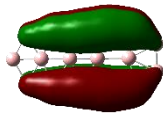
B₁₇(-)



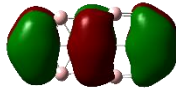
HOMO



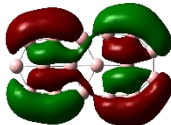
HOMO-1



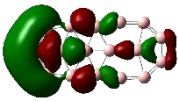
HOMO-2



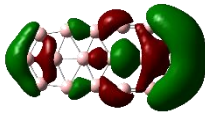
HOMO-3



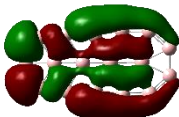
HOMO-4



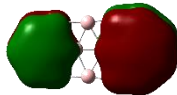
HOMO-5



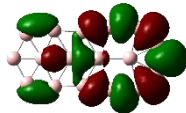
HOMO-6



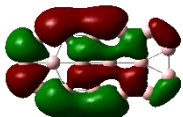
HOMO-7



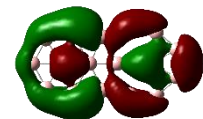
HOMO-8



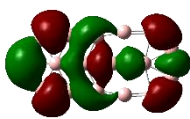
HOMO-9



HOMO-10



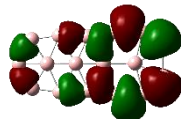
HOMO-11



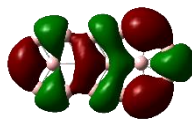
HOMO-12



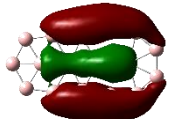
HOMO-13



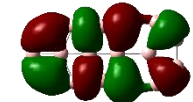
HOMO-14



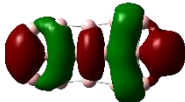
HOMO-15



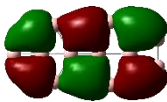
HOMO-16



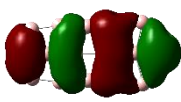
HOMO-17



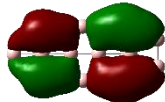
HOMO-18



HOMO-19



HOMO-20



HOMO-21



HOMO-22



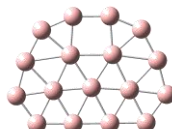
HOMO-23



HOMO-24

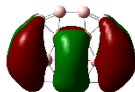


HOMO-25

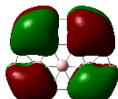


B₁₇(-)

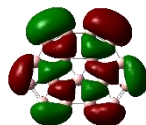
2nd structure



HOMO



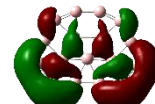
HOMO-1



HOMO-2



HOMO-3



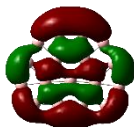
HOMO-4



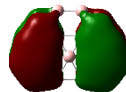
HOMO-5



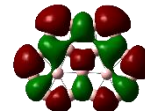
HOMO-6



HOMO-7



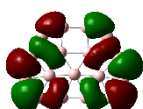
HOMO-8



HOMO-9



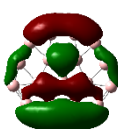
HOMO-10



HOMO-11



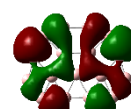
HOMO-12



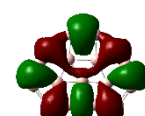
HOMO-13



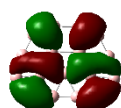
HOMO-14



HOMO-15



HOMO-16



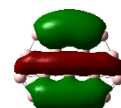
HOMO-17



HOMO-18



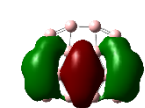
HOMO-19



HOMO-20



HOMO-21



HOMO-22



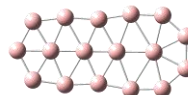
HOMO-23



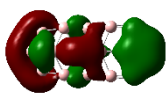
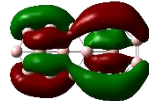
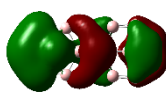
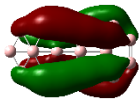
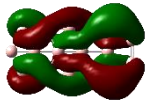
HOMO-24



HOMO-25



B₁₇(+)



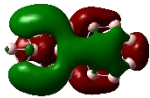
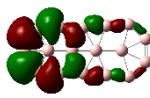
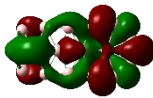
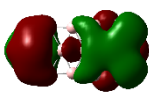
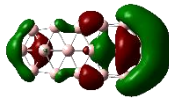
HOMO

HOMO-1

HOMO-2

HOMO-3

HOMO-4



HOMO-5

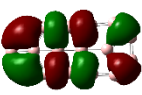
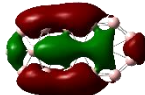
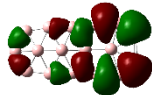
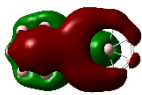
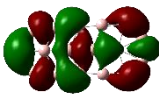
HOMO-6

HOMO-7

HOMO-8

HOMO-9

HOMO-10



HOMO-11

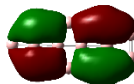
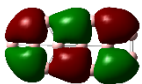
HOMO-12

HOMO-13

HOMO-14

HOMO-15

HOMO-16



HOMO-17

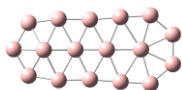
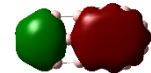
HOMO-18

HOMO-19

HOMO-20

HOMO-21

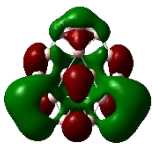
HOMO-22



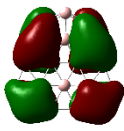
HOMO-23

HOMO-24

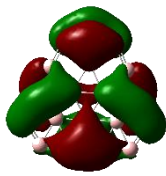
B₁₉(0)



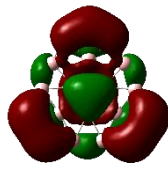
HOMO



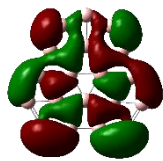
HOMO-1



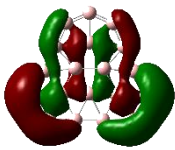
HOMO-2



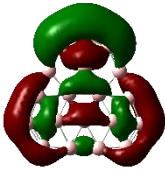
HOMO-3



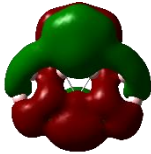
HOMO-4



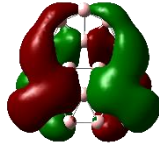
HOMO-5



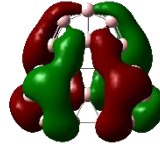
HOMO-6



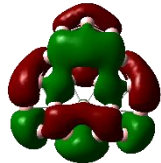
HOMO-7



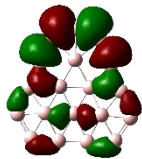
HOMO-8



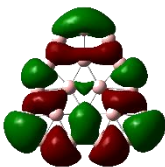
HOMO-9



HOMO-10



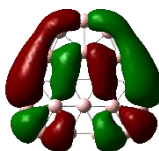
HOMO-11



HOMO-12



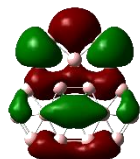
HOMO-13



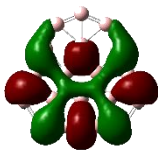
HOMO-14



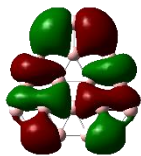
HOMO-15



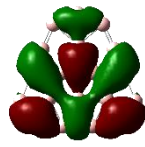
HOMO-16



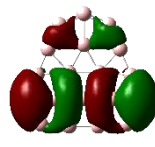
HOMO-17



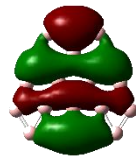
HOMO-18



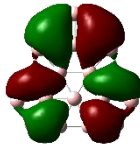
HOMO-19



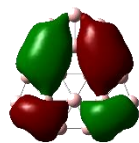
HOMO-20



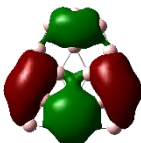
HOMO-21



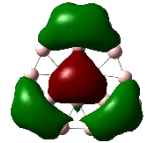
HOMO-22



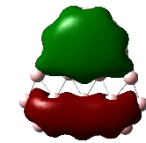
HOMO-23



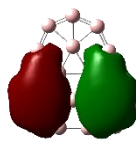
HOMO-24



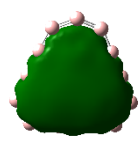
HOMO-25



HOMO-26

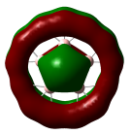


HOMO-27

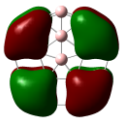


HOMO-28

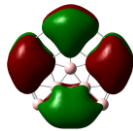
B₁₉(-)



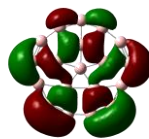
HOMO



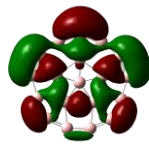
HOMO-1



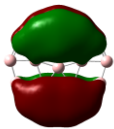
HOMO-2



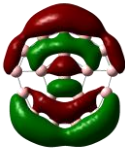
HOMO-3



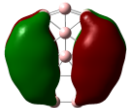
HOMO-4



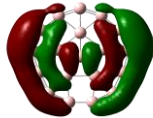
HOMO-5



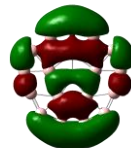
HOMO-6



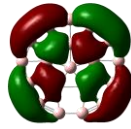
HOMO-7



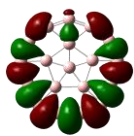
HOMO-8



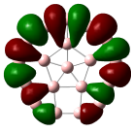
HOMO-9



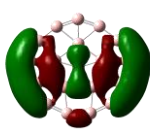
HOMO-10



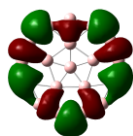
HOMO-11



HOMO-12



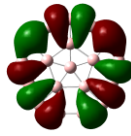
HOMO-13



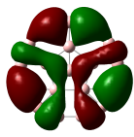
HOMO-14



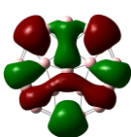
HOMO-15



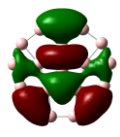
HOMO-16



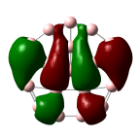
HOMO-17



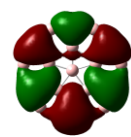
HOMO-18



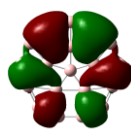
HOMO-19



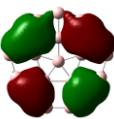
HOMO-20



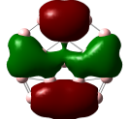
HOMO-21



HOMO-22



HOMO-23



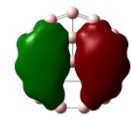
HOMO-24



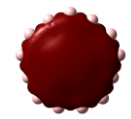
HOMO-5



HOMO-26



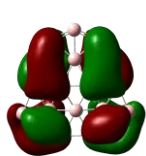
HOMO-27



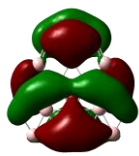
HOMO-28

B₁₉(+)

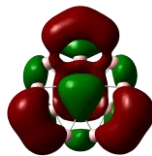
Not stale



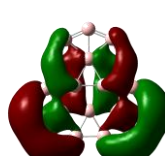
HOMO



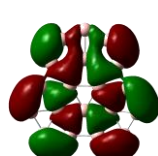
HOMO-1



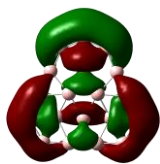
HOMO-2



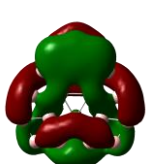
HOMO-3



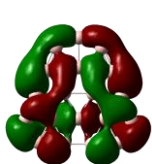
HOMO-4



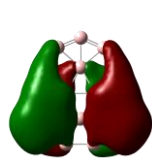
HOMO-5



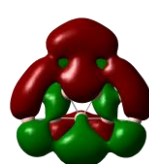
HOMO-6



HOMO-7



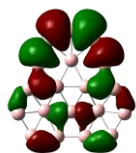
HOMO-8



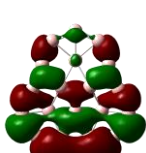
HOMO-9



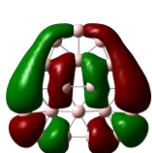
HOMO-10



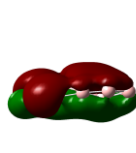
HOMO-11



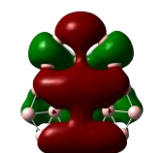
HOMO-12



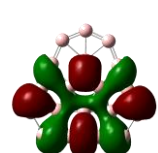
HOMO-13



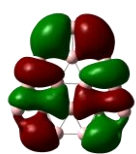
HOMO-14



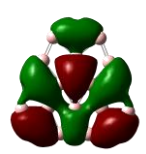
HOMO-15



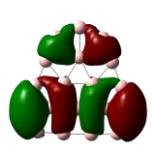
HOMO-16



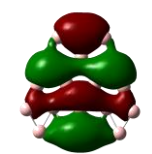
HOMO-17



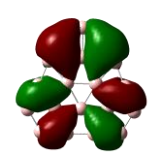
HOMO-18



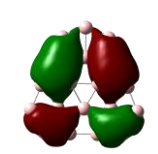
HOMO-19



HOMO-20



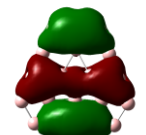
HOMO-21



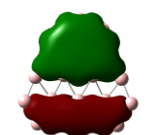
HOMO-22



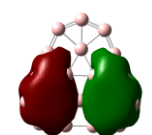
HOMO-23



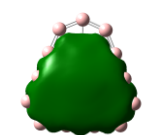
HOMO-24



HOMO-5



HOMO-26



HOMO-27