Electronic Supplementary Information

Structural Evolution and Electronic Properties of Boron Sulfides $(B_2S_3)_n$ (n=1-6): Insights from DFT Calculations

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1. Functional testing

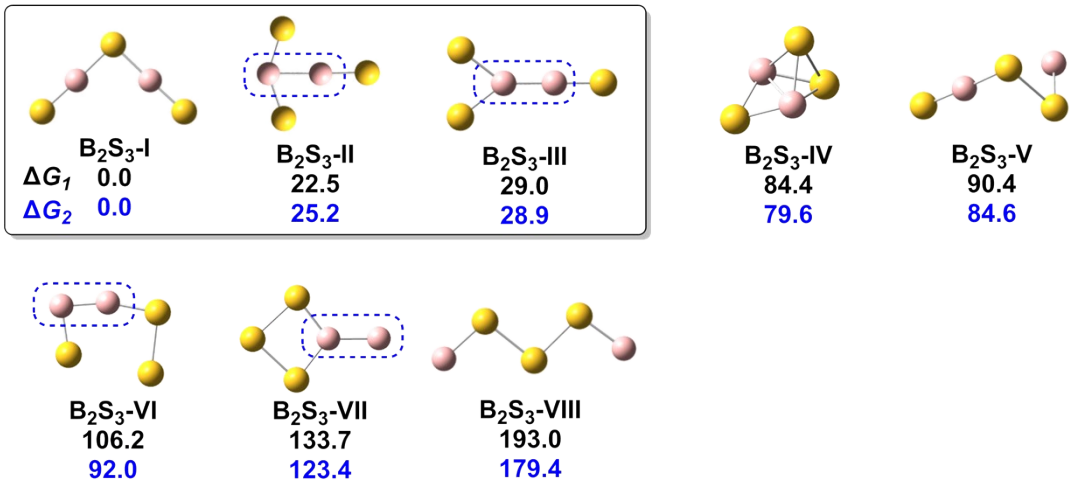

Fig. S1. Optimized the low-energy isomers of B_2S_3 cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol) and G4(MP2)-6X method (ΔG_2, in kcal/mol), respectively. The color of atoms: S-yellow; B-pink.

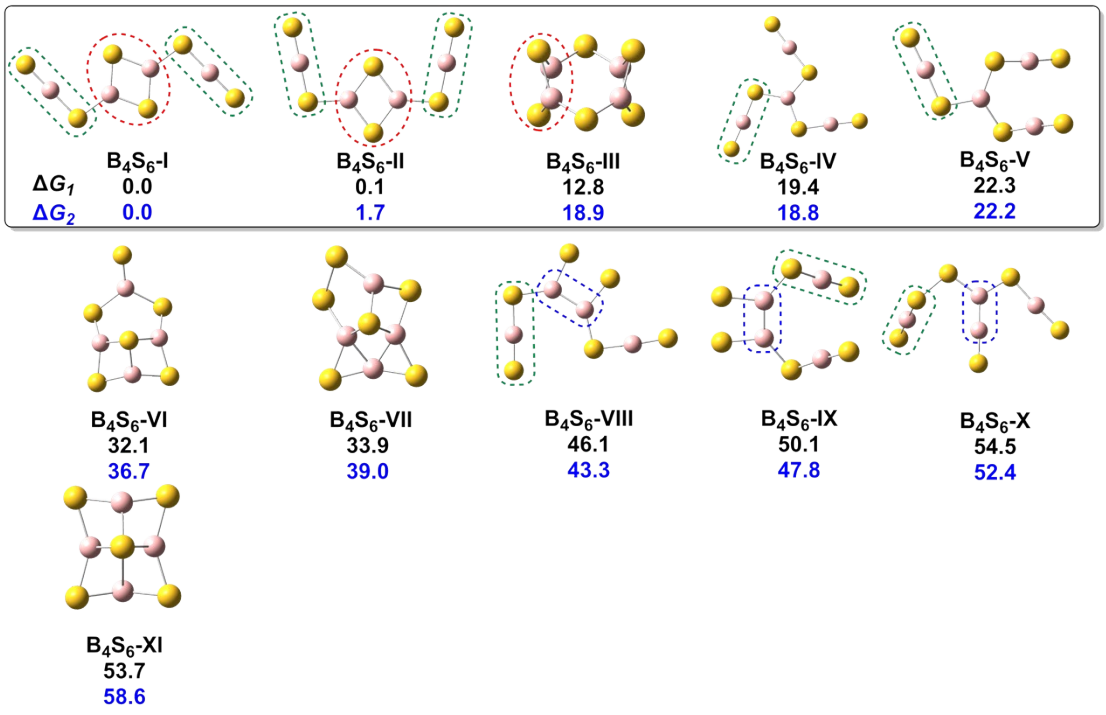

Fig. S2. Optimized the low-energy isomers of B_4S_6 cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol) and G4(MP2)-6X method (ΔG_2, in kcal/mol), respectively. The color of atoms: S-yellow; B-pink.

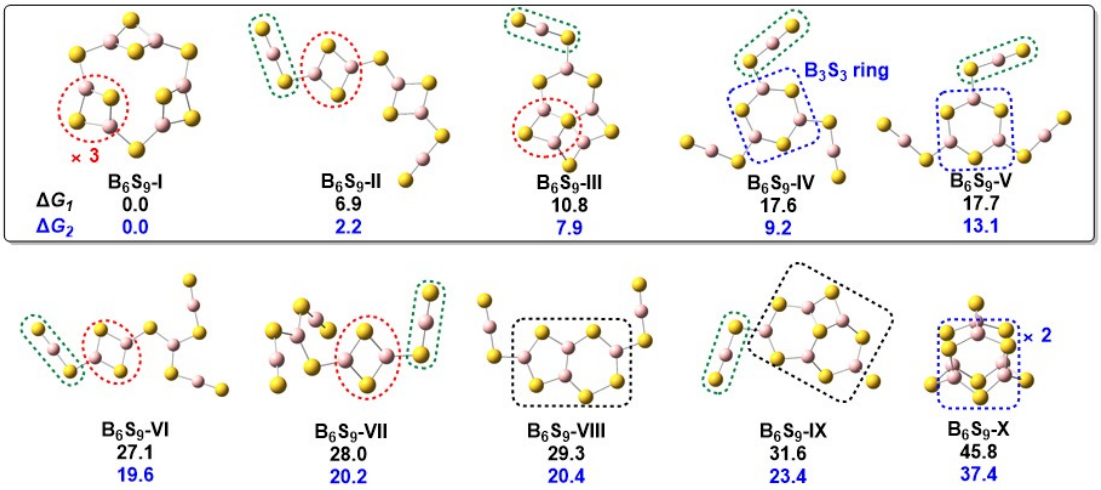

Fig. S3. Optimized the low-energy isomers of B_6S_9 cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol) and G4(MP2)-6X method (ΔG_2, in kcal/mol), respectively. The color of atoms: S-yellow; B-pink.

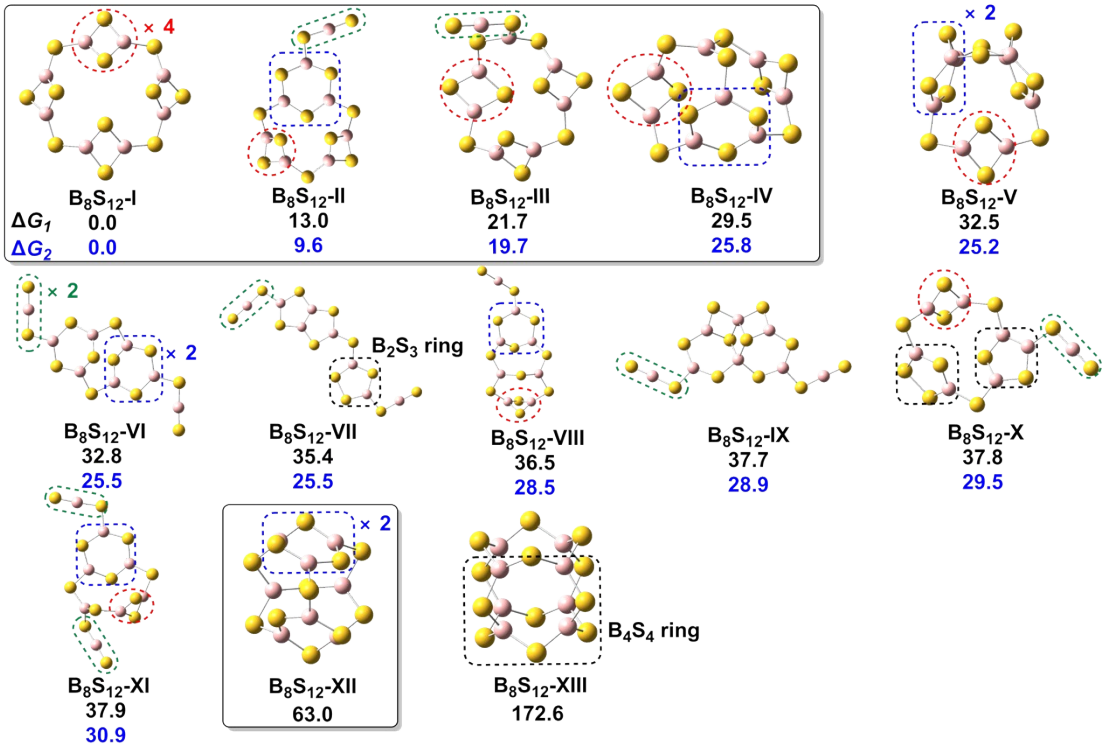

Fig. S4. Optimized the low-energy isomers of B_8S_{12} cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol) and G4(MP2)-6X method (ΔG_2, in kcal/mol), respectively. The color of atoms: S-yellow; B-pink.

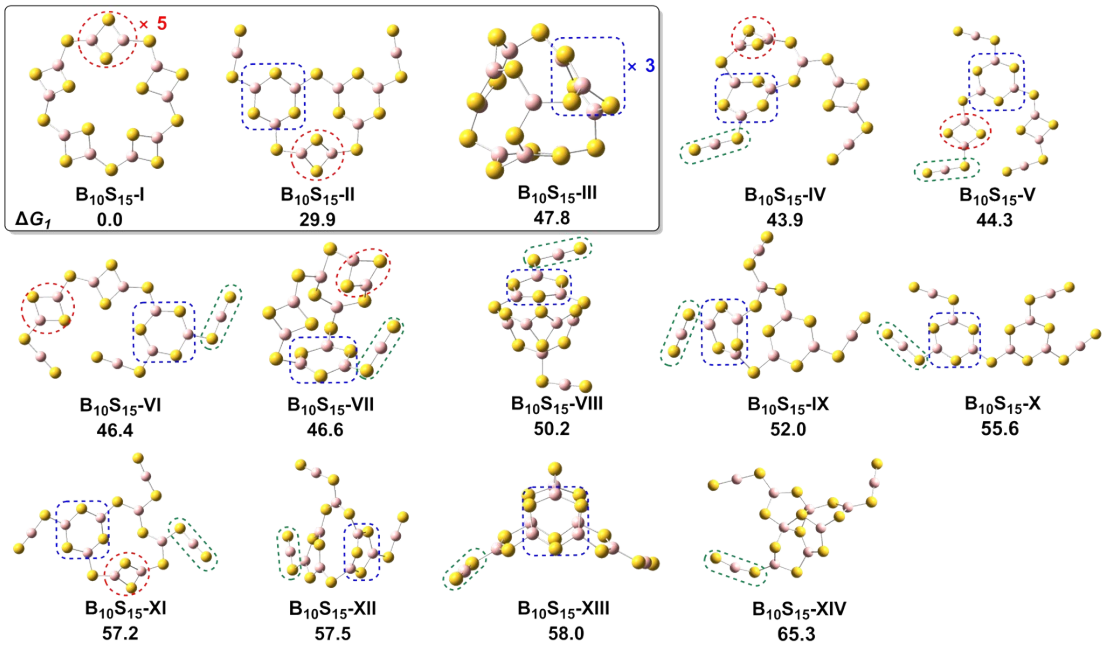

Fig. S5. Optimized the low-energy isomers of $B_{10}S_{15}$ cluster and their free energies calculated at the M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

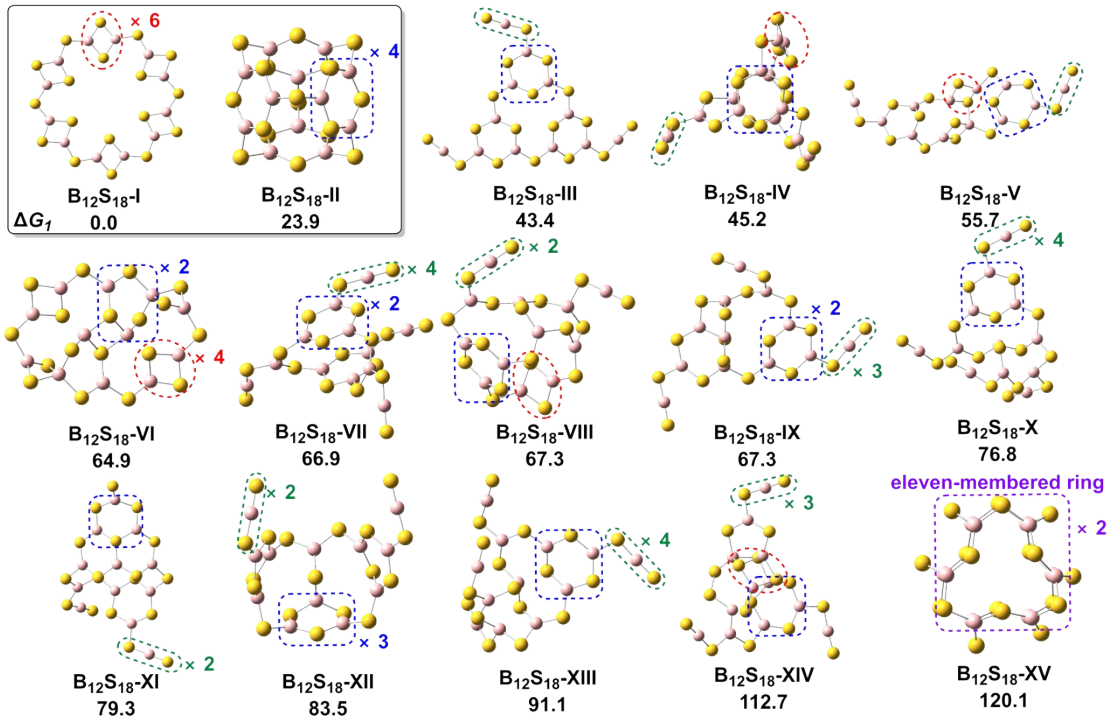

Fig. S6. Optimized the low-energy isomers of $B_{12}S_{18}$ cluster and their free energies calculated at the M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

2. Low-Energy Structures of cation clusters $(B_2S_3)_n^+$

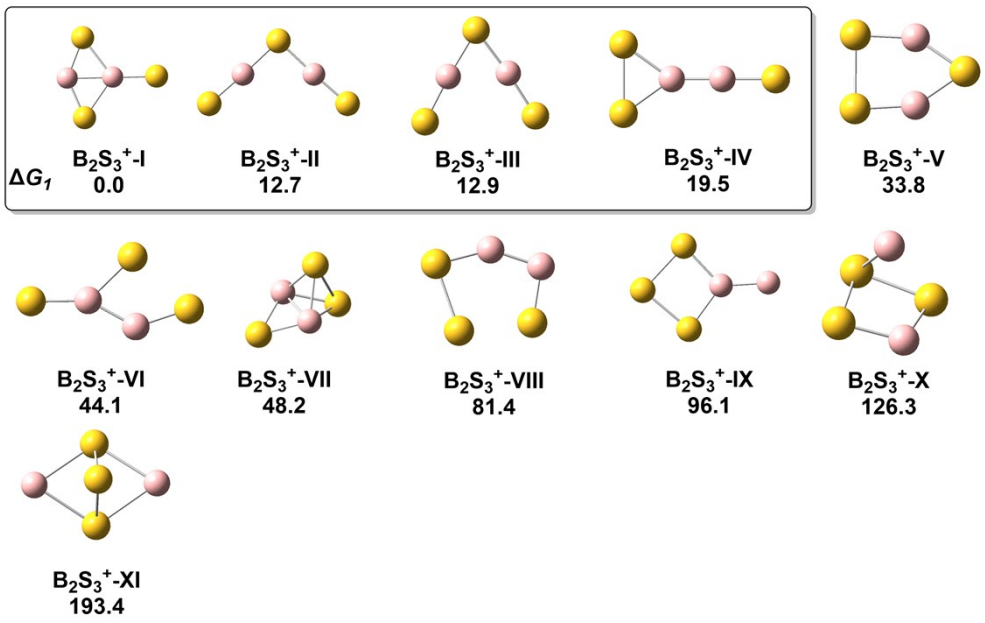

Fig. S7 Optimized the low-energy isomers of $B_2S_3^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

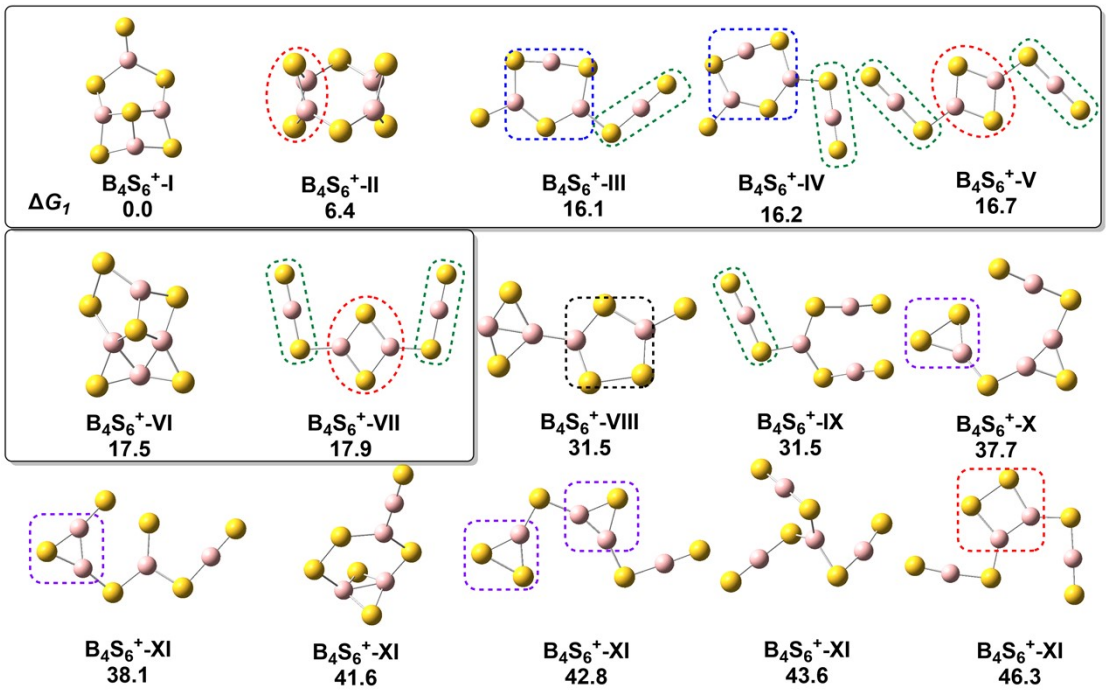

Fig. S8 Optimized the low-energy isomers of $B_4S_6^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

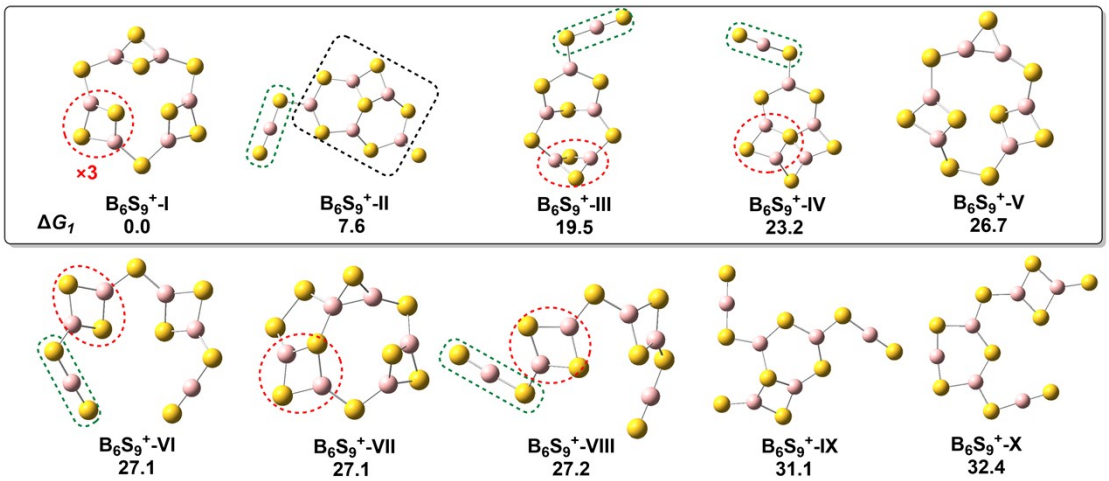

Fig. S9 Optimized the low-energy isomers of $B_6S_9^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

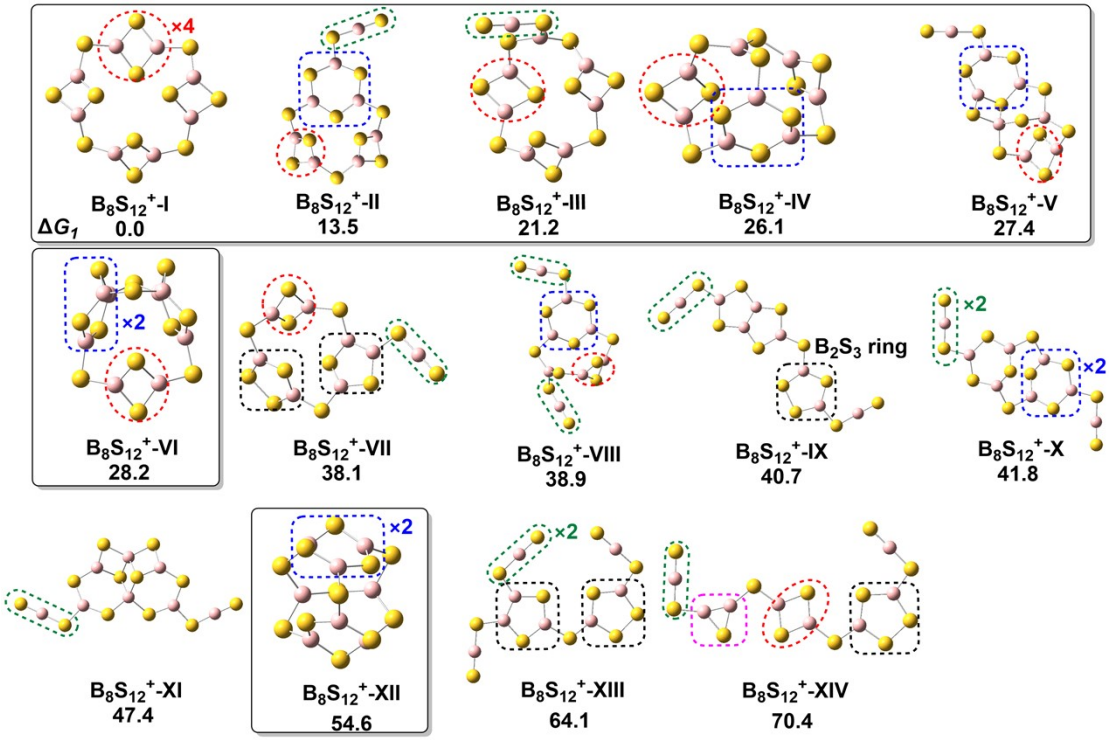

Fig. S10 Optimized the low-energy isomers of $B_8S_{12}^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

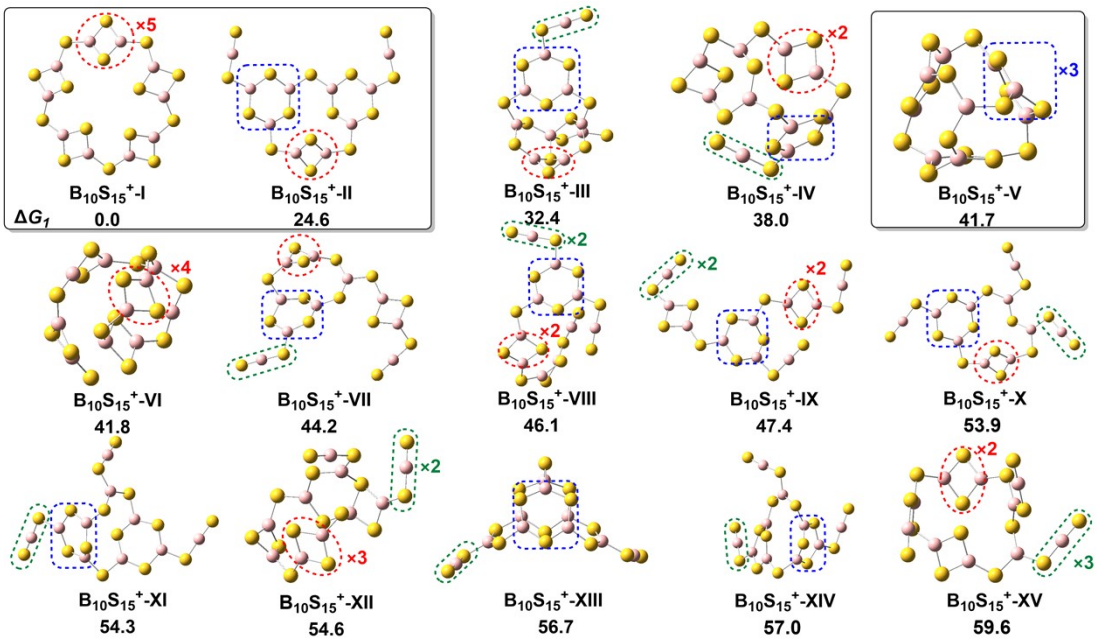

Fig. S11 Optimized the low-energy isomers of $B_{10}S_{15}^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

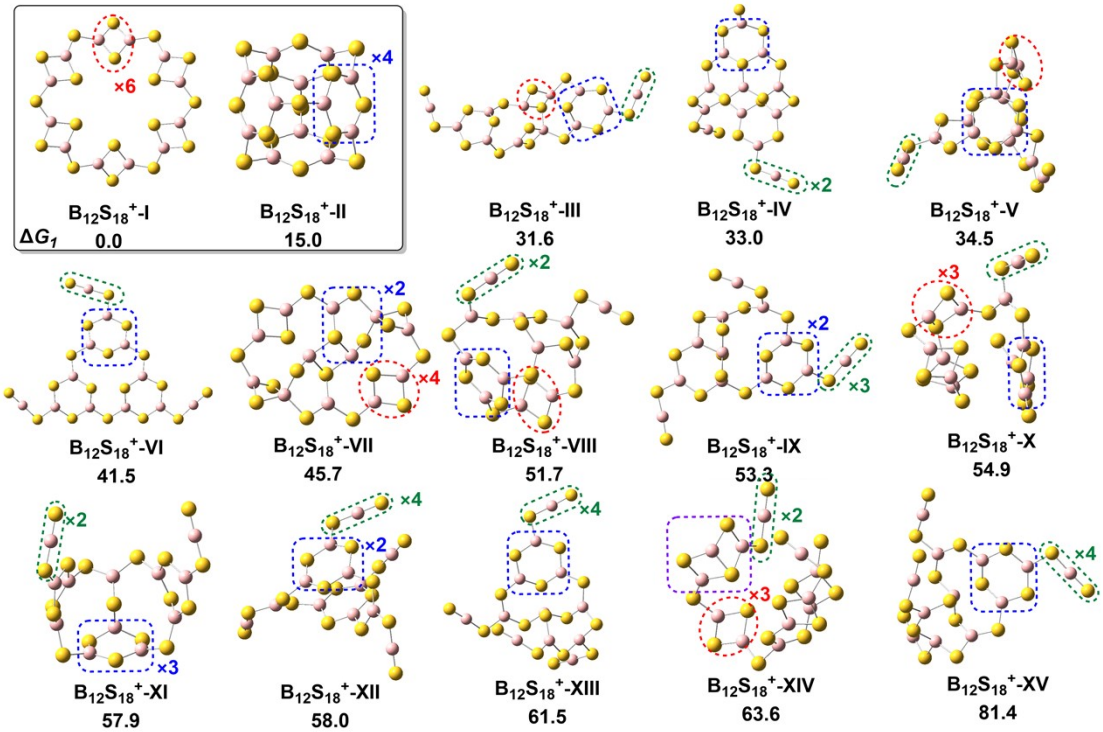

Fig. S12 Optimized the low-energy isomers of $B_{12}S_{18}^+$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

3. Low-Energy Structures of anion clusters $(B_2S_3)_n^-$

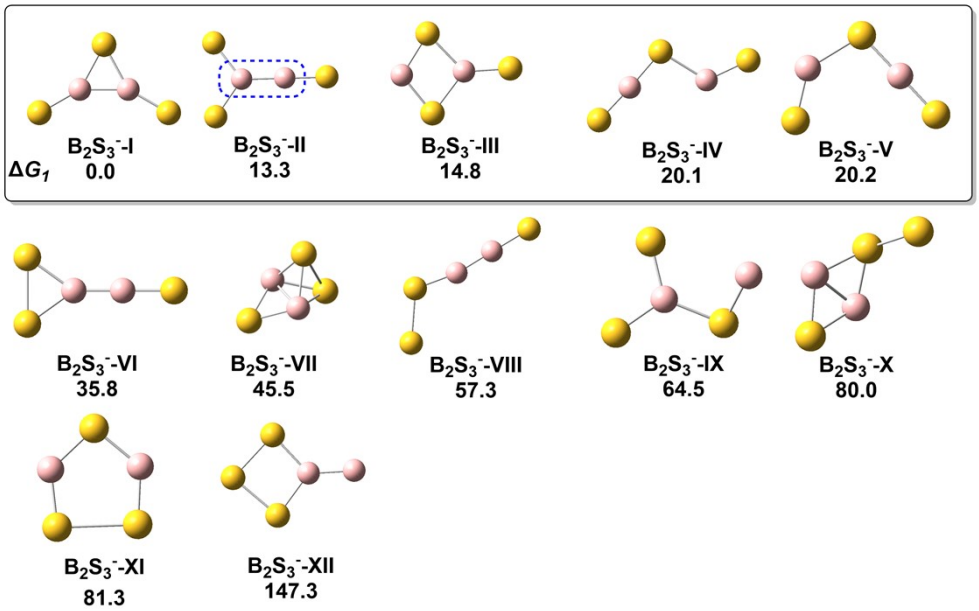

Fig. S13. Optimized the low-energy isomers of $B_2S_3^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

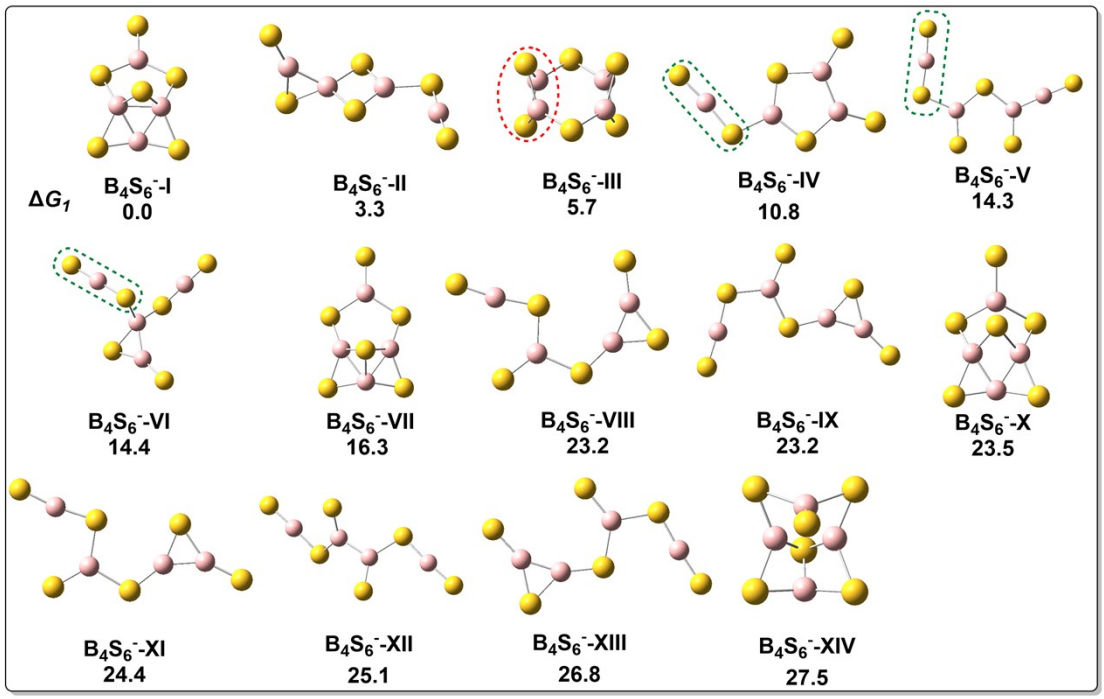

Fig. S14. Optimized the low-energy isomers of $B_4S_6^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

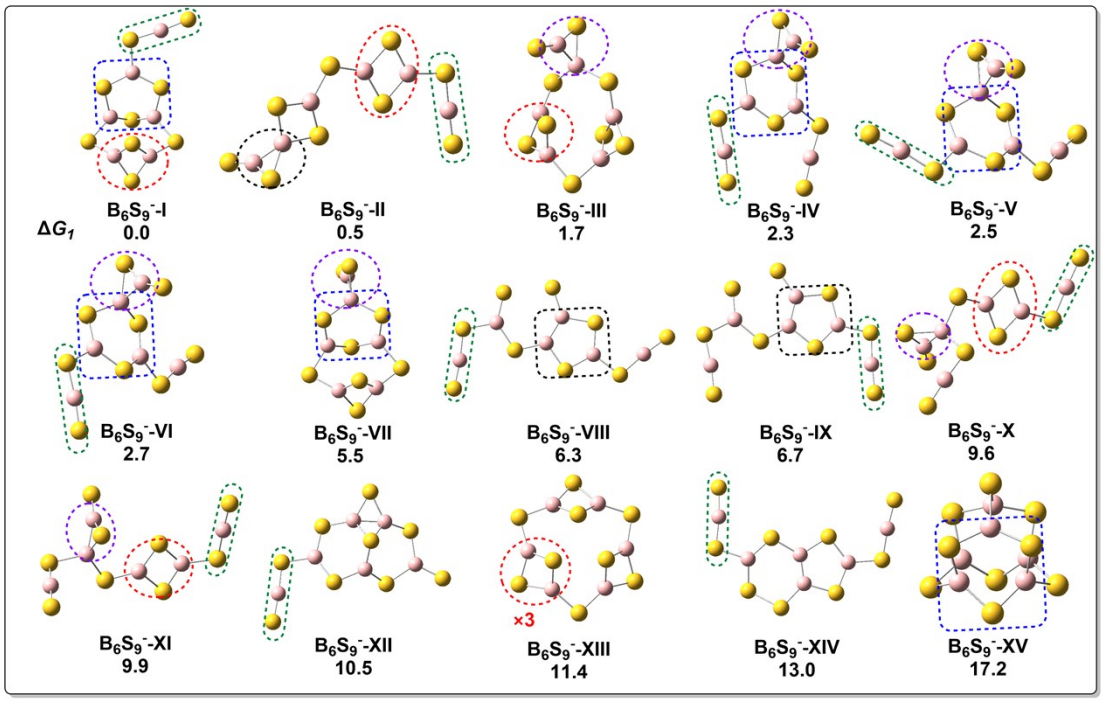

Fig. S15. Optimized the low-energy isomers of $B_6S_9^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

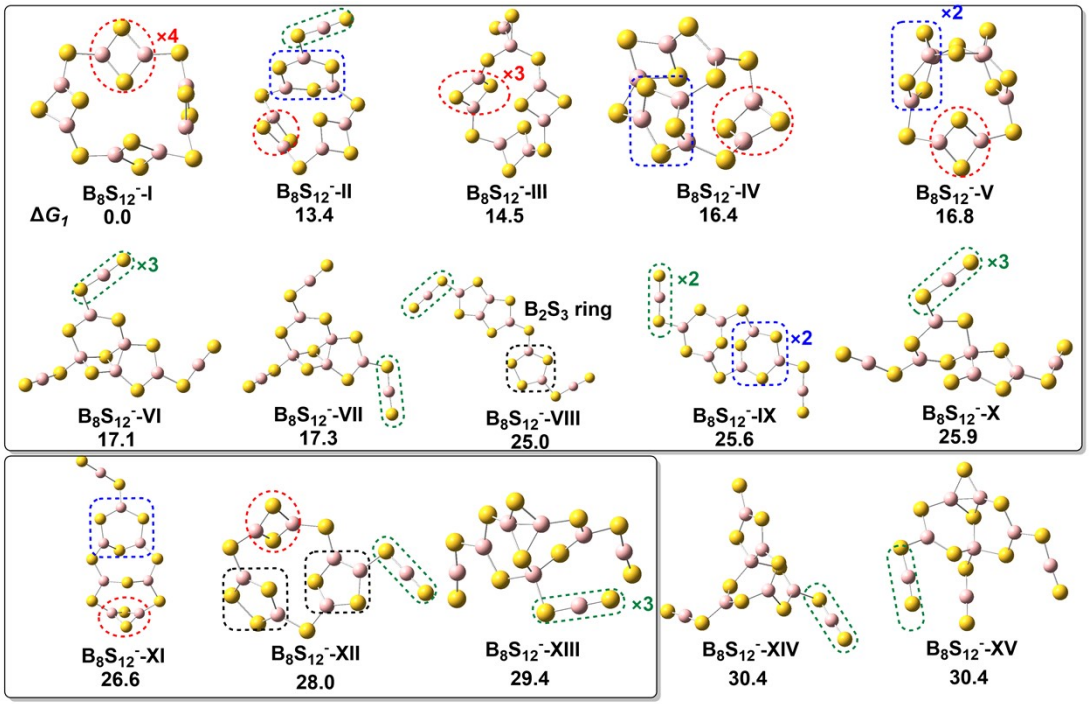

Fig. S16. Optimized the low-energy isomers of $B_8S_{12}^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

Fig. S17. Optimized the low-energy isomers of $B_{10}S_{15}^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

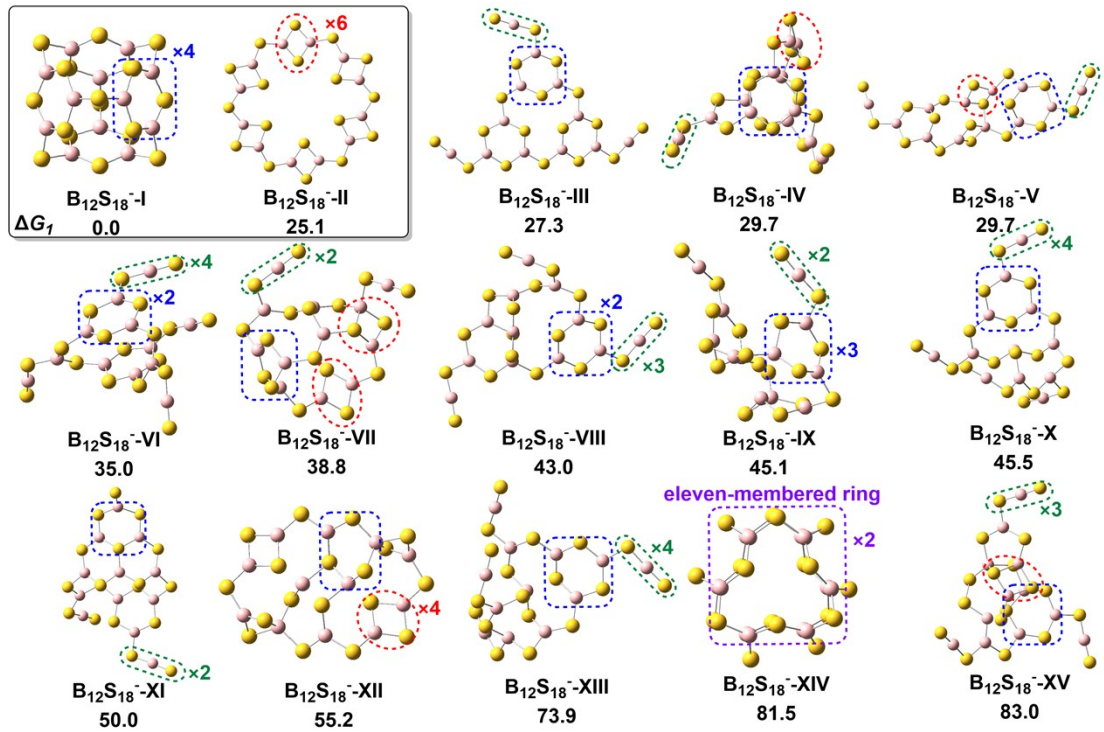

Fig. S18. Optimized the low-energy isomers of $B_{12}S_{18}^-$ cluster and their free energies calculated using M06-2X-D3/6-31G(d,p) level (ΔG_1, in kcal/mol). The color of atoms: S-yellow; B-pink.

4. AdNDP analysis

AdNDP, developed by Zubarev and Boldyrev, is a theoretical tool that combines the intuitive simplicity of Lewis theory with the adaptability of canonical molecular orbital theory to analyze chemical bonding.[1] The density matrix P is represented in the block form:

$$P = \begin{vmatrix} P_{11} & P_{12} & \cdots & P_{1N} \\ P_{21} & P_{22} & \cdots & P_{2N} \\ \cdots & \cdots & \cdots & \cdots \\ P_{i1} & P_{i2} & \cdots & P_{iN} \\ \cdots & \cdots & \cdots & \cdots \\ P_{N1} & P_{N2} & \cdots & P_{NN} \end{vmatrix}$$

where each block corresponds to a specific atomic center. By diagonalizing the sub-blocks of P, hybrid orbitals that maximize electron occupancy at that center can be obtained. Notably, the AdNDP method has proven effective for analyzing bonding in various systems, including boron clusters,[2, 3] boron oxide clusters,[4, 5] and so on. The delocalized orbitals of $B_{10}S_{15}$ and $B_{12}S_{18}$ clusters display analogous bonding characteristics, mainly including lone pair electrons on the S atoms, 2c-2e σ-bonds from B−S single bonds, delocalized 3c-2e π-bond contributed by B−S−B units, and 4c-2e π-bonds and 2c-2e π*-bonds from the planar or non-planar B_2S_2 rings.

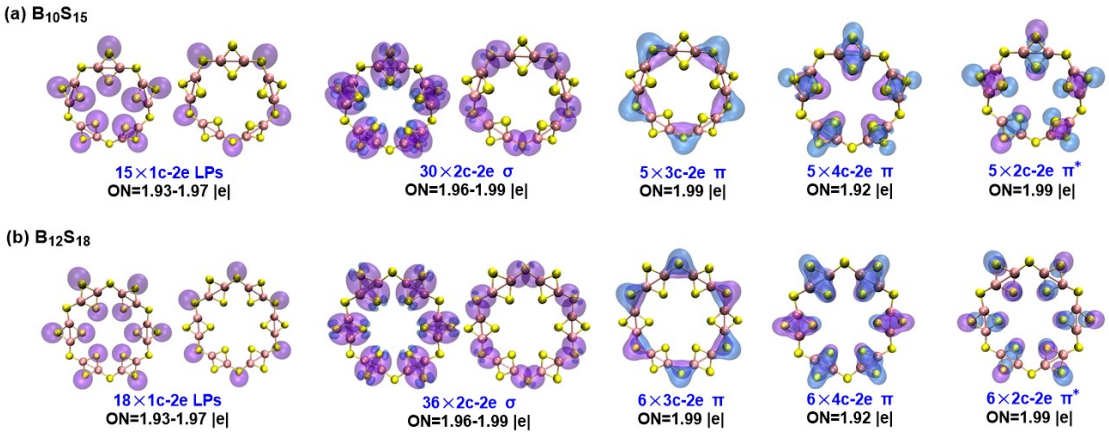

Fig. S7. AdNDP delocalized bonding patterns and their occupied numbers for (a) $B_{10}S_{15}$ and (b) $B_{12}S_{18}$. The color of atoms: S-yellow, B-pink.

5. Optimized structures of $[B_2S_3]_n[NH_3]_m$

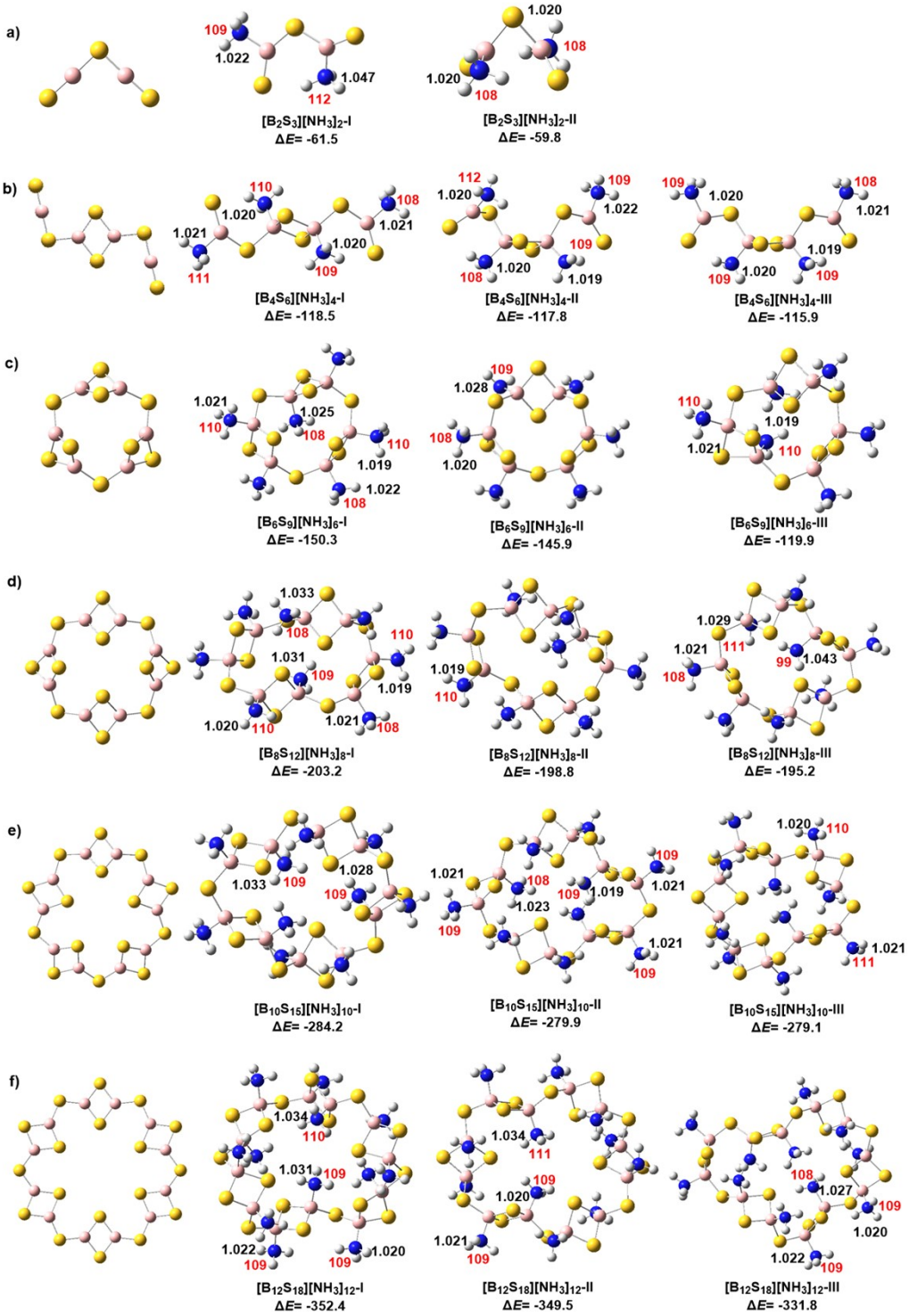

Fig. S8. The optimized structures of the studied $[B_2S_3]_n[NH_3]_m$, and the relative energies (ΔE, in kcal/mol). The key N−H bond lengths (Å) and H−N−H angles (°) are given in black and red, respectively. The color of atoms: S-yellow; B-pink; N-blue; H-white.

6. Optimized structures of $[B_2S_3]_n[CO]_m$

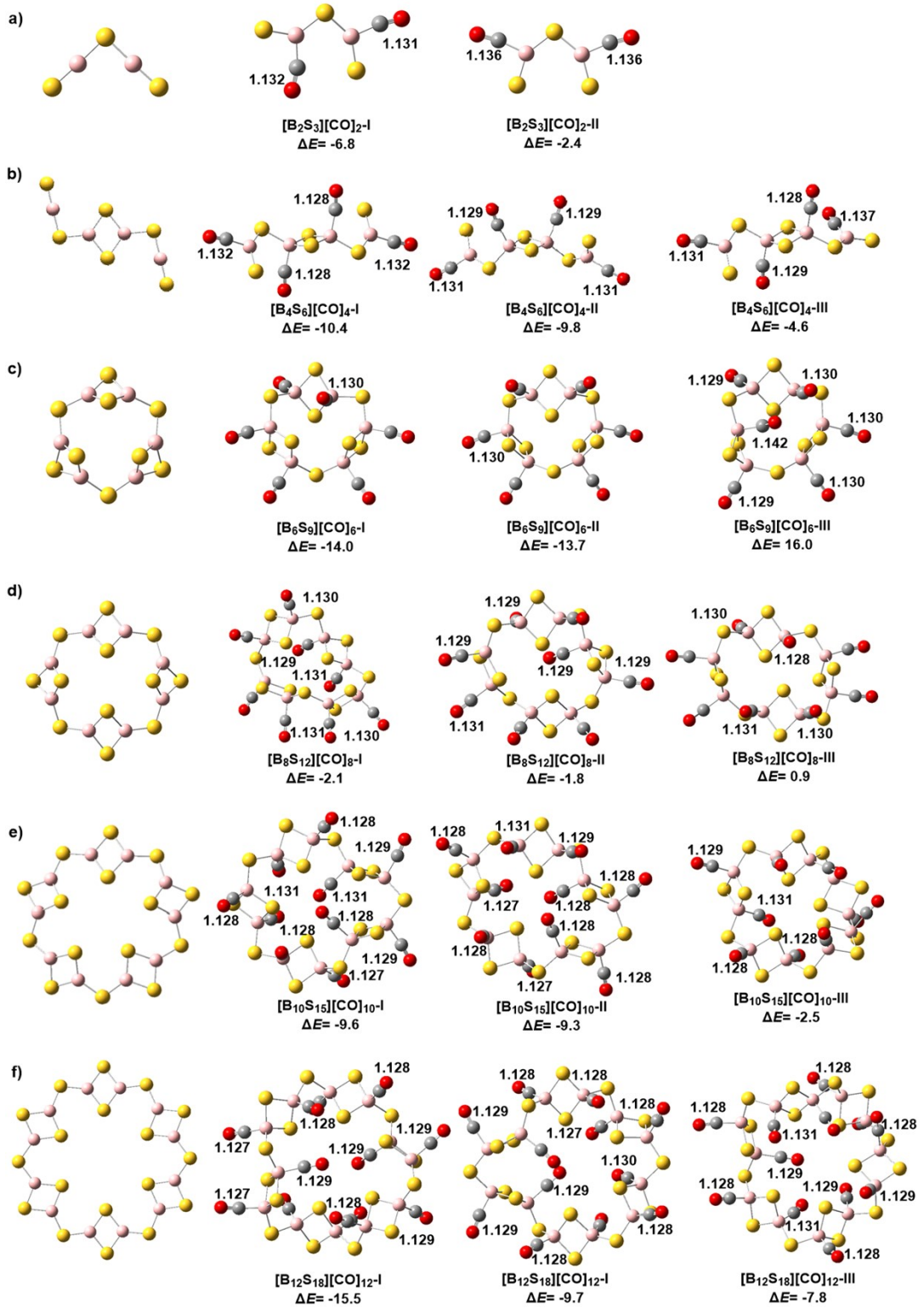

Fig. S9. The optimized structures of the studied $[B_2S_3]_n[CO]_m$, and the relative energies (ΔE, in kcal/mol). The key C−O bond lengths (Å) are given in black. The color of atoms: S-yellow; B-pink; C-gray; O-red.

7. Interaction analysis between [B_2S_3] with NH_3 and CO molecules

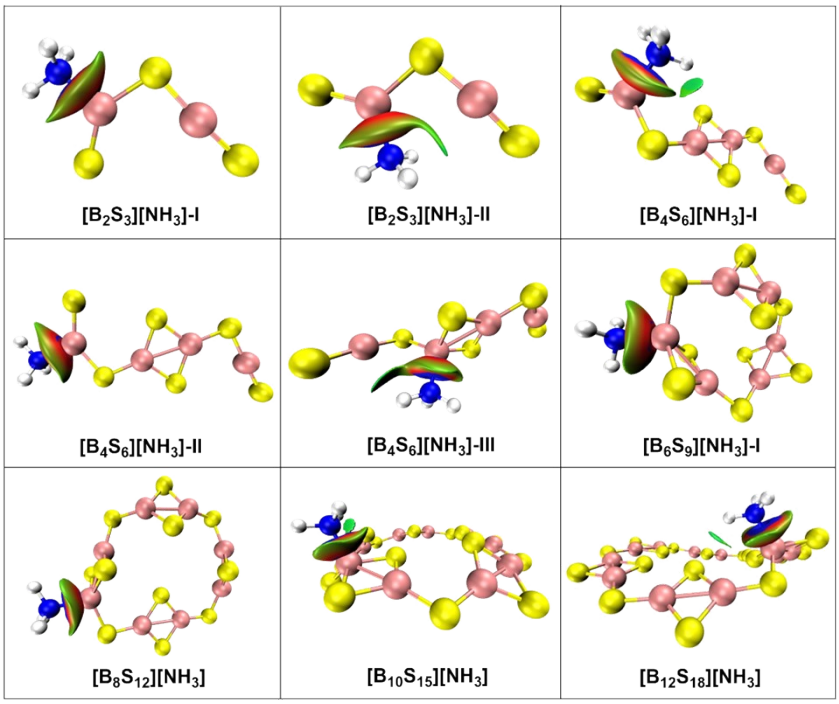

Fig. S10. The interaction between $[B_2S_3]_n$ and NH_3 molecular. The color of atoms: S-yellow; B-pink; N-blue; H-white.

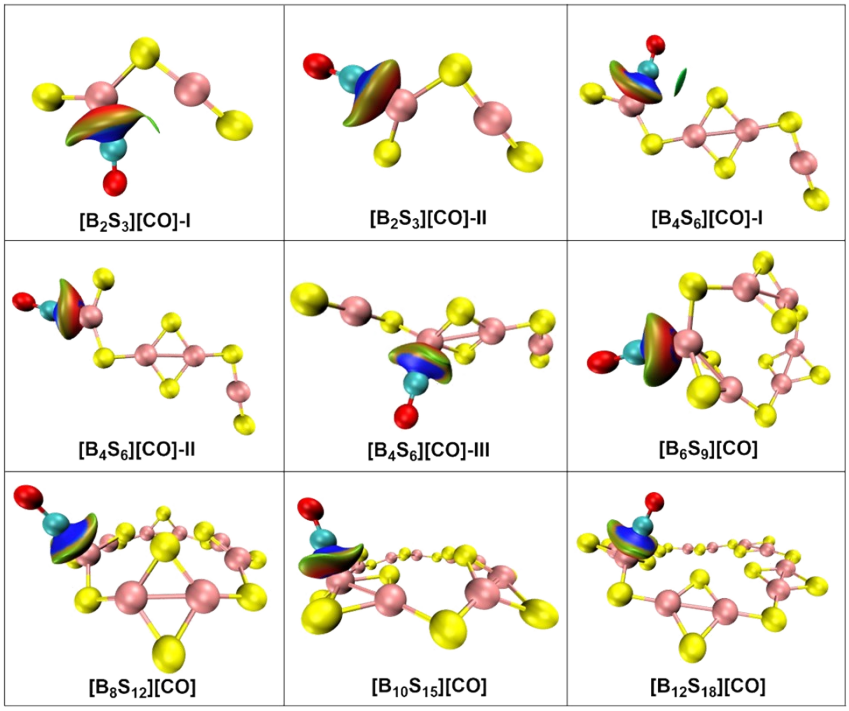

Fig. S11. The interaction between $[B_2S_3]_n$ and CO molecular. The color of atoms: S-yellow; B-pink; C-green; O-red.

8. Absolute free energies and electronic energies of all stationary points

Table S1. The calculated absolute free energies and electronic energies (E, in a.u.) at the M06-2X-D3/6-31G(d,p) level (G_1 and E_1, in a.u.) and G4(MP2)-6X method (G_2 and E_2, in a.u.).

Species	G_1	E_1	G_2	E_2
B_2S_3-I	-1244.250493	-1244.230932	-1243.03877553	-1243.01857364
B_2S_3-II	-1244.214713	-1244.195664	-1242.99857893	-1242.97890845
B_2S_3-III	-1244.204203	-1244.184928	-1242.99349642	-1242.97298520
B_2S_3-IV	-1244.11327	-1244.096429	-1242.91195480	-1242.89311611
B_2S_3-V	-1244.106472	-1244.084136	-1242.90690132	-1242.88485236
B_2S_3-VI	-1244.081242	-1244.061086	-1242.88715079	-1242.86706865
B_2S_3-VII	-1244.037476	-1244.016471	-1242.84205284	-1242.82108598
B_2S_3-VIII	-1243.943006	-1243.918285	-1242.75289940	-1242.72861803
B_4S_6-I	-2488.560729	-2488.544207	-2486.13421498	-2486.11524381
B_4S_6-II	-2488.560639	-2488.544106	-2486.13147818	-2486.11516030
B_4S_6-III	-2488.540332	-2488.540332	-2486.10414799	-2486.09493390
B_4S_6-IV	-2488.529875	-2488.529875	-2486.10419500	-2486.08686262
B_4S_6-V	-2488.525206	-2488.525206	-2486.09888257	-2486.08188150
B_4S_6-VI	-2488.509556	-2488.509556	-2486.07571582	-2486.06533028
B_4S_6-VII	-2488.506778	-2488.506778	-2486.07200184	-2486.06132920
B_4S_6-VIII	-2488.487219	-2488.487219	-2486.06523413	-2486.04742494
B_4S_6-IX	-2488.480928	-2488.480928	-2486.05797788	-2486.04028486
B_4S_6-X	-2488.473841	-2488.473841	-2486.05078946	-2486.03197398
B_4S_6-XI	-2488.475221	-2488.475221	-2486.04076648	-2486.03165330
B_6S_9-I	-3732.87902	-3732.877632	-3729.22639547	-3729.22418615
B_6S_9-II	-3732.867967	-3732.853432	-3729.22285807	-3729.20813043
B_6S_9-III	-3732.861848	-3732.856253	-3729.21376148	-3729.20690892
B_6S_9-IV	-3732.851043	-3732.837967	-3729.21165939	-3729.19778052

B_6S_9-V	-3732.850836	-3732.838029	-3729.20558207	-3729.19829731
B_6S_9-VI	-3732.835774	-3732.820077	-3729.19521809	-3729.17850349
B_6S_9-VII	-3732.834446	-3732.820251	-3729.19415650	-3729.18188074
B_6S_9-VIII	-3732.832305	-3732.821302	-3729.19383780	-3729.17803770
B_6S_9-IX	-3732.828684	-3732.821425	-3729.18907147	-3729.18074552
B_6S_9-X	-3732.805981	-3732.805873	-3729.16681406	-3729.16567579
B_8S_{12}-I	-4977.212695	-4977.215440	-4972.34461388	-4972.34669029
B_8S_{12}-II	-4977.192007	-4977.192138	-4972.329246588	-4972.32819397
B_8S_{12}-III	-4977.17814	-4977.177329	-4972.31314138	-4972.31096606
B_8S_{12}-IV	-4977.165677	-4977.171374	-4972.30349021	-4972.30782122
B_8S_{12}-V	-4977.160838	-4977.168393	-4972.30437794	-4972.30980182
B_8S_{12}-VI	-4977.160358	-4977.156415	-4972.30396897	-4972.30087039
B_8S_{12}-VII	-4977.156261	-4977.150443	-4972.30403439	-4972.29669021
B_8S_{12}-VIII	-4977.15458	-4977.157277	-4972.29914561	-4972.30065522
B_8S_{12}-IX	-4977.152547	-4977.150300	-4972.29858239	-4972.29642288
B_8S_{12}-X	-4977.152472	-4977.154163	-4972.29764221	-4972.29700590
B_8S_{12}-XI	-4977.152303	-4977.150204	-4972.29538763	-4972.29123152
B_8S_{12}-XII	-4977.112298	-4977.119983	---	---
B_8S_{12}-XIII	-4976.9377	-4976.943168	---	---
$B_{10}S_{15}$-I	-6221.534196	-6221.538542	---	---
$B_{10}S_{15}$-II	-6221.486567	-6221.489926	---	---
$B_{10}S_{15}$-III	-6221.457891	-6221.474483	---	---
$B_{10}S_{15}$-IV	-6221.464159	-6221.463381	---	---
$B_{10}S_{15}$-V	-6221.463541	-6221.456675	---	---
$B_{10}S_{15}$-VI	-6221.46027	-6221.457319	---	---
$B_{10}S_{15}$-VII	-6221.459864	-6221.469605	---	---
$B_{10}S_{15}$-VIII	-6221.454218	-6221.461206	---	---
$B_{10}S_{15}$-IX	-6221.451271	-6221.451719	---	---
$B_{10}S_{15}$-X	-6221.445583	-6221.438011	---	---

$B_{10}S_{15}$-XI	-6221.443071	-6221.441033	---	---
$B_{10}S_{15}$-XII	-6221.44261	-6221.443502	---	---
$B_{10}S_{15}$-XIII	-6221.44179	-6221.447044	---	---
$B_{10}S_{15}$-XIV	-6221.430196	-6221.434813	---	---
$B_{12}S_{18}$-I	-7465.849773	-7465.854227	---	---
$B_{12}S_{18}$-II	-7465.811727	-7465.836622	---	---
$B_{12}S_{18}$-III	-7465.780554	-7465.786502	---	---
$B_{12}S_{18}$-IV	-7465.777664	-7465.792309	---	---
$B_{12}S_{18}$-V	-7465.761034	-7465.774828	---	---
$B_{12}S_{18}$-VI	-7465.746419	-7465.772152	---	---
$B_{12}S_{18}$-VII	-7465.743109	-7465.75092	---	---
$B_{12}S_{18}$-VIII	-7465.742587	-7465.75747	---	---
$B_{12}S_{18}$-IX	-7465.742555	-7465.752533	---	---
$B_{12}S_{18}$-X	-7465.727377	-7465.735419	---	---
$B_{12}S_{18}$-XI	-7465.723341	-7465.733804	---	---
$B_{12}S_{18}$-XII	-7465.716728	-7465.726224	---	---
$B_{12}S_{18}$-XIII	-7465.70464	-7465.714494	---	---
$B_{12}S_{18}$-XIV	-7465.670205	-7465.683514	---	---
$B_{12}S_{18}$-XV	-7465.657026	-7465.680558	---	---

Table S2. The calculated absolute free energies (G_1, in a.u.) and electronic energies (E_1, in a.u.) at the M06-2X-D3/6-31G(d,p).

Species	G_1	E_1	Species	G_1	E_1
NH_3	-56.504905	-56.521673	**$[B_4S_6][NH_3]$-III**	-2545.084893	-2545.106710
$[B_2S_3][NH_3]$-I	-1300.783499	-1300.801746	**$[B_6S_9][NH_3]$**	-3789.430266	-3789.467033
$[B_2S_3][NH_3]$-II	-1300.778356	-1300.796553	**$[B_8S_{12}][NH_3]$**	-5033.751999	-5033.793189
$[B_4S_6][NH_3]$-I	-2545.100469	-2545.124659	**$[B_{10}S_{15}][NH_3]$**	-6278.069809	-6278.115307
$[B_4S_6][NH_3]$-II	-2545.087422	-2545.108419	**$[B_{12}S_{18}][NH_3]$**	-7522.386522	-7522.432946
CO	-113.284665	-113.270737	**$[B_4S_6][CO]$-III**	-2601.828683	-2601.816106
$[B_2S_3][CO]$-I	-1357.521347	-1357.506718	**$[B_6S_9][CO]$**	-3846.166866	-3846.169544
[B2S3][CO]-II	-1357.520684	-1357.506191	**$[B_8S_{12}][CO]$**	-5090.486560	-5090.494498
$[B_4S_6$-I$][CO]$-I	-2601.833603	-2601.822414	**$[B_{10}S_{15}][CO]$**	-6334.808916	-6334.817917
$[B_4S_6$-I$][CO]$-II	-2601.828858	-2601.817074	**$[B_{12}S_{18}][CO]$**	-7579.119279	-7579.134268
$[B_2S_3][NH_3]_2$-I	-1357.315615	-1357.372286	**$[B_8S_{12}][NH_3]_8$-II**	-5429.386609	-5429.705646
$[B_2S_3][NH_3]_2$-II	-1357.309953	-1357.369516	**$[B_8S_{12}][NH_3]_8$-III**	-5429.392673	-5429.712766
$[B_4S_6][NH_3]_4$-I	-2714.676738	-2714.815648	**$[B_{10}S_{15}][NH_3]_{10}$-I**	-6786.792026	-6787.200116
$[B_4S_6][NH_3]_4$-II	-2714.677433	-2714.818668	**$[B_{10}S_{15}][NH_3]_{10}$-II**	-6786.792168	-6787.201374
$[B_4S_6][NH_3]_4$-III	-2714.681554	-2714.819761	**$[B_{10}S_{15}][NH_3]_{10}$-III**	-6786.798536	-6787.208115
$[B_6S_9][NH_3]_6$-I	-4071.964286	-4072.198748	**$[B_{12}S_{18}][NH_3]_{12}$-I**	-8144.148507	-8144.642997
$[B_6S_9][NH_3]_6$-II	-4072.00821	-4072.240134	**$[B_{12}S_{18}][NH_3]_{12}$-II**	-8144.17559	-8144.671165
$[B_6S_9][NH_3]_6$-III	-4072.01411	-4072.247163	**$[B_{12}S_{18}][NH_3]_{12}$-III**	-8144.178582	-8144.675809
$[B_8S_{12}][NH_3]_8$-I	-5429.379044	-5429.699945			
$[B_2S_3][CO]_2$-I	-1470.786788	-1470.776218	**$[B_8S_{12}][CO]_8$-II**	-5883.342563	-5883.384182
$[B_2S_3][CO]_2$-II	-1470.793597	-1470.783296	**$[B_8S_{12}][CO]_8$-III**	-5883.341854	-5883.384722
$[B_4S_6][CO]_4$-I	-2941.630419	-2941.634411	**$[B_{10}S_{15}][CO]_{10}$-I**	-7354.189908	-7354.249817
$[B_4S_6][CO]_4$-II	-2941.637098	-2941.642837	**$[B_{10}S_{15}][CO]_{10}$-II**	-7354.200022	-7354.260744
$[B_4S_6][CO]_4$-III	-2941.638269	-2941.643761	**$[B_{10}S_{15}][CO]_{10}$-III**	-7354.199402	-7354.261212
$[B_6S_9][CO]_6$-I	-4412.446992	-4412.476632	**$[B_{12}S_{18}][CO]_{12}$-I**	-8825.039544	-8825.115475
$[B_6S_9][CO]_6$-II	-4412.498340	-4412.523832	**$[B_{12}S_{18}][CO]_{12}$-II**	-8825.042356	-8825.118439

$[B_6S_9][CO]_6$-III	-4412.496782	-4412.524437	**$[B_{12}S_{18}][CO]_{12}$-III**	-8825.051566	-8825.127731
$[B_8S_{12}][CO]_8$-I	-5883.342819	-5883.382783			

9. The bonding energy between $(B_2S_3)_n$ clusters and B_2S_3 monolayer

Table S3 The calculated bonding energy (E_{bond}, in eV) between $(B_2S_3)_n$ clusters and B_2S_3 monolayer (*Nanoscale*, 2021,13, 3627).

The number of B_2S_3	Species	E_{bond} (eV)	Species	E_{bond} (eV)
1	**B_2S_3**	6.00899447	**B_2S_3 monolayer (unit cell)**	4.245039642
2	**B_4S_6**	5.002760412	**B_2S_3 monolayer (2×1×1 supercell)**	4.284279641
3	**B_6S_9**	4.245475076	**B_2S_3 monolayer (2×2×1 supercell)**	4.284277196
4	**B_8S_{12}**	4.291735525	**B_2S_3 monolayer (3×1×1 supercell)**	4.284279515
5	**$B_{10}S_{15}$**	4.309766436	**B_2S_3 monolayer (5×1×1 supercell)**	4.284280219
6	**$B_{12}S_{18}$**	4.314446696	**B_2S_3 monolayer (3×2×1 supercell)**	4.284281377

Method. To ensure a direct comparison, we calculated the bonding energy using the following formula:

$$E_{bond}\left([B_2S_3]_n\right) = \frac{2nE(B) + 3nE(S) - E\left([B_2S_3]_n\right)}{N_{bond}}$$

where N_{bond} is the number of bonds.

All calculations are performed using density functional theory (DFT) and the Vienna ab initio simulation package (VASP).[6-8] The exchange-correction function was described by the Perdew-Burke-Ernzerhof (PBE) function within the generalized gradient approximation (GGA).[9] The crystal structures are completely relaxed until the energy is less than 10^{-5} eV and the residual force is less than 0.01 eV Å^{-1}. The plane wave energy cutoff is set to 500 eV and the Monkhorst–Pack mesh of 13×13×1 K-

points is employed for structural optimization. A vacuum space of 20 Å is necessary in the vertical direction for the monolayers.

Discussion. The results show that the bonding energy of $(B_2S_3)_n$ clusters is generally stronger than that of the B_2S_3 monolayer (except B_6S_9 cluster). For B_2S_3 and B_4S_6 clusters, their bonding energies are 6.008 eV and 5.003 eV, respectively, while the corresponding bonding energies in the B_2S_3 monolayer with the same number of units are 4.245 eV and 4.284 eV. This enhancement in clusters arises from the presence of terminal B−S (between double and triple bonds triple bonds), which strengthen the overall bonding. However, B_6S_9 cluster exhibits a lower bonding energy (4.245 eV) compared to the corresponding B_2S_3 monolayer consistent with previous studies, which suggest that B_6S_9 is relatively less stable and more prone to interactions with small molecules. As the cluster size increases, such as in B_8S_{12}, $B_{10}S_{15}$, and $B_{12}S_{18}$, the bonding energy gradually increases and remains higher than that of the corresponding B_2S_3 monolayer.

10. Cartesian coordinates

Table S4. Cartesian coordinates of all the studied molecules.

B_2S_3-I

B	-1.27821000	0.25478600	-0.00003900
B	1.27820700	0.25478300	0.00005200
S	-2.46491700	-0.82516700	-0.00006000
S	-0.00000100	1.49109200	-0.00002900
S	2.46492000	-0.82516500	0.00008500

B_2S_3-II

B	-1.40963800	0.00027600	0.00052300
B	0.43595500	0.00024900	0.00093300
S	2.08424600	-0.00053200	-0.00011200
S	-0.89046600	-1.58492500	-0.00017100
S	-0.88950400	1.58529300	-0.00017100

B_2S_3-III

B	1.38138800	-0.00094900	0.00020800
B	-0.26811300	-0.00125900	0.00023700
S	2.98256500	-0.00022500	0.00014400
S	-1.66408300	1.08893100	-0.00020400
S	-1.66638000	-1.08801500	-0.00007800

B_2S_3-IV

B	-0.26597100	0.00007200	-0.91856200
B	-0.26583800	0.00009500	0.91843400
S	0.99922200	1.05596100	0.00000100
S	0.99907600	-1.05604400	0.00000700
S	-1.83210700	0.00003100	0.00003100

B_2S_3-V

B	1.05085100	0.29063800	-0.01138500
B	-1.69154700	-0.56580300	1.43523700
S	2.51885400	-0.35613600	-0.00202100
S	-0.55413300	1.05972000	-0.01160800
S	-1.76450300	-0.61759500	-0.43132600

B_2S_3-VI

B	-1.92878400	1.12905700	0.00005600
B	-0.36140000	1.24213700	-0.00007400
S	-1.68428700	-0.50935000	-0.00000600
S	1.31725500	0.91129200	0.00000900
S	1.08271500	-1.14294000	0.00000300

B_2S_3-VII

B	2.95936600	-0.00006300	-0.00002300
B	1.18899100	-0.00009900	0.00000200
S	-1.46186100	0.00011800	-0.00001300
S	0.08284600	1.42437300	0.00001000
S	0.08265400	-1.42444100	0.00001000

B_2S_3- VIII

B	3.02401600	0.58705800	0.00000000
B	-3.02401900	0.58705200	0.00000000
S	1.58496500	-0.59077700	0.00000000
S	0.00000000	0.81464500	0.00000000
S	-1.58496400	-0.59077800	0.00000000

B_4S_6-I

B	-3.61878200	-0.39083800	0.00002300
B	-0.91360200	-0.58563000	-0.00005700
S	-4.74648700	0.75310600	0.00003600
S	-2.38049800	-1.65862000	-0.00004900
S	0.79750200	-1.23244300	-0.00007800
B	0.91361300	0.58565000	-0.00001400
B	3.61878400	0.39083700	0.00005600
S	-0.79749100	1.23246300	-0.00002000
S	2.38051700	1.65863300	0.00007400
S	4.74645200	-0.75314400	0.00003300

B_4S_6-II

B	1.08500600	-0.99526500	0.00028500
B	3.25274700	0.63640800	-0.00005100
S	-0.00036700	-2.46439200	-0.00022600
S	2.89895000	-1.10028100	0.00008900
S	3.58233600	2.20825600	-0.00005100
B	-3.25266400	0.63685000	0.00021000
B	-1.08550100	-0.99513100	0.00011000
S	-3.58123400	2.20886000	-0.00009100
S	-2.89940500	-1.09984000	0.00006600
S	-0.00015300	0.47150300	0.00004000

B_4S_6-III

B	-1.28346600	-0.98766000	-0.00036200

B	1.28328400	0.98755300	-0.00064500
B	1.28415100	-0.98698500	0.00014800
B	-1.28431400	0.98706700	-0.00038600
S	-0.00080100	2.34215500	0.00052700
S	-1.75181000	-0.00044300	1.46277500
S	-1.75141600	-0.00061600	-1.46351400
S	1.75181000	0.00023100	-1.46326700
S	1.75158900	0.00080200	1.46298400
S	0.00073600	-2.34212000	0.00088400

B_4S_6-IV

B	-2.48163500	-1.27232200	0.00002500
B	0.13928800	2.78541500	-0.00007400
S	-3.16078400	-2.72622200	-0.00007300
S	1.20883800	1.36995700	-0.00010300
S	-0.78175000	4.09950500	0.00002400
B	2.34282800	-1.51339200	0.00002800
B	0.00032900	0.00008500	0.00003800
S	3.94153300	-1.37335100	0.00001100
S	0.58216100	-1.73132800	0.00004800
S	-1.79025100	0.36150500	0.00008800

B_4S_6-V

B	-3.20186500	-0.24723000	0.04315000
B	1.09955900	1.67402200	-0.12956700
S	-4.31033300	0.83741500	0.45464000
S	-0.35634700	0.96866600	0.60248800
S	2.35061400	2.42066900	-0.80241100
B	2.27022100	-1.20995200	0.15546000
B	-0.43872200	-0.65257200	-0.22771500
S	3.50182900	-0.95368900	1.15298800
S	0.93912300	-1.62766100	-0.94039500
S	-2.04025900	-1.50923300	-0.41772500

B_4S_6-VI

B	0.48247000	-1.35927200	0.07373100
B	2.08076700	0.00013800	0.39240500
B	-1.97080700	-0.00031300	-0.23461600
B	0.48217700	1.35916700	0.07339800
S	-0.99278000	-1.61824800	-0.80376000
S	-3.46095400	0.00006500	0.51636900
S	0.56567800	0.00003400	1.46146200
S	2.27279400	-1.68764700	-0.23274900
S	-0.99320900	1.61793800	-0.80391400
S	2.27265600	1.68794600	-0.23269600

B_4S_6-VII

B	0.20965800	-0.87530900	0.14137300
B	1.84507600	-0.46133400	-0.39972400
B	-1.35373300	0.90859200	0.32438100
B	0.85263600	0.91642000	0.04461300
S	2.70971000	1.04592200	-0.21476400
S	-0.09747600	0.31480000	1.65520900
S	-0.45695700	2.01623900	-0.75444100
S	-1.37222900	-1.30603200	-0.80605000
S	1.59086400	-2.15015600	-0.02619900
S	-2.85942300	-0.07338800	0.11166900

B_4S_6-VIII

B	-1.08410200	1.14115000	-0.00028900
B	-2.83780600	-0.88265300	-0.00010300
S	-0.33395300	2.78153800	-0.00024600
S	-2.87899400	0.88690100	-0.00014100
S	-2.83346400	-2.49072700	0.00001500
B	2.52071700	-1.31065800	-0.00007600
B	0.36244000	0.24067000	-0.00036100
S	4.10584800	-1.04005000	-0.00045100
S	0.76238500	-1.52619600	0.00041900
S	1.50278800	1.64212500	0.00066300

B_4S_6-VIII

B	-1.08410200	1.14115000	-0.00028900
B	-2.83780600	-0.88265300	-0.00010300
S	-0.33395300	2.78153800	-0.00024600
S	-2.87899400	0.88690100	-0.00014100
S	-2.83346400	-2.49072700	0.00001500
B	2.52071700	-1.31065800	-0.00007600
B	0.36244000	0.24067000	-0.00036100
S	4.10584800	-1.04005000	-0.00045100
S	0.76238500	-1.52619600	0.00041900
S	1.50278800	1.64212500	0.00066300

B_4S_6-IX

B	1.41515500	-1.67061400	0.36613900
B	-1.01623200	-0.78852200	-0.32577100
S	2.55106500	-1.35915900	1.46200800
S	0.13232200	-2.12484100	-0.76760300
S	-2.80782400	-0.96250300	-0.48536000

B	-1.01646700	0.78822200	0.32646900
B	1.41528500	1.67087300	-0.36608900
S	-2.80825000	0.96187900	0.48540700
S	0.13123800	2.12581700	0.76606500
S	2.55215500	1.35881900	-1.46075200

B_4S_6-X

B	0.42944200	-0.78543200	0.63586400
B	-2.92980800	-0.28206300	-0.31245500
S	0.39908600	-2.33056900	1.05677700
S	-2.49075300	0.63371800	1.13892900
S	-3.32780000	-1.14223500	-1.60989500
B	3.08919200	0.37873500	-0.43155000
B	0.44225400	0.81905000	0.18497000
S	4.20676500	-0.77336000	-0.41261400
S	1.90251700	1.69624400	-0.47572800
S	-1.01202700	1.87548600	0.27852300

B_4S_6-XI

B	0.00088500	1.18906200	0.00011700
B	1.78436200	-0.00035200	-0.43042100
B	-0.00050300	-1.18976700	0.00150500
B	-1.78537000	0.00054500	0.42995300
S	-1.85108200	-1.71556200	-0.22182400
S	-0.36562300	-0.00071000	1.58547600
S	0.36562200	0.00071300	-1.58651500
S	1.84997900	-1.71663600	0.22122700
S	1.85116200	1.71545500	0.22213300
S	-1.84986100	1.71690100	-0.22085900

B_6S_9-I

B	2.69510627	0.95600399	-1.09356203
B	-1.67658015	0.51721595	-1.76044032
S	2.41316853	2.34848944	-2.35668739
S	-0.99766693	-1.06889664	-1.01660814
S	-0.88286124	1.49948389	-3.16659109
B	0.11072304	-0.69080232	2.12480650
B	-2.03211559	-0.36281287	0.38386474
S	1.13957061	-1.39602877	0.71978304
S	-1.77656976	-0.71264224	2.22354290
S	-3.16698454	0.79171885	-0.61268896
B	0.88780035	1.23263577	-2.56190141
B	2.27356441	-0.08740529	1.44884082
S	1.56001062	-0.35534683	-1.81597432
S	3.66015890	0.80411531	0.52436975
S	1.49588340	0.07800599	3.17564181

B_6S_9-II

B	-1.32427500	0.86710200	-0.00427500
B	1.52184400	1.48476100	-0.01170500
S	-3.13038900	1.18170400	0.02803300
S	-0.12833200	2.22575400	0.00382400
S	3.03572200	2.51551700	-0.01721200
B	5.10498600	-1.47189900	0.02227600
B	3.58835300	0.77854400	-0.00690800
S	4.90229300	-3.06543100	0.03247500
S	5.33828000	0.28428200	0.01105200
S	2.08681000	-0.25600500	-0.01222800
B	-5.61302200	-0.93286500	0.00437600
B	-2.91828600	-0.62429800	-0.01777500
S	-6.93421600	-0.01982000	0.04048400
S	-4.16270000	-1.94965500	-0.03422200
S	-1.11984400	-0.94801700	-0.04782800

B_6S_9-III

B	-2.89479800	-0.60834800	-0.50682900
B	-2.16718000	1.61990800	0.49039100
S	-2.80338100	-2.17921700	0.40845900
S	-3.80088700	0.92488400	-0.01758400
S	-1.14535400	2.82207300	-0.41813800
B	-1.19895000	-1.73716700	-0.34950100
B	4.35260300	-0.13471800	-0.01010300
S	0.40101000	-2.15712100	0.41848100
S	-1.55040800	-0.64015000	-1.75272800
S	5.37396400	1.10602500	-0.00857800
B	-0.13135200	1.51766100	0.36294900
B	1.62292000	-0.85981100	0.01104400
S	-1.08541800	0.85280300	1.75629400
S	1.42320600	0.90801800	-0.37549500
S	3.31750500	-1.57404300	-0.01007000

B_6S_9-IV

B	-0.56705996	1.25280891	-1.20411164
B	-2.72138565	2.15955843	-2.83439590
S	1.08668799	1.54966680	-0.56464252
S	-1.09821822	2.59171509	-2.29856278
S	-4.20223739	1.86616757	-3.38473990
B	3.95852039	1.76659716	0.72643986

B	1.58606395	0.20426361	0.51636297
S	4.72811369	3.10278186	0.27440592
S	3.21912299	0.26909183	1.29200693
S	0.69314412	-1.28276313	0.98883807
B	-0.92202132	-1.31409621	0.20204548
B	-1.12487747	-3.78476462	1.60176671
S	-1.68432463	-0.12299644	-0.90815674
S	-2.01767980	-2.71876570	0.51744572
S	-0.40117530	-4.82721611	2.58743391

B_6S_9-V

B	3.14513154	-0.08937003	3.25214442
B	-2.37162153	0.86751005	-1.87235712
S	3.42927026	-1.21141308	4.36649644
S	-2.62534745	0.64369281	-0.06937663
S	-1.07283951	1.99469120	-2.50884862
B	-0.13630772	-1.34269916	-0.20809054
B	-2.61712782	-1.00989325	-0.86367156
S	0.82330485	-0.94574509	1.25974670
S	-1.64610321	-2.39227754	-0.15053987
S	-3.12311910	-0.64407972	-2.58714320
B	1.65889336	0.62636752	0.93605573
B	0.18099419	1.08856070	-1.51211009
S	2.92524587	1.21161652	2.08194063
S	1.18644232	1.89704052	-0.26128364
S	0.24318392	-0.69400144	-1.86296266

B_6S_9-VI

B	-2.86280000	-0.78078600	0.06074100
B	-5.51855500	-0.23931100	0.05380100
S	-2.50540800	0.98847300	-0.15204100
S	-4.45292000	-1.64854900	0.19704200
S	-6.49019500	1.03280900	-0.07605700
B	2.10977300	0.04019800	-0.08340300
B	3.38704300	2.53546400	0.08727700
S	0.64177500	1.11338800	-0.13702300
S	3.76830600	0.80283300	0.01741800
S	3.14607000	4.12091700	0.15215400
B	-0.88328500	0.13610500	-0.06521900
B	3.67644500	-2.28130900	-0.05839800
S	-1.24882000	-1.64115200	0.13116800
S	1.97908500	-1.78052100	-0.17102700
S	5.19066300	-2.80393700	0.03999100

B_6S_9-VII

B	0.09225200	-0.38850700	-0.88179900
B	-0.34795700	2.70819300	-0.26444800
S	-1.70452800	-0.20407400	-1.04057500
S	1.18286200	-0.19970200	0.57797000
S	0.60671500	3.17279000	-1.47167800
B	-2.22377500	0.76309600	0.41438500
B	-4.19874400	-1.19999300	0.64286800
S	-1.40850100	2.26103300	1.08446800
S	-3.76682900	0.38627000	1.31503300
S	-4.67478200	-2.63107500	0.09357600
B	2.21425200	-0.86455300	-0.76939000
B	4.34645900	-0.87435200	0.90679900
S	1.13584600	-1.03777900	-2.23045200
S	3.97670800	-1.31155900	-0.76969400
S	4.68923100	-0.48086600	2.42622200

B_6S_9-VIII

B	-0.36916200	-1.80272900	0.00052100
B	-2.77741600	-0.61337500	-0.00023900
S	2.75939700	-2.24244500	0.00219100
S	-2.11729700	-2.31313100	0.00038700
S	-4.60020600	-0.48752400	0.00024200
B	2.74909300	-0.44662200	-0.00168400
B	4.32705400	1.88627100	0.00045800
S	1.41678800	0.78422400	-0.00315500
S	4.50780200	0.12668600	-0.00326500
S	4.25769700	3.49172000	0.00351300
B	-0.13058000	-0.13429200	-0.00093600
B	-4.81908800	1.27065900	0.00027600
S	0.84123000	-3.09752600	0.00125900
S	-1.66661500	0.83213500	-0.00096400
S	-5.08001600	2.85588700	0.00029400

B_6S_9-IX

B	-4.60696700	-0.67276800	0.01712200
B	-2.16891400	0.72314300	-0.02005200
S	-5.24319500	-2.14546000	0.01930000
S	-3.98034800	0.98776200	0.02188700
S	-1.50236000	-0.95233800	-0.07489800
B	2.44663000	1.27260100	0.05834900
B	0.37858200	2.06195500	0.29388700
S	3.66804000	0.34972100	-0.73819600
S	1.86304900	3.01459700	-0.05058400

S	-1.31205600	2.35256400	-0.18846100
B	3.18532100	-1.44948000	-0.16456500
B	0.32901200	-0.84394200	-0.02086700
S	4.20226000	-2.49986000	0.63950300
S	1.40442500	-1.95803300	-0.79147700
S	1.03654100	0.50995100	1.11171500

B_6S_9-X

B	1.60265200	-0.12959400	-1.25339700
B	1.60277000	-0.12981900	1.25329800
S	0.81315300	-1.71426000	-1.70439800
S	2.99029400	-0.24148000	-0.00012200
S	1.07818300	1.56108800	1.70469000
B	-0.68918800	1.45288000	-1.25358600
B	-0.68906900	1.45264500	1.25377100
S	1.07805400	1.56136000	-1.70457800
S	-1.28565900	2.71027600	0.00023700
S	-1.89128900	0.15293900	1.70476100
B	-0.91382600	-1.32298200	-1.25382700
B	-0.91371900	-1.32320800	1.25374100
S	-1.89142700	0.15320500	-1.70464600
S	-1.70448100	-2.46856600	-0.00011400
S	0.81329000	-1.71453800	1.70417000

B_8S_{12}-I

B	-1.07588600	-2.93995000	0.11087400
B	1.07589300	2.94008500	0.11093600
S	0.00000000	-1.79395000	1.03398700
S	0.00007500	1.79377700	1.03368500
S	2.77545200	-2.73142200	-0.49366600
B	-3.28182700	1.05191600	0.00580700
B	-1.07591400	2.93994900	0.11099300
S	-4.34971000	-0.00001200	-1.04157800
S	-2.77535400	2.73128300	-0.49391300
S	-0.00007800	4.30799200	-0.45793500
B	1.07593300	-2.93998300	0.11097900
B	-3.28178000	-1.05192500	0.00571600
S	0.00005100	-4.30785100	-0.45813200
S	-2.77531700	-2.73131200	-0.49403400
S	-2.71012900	-0.00007200	1.38075600
B	3.28165300	1.05191100	0.00567500
B	3.28182500	-1.05184200	0.00563800
S	4.34943300	0.00008700	-1.04192900
S	2.77538200	2.73143000	-0.49379100
S	2.71022600	0.00000000	1.38073200

B_8S_{12}-II

B	3.20211400	-1.93733500	-0.10482500
B	3.82249400	0.88442100	-0.09641100
S	2.14521600	-1.92794000	-1.58772200
S	4.39019900	-0.72144800	0.54984200
S	3.83801700	2.36863900	0.98391600
B	2.44034300	2.41468400	-0.17480700
B	-0.36205700	1.84516000	0.14272100
S	2.85332800	1.32479600	-1.57355800
S	0.81659500	3.23539900	0.12413100
S	0.26291400	0.17866600	0.48330600
B	-1.00304000	-1.07070400	0.13618800
B	1.30685600	-2.75090000	-0.19697700
S	-2.79943800	-0.83697200	-0.01650200
S	-0.51410500	-2.82397000	0.08810800
S	2.58890500	-3.29405100	0.96895800
B	-3.17508100	0.92854300	0.03478700
B	-5.81593900	-0.07062800	0.04379000
S	-2.08671700	2.37558200	-0.04212800
S	-4.93709800	1.46610100	0.04677300
S	-6.68772000	-1.42081600	0.04223000

B_8S_{12}-III

B	0.54027400	-2.51330300	-0.61617000
B	2.60088500	-0.56806500	-0.76351500
S	-0.78004700	-3.66719400	-1.11462500
S	1.66767300	-1.75835200	-1.81404400
S	3.68665000	-1.32143100	0.49507700
B	-1.00079200	2.48583100	-0.88971900
B	-2.96488200	1.54792700	0.85049600
S	0.43934000	3.48042400	-1.42688900
S	-2.37986300	3.12415300	0.08696800
S	-1.97253700	0.50398100	1.96630900
B	-3.18169000	-0.50698700	1.05645900
B	-1.34395200	-2.61797800	0.27384300
S	-4.48740300	0.64162300	0.46177600
S	-3.11374300	-2.21082500	0.43227000
S	0.15168900	-1.96036000	1.08243900
B	0.91600200	1.71815000	-1.40393400
B	4.26538100	0.08935500	1.40894000
S	-0.63366200	0.76005100	-1.38483200
S	2.63463200	1.22684900	-1.05805400

S	4.84001200	1.29516700	2.29973200	S	-0.24551000	1.80259800	1.64429200

B_8S_{12}-IV

B	-1.02916500	-2.08654600	0.40469600	B	6.32339800	-0.05295500	0.05150700
B	-2.98115800	-0.92868800	-0.90971600	B	1.57244300	-1.04232800	-0.45011200
S	2.14184500	0.43536700	-2.41855600	S	7.20604200	-1.39479300	0.04676100
S	-2.61348100	-2.65569500	-0.38382600	S	3.30187100	-0.89016100	0.07169500
S	-4.34626500	0.14489100	-0.36308900	S	0.69099900	0.17385000	-1.50296100
B	3.12192200	-0.04211500	-0.94930000	B	3.68198500	0.88617600	-0.00824900
B	1.91607600	1.65575600	-1.07924700	B	0.90780000	1.63721200	-0.42083600
S	0.52022300	-2.62481800	-0.36176400	S	5.41728000	1.47044800	0.05782800
S	3.31385300	1.47171100	0.05998000	S	2.49827700	2.26683100	0.16277600
S	0.35038600	2.63763000	-0.96174500	S	-0.63430900	2.56427000	0.00262200
B	0.34845500	-0.07592000	1.98704800	B	-6.32349400	0.05289100	-0.05074000
B	1.90616700	-1.82203100	0.50033900	B	-3.68200700	-0.88615100	0.00841000
S	-1.26649000	-0.88209300	1.74300300	S	-7.20614400	1.39471300	-0.04593700
S	1.94049200	-0.97746000	2.10495800	S	-5.41730800	-1.47046600	-0.05718500
S	3.49510300	-1.79113900	-0.46800900	S	-2.49833800	-2.26680900	-0.16286700
B	-2.78694900	1.09146100	-0.56025900	B	-0.90770300	-1.63722000	0.42035000
B	-0.45272500	2.20248000	0.60037600	B	-1.57238400	1.04238100	0.44968000
S	-1.76111400	0.15303600	-1.74020900	S	0.63424200	-2.56430600	-0.00343100
S	-2.28978900	2.34751200	0.66055200	S	-0.69065700	-0.17377700	1.50232500
S	0.50191800	1.74280900	2.13060100	S	-3.30196700	0.89019900	-0.07162900

B_8S_{12}-V

B	0.54474000	-2.45405600	0.13803700	B	7.50922900	-0.07330800	-0.00150400
B	2.83019700	-1.07975600	-0.08163100	B	5.01635200	1.12269600	0.00033400
S	-0.24538000	-1.80252900	1.64426800	S	8.19463400	-1.52716300	-0.00243600
S	2.36863400	-2.77037700	0.40388600	S	6.80451300	1.54793500	-0.00056500
S	1.89763800	0.00002400	-1.22160000	S	3.90221900	2.52968600	0.00169600
B	0.54467900	2.45378000	0.13795800	B	2.58342700	-0.15810500	0.00089700
B	2.83035200	1.07996200	-0.08189300	B	-7.34492700	1.23028400	-0.00084200
S	-0.14373400	2.64026700	-1.52226500	S	4.35796600	-0.55661500	-0.00015500
S	2.36850800	2.77044400	0.40383900	S	2.05150800	1.55676000	0.00179000
S	4.09992700	0.00010200	0.68279700	S	-7.65108900	2.80731400	-0.00105200
B	-1.93420300	-1.25021800	1.26936800	B	-2.66525900	-0.09599700	-0.00029000
B	-1.54488900	-1.44286600	-1.38502900	B	-0.24993700	-1.22760900	0.00065100
S	-2.63500300	-0.00003600	2.46596900	S	-4.18491700	0.87363300	-0.00082100
S	-2.92384900	-1.64274600	-0.20603900	S	-0.95215300	0.47036700	-0.00038700
S	-0.14358300	-2.64030200	-1.52225600	S	1.51056300	-1.64240100	0.00121500
B	-1.54503400	1.44284500	-1.38510500	B	-5.26084000	-0.61521800	-0.00033000
B	-1.93434600	1.25029800	1.26944200	B	-2.86562600	-1.76467300	0.00047600
S	-1.40851800	-0.00003600	-2.52969400	S	-7.08424000	-0.52310000	-0.00055400
S	-2.92397200	1.64259500	-0.20605600	S	-4.58092200	-2.32328300	0.00043800

S	-1.34383900	-2.71877900	0.00102000	S	3.66773600	0.65200300	0.38433500

B_8S_{12}-VIII

B	-3.50527500	1.15522700	-0.96584100	B	-1.32609100	-2.35204300	0.37757100
B	-1.10947700	1.43460500	0.34660800	B	1.24179700	-1.68467600	-0.31013800
S	-5.24773700	0.91948100	-0.50374000	S	-1.71715900	-0.97609300	1.49046200
S	-2.33889600	2.48603700	-0.70172100	S	0.37093400	-3.11167500	0.39806600
S	0.14603700	0.28319800	-0.84034800	S	0.32837300	-0.47985000	-1.34058600
B	0.38243700	-1.44324200	-0.16323600	B	-0.98864900	2.62173800	-0.47695200
B	6.00153200	-0.07180900	-0.19505600	B	1.37704500	0.89669900	-0.79278100
S	-0.98139100	-2.45449700	0.35064600	S	-2.17880400	1.59009900	-1.38728200
S	4.97192300	-1.49497600	-0.42159800	S	0.84656400	2.59833500	-0.47865100
S	6.99976100	1.17327500	-0.00958200	S	-2.57669500	-2.97276100	-0.74090200
B	1.33073500	1.26386100	0.21650000	B	5.63595800	0.44158300	0.27947200
B	3.28641900	-0.81669900	-0.14057900	B	2.93182900	0.36697100	-0.33432300
S	0.35994000	2.51881500	0.98543900	S	6.84017000	-0.52748900	0.72069700
S	3.10039700	0.92219200	0.35716100	S	4.32706900	1.53064200	-0.20987800
S	2.05689900	-2.15957600	-0.23783900	S	3.01555600	-1.39038100	0.08260100
B	-4.39037400	-0.68368500	-0.30435900	B	-2.89057700	2.09411300	0.22035200
B	-2.36356400	-1.15038600	0.58143800	B	-3.29737600	-0.48855300	0.75933400
S	-2.92146400	-0.57804700	-1.42800100	S	-1.94706000	3.56434000	0.76299600
S	-4.11939600	-1.85261000	1.01030900	S	-4.06099300	1.13270300	1.23596300
S	-1.91120700	0.33424700	1.63443900	S	-4.08668400	-1.55031800	-0.44677900

B_8S_{12}-IX

B	-2.12120300	1.57367000	-0.51864000	B	-0.90358800	-1.06057800	-0.23597300
B	0.00021400	2.28089100	0.00041000	B	-0.67369000	1.85407200	-0.69696200
S	-3.66770200	0.65182500	-0.38656000	S	-2.66006800	-1.04371200	0.20138800
S	-1.67227600	3.12877500	0.22111200	S	0.03009400	0.22840400	-1.09896600
S	1.67229200	3.12946800	-0.22041500	S	3.14349000	1.36070800	-0.66048700
B	-3.04622300	-0.96715800	0.17945800	B	1.89234000	2.44968500	0.09843100
B	-5.81484800	-1.51387500	0.15178600	B	2.63195500	0.79340100	0.99435600
S	-1.38925500	-1.56364600	0.56890100	S	0.43994600	3.30221400	-0.69707200
S	-4.28080700	-2.29011100	0.55879200	S	2.04798600	2.27739000	1.90046700
S	-7.24329300	-0.86681400	-0.20553900	S	2.14773300	-0.84329600	1.63716800
B	3.04591800	-0.96783700	-0.17897500	B	-3.30225600	0.61050100	-0.18011700
B	5.81466200	-1.51419000	-0.15296400	B	-5.76136400	-0.72708600	0.17305400
S	1.38867900	-1.56495100	-0.56613600	S	-2.43123000	2.19146500	-0.40970700
S	4.28035300	-2.29105400	-0.55777100	S	-5.11998700	0.89084900	-0.15590300
S	7.24336800	-0.86659800	0.20233900	S	-6.42365600	-2.16142100	0.46525700
B	0.00003300	-0.40605100	0.00079700	B	4.44254700	-1.80222700	-0.53268600
B	2.12157600	1.57398600	0.51848200	B	1.74612900	-1.86068600	0.15790800
S	0.56295400	0.93146200	1.35148600	S	5.87788900	-1.26557200	-0.05040400
S	-0.56209100	0.93106900	-1.35065500	S	2.89082100	-2.42324900	-1.13423600

S	0.03446000	-2.59411700	0.07186600

B_8S_{12}-XII

B	2.08145700	-1.36519500	0.86586800
B	-1.83837700	-1.37444400	-1.22087300
S	2.31416900	2.62168000	-0.48238100
S	2.31198700	-2.62343100	-0.47988200
S	0.56409400	-1.61493700	1.86256200
B	0.91168400	-1.70021900	-1.30512600
B	2.08234500	1.36518600	0.86440700
S	1.38587700	-0.00126100	-1.92849300
S	3.27837500	-0.00051400	0.93871800
S	-0.59203100	-2.69280100	-1.56640500
B	-0.12793900	0.00113200	2.28473600
B	-1.83762000	1.37459600	-1.22214200
S	-2.65612400	1.63486700	0.38891100
S	-2.65650200	-1.63338300	0.39036700
S	-1.88224300	0.00182500	2.93529000
B	0.91280600	1.69835200	-1.30649800
B	-2.47273700	0.00102400	1.16564900
S	-0.59015900	2.69181100	-1.56714400
S	0.56502000	1.61638800	1.86073700
S	-1.95234600	-0.00037900	-2.39166200

B_8S_{12}-XIII

B	-1.42233900	1.42233900	1.42233900
B	1.42233900	1.42233900	1.42233900
S	-2.25755500	0.00000000	2.25755500
S	0.00000000	2.25755500	2.25755500
S	2.25755500	2.25755500	0.00000000
B	1.42233900	1.42233900	-1.42233900
B	-1.42233900	1.42233900	-1.42233900
S	2.25755500	0.00000000	-2.25755500
S	0.00000000	2.25755500	-2.25755500
S	-2.25755500	2.25755500	0.00000000
B	-1.42233900	-1.42233900	-1.42233900
B	1.42233900	-1.42233900	-1.42233900
S	-2.25755500	0.00000000	-2.25755500
S	0.00000000	-2.25755500	-2.25755500
S	2.25755500	-2.25755500	0.00000000
B	1.42233900	-1.42233900	1.42233900
B	-1.42233900	-1.42233900	1.42233900
S	-2.25755500	-2.25755500	0.00000000
S	0.00000000	-2.25755500	2.25755500
S	2.25755500	0.00000000	2.25755500

$B_{10}S_{15}$-I

B	-2.64022700	-3.19163000	-0.06797000
B	0.18525800	3.98356400	0.02502700
S	-2.30942300	-1.60241400	-0.89965400
S	0.81336700	2.33993000	-0.46898800
S	-4.90276000	0.01598200	0.38288300
B	2.25439500	-3.33271800	0.01716800
B	2.27768000	3.31878700	0.01770700
S	1.63179100	-5.02298900	0.34000800
S	3.99157600	2.82400500	0.34222200
S	1.66544800	5.01283800	0.34043100
B	-3.92752600	-1.44578400	-0.06980800
B	0.15807000	-3.98447900	0.02462500
S	-4.38808600	-3.13341400	0.46761100
S	-1.52913100	-4.56538300	0.34760500
S	0.79633100	-2.34475700	-0.46961000
B	-2.61789800	3.20799600	-0.06816400
B	-3.91709300	1.47054000	-0.06987200
S	-4.36690600	3.16189900	0.46497000
S	-1.49845100	4.57536600	0.34630000
S	-2.29618000	1.61519800	-0.89647900
B	4.11263500	1.06642500	-0.09753100
B	4.10496600	-1.09261900	-0.09774500
S	3.97170000	-2.84943300	0.34106600
S	5.45559900	-0.01791700	0.50792400
S	2.96817000	-0.00893600	-1.02548700

$B_{10}S_{15}$-II

B	-4.36822800	0.85571200	0.20086500
B	-5.65478200	3.36460200	0.28427600
S	-2.92906700	1.90008500	-0.12233400
S	-6.00253000	1.64102500	0.50193600
S	-5.42621800	4.94368400	0.09891700
B	-1.52476700	0.85195200	-0.61446100
B	1.52463300	0.85201000	-0.61441500
S	0.00039300	-2.81878800	1.43853800
S	-0.00008900	1.86442900	-0.75625600
S	2.92883200	1.90018000	-0.12208700
B	-2.94992600	-1.68859500	-0.15413000
B	5.65449000	3.36487300	0.28477200
S	-1.57606300	-0.90159900	-1.03476200
S	-4.47013200	-0.94110200	0.46402800

S	5.42597500	4.94396100	0.09939900	S	-3.18575300	-2.59110200	0.40506200
B	2.95012700	-1.68847900	-0.15495300	B	2.84212800	2.02166000	0.56281200
B	4.36813600	0.85588800	0.20073800	B	-5.35708300	3.30367300	-0.75107700
S	1.57614400	-0.90139300	-1.03531700	S	3.08542800	3.75588800	1.12500400
S	4.47017100	-0.94097600	0.46355900	S	1.44398300	1.24548400	1.45085700
S	6.00229400	1.64129700	0.50236100	S	-4.27972700	4.46220800	-1.03432400
B	-1.07345100	-3.78277200	0.31949300	B	-1.37806600	-2.26430400	0.31728200
B	1.07381100	-3.78264800	0.31899000	B	0.80536500	-0.10803900	0.41831700
S	-2.84933900	-3.51847000	-0.03347500	S	-3.56651500	0.70276500	0.02518600
S	0.00005500	-5.04472200	-0.45217000	S	-0.77159500	-0.74122300	1.10624400
S	2.84956200	-3.51840600	-0.03458000	S	1.51271900	-0.70639700	-1.13055100
---				B	4.56730600	4.20975300	0.27040700
$B_{10}S_{15}$-III				B	3.29071700	-0.42958300	-0.70574800
B	-1.32899200	-2.08919800	1.31251200	S	5.90818300	4.67729600	-0.48221300
S	-2.94337900	-2.17866500	0.45872800	S	3.99784300	1.26030200	-0.58881200
S	-1.44417300	-1.14087000	2.89040100	S	2.12146200	-3.14497800	1.37597800
S	-0.98900300	-1.93659100	-2.16700700	B	1.20687800	-3.74909600	-0.07690500
B	0.28593700	-2.62595800	-1.08527900	B	3.13841600	-3.12010200	-0.14086300
S	0.24220400	-2.78447200	0.71743000	S	-0.55530200	-3.66445200	-0.51250400
S	1.93275000	-2.95928600	-1.89973300	S	2.45030300	-4.32986100	-1.29371600
B	-2.41721600	1.06501900	-1.08639200	S	4.41668100	-1.81422700	-0.48496900
S	-2.53316800	1.18223300	0.71627300	---			
S	-1.18218000	1.82433500	-2.16765000	**$B_{10}S_{15}$-V**			
B	-2.45241200	-1.52467300	-1.16520000	B	5.08819100	-4.10344300	-0.00170000
S	-3.52903900	-0.19432800	-1.90132300	B	2.93650800	-2.45959600	-0.03243800
B	-0.00079300	0.00094900	2.82329900	S	5.41073100	-5.67629400	-0.06567300
B	-1.14610100	2.19597600	1.31178400	S	4.74861300	-2.36629200	0.07339000
S	-0.26829100	1.82178300	2.89047300	S	1.85330400	-0.98549400	0.00247500
S	-0.41531500	3.63830100	0.45783000	B	0.75172400	-2.43405800	-0.12140100
S	2.29038500	1.60229000	0.71733600	B	-1.94893400	-1.07549800	-0.10376100
B	-0.09366900	2.88538200	-1.16545500	S	1.84697500	-3.90758500	-0.17864400
S	1.59710700	3.15229300	-1.90103300	S	-1.04342800	-2.66401900	-0.15580800
B	2.54699600	-1.36197800	-1.16380800	S	-3.72867100	-1.42256300	0.01562900
S	2.17423900	0.11106000	-2.16685800	B	4.59928500	2.89554100	0.23146000
S	3.35806500	-1.45987400	0.46047500	B	2.23704100	4.15990800	0.01039000
B	2.13243700	1.56012700	-1.08552000	S	5.11680800	1.37811000	0.36458100
B	2.47393500	-0.10562500	1.31348900	S	4.01284300	4.55932400	0.08138500
S	1.70975800	-0.67821300	2.89171000	S	1.43325300	2.52730000	0.09372200
---				B	-4.65240500	0.12462500	0.03839600
$B_{10}S_{15}$-IV				B	-6.83082700	-1.65844300	0.17873400
B	-5.38721400	0.69238500	-0.01967900	S	-4.06856200	1.83673000	-0.00255300
B	-4.08501200	-1.02420800	0.33922100	S	-6.48804700	0.07897800	0.13413500
S	-6.54831800	2.03084700	-0.44032000	S	-7.22283300	-3.21534200	0.22405800
S	-5.91796500	-0.99634500	0.41227700	B	-2.26079900	1.87345400	-0.11975600

B	0.09153000	3.75137000	-0.10308500
S	-1.07895800	0.50693700	-0.20428200
S	-1.70673900	3.62118500	-0.19661400
S	0.91117600	5.39344500	-0.17856400

$B_{10}S_{15}$-VI

B	5.09804900	-0.94105200	-0.14592900
B	7.54582100	0.36125500	-0.65698200
S	4.49664000	0.75895300	-0.15706400
S	6.88305200	-1.26759700	-0.44214100
S	8.22381300	1.80270800	-0.86284700
B	2.46411700	-2.15690000	0.40967800
B	-0.13153400	-3.10590300	0.88731100
S	4.21137100	-2.50233500	0.09794500
S	1.51799600	-3.71272900	0.65159700
S	-1.64652300	-2.61655400	1.09880000
B	-4.55730700	1.82614300	-0.03597100
B	-1.87201200	2.91774700	0.23856300
S	-4.02684300	0.08795600	-0.25565000
S	-3.62641200	3.36208500	0.18035200
S	-0.55965000	4.18068500	0.38441300
B	-5.84739500	0.09288100	-0.34369500
B	-5.80615000	-2.58777200	-0.77560800
S	-6.38815000	1.81697200	-0.10191900
S	-6.99900200	-1.28643000	-0.62603000
S	-4.73209800	-3.77422600	-0.91257300
B	0.29877800	2.56714500	0.28122700
B	2.71265700	0.78289900	0.18772300
S	-1.01717700	1.30196200	0.18343300
S	2.10903800	2.50894000	0.21943800
S	1.58362300	-0.58428100	0.52777200

$B_{10}S_{15}$-VII

B	1.28986300	-1.02024400	2.11602200
B	3.46379000	0.12866000	0.55141100
S	1.00072700	-2.34793700	0.90862200
S	2.63050100	0.19034800	2.15985300
S	4.14788000	1.75992000	-0.02723600
B	0.24989400	-3.57389500	-1.79213400
B	2.24457600	-2.31898700	-0.39435800
S	-1.36183300	-3.59907200	-1.88380900
S	2.01548600	-3.51527400	-1.79565400
S	3.68666300	-1.25342900	-0.60699700
B	-1.20124600	-0.28292100	2.04180500
B	-3.05142600	-0.92641600	-0.05194100
S	-0.02856400	-0.83866000	3.39497900
S	-2.38696200	-1.57717500	1.47803500
S	-2.14683700	0.27001700	-1.21507400
B	-3.89505100	0.71802400	-0.73631700
B	-1.98394500	1.89837100	-0.00838200
S	-4.78123600	-0.87689600	-0.59769800
S	-3.89286700	2.26036800	0.12423900
S	-1.05423600	1.43700700	1.60108300
B	2.60619600	2.16405600	-0.88827800
B	0.55017000	2.77201000	-1.17280100
S	1.18269600	1.04816700	-1.21230600
S	2.03219600	3.83809300	-1.33651800
S	-1.12887300	3.34244400	-0.88684000

$B_{10}S_{15}$-VIII

B	4.21826300	0.47488200	-0.32727200
B	6.64147600	-0.96270600	-0.13543400
S	3.38389700	2.01036500	-0.82224400
S	6.03456100	0.63815500	-0.58646500
S	7.27401600	-2.38638100	0.25922700
B	-3.01113200	1.71722800	1.37144500
B	-1.03143100	2.48815500	-0.56704100
S	-3.62771100	0.30118100	0.31817600
S	-1.91265100	3.05615000	0.95983200
S	-1.50371200	1.37664700	-1.87492700
B	1.64616900	1.92820900	-0.31400200
B	1.78509000	-0.92388400	0.57349500
S	0.61361000	3.34744400	-0.79447200
S	0.87567200	0.64709400	0.72372700
S	3.55015700	-1.12365400	0.19322800
B	-2.93154200	-0.24786200	1.96360800
B	-0.82857500	-1.76995500	0.73322400
S	-3.41242900	1.13351400	3.04422200
S	-1.71671800	-1.49392700	2.33482300
S	-1.34076700	-1.59673400	-0.96053200
B	-2.52572700	-0.12381800	-1.26017700
B	-4.50125000	-1.91872600	-1.92805500
S	0.89465800	-2.45244100	0.98712600
S	-3.75257700	-0.52381800	-2.68779300
S	-5.19167700	-3.14032100	-1.12823700

$B_{10}S_{15}$-IX

B	-1.34656700	0.38746500	1.76957200

B	1.69912900	0.39163900	-0.42251800
S	-1.29464900	-1.34311700	2.35835300
S	0.31830500	-0.72369700	-0.73064800
S	1.31445200	2.21234200	-0.55254100
B	-6.05617600	-0.96401600	-1.17727000
B	-3.71135400	-0.15273900	0.11989100
S	-6.77270500	-2.24294700	-1.83344700
S	-5.32594200	0.48616500	-0.46800700
S	-2.67334000	1.17212600	0.80626100
B	3.64789200	-1.80549300	-0.31276900
B	6.35844700	-1.05661700	-0.53425600
S	3.44345100	0.00036600	-0.21717400
S	5.33961300	-2.50469700	-0.45716700
S	7.34947400	0.20466900	-0.61239000
B	-1.74886700	-2.16414300	0.79834100
B	0.76475200	-2.40995700	-0.17188400
S	-3.20624000	-1.85941500	-0.22939900
S	-0.60373200	-3.53221600	0.25661000
S	2.42623200	-3.13147900	-0.13371800
B	-0.13935100	5.00418500	-0.40541200
B	0.27343100	2.55246400	0.87744000
S	0.16741700	5.78949200	-1.77240100
S	-0.50650100	4.18517200	1.12523800
S	0.10499700	1.35511700	2.29132400

$B_{10}S_{15}$-X

B	-7.20192100	-1.23355100	0.94022800
B	-4.42690100	-1.44092100	0.52552600
S	-8.45685100	-0.25322500	0.73630200
S	-5.86314700	-2.36696000	1.19816500
S	-4.69433900	0.21438000	-0.15039600
B	-4.78890800	3.03001300	-1.43293400
B	7.20045800	-1.23385600	-0.94433000
S	-6.30490900	3.55133000	-1.34913400
S	8.45563500	-0.25360000	-0.74159900
S	5.86131700	-2.36715400	-1.20090800
B	4.42596600	-1.44123500	-0.52622800
B	4.79072500	3.02890700	1.43349100
S	2.90570400	-2.40765500	-0.70329500
S	4.69426100	0.21392400	0.14968500
S	6.30665200	3.55015300	1.34798900
B	1.51002800	-1.50514400	0.01544300
B	3.12859000	0.85288300	0.78608300
S	-0.00028300	-2.54266100	0.00220600
S	1.47919200	0.10672300	0.83130100
S	3.09692900	2.51962400	1.55818300
B	-1.51022200	-1.50479600	-0.01241200
B	-3.12774800	0.85361600	-0.78420700
S	-2.90694400	-2.40746400	0.70422400
S	-1.47822400	0.10763100	-0.82717300
S	-3.09501700	2.52060600	-1.55575700

$B_{10}S_{15}$-XI

B	-1.37186700	1.34148200	-0.58969700
B	-2.39986500	-1.41633700	-0.52110700
S	-0.04712600	2.62017700	-0.68792200
S	-1.15876600	-0.31747200	-1.25607600
S	-4.02319400	-1.00879600	0.15551000
B	-6.84536500	0.14856300	0.80441300
B	-4.16791100	0.79570200	0.22666800
S	-7.86457100	-1.08242700	0.96486100
S	-5.78527800	1.55936200	0.64544600
S	-2.87847300	2.06736700	0.11056600
B	1.64040500	1.92906500	-0.65967900
B	2.20794900	4.63408200	-0.05582700
S	1.97441500	0.16574700	-0.97492800
S	3.02537500	3.09681800	-0.40397300
S	1.58912000	6.07870000	0.27238900
B	-0.25308200	-3.23386700	-0.19086500
B	1.85087700	-2.88599000	-0.02544200
S	-2.02010700	-3.20952200	-0.65439400
S	1.06269200	-4.19741900	-1.01813000
S	3.59162200	-2.33024200	-0.19740400
B	3.49729300	-0.50948000	-0.22590500
B	5.97523300	-0.70659600	1.02450000
S	0.57327000	-2.25500000	1.11108500
S	4.91956000	0.51348100	0.28307800
S	6.99969000	-1.73096900	1.71643900

$B_{10}S_{15}$-XII

B	-2.08169300	-2.06857200	1.04692200
B	-2.96156600	-1.53896100	3.64698300
S	-2.39009800	-0.29799900	0.82046400
S	-2.33547800	-2.87785900	2.66634600
S	-3.53126700	-0.36852200	4.58625200
B	-2.54734200	-0.01142400	-0.96297500
B	0.96696100	0.71871300	-0.52619900
S	-1.78024300	4.48868000	-0.74997900

S	0.20465300	2.23957800	0.13764400
S	2.36842100	0.18763900	0.49806500
B	-1.48028400	-2.39802900	-1.79939300
B	5.24715500	-0.54367900	1.46501400
S	-2.77810900	-1.22523400	-2.30203300
S	-1.26183100	-3.15053100	-0.16091200
S	5.71049900	0.52845600	2.56670200
B	0.93571700	-1.74266600	-2.14369600
B	3.15556300	-1.23931400	-0.29215000
S	0.39398600	0.00094500	-2.08107200
S	2.46316300	-2.43163600	-1.47915000
S	4.82161600	-1.77370900	0.26127700
B	-0.24285000	5.28029200	-0.35347000
B	-1.35862200	2.69954500	-0.70165500
S	1.09341000	6.10727400	-0.01820100
S	-2.67544600	1.74315300	-1.50969300
S	-0.18860000	-2.90645600	-3.04176600

$B_{10}S_{15}$-XIII

B	0.92966800	-0.80614900	1.96561100
B	-0.14289100	1.92930200	1.89539200
S	2.33691200	-1.96685700	1.74818200
S	1.31597700	0.93447400	2.30002200
S	-0.93674300	3.05530300	-1.34328600
B	3.47170700	-1.37670300	0.45073500
B	1.87051600	0.88587200	-0.87515000
S	4.98804800	-2.43834600	0.50952200
S	3.43907300	-0.09829100	-0.82655900
S	0.19567700	3.73111900	1.53624300
B	-1.87323900	-0.39425500	1.39427500
B	5.85705000	-1.99640300	-0.96682400
S	-0.66482700	-1.65129000	1.85470500
S	-3.37288800	-1.11917100	0.60405900
S	2.18599200	2.65139400	-0.67231800
B	-3.57213600	-0.43548000	-1.06286900
B	-1.01194100	1.25784900	-1.49564200
S	6.71683700	-1.66278500	-2.28381500
S	-2.64450900	0.68216500	-2.15343900
S	0.30704600	0.02082600	-1.24694400
B	0.49361000	3.16916800	-0.20707800
B	-6.01523300	-1.86083700	-0.78789200
S	-1.85494700	1.40202900	1.62944100
S	-6.93853200	-2.67370600	0.24805400
S	-5.07534000	-0.98322900	-2.00091600

$B_{10}S_{15}$-XIV

B	-3.28460600	4.10774100	0.05251900
B	-0.99006700	2.53190400	-0.17058500
S	-4.84454800	4.00361500	0.43288800
S	-1.57759900	4.27120400	-0.37142400
S	0.76818300	2.36056200	-0.55545100
B	1.63685100	-1.61399700	1.30367600
B	-1.01735300	-0.23035700	0.27484800
S	1.27424900	-3.03295900	0.30410200
S	0.55220800	-0.08275000	1.50251000
S	-2.13597200	1.24034600	0.38338400
B	-4.89453700	-1.58743200	0.00850700
B	-2.55868100	-2.61916700	-0.89604300
S	-5.41290500	-0.74789400	1.27389600
S	-4.29950800	-2.51221300	-1.38456300
S	-1.24197600	-3.39007800	-1.80650100
B	1.22703500	0.54550500	-0.26829200
B	-0.24638600	-2.36008600	-0.55701000
S	3.07839800	0.36107400	-0.62786600
S	-0.02335000	-0.55160700	-1.35681700
S	-1.77858600	-1.96772000	0.69069300
B	3.94017400	-0.40080700	0.76068800
B	6.15606600	0.90753700	-0.39074800
S	3.26471900	-1.41875400	2.11894800
S	5.77694300	-0.27833000	0.86800600
S	6.60958900	1.97024100	-1.50854300

$B_{12}S_{18}$-I

B	-4.10970000	2.70842100	0.00999700
S	-3.66014600	4.43566300	0.30194900
S	-3.12146600	1.17049000	-0.07033700
S	-5.85208600	2.21103900	-0.22346400
B	-4.87133400	0.66984300	-0.25698300
S	-5.67002900	-0.94330600	-0.43206300
B	-4.37876900	-2.20822100	-0.37005800
S	-2.56616300	-2.11504000	-0.13867600
S	-4.79034300	-3.98428100	-0.49053500
B	-2.99577900	-3.89349200	-0.16148100
S	-2.02166900	-5.38778400	0.13723800
B	-0.29840000	-4.88405000	0.35809900
S	1.00619100	-6.11171100	0.71562800
S	0.54411300	-3.26770200	0.19945000
B	1.85721900	-4.52272100	0.41849900

B	4.10989700	-2.70801000	0.01179200
S	3.66025800	-4.43571600	0.30082600
S	3.12191800	-1.16976000	-0.06489700
S	5.85181700	-2.21097400	-0.22587800
B	4.87143000	-0.66949000	-0.25576500
S	5.67001500	0.94350900	-0.43262400
B	4.37867500	2.20832800	-0.37056000
S	2.56622900	2.11494700	-0.13818000
S	4.78985700	3.98435500	-0.49275500
B	2.99542100	3.89348100	-0.16296800
S	2.02147600	5.38767800	0.13677200
B	0.29854200	4.88359900	0.35948900
S	-1.00588200	6.11102600	0.71843000
S	-0.54413100	3.26747800	0.19946300
B	-1.85706400	4.52259700	0.41883000

$B_{12}S_{18}$-II

B	1.21423200	-2.60652500	-1.61006500
S	1.67513100	-1.27419300	-2.74358900
B	-1.40478000	-2.58597900	-1.47844900
S	-1.83443300	-2.92533900	0.24552200
S	-0.13820900	-3.73316500	-2.21985700
B	2.70235700	-0.05774400	-1.88471500
B	1.40026500	2.21575100	-1.99610800
S	3.45028300	-0.13768700	-0.23947000
S	2.94901800	1.55155300	-2.78986900
S	-0.13122300	1.88217500	-2.89934000
B	1.61897100	-0.64463500	2.79503900
S	1.78375100	1.15565900	2.73034700
B	2.82033300	-1.57647300	0.65810200
S	1.80732000	-2.95232300	0.06368700
S	3.19008900	-1.59588300	2.48367500
B	0.14766100	1.92524700	2.66988900
B	0.04483000	3.26840300	0.42048900
S	-1.48533700	1.17923900	2.89219400
S	0.13824300	3.73327100	2.22186700
S	1.64089200	3.02136400	-0.39432100
B	-2.76461300	-1.53626800	0.93685600
S	-3.45885200	-0.08710800	0.10589000
B	-1.34130600	-0.62324900	2.94074500
S	0.13940200	-1.65867200	3.02936700
S	-2.94959500	-1.55096500	2.79023700
B	-2.87719100	-0.01687800	-1.60567900
B	-1.55999300	2.23798800	-1.84845200
S	-1.95922800	-1.24779000	-2.56203000
S	-3.18946600	1.59624300	-2.48329700
S	-1.62802600	3.04373600	-0.23028000

$B_{12}S_{18}$-III

B	-3.19074900	6.58108600	-0.46250500
B	-1.09932500	4.71694900	-0.13254200
S	-4.78877300	6.73799600	-0.50540900
S	-1.42136000	6.50361300	-0.42534200
S	0.68625300	4.39567800	-0.12751500
B	-1.88473000	1.94223900	0.47628600
B	7.80188600	-0.67465000	-0.67035800
S	-2.49630200	3.57259800	-0.04036100
S	-3.25412900	0.71703100	0.45459000
S	8.72809600	0.63289700	-0.78463000
B	-2.68936600	-1.03184100	0.45233400
B	-0.59875800	-3.13240600	0.40523800
S	4.86086800	0.22371700	-0.16446500
S	-1.04721000	-1.50150900	1.03397200
S	-1.70666800	-4.44213900	-0.18041700
B	5.15761900	-1.55839600	-0.23762700
B	0.98122300	2.69521000	0.42668600
S	1.96223100	-0.70076000	0.99126500
S	2.77853900	2.30959600	0.37289300
S	-0.22773800	1.50428300	1.03880600
B	3.15641500	0.51192000	0.39433400
B	2.38058500	-2.34918400	0.38982000
S	6.86127100	-2.17154900	-0.56069500
S	3.99310300	-2.94864500	-0.18203300
S	1.14634600	-3.71072800	0.36960500
B	-3.40829900	-3.81319400	-0.20938100
B	-6.14651100	-4.35106700	-0.62109800
S	-4.03252400	-2.11942000	-0.10692000
S	-4.58593600	-5.18568200	-0.54250700
S	-7.59981300	-3.67218600	-0.70683300

$B_{12}S_{18}$-IV

B	0.86424900	-0.58223400	-2.53080800
B	-0.48720900	1.86309200	-1.51946800
S	2.50555200	0.14385400	-2.67444100
S	-0.71533300	0.14036300	-2.03558900
S	-1.92931400	2.88690700	-1.05899700
B	0.77073300	0.36949400	2.60457700
B	3.99718000	2.02002200	0.19207700

S	1.24173700	-1.36291800	2.70446100
S	1.88948700	1.62459100	3.41637600
S	4.32652000	2.95126800	1.72810700
B	0.55892500	-3.20533600	-1.49672600
B	-0.20371300	-5.30856300	0.14807200
S	0.65738400	-2.36078900	-3.08758400
S	-0.36634700	-4.78304200	-1.53557400
S	-0.13395400	-5.78959600	1.68102800
B	-3.32077500	1.87302300	-0.43908600
B	-6.07563300	1.82718900	0.18000700
S	-3.38085800	0.28400200	0.42045500
S	-4.90896100	2.72712900	-0.80493400
S	-7.20298900	1.07031600	1.03946400
B	2.45591500	1.79650100	-1.91794100
B	3.14024800	1.60734300	2.11474900
S	1.04356900	2.82959000	-1.46473100
S	3.24795800	0.43626000	0.71191300
S	4.08127500	2.62138100	-1.52329400
B	0.41424300	-2.00344700	1.18847500
B	-1.70929300	-0.17239400	1.05436500
S	1.56167900	-2.63202000	-0.04144800
S	-1.39017100	-1.94117200	0.89084600
S	-0.65375800	1.12741000	1.76572500

$B_{12}S_{18}$-V

B	8.82681700	0.55527400	0.66891800
B	6.24260400	-0.45614100	0.23638100
S	9.67454500	1.91759100	0.72984900
S	7.95617500	-0.98761900	0.61708700
S	5.16257600	-1.90807100	0.02082100
B	4.08990500	1.41612000	-0.06720400
B	1.63271300	1.44415700	-0.27154500
S	5.89059000	1.30397500	-0.06399900
S	3.04431200	2.63074100	-0.80408800
S	0.22433900	2.06338100	0.74542800
B	-3.60321800	0.66751200	0.20941300
B	-4.01359300	-1.62256900	1.02898300
S	-2.37169900	1.16928900	-0.98491400
S	-3.18537900	-0.17502700	1.80066900
S	-5.83352500	-1.83223200	1.21884400
B	0.63286200	-1.39397200	-1.00439500
B	3.43762700	-1.33773100	-0.11881200
S	-0.68383500	-2.41749700	-1.94649600
S	2.27098600	-2.35546500	-0.97026900
S	2.93654000	0.20965900	0.78139000
B	-0.67249600	0.77198700	-0.26535100
B	-1.55284900	-2.14547300	-0.42520200
S	0.69642000	0.45179300	-1.66591800
S	-0.42413300	-1.08489100	0.62140600
S	-3.19169600	-2.84505300	-0.02742100
B	-6.36021000	-0.21198400	0.58903600
B	-8.41545100	1.60207300	-0.03198400
S	-5.34202800	1.03175600	-0.26324400
S	-8.18552300	0.00085500	0.68534400
S	-8.71513700	3.04892300	-0.66581300

$B_{12}S_{18}$-VI

B	4.20039200	-1.63196400	0.39186600
B	4.80520200	1.13307500	0.33586400
S	4.17841500	-3.41734100	0.01273600
S	5.59512200	-0.56601600	0.19478400
S	3.47669200	1.49089100	1.48034100
B	-4.19976000	1.63234400	-0.39304200
B	-4.80535900	-1.13214100	-0.33818200
S	-4.17778900	3.41755600	-0.01303300
S	-5.59536100	0.56680900	-0.19815100
S	-3.47554600	-1.49016100	-1.48093100
B	-0.38959600	-2.85605100	-0.32523800
B	2.41364700	-3.01782600	0.03444600
S	-1.84478900	-3.59303300	0.29331900
S	1.07629700	-3.94134100	-0.67446400
S	2.37574200	-1.37604900	0.92791200
B	0.38949300	2.85513800	0.32680100
B	-2.41318800	3.01715400	-0.03344500
S	1.84397500	3.59276100	-0.29260500
S	-1.07644900	3.93987100	0.67773700
S	-2.37480000	1.37611400	-0.92773000
B	1.31509600	-0.10994400	-0.26215300
B	3.06834100	2.08175800	-0.34369300
S	0.26537400	1.06906800	0.94889900
S	2.29592700	0.72339900	-1.52595200
S	4.87985000	2.38222800	-0.94996300
B	-1.31449000	0.10911500	0.26350100
B	-3.06905000	-2.08150300	0.34344000
S	-0.26491200	-1.07010800	-0.94728700
S	-2.29684500	-0.72335200	1.52630900
S	-4.88113000	-2.38103300	0.94802900

$B_{12}S_{18}$-VII

B	-1.47237200	-0.14897100	1.96094900
B	1.45704600	0.01103800	1.75582500
S	-1.75171000	1.61452500	1.71454100
S	0.07917100	-1.03605600	2.27313400
S	3.09708700	-0.78876500	1.55315800
B	0.56477900	1.28033400	-2.01063400
B	3.03130800	2.60306800	-1.99693900
S	-1.23997700	1.42321200	-1.95272500
S	1.33336200	2.89444900	-2.42642100
S	4.57433000	2.39148000	-1.60533200
B	-4.06481600	-0.79554000	0.65835900
B	-6.59445400	-1.16998800	-0.52635600
S	-2.95524500	-1.23516000	2.03872700
S	-5.79151200	-1.28834200	1.04945100
S	-7.40363200	-1.09206100	-1.91230200
B	2.85902600	-2.39312000	0.70816500
B	4.03249900	-4.83476400	-0.06636500
S	1.54514400	-2.97742300	-0.40510300
S	4.23082900	-3.54008400	1.12793800
S	3.92303200	-6.05390800	-1.10708700
B	-0.15954800	2.46555800	1.50193900
B	1.21006500	4.82447900	0.82826800
S	1.52150800	1.80497200	1.48021800
S	-0.43239400	4.24907200	1.16649400
S	2.66970900	5.40403500	0.49088400
B	-1.93657700	-0.11632600	-1.30097000
B	0.63609100	-1.50784900	-1.04014600
S	-3.73435000	0.02737300	-0.93081400
S	-1.16363900	-1.72849900	-1.04654700
S	1.63483600	-0.13691900	-1.65574400

$B_{12}S_{18}$-VIII

B	-1.93301700	-3.51407800	-1.10686600
B	-1.92017200	-0.56576100	1.95222100
S	-0.63943800	-2.23097100	-1.36834300
S	-2.81068100	-2.09665100	1.56412600
S	-2.55889800	1.11340500	1.78847000
B	2.35165600	-2.12579000	0.04250900
B	0.13404100	-3.67203100	-0.54125700
S	2.46305400	-0.54745200	1.08720200
S	1.59790300	-3.72231600	0.51496700
S	-1.05214800	-5.05445400	-0.70187900
B	-3.59062200	1.16276100	0.29399200
B	-3.60589500	-1.74927400	-0.03774100
S	-3.92502800	2.89563600	-0.26712000
S	-4.19212800	-0.18884300	-0.74125700
S	-3.74902900	-3.25114000	-1.10290800
B	0.04432500	5.01707700	-0.23988900
B	-2.13746300	3.30529500	-0.42074300
S	1.57996200	5.13685300	-0.70147200
S	-1.62826200	4.88680600	0.33371400
S	-1.10586200	2.22115400	-1.47739500
B	3.00504300	0.14541400	-0.73121700
B	5.60910700	0.22211900	0.16387200
S	3.22768500	-1.66914700	-1.40607000
S	4.51579800	1.29118900	-0.69980200
S	6.56484900	-0.78526500	0.98803300
B	0.46051800	1.75879400	-0.62981900
B	0.81809800	0.18076800	1.60071900
S	1.59370000	0.94112800	-1.72913700
S	0.57261700	1.92892500	1.21676200
S	-0.21522600	-0.92051100	2.59405400

$B_{12}S_{18}$-IX

B	-1.30111500	1.06850300	1.16963500
B	-1.96939200	-1.22263900	0.72347400
S	-0.78670400	2.77569100	1.32116200
S	-1.90320100	-0.12463200	2.31763500
S	-3.65429600	-1.97888200	0.27175200
B	-6.58209400	-2.87308700	-0.27876500
B	-4.67206900	-0.82067200	-0.62064500
S	-6.84518700	-4.31012600	0.39029800
S	-6.40171500	-1.29364300	-1.05963200
S	-4.40610000	0.90013000	-1.26494600
B	3.07568100	0.01360500	0.26799100
B	0.98219900	-2.08661000	0.63893900
S	4.34177700	-1.10999400	-0.35554400
S	1.45255700	-0.34090700	0.95481000
S	-0.71781200	-2.67674200	0.65896400
B	3.78351600	-2.81383800	-0.06046300
B	6.46807000	-3.34525700	-0.75898900
S	2.16045200	-3.45985900	0.38050500
S	4.97617000	-4.19214600	-0.32289100
S	7.85997000	-2.65348800	-1.16750400
B	1.19201400	5.44086600	0.40959000
B	2.32587700	2.91046800	0.09780900
S	-0.06365400	6.30282500	-0.11168900

S	2.52438100	4.46695100	1.04707900	S	5.29966800	-1.78453800	-1.14657200
S	3.69172800	1.75436300	0.39289900	S	2.40868600	-2.86083600	-1.34523500
B	-0.51292500	2.88636100	-0.51972000	B	3.82175900	1.17352300	0.32309700
B	-2.68178300	1.32102500	-1.12352800	B	1.42258000	-0.63885300	1.29787600
S	1.10288200	2.69886200	-1.27681100	S	5.44355100	1.32873300	-0.27209100
S	-2.01810100	2.92735900	-1.62864000	S	3.19519700	-0.55073700	0.81192700
S	-1.34688900	0.16463500	-0.53036200	S	0.51485900	0.75552300	1.97503600
---				B	-1.69730700	0.73449300	-0.82088400
$B_{12}S_{18}$-X				B	1.21302300	2.29690800	1.28288500
B	-2.38967300	2.30874200	2.71475900	S	-3.18465500	0.79278200	0.20190800
B	-2.57841200	-0.27576000	1.79392900	S	-0.71357400	2.23323100	-1.15176400
S	-1.58622000	3.68305400	2.44253300	S	2.78534000	2.66884400	0.52026000
S	-3.36915700	0.87086200	3.01888200	B	-6.13072800	-2.45094300	1.03013200
S	-3.72258000	-1.45511700	1.08309400	B	-3.94545200	-0.85862300	0.25201200
B	-4.37053700	-2.78239900	-1.92818400	S	-6.65082300	-3.96753900	1.11469000
B	-2.73560600	-2.83338500	0.24308600	S	-5.62915800	-0.75171600	0.97327100
S	-4.69317200	-1.63740200	-3.02036300	S	-3.25100000	-2.48004700	-0.15799600
S	-3.88924400	-3.99038900	-0.74953200	B	-1.63418600	-2.22521300	-0.91964300
S	-1.55497000	-3.87239500	1.38650500	B	0.89951500	-2.88527500	-0.37519500
B	4.48024900	0.19841700	-0.14258700	S	-0.93299100	-0.70687300	-1.62670700
B	7.01160800	-1.01864600	-0.08803200	S	-0.56573300	-3.72535500	-1.11495700
S	3.50163300	1.73168000	-0.17509400	S	0.57851200	-2.22961400	1.32394100
S	6.26451400	0.58458600	-0.23821900	B	-3.43574400	4.00505700	-1.23400800
S	7.74646800	-2.43859500	0.03950200	B	-1.13441000	3.41689600	0.21096400
B	2.15430100	-1.61829400	-0.01959800	S	-4.23253700	3.64952100	-2.58301500
B	1.76193600	1.35257200	-0.46028800	S	-2.63506600	4.45408700	0.28402600
S	3.95538300	-1.51955200	0.10399700	S	0.06877800	3.75570400	1.51401400
S	1.16435600	-0.34066400	-0.95823800	---			
S	0.69392900	2.78266200	-0.37357200	**$B_{12}S_{18}$-XII**			
B	-0.75903400	-0.40433100	-0.40085000	B	1.77981600	-5.37966300	0.84226800
B	-0.35288100	-3.08475100	0.39154500	B	2.73466200	-2.74360800	0.97776300
S	-0.79482400	-0.10079100	1.46189700	S	0.99996900	-6.41483900	-0.10657200
S	-1.24308600	-2.19060200	-0.98463400	S	2.64574700	-4.29836500	1.94733600
S	1.46402300	-3.12078400	0.66302100	S	3.42550000	-1.37824200	1.95354600
B	-0.96762200	2.40337600	-1.08507000	B	2.59638300	-1.14214000	-1.46772100
B	-1.07084400	5.22285600	-1.06355100	B	0.30109000	0.06033200	-2.18741100
S	-1.69986400	0.81771000	-1.49453500	S	1.95512300	-2.63106100	-0.65565000
S	-2.04012700	3.81742900	-1.53767500	S	1.69809300	-0.71832600	-3.06365700
S	-0.25440100	6.54443500	-0.65355500	S	-1.37661300	-0.18786500	-2.81696600
---				B	-2.41758500	0.54486800	-1.44590600
$B_{12}S_{18}$-XI				B	-2.56159000	2.54296200	0.57797400
B	6.24652700	-0.42741000	-0.15587000	S	3.13202700	2.90668700	-0.97061900
B	3.66187300	-1.78042100	-0.57461300	S	-2.39891300	2.33678000	-1.22932600
S	7.72361600	-0.69371300	0.58027900	S	-3.83703900	1.72106700	1.59109000

B	1.33153300	2.59548900	-0.97429200
B	3.85704600	-0.03978700	0.81000900
S	1.48909100	3.08474800	1.83776700
S	4.17912600	1.55388500	1.71353500
S	4.05460400	-0.17540400	-0.99460200
B	2.94148600	2.58251200	0.80708100
B	0.10252500	3.66576200	0.75680700
S	0.60486500	0.89323400	-0.54936700
S	0.25139000	4.07997700	-1.00439900
S	-1.53509900	3.67026200	1.60658700
B	-4.32133400	0.20296700	0.73419100
B	-5.97061300	-2.06971400	0.58596500
S	-3.40998200	-0.68087900	-0.57000100
S	-5.79328500	-0.57031200	1.51301900
S	-6.20129700	-3.44759200	-0.20694800

$B_{12}S_{18}$-XIII

B	3.83160400	1.02029300	-0.37603000
B	5.59404300	2.12421400	1.51763000
S	2.95709300	0.52047300	1.11944900
S	5.41959900	1.94432600	-0.23492400
S	5.82562300	2.33184300	3.09413200
B	-5.48148900	-1.72431500	1.19375500
B	-3.59655400	0.35280100	1.12740200
S	-5.66181000	-3.30278700	1.42337200
S	-5.37365500	0.02698500	0.90889200
S	-3.11694900	2.12925100	0.83513800
B	-2.01226900	4.74319300	-0.51819600
B	-2.61866100	2.04416400	-0.89351200
S	-2.01379000	5.87864500	0.61860200
S	-1.99237200	3.50947700	-1.79152100
S	-2.69944000	0.46966900	-1.85477300
B	2.24312300	-4.61629700	-0.21533100
B	1.82344400	-0.08760900	-2.08638200
S	0.64227900	-4.51253900	-0.96876100
S	3.67488800	-4.75498900	0.49880400
S	3.37677900	0.85692800	-2.14695700
B	1.43021400	-0.45878800	0.61959300
B	0.43426900	-2.70650700	-1.15621900
S	0.62224000	-1.45050200	2.03813600
S	1.94568600	-1.60269500	-0.92944300
S	0.33411400	0.42728900	-2.88405700
B	-0.94433000	-0.19926000	-1.57715400
B	-0.82891700	-0.58211400	1.46124200
S	-1.17446200	-2.09759100	-1.50919900
S	-0.18435900	0.57083400	0.15230400
S	-2.54223800	-0.91642200	1.91305800

$B_{12}S_{18}$-XIV

B	-4.83027500	-4.70240900	0.04046800
B	-2.57549000	-3.04087200	-0.29882200
S	-6.40595300	-4.69675100	0.35103200
S	-3.09375900	-4.80196000	-0.30086900
S	-0.87543700	-2.85893000	-0.85605400
B	6.85781100	-1.75688200	0.55070500
B	4.61337600	-0.38733400	-0.40367200
S	7.30246100	-2.83391900	1.65981600
S	6.42749500	-0.57347800	-0.68815000
S	3.89201400	0.83162700	-1.55114700
B	-0.27900300	-1.13269400	-0.44113600
B	2.02574600	0.91248900	-1.18055500
S	0.41536500	-1.03767400	1.51092100
S	1.45054800	-0.97710300	-1.25302500
S	0.99969500	2.03216700	-2.27438000
B	-1.34449600	2.06686400	-0.06326900
B	-2.23687800	5.15736600	0.65563900
S	-1.50245500	0.25590900	-0.95546400
S	-3.67708300	4.21234900	0.23667200
S	-1.00550600	6.08266600	1.11282900
B	0.32248700	0.83261400	1.48137800
B	2.10077300	-0.66104800	0.57199000
S	-1.06477700	1.81186800	1.90465800
S	1.97370600	1.31869300	0.77966200
S	3.78455200	-1.34277900	0.90772000
B	-3.15806400	-0.16020600	-0.24275800
B	-2.98383500	2.54552600	-0.01607400
S	-3.77885600	-1.77583900	0.23369000
S	-4.27598800	1.24719300	-0.08203800
S	-0.10106800	3.20801600	-0.94021600

$B_{12}S_{18}$-XV

S	-3.88964000	-1.59621000	-0.00179800
S	-1.93832300	0.00026300	2.09057500
B	-2.54511700	-1.51814600	1.26587500
B	-2.54323000	-1.51867900	-1.26743400
S	-1.93358500	0.00002900	-2.08947600
S	0.75584200	-4.00037800	0.00064500
S	-1.80154500	-3.15657500	1.67784300

B	-0.01247300	-2.95004700	1.30248100
B	-0.01094500	-2.95066800	-1.30225400
S	-1.79981100	-3.15706600	-1.67974000
S	-3.88944700	1.59649100	-0.00160100
S	-1.80124200	3.15716100	1.67816100
B	-2.54498400	1.51871300	1.26602500
B	-2.54297400	1.51845300	-1.26726900
S	-1.79945100	3.15681600	-1.67937700
S	3.44652800	1.72407400	0.00107200
S	3.36623700	-0.00008000	2.58570000
B	2.51913000	1.28113900	1.52023300
B	2.52081000	1.28121700	-1.51916200
S	3.36849200	-0.00045100	-2.58364900
S	0.75632100	4.00036000	0.00027500
S	0.93828500	1.76050600	2.28138900
B	-0.01227000	2.95037100	1.30210300
B	-0.01034500	2.95054600	-1.30257400
S	0.94101400	1.76125900	-2.28197000
S	3.44626600	-1.72476800	0.00129800
S	0.93827900	-1.76047600	2.28179900
B	2.51919500	-1.28159900	1.52043600
B	2.52057700	-1.28150000	-1.51879600
S	0.94034900	-1.76089100	-2.28103900

NH_3

N	0.00000000	0.00000000	0.11688900
H	0.00000000	0.93755700	-0.27274200
H	-0.81194900	-0.46877900	-0.27274200
H	0.81194900	-0.46877900	-0.27274200

$[B_2S_3][NH_3]$-I

B	1.55665000	0.54803900	0.00008400
B	-1.15837000	-0.13980700	0.00006900
S	2.91336800	-0.34629800	-0.00035500
S	-2.83521700	-0.10545900	-0.00040700
S	0.01129300	1.35118400	0.00032800
N	-0.38923600	-1.54680100	0.00058200
H	0.21415300	-1.67346200	-0.81744100
H	-1.12471600	-2.25727100	-0.00007600
H	0.21271100	-1.67363900	0.81961500

$[B_2S_3][NH_3]$-II

B	-1.26076700	0.01005200	0.00005600
B	1.47135200	-0.44203600	0.00000500
S	-1.18827200	1.68639600	0.00004300
S	2.89502400	0.30981000	-0.00005700
S	-0.01499200	-1.39272800	0.00008300
N	-2.71462500	-0.70942900	-0.00012200
H	-2.86238300	-1.29231500	-0.82701900
H	-3.39363800	0.05495000	-0.00021600
H	-2.86269800	-1.29236100	0.82667500

$[B_4S_6][NH_3]$-I

B	-3.52180500	-0.37605800	-0.54903700
B	-0.93323800	-0.35400400	0.21601900
S	-4.73569400	0.44566400	0.15167300
S	-2.09851200	-1.23190800	-1.06683400
S	0.82956900	-1.08599500	0.20549500
B	1.06925200	0.68567100	-0.04396400
B	3.76463300	0.26103200	-0.09463600
S	-0.54096700	1.49622400	-0.05975700
S	2.64571900	1.61331300	-0.26532100
S	4.79491700	-0.96618500	0.07098900
N	-1.57890900	-0.53145700	1.67997300
H	-1.69122900	-1.51973000	1.91624800
H	-2.50336100	-0.08385800	1.72738200
H	-0.96775800	-0.09724100	2.37472100

$[B_4S_6][NH_3]$-II

B	-3.53743800	-0.23629500	0.00010700
B	-0.61741600	-0.44614700	-0.00019700
S	-3.75980700	1.43125400	0.00004900
S	-2.11298500	-1.43866200	-0.00001700
S	1.06224000	-1.20674100	-0.00028300
B	1.29732500	0.59640600	-0.00015900
B	3.99682200	0.22132200	0.00028900
S	-0.35628000	1.36060000	-0.00023600
S	2.84833100	1.56461500	0.00015200
S	5.06102200	-0.98569500	0.00013100
N	-4.86811100	-1.17283500	0.00030200
H	-4.92040300	-1.77296600	-0.82572100
H	-5.65981100	-0.52584700	0.00084400
H	-4.91980300	-1.77371200	0.82582800

$[B_4S_6][NH_3]$-III

B	-3.44720100	-0.13281800	0.22024400
B	-0.62869000	-0.54537400	-0.08782000
S	-4.83095800	0.04631900	-0.70755500

S	-2.10876200	-1.47190200	0.20048600	B	0.28044100	-2.95942700	-0.23599800
S	1.08578100	-1.23102400	-0.12638500	B	-3.66733100	-0.01843800	0.15543400
B	1.28097200	0.56357900	-0.18672600	S	-1.18432100	-4.05276100	-0.30510100
B	3.97877000	0.29581700	0.01273400	S	-3.56580300	-1.92964300	0.10543800
S	-0.39763700	1.28070600	-0.32020000	S	-2.52585000	1.00988000	1.30577000
S	2.78171300	1.59530000	-0.10168600	B	3.64310300	-0.05690600	0.20461600
S	5.07841300	-0.87141500	0.11681800	B	2.96796900	-2.05576800	0.10964700
N	-3.17873500	0.88453700	1.44285600	S	4.41322200	-1.39422700	-0.78707100
H	-3.18526200	0.39469200	2.33993900	S	3.77155300	1.69386600	-0.26484400
H	-3.93978800	1.56686400	1.42477300	S	2.60250900	-0.87963900	1.45260500
H	-2.27984800	1.37292000	1.35950300	N	-5.19354300	0.23064000	0.64290300
---				H	-5.86297700	-0.19064600	-0.00498600
$[B_6S_9][NH_3]$				H	-5.36867500	1.23677500	0.68274600
B	-0.82059800	1.99937100	0.49000900	H	-5.35204100	-0.16570600	1.57180500
B	2.78023700	-0.15119400	-0.42127500	---			
S	0.23297400	3.42851500	0.02069300	**$[B_{10}S_{15}][NH_3]$**			
S	3.13757500	-1.37212900	0.87333000	B	-4.04981900	-1.19437200	0.01462800
S	2.96029000	1.69621500	-0.35902800	B	3.92792200	-1.52778700	-0.22524800
B	-1.13748300	-1.79940800	0.06023800	S	-2.35399100	-1.36411400	0.67483700
B	1.69698700	-1.90059500	-0.15217300	S	3.05061700	-0.33768600	0.84889200
S	-2.41909400	-1.33237000	1.26277400	S	-1.89777500	-4.55131100	-0.08829500
S	0.30577600	-2.83898300	0.55229500	B	-2.52686000	3.34718200	-0.10324000
S	1.85605400	-1.01019400	-1.73541800	B	4.00991200	0.66719100	-0.37332300
B	1.32065400	1.99316800	0.35804000	S	-4.22436800	3.36177200	-0.80586300
B	-2.70013200	-0.14770200	-0.21281200	S	3.85547600	2.39320600	-0.76882100
S	0.30429500	0.81367100	1.31137100	S	5.09331800	-0.55252800	-1.22451100
S	-2.53836900	1.75665100	0.00645800	B	-2.86372100	-3.03095500	0.13914800
S	-1.49758700	-0.93220400	-1.48146200	B	-3.95449700	1.70956000	-0.07726300
N	-4.21743400	-0.31750000	-0.74730400	S	-4.63599200	-2.90357100	-0.29528000
H	-4.36830300	0.21740300	-1.60560600	S	-4.99600200	0.26890100	-0.47489200
H	-4.89366000	-0.00337500	-0.04794700	S	-2.43090000	1.82807000	0.91215000
H	-4.38493100	-1.30648800	-0.94166800	B	1.97458100	-3.64610500	0.08280500
---				B	-0.16120600	-4.10786100	0.18954100
$[B_8S_{12}][NH_3]$				S	1.20559500	-5.30215200	-0.04750900
B	-1.84035400	-2.34357600	-0.10970800	S	3.68198400	-3.32053600	-0.42585300
B	2.21898800	2.48668100	0.27028000	S	0.63160000	-2.50297300	0.55760300
S	-0.36732100	-1.26114000	-0.09640700	B	2.45315200	2.99471400	0.39392900
S	0.79685200	1.83504200	1.20125600	B	0.34323800	3.81680000	-0.01718200
S	1.99890400	-3.52813400	-0.37798600	S	-1.26447500	4.57029600	-0.49454400
B	-2.35756300	1.82945700	-0.29812800	S	1.87653300	4.78070200	0.01955600
B	0.20859900	3.13230400	0.05842500	S	0.76315400	2.10000200	0.34876300
S	-3.40714200	0.95116400	-1.47738400	N	3.01996800	2.94005300	1.90902700
S	-1.37371100	3.30754700	-0.78765900	H	3.86727300	3.50371900	2.00117500
S	1.69543600	4.08763500	-0.43878700	H	3.24153200	1.97917500	2.18771200

H	2.31148900	3.30566100	2.54923400

$[B_{12}S_{18}][NH_3]$

B	-4.37747900	1.91913500	-0.74203100
S	-4.29131900	3.73132400	-0.73204200
S	-3.20656000	0.66468800	-0.10515500
S	-5.81980500	1.00182300	-1.35734600
B	-4.74373200	-0.26260700	-0.56508300
S	-5.18442300	-1.94492000	-0.21022500
B	-3.68238200	-2.57302400	0.80059200
S	-1.93132500	-2.45139400	0.03741300
S	-3.74109200	-4.44821900	1.17247700
B	-2.09561400	-4.19549900	0.46321200
S	-0.91729500	-5.58538300	0.23849200
B	0.67925800	-4.84827800	-0.12576100
S	2.17975000	-5.85535700	-0.45535000
S	1.24931000	-3.10244700	-0.16143600
B	2.73973200	-4.12049200	-0.41442000
B	4.60723500	-1.87599100	-0.43380400
S	4.49251200	-3.67270800	-0.56964000
S	3.35315100	-0.56236800	-0.17998600
S	6.22361000	-1.01873400	-0.50077000
B	4.97705400	0.27402800	-0.17431300
S	5.46457000	1.99086700	0.13902100
B	3.96042900	2.96832700	0.35871600
S	2.18094900	2.56369300	0.20403000
S	4.04424500	4.75643500	0.73266800
B	2.27806600	4.37098200	0.47314700
S	1.03277200	5.68592500	0.44826100
B	-0.58088100	4.91680000	0.17602000
S	-2.09890000	5.91646200	-0.01920000
S	-1.09720400	3.17035000	0.01828100
B	-2.60637000	4.17487000	-0.24839800
N	-3.67285000	-1.77108100	2.20396300
H	-2.91895100	-2.12789900	2.79526600
H	-4.55947800	-1.88729800	2.69819600
H	-3.51534500	-0.76907000	2.04752400

CO

C	0.00000000	0.00000000	-0.64659400
O	0.00000000	0.00000000	0.48494500

$[B_2S_3][CO]$-I

B	1.61933700	-0.63808200	-0.00007600
B	-1.06569600	-0.23412200	-0.00038100
S	2.89441100	0.34904600	-0.00154700
S	-2.75122600	-0.13965500	-0.00177800
S	0.16010900	-1.61980400	0.00191700
C	-0.60567100	1.27987900	0.00089600
O	-0.49836100	2.40604400	0.00243000

$[B_2S_3][CO]$-II

B	1.34169100	-0.15482700	-0.00080300
B	-1.48944600	-0.42888500	0.00025100
S	1.53456500	1.54088700	-0.00581400
S	-3.13425400	-0.83088900	-0.00347400
S	0.05109200	-1.42309500	0.00192000
C	-1.48925900	1.16177500	0.00439500
O	-1.79485100	2.25159200	0.00757800
C	2.84707100	-0.66692000	0.00166700
O	3.96603500	-0.83172000	0.00295600

$[B_4S_6][CO]$-I

B	-3.59569500	0.78252200	0.02692800
B	-1.03407200	-0.15952100	-0.42263000
S	-4.21616200	-0.72653600	0.54773500
S	-2.06014000	1.42188800	-0.65368800
S	0.68383200	-0.12764400	-1.24462000
B	1.13700600	-0.65854000	0.53119300
B	3.73691700	0.74710600	0.38855100
S	-0.59159300	-0.77179400	1.32168800
S	2.45925400	0.22271800	1.56168500
S	5.29546100	1.43786900	0.49626400
C	-4.81321700	1.77996300	0.24642100
O	-5.77554400	2.33028300	0.46769100
C	-1.80448200	-1.41181900	-1.12310100
O	-2.12605300	-2.35136100	-1.65992800
C	1.61061900	-2.20212900	0.41852100
O	1.89523300	-3.29220600	0.34262600
C	3.62764100	0.72828800	-1.17903400
O	3.74704300	0.78482700	-2.30814800

$[B_4S_6][CO]$-II

B	-3.25206200	-0.18861900	-0.00001500
B	-0.39262300	-0.43811900	-0.00037800
S	-3.55843200	1.48024000	-0.00014300
S	-1.90192300	-1.42496700	-0.00019700
S	1.27456000	-1.21153500	-0.00045600

B	1.53084200	0.59005600	-0.00016000
B	4.21919900	0.18854000	0.00028100
S	-0.12190100	1.36627300	-0.00030800
S	3.08284900	1.54540400	0.00035500
S	5.26220600	-1.03463800	0.00026100
C	-4.72946900	-0.75962700	0.00045400
O	-5.84346400	-0.96674400	0.00080600

$[B_4S_6][CO]$-III

B	-3.33571300	-0.42201800	-0.00013800
B	-0.43151700	-0.55039000	0.00031300
S	-5.01864700	-0.63484400	-0.00065100
S	-1.90434200	-1.56868000	0.00012800
S	1.26858800	-1.24769600	0.00079200
B	1.46771000	0.55411400	0.00024900
B	4.16479900	0.26387900	-0.00008700
S	-0.21350200	1.27589200	0.00002900
S	2.97329500	1.57505700	-0.00017100
S	5.25555600	-0.91538100	-0.00051000
C	-3.26804600	1.14630000	0.00020000
O	-3.43666000	2.26809100	0.00040200

$[B_6S_9][CO]$

B	-0.58871400	2.08549800	0.53086600
B	2.85369100	-0.28991700	-0.48879200
S	0.51643500	3.44084400	-0.01684900
S	3.18474000	-1.47661800	0.84476800
S	3.11028500	1.54780100	-0.50228200
B	-1.07847500	-1.72091700	0.14900600
B	1.71699800	-1.98771500	-0.14319400
S	-2.30641600	-1.17261200	1.37631000
S	0.29271300	-2.85439900	0.60112000
S	1.88018400	-1.16554300	-1.75979100
B	1.53500000	1.95023000	0.29779100
B	-2.52919100	0.06482500	-0.07141200
S	0.50075300	0.85197600	1.32789500
S	-2.34747300	1.94770300	0.12589300
S	-1.40924500	-0.79530800	-1.37188900
C	-4.01330200	-0.22368800	-0.59840300
O	-5.02729500	-0.54367500	-0.97296200

$[B_8S_{12}][CO]$

B	1.10026900	-2.72433100	-0.23122900
B	-1.58903000	2.92196300	0.27808700
S	1.08465200	-1.20053600	0.74336900
S	-1.41480600	1.29070500	1.07309200
S	3.49625600	0.20854700	-1.04704300
B	-3.26882700	-1.52894700	0.07545400
B	-3.07225900	1.35976100	0.31697900
S	-3.35791700	-2.98673800	-1.02300700
S	-4.15519600	0.02636700	-0.27317900
S	-3.37091000	3.11711000	-0.10127100
B	2.84556100	-1.22499900	0.01840800
B	-1.77437200	-3.01345000	-0.10390100
S	2.78981700	-2.91803500	-0.87390700
S	-0.27158800	-3.82248500	-0.72935600
S	-2.00242800	-1.90714800	1.33047500
B	1.26762000	3.19568900	-0.13506700
B	2.76018900	1.71164000	-0.38786500
S	2.59895600	3.24908800	-1.37980800
S	-0.32925400	4.05376200	-0.37003900
S	1.79453300	2.00467500	1.14186300
C	3.82426800	-1.42915900	1.27321700
O	4.48934900	-1.59458400	2.16842000

$[B_{10}S_{15}][CO]$

B	-0.74378500	-4.06511600	0.18959300
B	2.76438100	2.58295200	0.13515600
S	0.25733200	-2.57536700	0.53764300
S	0.97114200	1.92619200	0.12921200
S	3.16097600	-3.79980600	-0.47038100
B	-4.22625200	-0.68249200	0.04704600
B	0.76156500	3.69752100	-0.18488500
S	-5.03080800	-2.29795500	-0.26502300
S	-0.73740100	4.67963700	-0.55144700
S	2.42443800	4.42876100	-0.21053700
B	1.43153900	-3.89004200	0.05841400
B	-3.28835300	-2.65503300	0.16387400
S	0.44990300	-5.43032800	-0.05287800
S	-2.52556000	-4.28347300	-0.07275400
S	-2.56666000	-1.07016500	0.70547300
B	4.06996400	0.06299200	-0.42197700
B	3.67041900	-2.06781000	-0.25163700
S	5.00280700	-1.29564500	-1.22643500
S	4.13734300	1.78560000	-0.90350400
S	2.97185100	-0.75157300	0.80690600
B	-2.13862900	3.62569100	-0.11693500
B	-3.75545700	2.18395400	-0.05357800

S	-4.97799300	0.89412400	-0.43612400
S	-3.84209200	3.87259900	-0.74704700
S	-2.19030100	2.09516400	0.87737200
C	3.20821800	2.52643700	1.68036900
O	3.49301400	2.50425600	2.77059800

$[B_{12}S_{18}][CO]$

B	-2.44651500	-4.25631200	-0.25415200
S	-4.13537100	-3.87635600	-0.78093700
S	-0.97254800	-3.20103700	0.00841000
S	-1.89365700	-5.97654200	0.01882100
B	-0.40646400	-4.92906500	0.19885500
S	1.22720600	-5.65069400	0.48140700
B	2.43758000	-4.30434200	0.48796500
S	2.29331300	-2.50349600	0.19621700
S	4.21394200	-4.64097900	0.74788200
B	4.08206900	-2.86197300	0.34938100
S	5.56081700	-1.84954700	0.10708900
B	5.02641700	-0.15140000	-0.22136000
S	6.23548800	1.17270900	-0.56820100
S	3.38058300	0.64406100	-0.21501100
B	4.60080700	1.98700500	-0.46760800
B	2.68410200	4.18689200	-0.38962000
S	4.44286900	3.78566700	-0.56089100
S	1.20923900	3.12861700	-0.19716100
S	2.08718800	5.91157800	-0.34933300
B	0.61105400	4.85857700	-0.08500800
S	-1.00862900	5.54768000	0.29740300
B	-2.16669900	4.13824700	0.37692200
S	-1.97805500	2.41795100	-0.14907600
S	-3.85279300	4.31899900	1.02560600
B	-3.75153500	2.47295900	0.55576900
S	-5.23734200	1.76938900	-0.38470900
B	-4.73336700	0.07980200	-0.67521200
S	-5.76024800	-1.22110600	-1.45866000
S	-3.18035900	-0.76409800	-0.16054700
B	-4.28651400	-2.07142100	-0.80878000
C	-3.64808800	1.71015500	1.97379200
O	-3.55905300	1.22369000	2.98607100

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