

From a Möbius-aromatic interlocked $\text{Mn}_2\text{B}_{10}\text{H}_{10}$ wheel to the metal-doped boranaphthalenes $\text{M}_2@B_{10}\text{H}_8$ and M_2B_5 2D-sheets (M = Mn and Fe): a Molecules to Materials continuum using DFT Study

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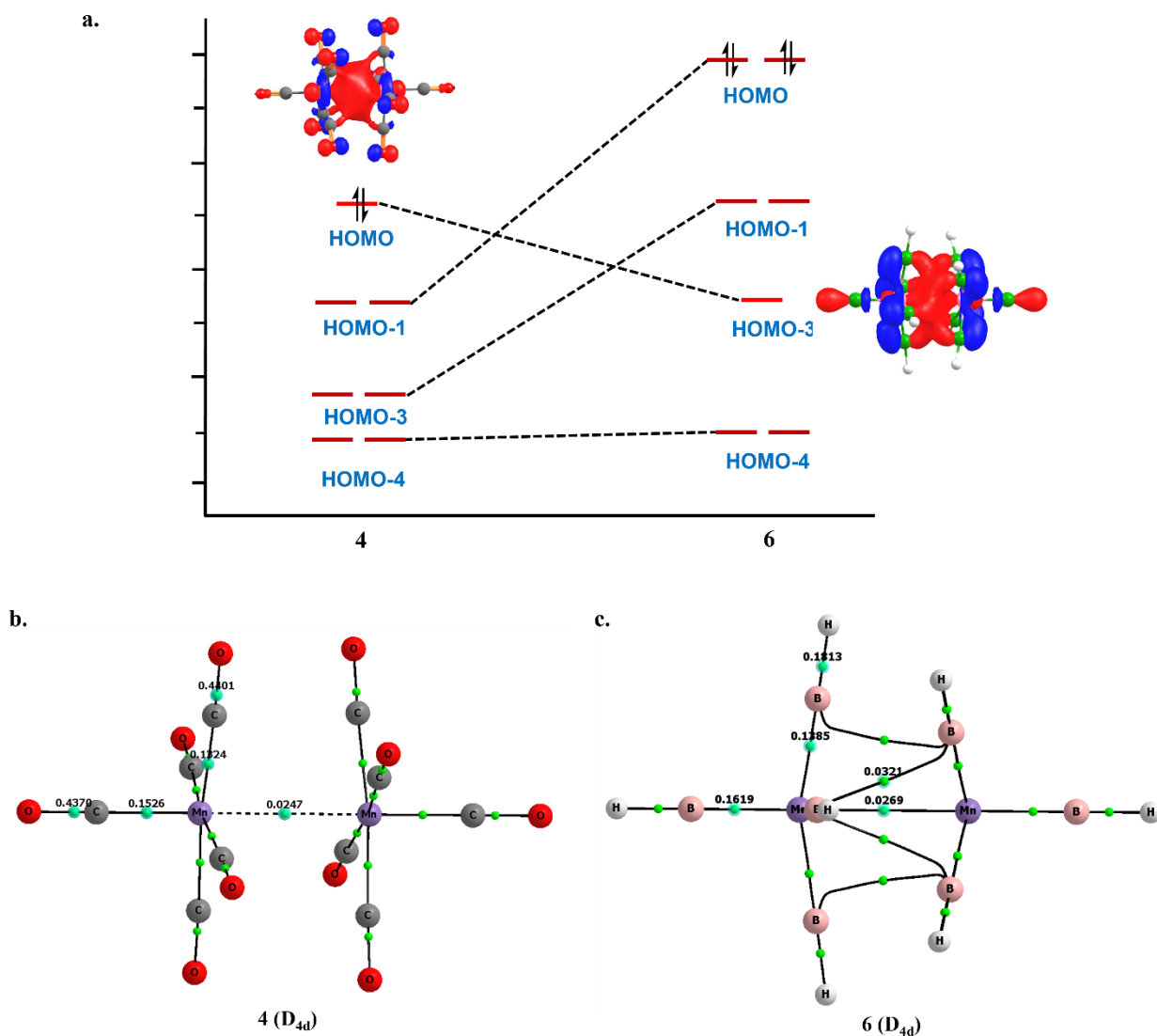


Figure S1. (a) Correlation diagram connecting important molecular orbitals of $\text{Mn}_2(\text{CO})_{10}$ (4, D_{4d}) and $\text{Mn}_2(\text{BH})_{10}$ (6, D_{4d}) at BP86/def2-tzvp level of theory. QTAIM analysis of (b) 4 and (c) 6. Black lines indicate bond path and green dots correspond to BCPs with electron densities shown for unique bonds.

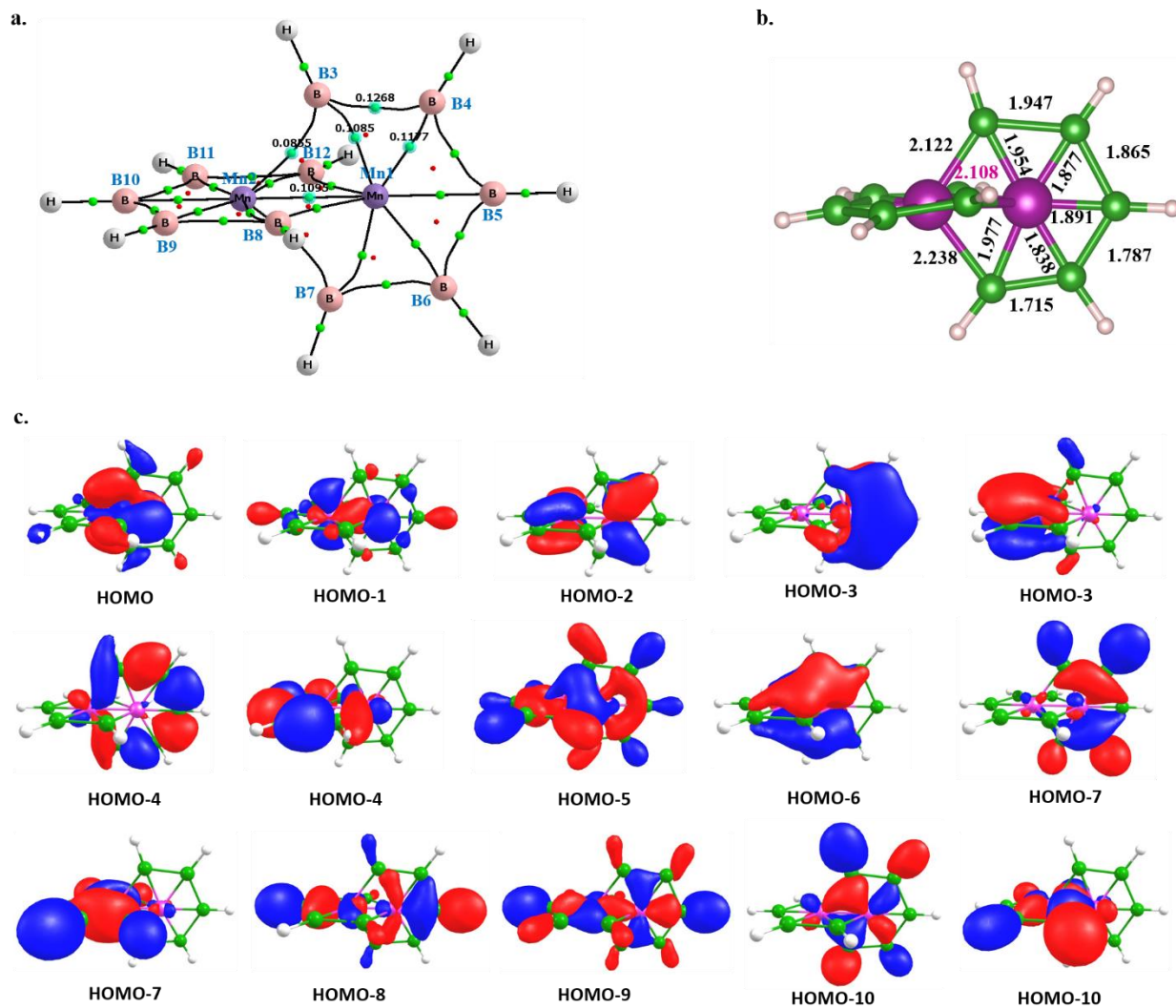


Figure S2. (a) QTAIM analysis of **7**. Black lines indicate bond path, green dots and red dots correspond to BCPs and RCPs respectively with electron densities shown for unique bonds. (b) Snapshot of the equilibrium structure of **7** at 300K after 20ps AIMD simulation (c) Important molecular orbitals of **7** obtained at BP86/def2-tzvp level of theory. HOMO-3, HOMO-4, HOMO-10 are doubly degenerate orbitals.

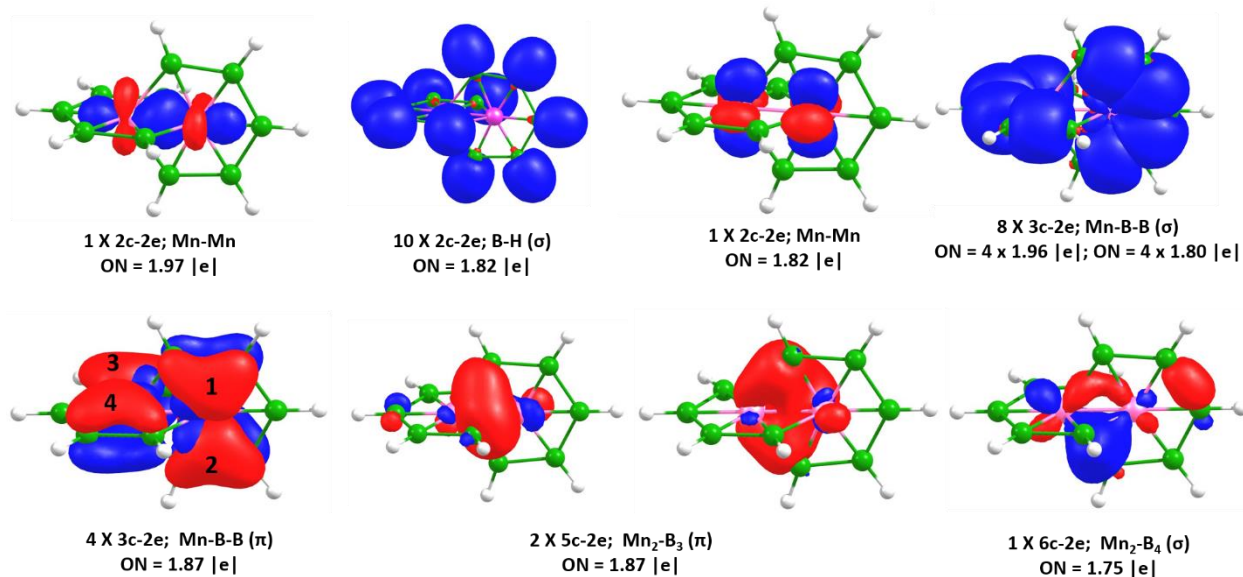


Figure S3. Different nc-2e bonding orbital obtained from AdNDP analysis of 7. ON stands for occupation number. In the ideal cases ON = 2 |e| for nc-2e bonds. [The total number of available electron pairs (e.p.) in 7, 27 (7 e.p. from 2Mn, 15 e.p. from 10B and 5 e.p. from 10H), is distributed in the following bonding orbitals: twelve 2c-2e (2 Mn-Mn bond and 8 B-H, σ), twelve 3c-2e (Fe-B-B, $8\sigma + 4\pi$), two 5c-2e (Fe₂-B₃, σ) and one 6c-2e (Fe₂-B₄, σ).]

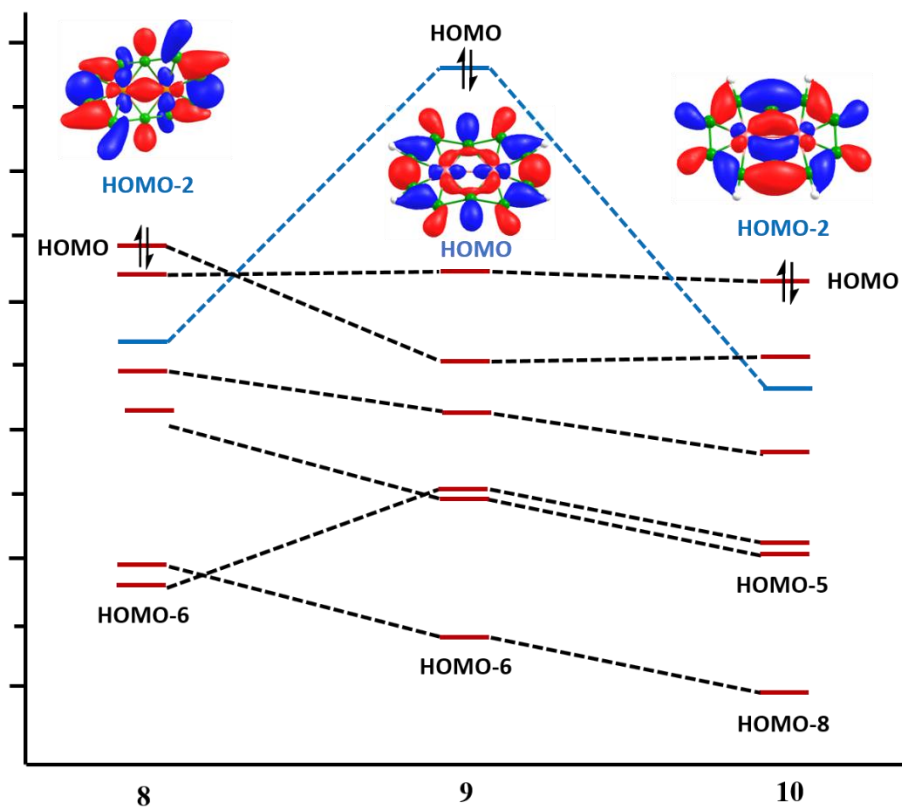


Figure S4. Correlation diagram connecting important molecular orbitals of twisted $\text{Fe}_2@B_{10}H_{10}$ (8), planar $\text{Fe}_2@B_{10}H_{10}$ (9) and $\text{Fe}_2@B_{10}H_8$ (10) at BP86/def2-tzvp level of theory. The maximum effect on the molecular orbital is highlighted with blue color.

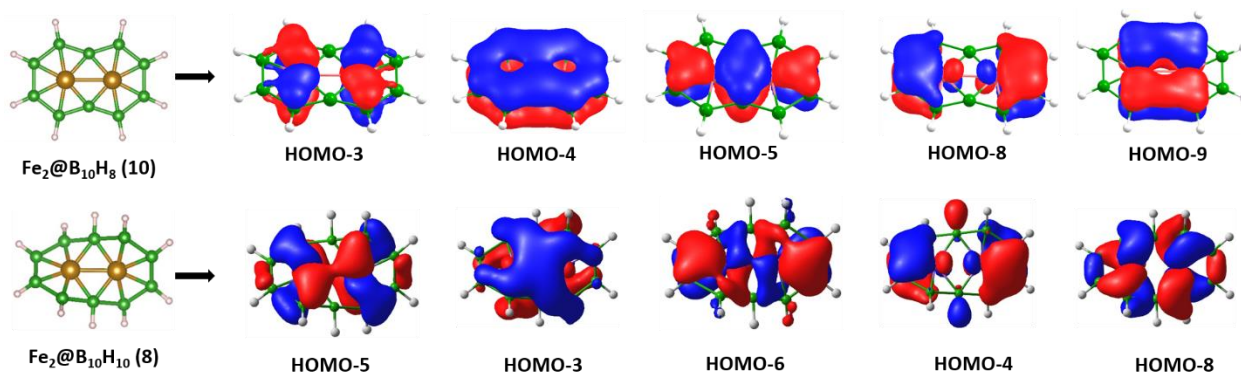


Figure S5. Comparison of π - molecular orbitals of 10 and 8.

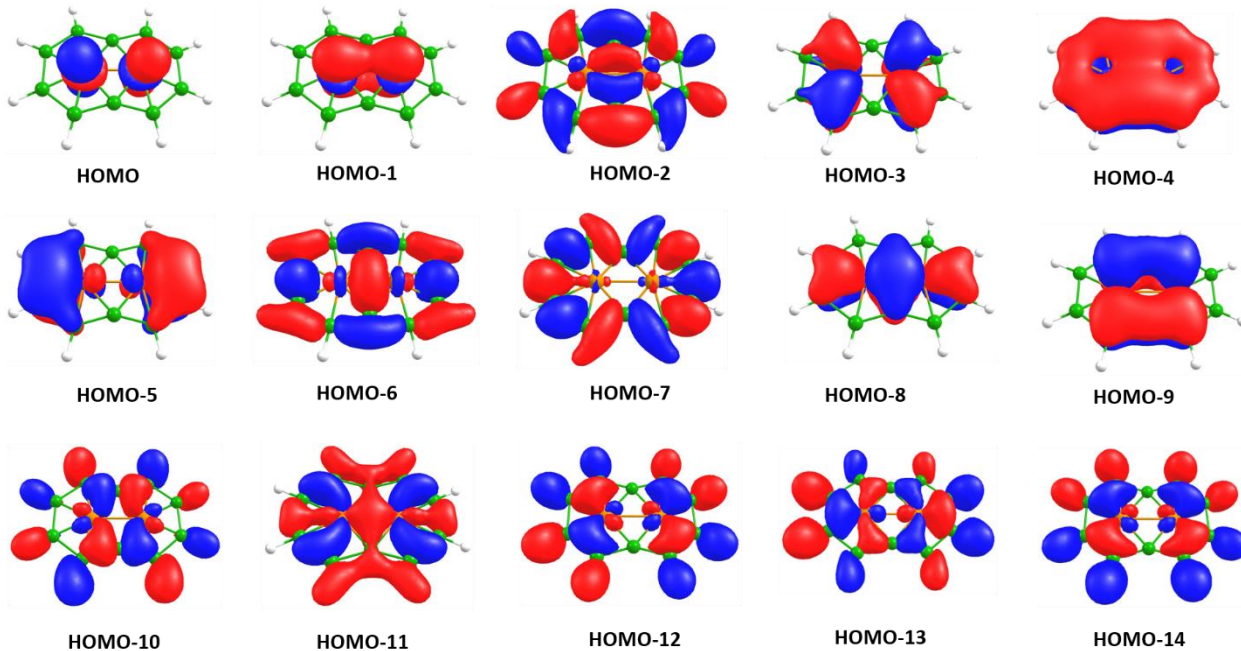


Figure S6. Important molecular orbitals of 10 obtained at BP86/def2-tzvp level of theory.

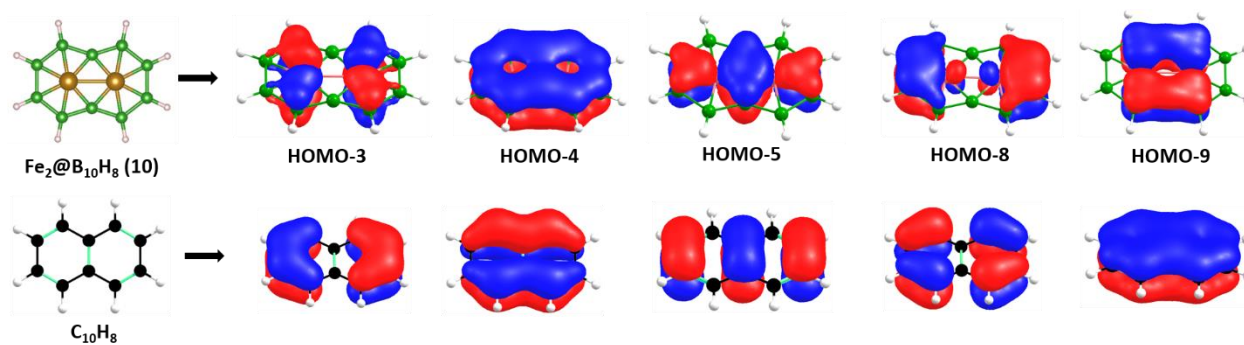


Figure S7. Comparison of π - molecular orbitals of 10 and Naphthalene.

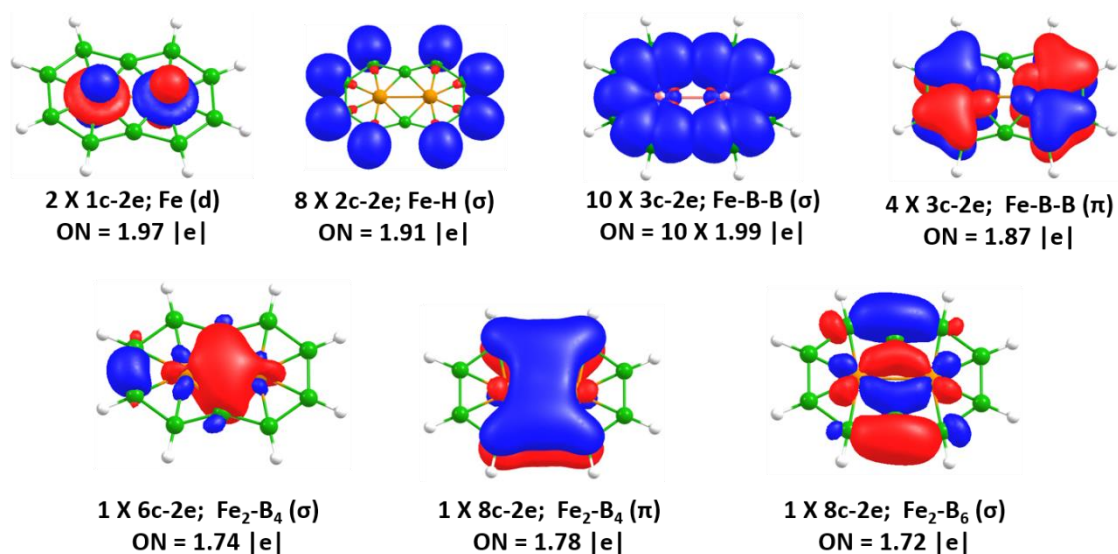


Figure S8. Different nc-2e bonding orbitals obtained from AdNDP analysis of 10. ON stands for occupation number. In the ideal cases ON = 2 |e| for nc-2e bonds. [The total number of available electron pairs (e.p.) in 10, 27 (8 e.p. from 2Fe, 15 e.p. from 10B and 4 e.p. from 8H), is distributed in the following bonding orbitals: two 1c-2e (Fe-d), eight 2c-2e (Fe-H, σ), fourteen 3c-2e (Fe-B-B, $10\sigma + 4\pi$), one 6c-2e (Fe_2-B_4 , σ) and two 8c-2e (Fe_2-B_6 , $\sigma + \pi$).]

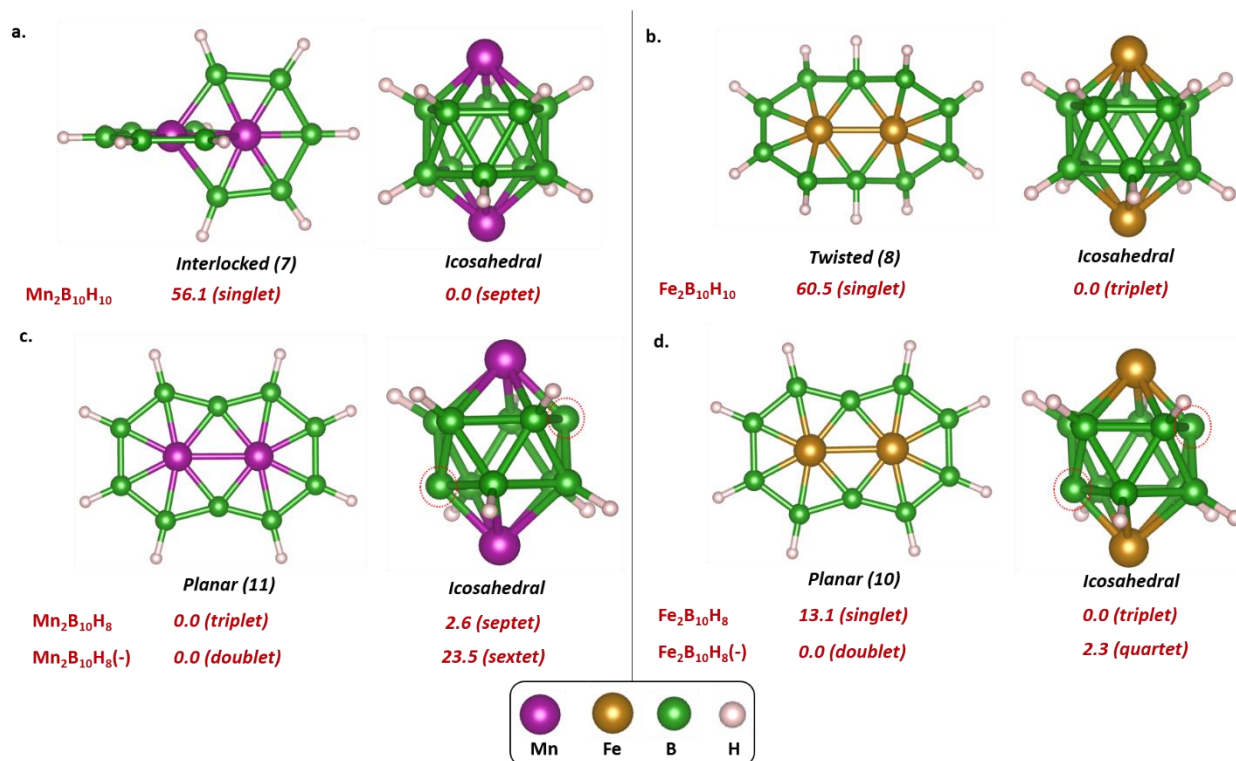


Figure S9. Relative energy comparison (in kcal/mol) between most stable isomers of (a) Interlocked Mn₂B₁₀H₁₀ (7), (b) Twisted Fe₂B₁₀H₁₀ (8), (c) Planar Mn₂B₁₀H₈ (11) and its monoanion, and (d) Planar Fe₂B₁₀H₈ (10) and its monoanion with their corresponding icosahedral isomers at BP86/def2-tzvp level of theory. The most stable spin states of all the complexes are given in the parenthesis (e.g. singlet, doublet, ...). Relative energy for other spin states are given in Table S1 and S2.

Table S1. Relative energy comparison (in kcal/mol) between different isomers of (a) Interlocked Mn₂B₁₀H₁₀ (7), (b) Twisted Fe₂B₁₀H₁₀ (8), (c) Planar Mn₂B₁₀H₈ (11) and (d) Planar Fe₂B₁₀H₈ (10) with their corresponding icosahedral isomers at BP86/def2-tzvp level of theory. Ih stands for Icosahedral. All the structures are given in Figure S8. Relative energies are evaluated w.r.t. their most stable isomers, for example, septet state of Icosahedral Mn₂B₁₀H₁₀ is the most stable isomer and thus rest of the energy values for icosahedral and interlocked structures are evaluated w.r.t. it.

| | Mn ₂ B ₁₀ H ₁₀ (7) | | Fe ₂ B ₁₀ H ₁₀ (8) | | Mn ₂ B ₁₀ H ₈ (11) | | Fe ₂ B ₁₀ H ₈ (10) | |
|---------|---|------|---|------|---|------|---|------|
| | Interlocked | Ih | Twisted | Ih | Planar | Ih | Planar | Ih |
| singlet | 56.1 | 20.0 | 60.5 | - | 15.2 | 11.4 | 13.1 | - |
| triplet | - | 14.3 | 66.0 | 0.0 | 0.0 | 8.5 | 21.5 | 0.0 |
| quintet | 97.4 | 1.6 | 84.6 | 13.0 | 25.0 | 3.5 | 35.2 | 1.9 |
| septet | - | 0.0 | 87.3 | 15.9 | 65.4 | 2.6 | 66.9 | 17.4 |

Table S2. Relative energy comparison (in kcal/mol) between different isomers of (c) monoanion of Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (11) and (d) monoanion of Planar $\text{Fe}_2\text{B}_{10}\text{H}_8$ (10) with their corresponding icosahedral isomers at BP86/def2-tzvp level of theory. Ih stands for Icosahedral. All the structures are given in Figure S8. Relative energies are evaluated w.r.t. their most stable isomers.

| | $\text{Mn}_2\text{B}_{10}\text{H}_8(-)$ | | $\text{Fe}_2\text{B}_{10}\text{H}_8(-)$ | |
|---------|---|------|---|-----|
| | Planar | Ih | Planar | Ih |
| doublet | 0.0 | 27.9 | 0.0 | 3.7 |
| quartet | 3.3 | 24.6 | 8.8 | 2.3 |
| sextet | 34.5 | 23.5 | 26.4 | 4.3 |

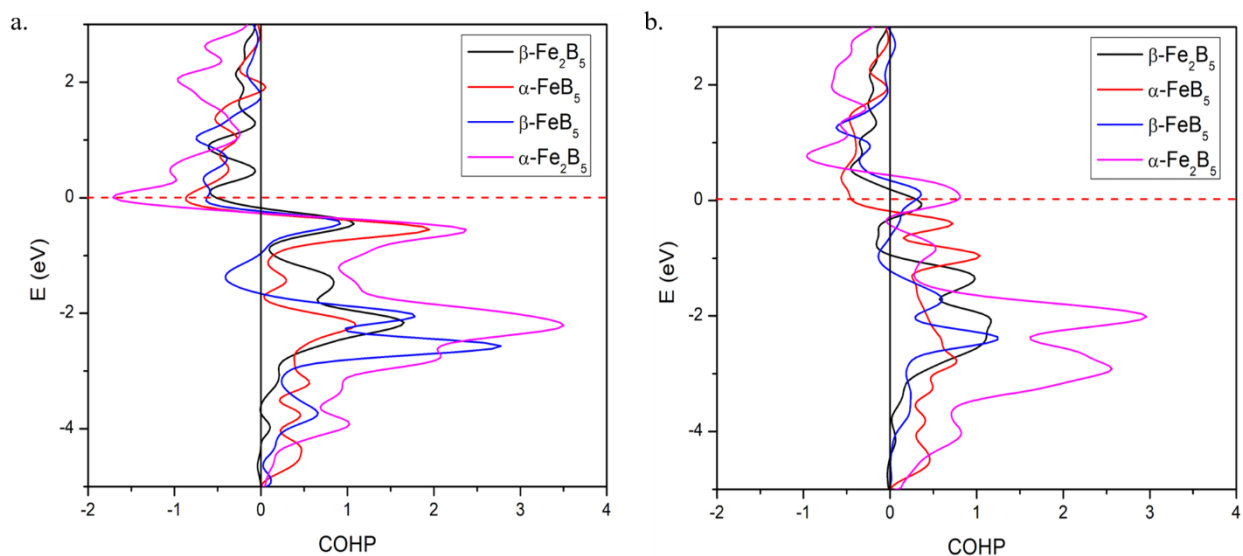


Figure S9. (a) Projected COHP plot for different metal boride monolayers in their (a) nonmagnetic states, (b) magnetic states.

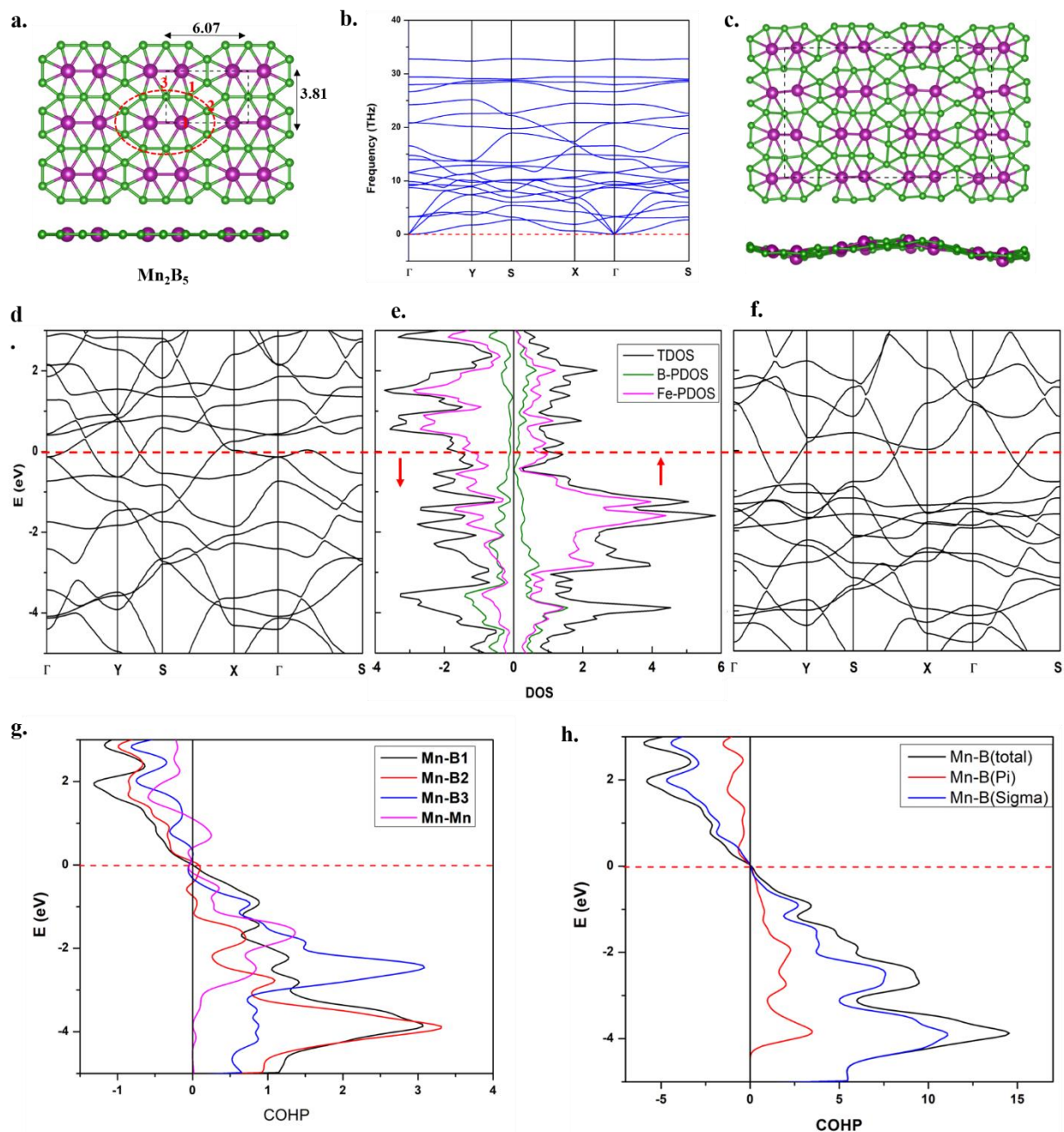


Figure S10. (a) Optimized Mn_2B_5 monolayer considering $\beta\text{-Mn}_2\text{B}_5$ monolayer ($\text{Mn1-B1} = 1.97 \text{ \AA}$, $\text{Mn1-B2} = 2.04 \text{ \AA}$, $\text{Mn2-B3} = 2.22 \text{ \AA}$, $\text{Mn-Mn} = 2.31 \text{ \AA}$). Unit cell is indicated by black dotted line along with the lattice parameters in \AA . Parent building is highlighted using red circle. (b) Phonon spectra (c) Snapshot of the equilibrium structure of Mn_2B_5 monolayer at 1000K after 6ps AIMD simulation (d) Spin polarized band structure for the spin down channel, (e) Total and projected DOS and (f) Spin polarized band structure for the spin up channel, (g) Projected COHP plot for different Fe-B bonds and Fe-Fe bonds in the unit cell and (h) Projected COHP plot for total Mn-B and its sigma and pi decomposition.

Cartesian coordinates of all the optimized geometries at BP86-D3(BJ)/def2-tzvp level of theory.

1

Total energy including ZPVE: -1654.9918 a. u.

Total free energy including ZPVE: -1655.0278 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | -0.025234000 | 0.000019000 | 0.050964000 |
| B | -1.654596000 | -0.000263000 | 1.218629000 |
| B | -0.076154000 | -0.000412000 | 1.846491000 |
| H | -2.551766000 | -0.000551000 | 2.008986000 |
| H | 0.473968000 | -0.001096000 | 2.906841000 |
| C | -1.915828000 | 0.000056000 | -0.258998000 |
| C | 1.077527000 | -1.370210000 | -0.263880000 |
| C | 1.077556000 | 1.370291000 | -0.263715000 |
| O | 1.795605000 | 2.270253000 | -0.369917000 |
| O | 1.795612000 | -2.270087000 | -0.370593000 |
| O | -2.347203000 | 0.000297000 | -1.365355000 |

2

Total energy including ZPVE: -1391.0473 a. u.

Total free energy including ZPVE: -1391.0788 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 0.000001000 | -0.256009000 | -0.367261000 |
| B | 1.825654000 | -0.024503000 | -0.065737000 |
| B | 0.823779000 | 1.361265000 | 0.280074000 |
| B | -0.823432000 | 1.361472000 | 0.280024000 |
| B | -1.825621000 | -0.024045000 | -0.065842000 |
| B | -0.000370000 | -1.579733000 | 0.756057000 |
| H | -0.000625000 | -2.359931000 | 1.665670000 |
| H | 2.994444000 | -0.244398000 | 0.071309000 |
| H | 1.615591000 | 2.015761000 | 0.908863000 |
| H | -1.615029000 | 2.016200000 | 0.908840000 |
| H | -2.994457000 | -0.243684000 | 0.071222000 |

3

Total energy including ZPVE: -1197.2782 a. u.

Total free energy including ZPVE: -1197.3089 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Cr | -0.000417000 | 0.000302000 | -0.419559000 |
| B | -1.785503000 | 0.262429000 | 0.190744000 |
| B | 1.121020000 | 1.413976000 | 0.191160000 |
| B | -0.664474000 | 1.678002000 | 0.190623000 |
| B | 1.785740000 | -0.263113000 | 0.190025000 |
| B | -1.118910000 | -1.415608000 | 0.191228000 |
| B | 0.665590000 | -1.677502000 | 0.190603000 |
| H | -2.845522000 | 0.417618000 | 0.724171000 |
| H | -1.060297000 | 2.673492000 | 0.724152000 |
| H | 2.845032000 | -0.419235000 | 0.724751000 |
| H | 1.784581000 | 2.254337000 | 0.725841000 |
| H | 1.059310000 | -2.673746000 | 0.724335000 |
| H | -1.790416000 | -2.250636000 | 0.724264000 |

4

Total energy including ZPVE: -1416.5791 a. u.

Total free energy including ZPVE: -1416.6096 a. u.

| | | | |
|----|--------------|--------------|-------------|
| Fe | 0.000000000 | 0.000000000 | 0.000000000 |
| B | 1.586207000 | 0.915798000 | 0.000000000 |
| B | 0.000000000 | 1.831597000 | 0.000000000 |
| H | 2.620914000 | 1.513177000 | 0.000000000 |
| H | -0.000005000 | 3.026372000 | 0.000000000 |
| B | -1.586208000 | 0.915797000 | 0.000000000 |
| B | 1.586208000 | -0.915797000 | 0.000000000 |
| B | -1.586207000 | -0.915798000 | 0.000000000 |
| B | 0.000000000 | -1.831597000 | 0.000000000 |
| H | -2.620914000 | -1.513177000 | 0.000000000 |
| H | -2.620913000 | 1.513179000 | 0.000000000 |
| H | 2.620913000 | -1.513179000 | 0.000000000 |
| H | 0.000005000 | -3.026372000 | 0.000000000 |

5

Total energy including ZPVE: -3436.4722 a. u.

Total free energy including ZPVE: -3436.5268 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.449424000 |
| Mn | 0.000000000 | 0.000000000 | -1.449424000 |
| C | 0.000000000 | 1.843124000 | 1.331815000 |
| C | 1.303286000 | 1.303286000 | -1.331815000 |
| C | 1.843124000 | 0.000000000 | 1.331815000 |
| C | 1.303286000 | -1.303286000 | -1.331815000 |
| C | 0.000000000 | -1.843124000 | 1.331815000 |
| C | -1.303286000 | -1.303286000 | -1.331815000 |
| C | -1.843124000 | 0.000000000 | 1.331815000 |
| C | -1.303286000 | 1.303286000 | -1.331815000 |
| C | 0.000000000 | 0.000000000 | 3.249176000 |
| C | 0.000000000 | 0.000000000 | -3.249176000 |
| O | 0.000000000 | 0.000000000 | 4.405142000 |
| O | 0.000000000 | 2.995441000 | 1.301006000 |
| O | 2.118097000 | 2.118097000 | -1.301006000 |
| O | 2.995441000 | 0.000000000 | 1.301006000 |
| O | 0.000000000 | -2.995441000 | 1.301006000 |
| O | -2.118097000 | -2.118097000 | -1.301006000 |
| O | -2.995441000 | 0.000000000 | 1.301006000 |
| O | -2.118097000 | 2.118097000 | -1.301006000 |
| O | 2.118097000 | -2.118097000 | -1.301006000 |
| O | 0.000000000 | 0.000000000 | -4.405142000 |

6

Total energy including ZPVE: -2556.5870 a. u.

Total free energy including ZPVE: -2556.6279 a. u.

| | | | |
|----|--------------|-------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.408008000 |
| Mn | 0.000000000 | 0.000000000 | -1.408008000 |
| B | -0.685341000 | 1.665070000 | 1.091247000 |
| B | 0.000000000 | 0.000000000 | 3.170820000 |
| B | 1.665070000 | 0.685341000 | 1.091247000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -1.665070000 | -0.685341000 | 1.091247000 |
| B | 0.685341000 | -1.665070000 | 1.091247000 |
| B | -0.685341000 | -1.665070000 | -1.091247000 |
| B | 1.665070000 | -0.685341000 | -1.091247000 |
| B | 0.000000000 | 0.000000000 | -3.170820000 |
| B | 0.685341000 | 1.665070000 | -1.091247000 |
| B | -1.665070000 | 0.685341000 | -1.091247000 |
| H | -1.136455000 | 2.757627000 | 0.887449000 |
| H | -2.757627000 | -1.136455000 | 0.887449000 |
| H | 2.757627000 | 1.136455000 | 0.887449000 |
| H | 1.136455000 | -2.757627000 | 0.887449000 |
| H | 0.000000000 | 0.000000000 | 4.369133000 |
| H | -2.757627000 | 1.136455000 | -0.887449000 |
| H | 1.136455000 | 2.757627000 | -0.887449000 |
| H | 0.000000000 | 0.000000000 | -4.369133000 |
| H | 2.757627000 | -1.136455000 | -0.887449000 |
| H | -1.136455000 | -2.757627000 | -0.887449000 |

7

Total energy including ZPVE: -2556.8661 a. u.

Total free energy including ZPVE: -2556.9049 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Mn | -1.056493000 | -0.000016000 | -0.000027000 |
| Mn | 1.056486000 | -0.000027000 | 0.000035000 |
| B | -0.253216000 | -1.240188000 | 1.232073000 |
| B | -2.066792000 | -1.119934000 | 1.112684000 |
| B | -2.944862000 | 0.000051000 | -0.000071000 |
| B | -2.066620000 | 1.120017000 | -1.112767000 |
| B | -0.252994000 | 1.240132000 | -1.232018000 |
| B | 0.253087000 | 1.232177000 | 1.240025000 |
| B | 0.253143000 | -1.232192000 | -1.240028000 |
| B | 2.944861000 | -0.000012000 | 0.000076000 |
| B | 2.066744000 | -1.112778000 | -1.119875000 |
| B | 2.066692000 | 1.112766000 | 1.119958000 |
| H | 0.188929000 | -2.025653000 | 2.012358000 |
| H | -2.746188000 | -1.818229000 | 1.806375000 |
| H | -0.188964000 | -2.012555000 | -2.025439000 |
| H | -2.745915000 | 1.818061000 | -1.806808000 |
| H | -4.141423000 | 0.000538000 | 0.000286000 |
| H | 2.745977000 | 1.806786000 | 1.818033000 |
| H | 2.746094000 | -1.806572000 | -1.818112000 |
| H | 4.141423000 | 0.000298000 | -0.000229000 |
| H | 0.189120000 | 2.025625000 | -2.012295000 |
| H | -0.189083000 | 2.012586000 | 2.025353000 |

8

Total energy including ZPVE: -2782.3604 a. u.

Total free energy including ZPVE: -2782.4008 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 1.178861000 | -0.000950000 | 0.000654000 |
| Fe | -1.178734000 | 0.000177000 | 0.000742000 |
| B | 1.538996000 | -1.608988000 | -0.931645000 |
| B | 2.925854000 | 0.702580000 | 0.418226000 |
| B | -0.002338000 | -1.594303000 | -0.002976000 |

| | | | |
|---|--------------|--------------|--------------|
| B | 2.926868000 | -0.701066000 | -0.417400000 |
| B | 1.538146000 | 1.609123000 | 0.932228000 |
| B | -1.535898000 | 1.606028000 | -0.936541000 |
| B | -0.000283000 | 1.593717000 | 0.001094000 |
| B | -2.927250000 | -0.698814000 | 0.419788000 |
| B | -1.540814000 | -1.606773000 | 0.934303000 |
| B | -2.925677000 | 0.702174000 | -0.419764000 |
| H | 1.596416000 | -2.496932000 | -1.727980000 |
| H | 3.833011000 | -1.374394000 | -0.826096000 |
| H | -0.003026000 | -2.808711000 | -0.009581000 |
| H | 1.593243000 | 2.498827000 | 1.726814000 |
| H | 3.832694000 | 1.376151000 | 0.825075000 |
| H | -3.829424000 | 1.377797000 | -0.830113000 |
| H | -1.590376000 | -2.499593000 | 1.725656000 |
| H | -3.833576000 | -1.371581000 | 0.829272000 |
| H | -0.001270000 | 2.808262000 | -0.000417000 |
| H | -1.589032000 | 2.491877000 | -1.735485000 |

9

Total energy including ZPVE: -2782.3334 a. u.

Total free energy including ZPVE: -2782.3691 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Fe | 0.000000000 | 1.227525000 | 0.000000000 |
| B | 0.000000000 | 3.014011000 | 0.808456000 |
| B | 0.000000000 | 3.014011000 | -0.808456000 |
| B | 0.000000000 | 1.711033000 | -1.916081000 |
| B | 0.000000000 | 1.711033000 | 1.916081000 |
| Fe | 0.000000000 | -1.227525000 | 0.000000000 |
| B | 0.000000000 | -3.014011000 | -0.808456000 |
| B | 0.000000000 | -3.014011000 | 0.808456000 |
| B | 0.000000000 | -1.711033000 | 1.916081000 |
| B | 0.000000000 | -1.711033000 | -1.916081000 |
| B | 0.000000000 | 0.000000000 | 1.539803000 |
| B | 0.000000000 | 0.000000000 | -1.539803000 |
| H | 0.000000000 | -2.031317000 | 3.070270000 |
| H | 0.000000000 | -3.980952000 | 1.517510000 |
| H | 0.000000000 | -3.980952000 | -1.517510000 |
| H | 0.000000000 | -2.031317000 | -3.070270000 |
| H | 0.000000000 | 2.031317000 | -3.070270000 |
| H | 0.000000000 | 3.980952000 | -1.517510000 |
| H | 0.000000000 | 3.980952000 | 1.517510000 |
| H | 0.000000000 | 2.031317000 | 3.070270000 |
| H | 0.000000000 | 0.000000000 | 2.748887000 |
| H | 0.000000000 | 0.000000000 | -2.748887000 |

MnB6⁻ (-109 cm⁻¹)

Total energy including ZPVE: -1300.1637 a. u.

Total free energy including ZPVE: 1300.1955 a. u.

| | | | |
|---|--------------|-------------|-------------|
| B | 0.000000000 | 0.771835000 | 0.000000000 |
| B | 1.416004000 | 1.659815000 | 0.000000000 |
| B | 1.562955000 | 0.063310000 | 0.000000000 |
| B | -1.562955000 | 0.063310000 | 0.000000000 |
| B | -1.416004000 | 1.659815000 | 0.000000000 |

| | | | |
|----|------------|-------------|------------|
| B | 0.00000000 | 2.42978800 | 0.00000000 |
| Mn | 0.00000000 | -1.32957500 | 0.00000000 |

10

Total energy including ZPVE: -2781.1948 a. u.

Total free energy including ZPVE: -2781.2321 a. u.

| | | | |
|----|------------|-------------|-------------|
| Fe | 0.00000000 | 0.00000000 | 1.24409000 |
| B | 0.00000000 | 0.86701800 | 2.95558700 |
| B | 0.00000000 | -0.86701800 | 2.95558700 |
| B | 0.00000000 | -1.91603800 | 1.60554300 |
| B | 0.00000000 | 1.91603800 | 1.60554300 |
| Fe | 0.00000000 | 0.00000000 | -1.24409000 |
| B | 0.00000000 | -0.86701800 | -2.95558700 |
| B | 0.00000000 | 0.86701800 | -2.95558700 |
| B | 0.00000000 | 1.91603800 | -1.60554300 |
| B | 0.00000000 | -1.91603800 | -1.60554300 |
| B | 0.00000000 | 1.47549500 | 0.00000000 |
| B | 0.00000000 | -1.47549500 | 0.00000000 |
| H | 0.00000000 | 3.08953200 | -1.84410100 |
| H | 0.00000000 | 1.36240300 | -4.04714300 |
| H | 0.00000000 | -1.36240300 | -4.04714300 |
| H | 0.00000000 | -3.08953200 | -1.84410100 |
| H | 0.00000000 | -3.08953200 | 1.84410100 |
| H | 0.00000000 | -1.36240300 | 4.04714300 |
| H | 0.00000000 | 1.36240300 | 4.04714300 |
| H | 0.00000000 | 3.08953200 | 1.84410100 |

11 (Singlet)

Total energy including ZPVE: -2555.6824 a. u.

Total free energy including ZPVE: -2555.7191 a. u.

| | | | |
|----|------------|-------------|-------------|
| Mn | 0.00000000 | 0.00000000 | 1.21353700 |
| B | 0.00000000 | 0.87185100 | 2.96218700 |
| B | 0.00000000 | -0.87185100 | 2.96218700 |
| B | 0.00000000 | -1.93905700 | 1.61668800 |
| B | 0.00000000 | 1.93905700 | 1.61668800 |
| Mn | 0.00000000 | 0.00000000 | -1.21353700 |
| B | 0.00000000 | -0.87185100 | -2.96218700 |
| B | 0.00000000 | 0.87185100 | -2.96218700 |
| B | 0.00000000 | 1.93905700 | -1.61668800 |
| B | 0.00000000 | -1.93905700 | -1.61668800 |
| B | 0.00000000 | 1.53446400 | 0.00000000 |
| B | 0.00000000 | -1.53446400 | 0.00000000 |
| H | 0.00000000 | 3.10724000 | -1.88154100 |
| H | 0.00000000 | 1.35953700 | -4.05675400 |
| H | 0.00000000 | -1.35953700 | -4.05675400 |
| H | 0.00000000 | -3.10724000 | -1.88154100 |
| H | 0.00000000 | -3.10724000 | 1.88154100 |
| H | 0.00000000 | -1.35953700 | 4.05675400 |
| H | 0.00000000 | 1.35953700 | 4.05675400 |
| H | 0.00000000 | 3.10724000 | 1.88154100 |

11 (Triplet)

Total energy including ZPVE: -2555.7064 a. u.
Total free energy including ZPVE: -2555.7439 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.242665000 |
| B | 0.000000000 | 0.876836000 | 2.978638000 |
| B | 0.000000000 | -0.876836000 | 2.978638000 |
| B | 0.000000000 | -1.945532000 | 1.620266000 |
| B | 0.000000000 | 1.945532000 | 1.620266000 |
| Mn | 0.000000000 | 0.000000000 | -1.242665000 |
| B | 0.000000000 | -0.876836000 | -2.978638000 |
| B | 0.000000000 | 0.876836000 | -2.978638000 |
| B | 0.000000000 | 1.945532000 | -1.620266000 |
| B | 0.000000000 | -1.945532000 | -1.620266000 |
| B | 0.000000000 | 1.531644000 | 0.000000000 |
| B | 0.000000000 | -1.531644000 | 0.000000000 |
| H | 0.000000000 | 3.106697000 | -1.912275000 |
| H | 0.000000000 | 1.371064000 | -4.069834000 |
| H | 0.000000000 | -1.371064000 | -4.069834000 |
| H | 0.000000000 | -3.106697000 | -1.912275000 |
| H | 0.000000000 | -3.106697000 | 1.912275000 |
| H | 0.000000000 | -1.371064000 | 4.069834000 |
| H | 0.000000000 | 1.371064000 | 4.069834000 |
| H | 0.000000000 | 3.106697000 | 1.912275000 |

Cartesian coordinates of all the optimized geometries using BP86 functional with LANL2DZ basis set for Mn, Fe, and 6-31G(d,p) basis set for other atoms.

Fe(CO)₃(PMe₃)(BPh)

Total energy including ZPVE: -1181.0115 a. u.
Total free energy including ZPVE: -1181.0662 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | -0.584509000 | -0.061686000 | 0.010646000 |
| C | -0.559855000 | -1.065357000 | -1.439520000 |
| C | -0.416587000 | 1.685742000 | -0.111031000 |
| O | -0.515230000 | -1.733619000 | -2.407270000 |
| O | -0.274251000 | 2.853533000 | -0.191270000 |
| C | -0.573617000 | -0.840757000 | 1.593349000 |
| O | -0.536418000 | -1.358377000 | 2.649387000 |
| P | -2.849023000 | 0.069856000 | -0.013090000 |
| C | -3.580269000 | 0.882334000 | -1.508267000 |
| C | -3.753562000 | -1.544867000 | 0.057767000 |
| C | -3.610336000 | 1.022959000 | 1.381000000 |
| H | -3.271725000 | 0.324619000 | -2.406434000 |
| H | -4.681770000 | 0.917088000 | -1.456429000 |
| H | -3.182865000 | 1.906389000 | -1.589085000 |
| H | -3.209714000 | 2.048954000 | 1.375221000 |
| H | -4.710041000 | 1.056876000 | 1.298936000 |
| H | -3.327415000 | 0.551816000 | 2.335465000 |
| H | -3.469981000 | -2.074709000 | 0.980690000 |
| H | -4.846679000 | -1.397878000 | 0.038485000 |
| H | -3.450744000 | -2.165677000 | -0.800026000 |
| B | 1.184619000 | -0.071589000 | 0.009845000 |
| C | 2.708220000 | -0.029744000 | 0.003255000 |

| | | | |
|---|-------------|--------------|--------------|
| C | 3.471793000 | -1.226821000 | 0.003473000 |
| C | 3.390277000 | 1.216373000 | -0.003772000 |
| C | 4.871488000 | -1.177086000 | -0.003340000 |
| H | 2.960125000 | -2.195029000 | 0.008676000 |
| C | 4.790155000 | 1.259503000 | -0.010109000 |
| H | 2.814647000 | 2.147868000 | -0.005097000 |
| C | 5.530675000 | 0.064573000 | -0.009928000 |
| H | 5.451036000 | -2.105956000 | -0.003534000 |
| H | 5.306265000 | 2.225069000 | -0.015466000 |
| H | 6.625234000 | 0.101115000 | -0.015112000 |

Fe(CO)₄(PMe₃)

Total energy including ZPVE: -1037.9638 a. u.

Total free energy including ZPVE: -1038.0096 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 0.167125000 | -0.016420000 | 0.310302000 |
| C | -0.114886000 | -1.502194000 | -0.621320000 |
| C | 0.327407000 | 1.543052000 | -0.524285000 |
| O | -0.304609000 | -2.484351000 | -1.235325000 |
| O | 0.429300000 | 2.574506000 | -1.075110000 |
| C | 0.096547000 | -0.068178000 | 2.084115000 |
| O | 0.046352000 | -0.102660000 | 3.256216000 |
| P | -2.065696000 | 0.308580000 | 0.310524000 |
| C | -2.828406000 | 0.452921000 | -1.366774000 |
| C | -3.046601000 | -1.033201000 | 1.118375000 |
| C | -2.632721000 | 1.840069000 | 1.175388000 |
| H | -2.618980000 | -0.464330000 | -1.938534000 |
| H | -3.918763000 | 0.604028000 | -1.298892000 |
| H | -2.371719000 | 1.302332000 | -1.898148000 |
| H | -2.174360000 | 2.717449000 | 0.693243000 |
| H | -3.731048000 | 1.932831000 | 1.142211000 |
| H | -2.298304000 | 1.808434000 | 2.223892000 |
| H | -2.729939000 | -1.130581000 | 2.168337000 |
| H | -4.126934000 | -0.815892000 | 1.078051000 |
| H | -2.843354000 | -1.986793000 | 0.606959000 |
| C | 1.918370000 | -0.268842000 | 0.306457000 |
| O | 3.073838000 | -0.434864000 | 0.303611000 |

Mn₂(BPh)₁₀

Total energy including ZPVE: -2772.1343 a. u.

Total free energy including ZPVE: -2772.2472 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Mn | -1.073659000 | -0.000140000 | -0.000159000 |
| Mn | 1.073642000 | -0.000077000 | 0.000172000 |
| B | -0.201278000 | 1.238631000 | -1.218540000 |
| B | -2.957572000 | -0.000031000 | -0.000412000 |
| B | 0.201321000 | 1.238776000 | 1.218484000 |
| B | -2.059151000 | 1.152120000 | -1.116402000 |
| B | -2.059630000 | -1.152272000 | 1.115851000 |
| B | 0.201763000 | -1.239170000 | -1.218176000 |
| B | -0.201831000 | -1.239139000 | 1.218291000 |

| | | | |
|---|--------------|--------------|--------------|
| B | 2.957564000 | 0.000226000 | 0.000304000 |
| B | 2.059149000 | 1.152215000 | 1.116419000 |
| B | 2.059665000 | -1.152154000 | -1.115836000 |
| C | -0.415764000 | 2.304933000 | 2.168743000 |
| C | -0.026637000 | 3.667266000 | 2.068172000 |
| C | -1.397226000 | 1.976049000 | 3.140171000 |
| C | -0.611074000 | 4.653116000 | 2.876448000 |
| H | 0.743654000 | 3.953952000 | 1.344780000 |
| C | -1.949356000 | 2.953913000 | 3.979241000 |
| H | -1.736184000 | 0.938442000 | 3.225721000 |
| C | -1.567703000 | 4.299730000 | 3.842247000 |
| H | -0.303974000 | 5.698606000 | 2.764110000 |
| H | -2.693270000 | 2.667760000 | 4.731024000 |
| H | -2.012020000 | 5.067062000 | 4.485270000 |
| C | 2.912852000 | 2.081656000 | 2.029354000 |
| C | 3.901043000 | 2.943379000 | 1.486099000 |
| C | 2.723880000 | 2.105108000 | 3.436332000 |
| C | 4.658118000 | 3.790905000 | 2.306908000 |
| H | 4.081496000 | 2.938482000 | 0.406249000 |
| C | 3.497100000 | 2.933951000 | 4.261226000 |
| H | 1.949282000 | 1.474563000 | 3.886549000 |
| C | 4.464396000 | 3.783365000 | 3.698559000 |
| H | 5.409988000 | 4.450559000 | 1.860258000 |
| H | 3.335266000 | 2.926763000 | 5.344644000 |
| H | 5.063144000 | 4.437535000 | 4.341558000 |
| C | 4.509937000 | 0.000509000 | 0.000316000 |
| C | 5.243608000 | 0.522366000 | -1.097030000 |
| C | 5.243831000 | -0.521044000 | 1.097653000 |
| C | 6.645225000 | 0.527052000 | -1.095605000 |
| H | 4.702573000 | 0.924516000 | -1.960787000 |
| C | 6.645450000 | -0.525164000 | 1.096214000 |
| H | 4.702970000 | -0.923388000 | 1.961428000 |
| C | 7.350691000 | 0.001085000 | 0.000301000 |
| H | 7.190135000 | 0.936622000 | -1.953227000 |
| H | 7.190533000 | -0.934506000 | 1.953835000 |
| H | 8.446055000 | 0.001308000 | 0.000296000 |
| C | 2.913696000 | -2.081582000 | -2.028467000 |
| C | 3.901947000 | -2.942961000 | -1.484763000 |
| C | 2.725022000 | -2.105457000 | -3.435473000 |
| C | 4.659362000 | -3.790563000 | -2.305178000 |
| H | 4.082181000 | -2.937720000 | -0.404879000 |
| C | 3.498570000 | -2.934387000 | -4.259973000 |
| H | 1.950396000 | -1.475185000 | -3.886021000 |
| C | 4.465916000 | -3.783453000 | -3.696869000 |
| H | 5.411277000 | -4.449942000 | -1.858196000 |
| H | 3.336960000 | -2.927538000 | -5.343427000 |
| H | 5.064922000 | -4.437686000 | -4.339563000 |
| C | -0.414871000 | -2.305512000 | -2.168516000 |
| C | -1.396254000 | -1.976816000 | -3.140086000 |
| C | -0.025406000 | -3.667750000 | -2.067970000 |
| C | -1.947971000 | -2.954761000 | -3.979338000 |
| H | -1.735487000 | -0.939294000 | -3.225585000 |
| C | -0.609421000 | -4.653686000 | -2.876441000 |
| H | 0.744810000 | -3.954291000 | -1.344443000 |
| C | -1.565968000 | -4.300480000 | -3.842393000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.691838000 | -2.668744000 | -4.731220000 |
| H | -0.302069000 | -5.699105000 | -2.764131000 |
| H | -2.009945000 | -5.067882000 | -4.485567000 |
| C | 0.415721000 | 2.304715000 | -2.168939000 |
| C | 0.026703000 | 3.667078000 | -2.068402000 |
| C | 1.397005000 | 1.975690000 | -3.140498000 |
| C | 0.611074000 | 4.652828000 | -2.876848000 |
| H | -0.743444000 | 3.953869000 | -1.344899000 |
| C | 1.949070000 | 2.953456000 | -3.979725000 |
| H | 1.735888000 | 0.938056000 | -3.226026000 |
| C | 1.567528000 | 4.299308000 | -3.842773000 |
| H | 0.304063000 | 5.698347000 | -2.764539000 |
| H | 2.692848000 | 2.667197000 | -4.731603000 |
| H | 2.011791000 | 5.066562000 | -4.485925000 |
| C | -2.912825000 | 2.081750000 | -2.029158000 |
| C | -3.900684000 | 2.943639000 | -1.485557000 |
| C | -2.724195000 | 2.105294000 | -3.436172000 |
| C | -4.657765000 | 3.791431000 | -2.306084000 |
| H | -4.080862000 | 2.938656000 | -0.405661000 |
| C | -3.497417000 | 2.934423000 | -4.260780000 |
| H | -1.949864000 | 1.474606000 | -3.886645000 |
| C | -4.464373000 | 3.784005000 | -3.697782000 |
| H | -5.409377000 | 4.451209000 | -1.859181000 |
| H | -3.335851000 | 2.927321000 | -5.344238000 |
| H | -5.063120000 | 4.438386000 | -4.340566000 |
| C | -4.509947000 | 0.000163000 | -0.000658000 |
| C | -5.243785000 | 0.521839000 | 1.096663000 |
| C | -5.243673000 | -0.521282000 | -1.098157000 |
| C | -6.645402000 | 0.526466000 | 1.095055000 |
| H | -4.702879000 | 0.923877000 | 1.960552000 |
| C | -6.645292000 | -0.525461000 | -1.096904000 |
| H | -4.702679000 | -0.923495000 | -1.961909000 |
| C | -7.350698000 | 0.000616000 | -0.001015000 |
| H | -7.190445000 | 0.935890000 | 1.952662000 |
| H | -7.190246000 | -0.934714000 | -1.954650000 |
| H | -8.446063000 | 0.000794000 | -0.001157000 |
| C | -2.913690000 | -2.081644000 | 2.028515000 |
| C | -3.902012000 | -2.943027000 | 1.484965000 |
| C | -2.724958000 | -2.105347000 | 3.435524000 |
| C | -4.659461000 | -3.790462000 | 2.305524000 |
| H | -4.082258000 | -2.937941000 | 0.405081000 |
| C | -3.498543000 | -2.934100000 | 4.260165000 |
| H | -1.950258000 | -1.475084000 | 3.885957000 |
| C | -4.465979000 | -3.783166000 | 3.697209000 |
| H | -5.411431000 | -4.449851000 | 1.858652000 |
| H | -3.336893000 | -2.927121000 | 5.343612000 |
| H | -5.065021000 | -4.437257000 | 4.340013000 |
| C | 0.414919000 | -2.305384000 | 2.168668000 |
| C | 0.025521000 | -3.667645000 | 2.068215000 |
| C | 1.396313000 | -1.976575000 | 3.140193000 |
| C | 0.609621000 | -4.653509000 | 2.876717000 |
| H | -0.744717000 | -3.954263000 | 1.344741000 |
| C | 1.948110000 | -2.954444000 | 3.979476000 |
| H | 1.735484000 | -0.939029000 | 3.225630000 |
| C | 1.566182000 | -4.300196000 | 3.842612000 |

| | | | |
|---|-------------|--------------|-------------|
| H | 0.302315000 | -5.698949000 | 2.764476000 |
| H | 2.691983000 | -2.668353000 | 4.731324000 |
| H | 2.010235000 | -5.067535000 | 4.485809000 |

Cartesian coordinates of all the optimized geometries at BP86/def2-tzvp level of theory.

Interlocked Mn₂B₁₀H₁₀ (singlet)

Total thermal enthalpies: -2556.794707 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.055622000 | -0.000026000 | -0.000002000 |
| Mn | -1.055625000 | -0.000053000 | -0.000045000 |
| B | 0.265540000 | -1.240598000 | -1.239272000 |
| B | 2.947555000 | 0.000019000 | 0.000063000 |
| B | -0.265386000 | -1.239194000 | 1.240568000 |
| B | 2.074961000 | -1.114399000 | -1.113229000 |
| B | 2.074759000 | 1.114454000 | 1.113262000 |
| B | -0.265325000 | 1.239470000 | -1.240247000 |
| B | 0.265189000 | 1.240546000 | 1.239072000 |
| B | -2.947555000 | -0.000043000 | -0.000057000 |
| B | -2.074883000 | -1.113343000 | 1.114322000 |
| B | -2.074844000 | 1.113369000 | -1.114304000 |
| H | -0.173465000 | -2.024882000 | -2.022762000 |
| H | 2.753812000 | -1.811059000 | -1.809023000 |
| H | 0.173511000 | -2.022635000 | 2.024964000 |
| H | 2.753428000 | 1.811194000 | 1.809150000 |
| H | 4.144071000 | 0.000109000 | 0.000172000 |
| H | -2.753581000 | 1.809147000 | -1.811088000 |
| H | -2.753630000 | -1.809306000 | 1.810911000 |
| H | -4.144071000 | -0.000176000 | -0.000258000 |
| H | -0.173637000 | 2.024935000 | 2.022558000 |
| H | 0.173560000 | 2.023224000 | -2.024336000 |

Interlocked Mn₂B₁₀H₁₀ (quintet)

Total thermal enthalpies: -2556.794707 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.204439000 | 0.002097000 | -0.002612000 |
| Mn | -1.204448000 | 0.001074000 | 0.001798000 |
| B | 0.493936000 | -1.241793000 | -1.233069000 |
| B | 3.124984000 | -0.002299000 | 0.002024000 |
| B | -0.493582000 | -1.241472000 | 1.233269000 |
| B | 2.328354000 | -1.098007000 | -1.090772000 |
| B | 2.327770000 | 1.095628000 | 1.092659000 |
| B | -0.493372000 | 1.240770000 | -1.233255000 |
| B | 0.493069000 | 1.240554000 | 1.233393000 |
| B | -3.124992000 | -0.002007000 | -0.000922000 |
| B | -2.328043000 | -1.097906000 | 1.091413000 |
| B | -2.328070000 | 1.095638000 | -1.092134000 |
| H | -0.020829000 | -2.005852000 | -1.990924000 |
| H | 2.828057000 | -1.871125000 | -1.857529000 |
| H | 0.021433000 | -2.004755000 | 1.991716000 |
| H | 2.828128000 | 1.865239000 | 1.862526000 |
| H | 4.322613000 | -0.005385000 | 0.006146000 |
| H | -2.828809000 | 1.866093000 | -1.860916000 |
| H | -2.827415000 | -1.869915000 | 1.859496000 |
| H | -4.322630000 | -0.004093000 | -0.003834000 |

| | | | |
|---|--------------|-------------|--------------|
| H | -0.021065000 | 2.002031000 | 1.994360000 |
| H | 0.020483000 | 2.002969000 | -1.993710000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (singlet)

Total thermal enthalpies: -2555.622742 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.215759000 |
| B | 0.000000000 | 0.872099000 | 2.966117000 |
| B | 0.000000000 | -0.872099000 | 2.966117000 |
| B | 0.000000000 | -1.940824000 | 1.619866000 |
| B | 0.000000000 | 1.940824000 | 1.619866000 |
| Mn | 0.000000000 | 0.000000000 | -1.215759000 |
| B | 0.000000000 | -0.872099000 | -2.966117000 |
| B | 0.000000000 | 0.872099000 | -2.966117000 |
| B | 0.000000000 | 1.940824000 | -1.619866000 |
| B | 0.000000000 | -1.940824000 | -1.619866000 |
| B | 0.000000000 | 1.536425000 | 0.000000000 |
| B | 0.000000000 | -1.536425000 | 0.000000000 |
| H | 0.000000000 | 3.108941000 | -1.886482000 |
| H | 0.000000000 | 1.360429000 | -4.060600000 |
| H | 0.000000000 | -1.360429000 | -4.060600000 |
| H | 0.000000000 | -3.108941000 | -1.886482000 |
| H | 0.000000000 | -3.108941000 | 1.886482000 |
| H | 0.000000000 | -1.360429000 | 4.060600000 |
| H | 0.000000000 | 1.360429000 | 4.060600000 |
| H | 0.000000000 | 3.108941000 | 1.886482000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (triplet)

Total thermal enthalpies: -2555.646943 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.245181000 |
| B | 0.000000000 | 0.877143000 | 2.982428000 |
| B | 0.000000000 | -0.877143000 | 2.982428000 |
| B | 0.000000000 | -1.947188000 | 1.623128000 |
| B | 0.000000000 | 1.947188000 | 1.623128000 |
| Mn | 0.000000000 | 0.000000000 | -1.245181000 |
| B | 0.000000000 | -0.877143000 | -2.982428000 |
| B | 0.000000000 | 0.877143000 | -2.982428000 |
| B | 0.000000000 | 1.947188000 | -1.623128000 |
| B | 0.000000000 | -1.947188000 | -1.623128000 |
| B | 0.000000000 | 1.533745000 | 0.000000000 |
| B | 0.000000000 | -1.533745000 | 0.000000000 |
| H | 0.000000000 | 3.107852000 | -1.918358000 |
| H | 0.000000000 | 1.371884000 | -4.073551000 |
| H | 0.000000000 | -1.371884000 | -4.073551000 |
| H | 0.000000000 | -3.107852000 | -1.918358000 |
| H | 0.000000000 | -3.107852000 | 1.918358000 |
| H | 0.000000000 | -1.371884000 | 4.073551000 |
| H | 0.000000000 | 1.371884000 | 4.073551000 |
| H | 0.000000000 | 3.107852000 | 1.918358000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (quintet)

Total thermal enthalpies: -2555.607074 a. u.

(One imaginary frequency -50.5)

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.321710000 |
| B | 0.000000000 | 0.869399000 | 3.041133000 |
| B | 0.000000000 | -0.869399000 | 3.041133000 |
| B | 0.000000000 | -1.917847000 | 1.658298000 |
| B | 0.000000000 | 1.917847000 | 1.658298000 |
| Mn | 0.000000000 | 0.000000000 | -1.321710000 |
| B | 0.000000000 | -0.869399000 | -3.041133000 |
| B | 0.000000000 | 0.869399000 | -3.041133000 |
| B | 0.000000000 | 1.917847000 | -1.658298000 |
| B | 0.000000000 | -1.917847000 | -1.658298000 |
| B | 0.000000000 | 1.486335000 | 0.000000000 |
| B | 0.000000000 | -1.486335000 | 0.000000000 |
| H | 0.000000000 | 3.102264000 | -1.842777000 |
| H | 0.000000000 | 1.431690000 | -4.099848000 |
| H | 0.000000000 | -1.431690000 | -4.099848000 |
| H | 0.000000000 | -3.102264000 | -1.842777000 |
| H | 0.000000000 | -3.102264000 | 1.842777000 |
| H | 0.000000000 | -1.431690000 | 4.099848000 |
| H | 0.000000000 | 1.431690000 | 4.099848000 |
| H | 0.000000000 | 3.102264000 | 1.842777000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (septet)

Total thermal enthalpies: -2555.542708 a. u.

(Three imaginary frequencies)

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.284071000 |
| B | 0.000000000 | 0.895598000 | 3.043812000 |
| B | 0.000000000 | -0.895598000 | 3.043812000 |
| B | 0.000000000 | -1.960322000 | 1.678128000 |
| B | 0.000000000 | 1.960322000 | 1.678128000 |
| Mn | 0.000000000 | 0.000000000 | -1.284071000 |
| B | 0.000000000 | -0.895598000 | -3.043812000 |
| B | 0.000000000 | 0.895598000 | -3.043812000 |
| B | 0.000000000 | 1.960322000 | -1.678128000 |
| B | 0.000000000 | -1.960322000 | -1.678128000 |
| B | 0.000000000 | 1.577264000 | 0.000000000 |
| B | 0.000000000 | -1.577264000 | 0.000000000 |
| H | 0.000000000 | 3.150892000 | -1.828438000 |
| H | 0.000000000 | 1.345290000 | -4.155983000 |
| H | 0.000000000 | -1.345290000 | -4.155983000 |
| H | 0.000000000 | -3.150892000 | -1.828438000 |
| H | 0.000000000 | -3.150892000 | 1.828438000 |
| H | 0.000000000 | -1.345290000 | 4.155983000 |
| H | 0.000000000 | 1.345290000 | 4.155983000 |
| H | 0.000000000 | 3.150892000 | 1.828438000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (-) (doublet)

Total thermal enthalpies: -2555.752564 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.229978000 |
| B | 0.000000000 | 0.871104000 | 2.973996000 |
| B | 0.000000000 | -0.871104000 | 2.973996000 |
| B | 0.000000000 | -1.935563000 | 1.625198000 |
| B | 0.000000000 | 1.935563000 | 1.625198000 |
| Mn | 0.000000000 | 0.000000000 | -1.229978000 |
| B | 0.000000000 | -0.871104000 | -2.973996000 |
| B | 0.000000000 | 0.871104000 | -2.973996000 |
| B | 0.000000000 | 1.935563000 | -1.625198000 |
| B | 0.000000000 | -1.935563000 | -1.625198000 |
| B | 0.000000000 | 1.524829000 | 0.000000000 |
| B | 0.000000000 | -1.524829000 | 0.000000000 |
| H | 0.000000000 | 3.107789000 | -1.895414000 |
| H | 0.000000000 | 1.373066000 | -4.069590000 |
| H | 0.000000000 | -1.373066000 | -4.069590000 |
| H | 0.000000000 | -3.107789000 | -1.895414000 |
| H | 0.000000000 | -3.107789000 | 1.895414000 |
| H | 0.000000000 | -1.373066000 | 4.069590000 |
| H | 0.000000000 | 1.373066000 | 4.069590000 |
| H | 0.000000000 | 3.107789000 | 1.895414000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (-) (quartet)

Total thermal enthalpies: -2555.747254 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.272855000 |
| B | 0.000000000 | 0.882194000 | 3.005119000 |
| B | 0.000000000 | -0.882194000 | 3.005119000 |
| B | 0.000000000 | -1.943041000 | 1.635436000 |
| B | 0.000000000 | 1.943041000 | 1.635436000 |
| Mn | 0.000000000 | 0.000000000 | -1.272855000 |
| B | 0.000000000 | -0.882194000 | -3.005119000 |
| B | 0.000000000 | 0.882194000 | -3.005119000 |
| B | 0.000000000 | 1.943041000 | -1.635436000 |
| B | 0.000000000 | -1.943041000 | -1.635436000 |
| B | 0.000000000 | 1.513534000 | 0.000000000 |
| B | 0.000000000 | -1.513534000 | 0.000000000 |
| H | 0.000000000 | 3.110227000 | -1.921649000 |
| H | 0.000000000 | 1.382108000 | -4.100090000 |
| H | 0.000000000 | -1.382108000 | -4.100090000 |
| H | 0.000000000 | -3.110227000 | -1.921649000 |
| H | 0.000000000 | -3.110227000 | 1.921649000 |
| H | 0.000000000 | -1.382108000 | 4.100090000 |
| H | 0.000000000 | 1.382108000 | 4.100090000 |
| H | 0.000000000 | 3.110227000 | 1.921649000 |

Planar $\text{Mn}_2\text{B}_{10}\text{H}_8$ (-) (sextet)

Total thermal enthalpies: -2555.697595 a. u.

(Two imaginary frequencies)

| | | | |
|----|-------------|-------------|-------------|
| Mn | 0.000000000 | 0.000000000 | 1.310290000 |
| B | 0.000000000 | 0.902051000 | 3.042869000 |

| | | | |
|----|------------|-------------|-------------|
| B | 0.00000000 | -0.90205100 | 3.04286900 |
| B | 0.00000000 | -1.93474300 | 1.67393400 |
| B | 0.00000000 | 1.93474300 | 1.67393400 |
| Mn | 0.00000000 | 0.00000000 | -1.31029000 |
| B | 0.00000000 | -0.90205100 | -3.04286900 |
| B | 0.00000000 | 0.90205100 | -3.04286900 |
| B | 0.00000000 | 1.93474300 | -1.67393400 |
| B | 0.00000000 | -1.93474300 | -1.67393400 |
| B | 0.00000000 | 1.53441700 | 0.00000000 |
| B | 0.00000000 | -1.53441700 | 0.00000000 |
| H | 0.00000000 | 3.13149200 | -1.81325600 |
| H | 0.00000000 | 1.35466400 | -4.16119400 |
| H | 0.00000000 | -1.35466400 | -4.16119400 |
| H | 0.00000000 | -3.13149200 | -1.81325600 |
| H | 0.00000000 | -3.13149200 | 1.81325600 |
| H | 0.00000000 | -1.35466400 | 4.16119400 |
| H | 0.00000000 | 1.35466400 | 4.16119400 |
| H | 0.00000000 | 3.13149200 | 1.81325600 |

Icosahedral Mn₂B₁₀H₁₀ (singlet)

Total thermal enthalpies: -2556.852187 a. u.

| | | | |
|----|-------------|-------------|-------------|
| B | 0.77329800 | 0.81203400 | 1.29830400 |
| B | -0.77324800 | -1.48570500 | 0.37106700 |
| B | 0.77314300 | 0.10592200 | -1.52765500 |
| B | -0.77317300 | 1.42013300 | 0.57265900 |
| B | -0.77329800 | -0.81203500 | -1.29830400 |
| B | -0.77317000 | 0.98382800 | -1.17340300 |
| H | -1.32781500 | -0.18071500 | 2.60070100 |
| H | 1.32770700 | -2.41762000 | -0.97540100 |
| H | 1.32796500 | 2.52930300 | -0.63159100 |
| B | 0.77317300 | -1.42013200 | -0.57265900 |
| B | 0.77317100 | -0.98382800 | 1.17340300 |
| B | -0.77314300 | -0.10592200 | 1.52765500 |
| B | 0.77324800 | 1.48570500 | -0.37106700 |
| H | -1.32796500 | -2.52930300 | 0.63159100 |
| H | 1.32781500 | 0.18071400 | -2.60070000 |
| H | -1.32759000 | 1.67508800 | -1.99769100 |
| H | -1.32770700 | 2.41762100 | 0.97540100 |
| H | 1.32773000 | 1.38243200 | 2.21038300 |
| H | 1.32759100 | -1.67508800 | 1.99769100 |
| H | -1.32773500 | -1.38243500 | -2.21038800 |
| Mn | -2.07021800 | 0.00000900 | 0.00003900 |
| Mn | 2.07021900 | -0.00000900 | -0.00003900 |

Icosahedral Mn₂B₁₀H₁₀ (triplet)

Total thermal enthalpies: -2556.861339 a. u.

| | | | |
|---|-------------|-------------|-------------|
| B | 0.74602900 | 0.00760200 | -1.36641500 |
| B | -0.75907500 | 1.51303900 | 0.45839900 |
| B | 0.75032200 | -0.89507600 | 1.26178500 |
| B | -0.75033100 | -0.88135100 | -1.27125900 |
| B | -0.74602900 | -0.00760200 | 1.36641500 |
| B | -0.75916400 | -1.51811700 | 0.44197600 |
| H | -1.30372700 | 1.50677900 | -2.14193200 |

| | | | |
|----|--------------|--------------|--------------|
| H | 1.303700000 | 1.483414000 | 2.158060000 |
| H | 1.344337000 | -2.537917000 | -0.719198000 |
| B | 0.750331000 | 0.881351000 | 1.271259000 |
| B | 0.759164000 | 1.518117000 | -0.441976000 |
| B | -0.750322000 | 0.895076000 | -1.261785000 |
| B | 0.759075000 | -1.513039000 | -0.458399000 |
| H | -1.344337000 | 2.537917000 | 0.719198000 |
| H | 1.303727000 | -1.506779000 | 2.141932000 |
| H | -1.343494000 | -2.546301000 | 0.691470000 |
| H | -1.303700000 | -1.483414000 | -2.158060000 |
| H | 1.343494000 | 2.546301000 | -0.691470000 |
| Mn | -2.079793000 | -0.000420000 | 0.087932000 |
| Mn | 2.079793000 | 0.000420000 | -0.087932000 |

Icosahedral Mn₂B₁₀H₁₀ (quintet)

Total thermal enthalpies: -2556.881507 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | 0.749664000 | 1.394397000 | 0.651630000 |
| B | -0.749685000 | -1.050562000 | 1.124692000 |
| B | 0.749594000 | -0.745104000 | -1.346619000 |
| B | -0.749468000 | 1.510992000 | -0.292563000 |
| B | -0.749664000 | -1.394397000 | -0.651630000 |
| B | -0.749608000 | 0.188818000 | -1.527381000 |
| H | -1.403878000 | 1.237791000 | 2.237330000 |
| H | 1.403703000 | -2.510380000 | 0.485876000 |
| H | 1.403894000 | 1.745506000 | -1.868501000 |
| B | 0.749468000 | -1.510992000 | 0.292563000 |
| B | 0.749608000 | -0.188818000 | 1.527381000 |
| B | -0.749594000 | 0.745104000 | 1.346619000 |
| B | 0.749685000 | 1.050562000 | -1.124691000 |
| H | -1.403894000 | -1.745507000 | 1.868501000 |
| H | 1.403879000 | -1.237791000 | -2.237330000 |
| H | -1.403634000 | 0.313808000 | -2.537729000 |
| H | -1.403703000 | 2.510380000 | -0.485876000 |
| H | 1.403593000 | 2.316759000 | 1.082671000 |
| H | 1.403635000 | -0.313808000 | 2.537729000 |
| H | -1.403594000 | -2.316758000 | -1.082670000 |
| Mn | -2.106346000 | 0.000045000 | 0.000004000 |
| Mn | 2.106346000 | -0.000045000 | -0.000004000 |

Icosahedral Mn₂B₁₀H₁₀ (septet)

Total thermal enthalpies: -2556.884106 a. u.

| | | | |
|---|--------------|--------------|--------------|
| B | 0.739409000 | 0.516357000 | -1.411617000 |
| B | -0.725304000 | 1.268691000 | 0.916297000 |
| B | 0.730999000 | -1.322373000 | 0.847889000 |
| B | -0.747092000 | -0.440378000 | -1.434138000 |
| B | -0.739409000 | -0.516357000 | 1.411618000 |
| B | -0.753908000 | -1.606524000 | -0.035260000 |
| H | -1.337174000 | 2.116287000 | -1.527107000 |
| H | 1.405472000 | 0.666085000 | 2.426361000 |
| H | 1.342573000 | -2.018093000 | -1.635624000 |
| B | 0.747092000 | 0.440379000 | 1.434138000 |
| B | 0.753908000 | 1.606525000 | 0.035260000 |
| B | -0.730999000 | 1.322373000 | -0.847889000 |

| | | | |
|----|--------------|--------------|--------------|
| B | 0.725303000 | -1.268691000 | -0.916297000 |
| H | -1.342576000 | 2.018091000 | 1.635623000 |
| H | 1.337173000 | -2.116287000 | 1.527107000 |
| H | -1.296117000 | -2.683065000 | -0.068425000 |
| H | -1.405472000 | -0.666085000 | -2.426360000 |
| H | 1.401318000 | 0.782768000 | -2.391205000 |
| H | 1.296114000 | 2.683067000 | 0.068425000 |
| H | -1.401318000 | -0.782767000 | 2.391202000 |
| Mn | -2.188712000 | 0.002687000 | 0.000757000 |
| Mn | 2.188712000 | -0.002687000 | -0.000757000 |

Icosahedral $Mn_2B_{10}H_8$ (singlet)

Total thermal enthalpies: -2555.628779 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | 0.730081000 | 0.007280000 | -1.315628000 |
| B | -0.774533000 | 1.546758000 | 0.437656000 |
| B | 0.746237000 | -0.920836000 | 1.241695000 |
| B | -0.746181000 | -0.907401000 | -1.251671000 |
| B | -0.730081000 | -0.007280000 | 1.315628000 |
| B | -0.774612000 | -1.551599000 | 0.420825000 |
| H | -1.315389000 | 1.477001000 | -2.148547000 |
| H | 1.315089000 | 1.453698000 | 2.164648000 |
| H | 1.333505000 | -2.580411000 | -0.723840000 |
| B | 0.746181000 | 0.907401000 | 1.251671000 |
| B | 0.774612000 | 1.551599000 | -0.420825000 |
| B | -0.746237000 | 0.920836000 | -1.241695000 |
| B | 0.774533000 | -1.546758000 | -0.437656000 |
| H | -1.333505000 | 2.580411000 | 0.723840000 |
| H | 1.315389000 | -1.477001000 | 2.148547000 |
| H | -1.332899000 | -2.588618000 | 0.695864000 |
| H | -1.315089000 | -1.453698000 | -2.164648000 |
| H | 1.332899000 | 2.588618000 | -0.695864000 |
| Mn | -2.063437000 | -0.000484000 | 0.081344000 |
| Mn | 2.063437000 | 0.000484000 | -0.081344000 |

Icosahedral $Mn_2B_{10}H_8$ (triplet)

Total thermal enthalpies: -2555.633457 a. u.

| | | | |
|---|--------------|--------------|--------------|
| B | 0.746029000 | 0.007602000 | -1.366415000 |
| B | -0.759075000 | 1.513039000 | 0.458399000 |
| B | 0.750322000 | -0.895076000 | 1.261785000 |
| B | -0.750331000 | -0.881351000 | -1.271259000 |
| B | -0.746029000 | -0.007602000 | 1.366415000 |
| B | -0.759164000 | -1.518117000 | 0.441976000 |
| H | -1.303727000 | 1.506779000 | -2.141932000 |
| H | 1.303700000 | 1.483414000 | 2.158060000 |
| H | 1.344337000 | -2.537917000 | -0.719198000 |
| B | 0.750331000 | 0.881351000 | 1.271259000 |
| B | 0.759164000 | 1.518117000 | -0.441976000 |
| B | -0.750322000 | 0.895076000 | -1.261785000 |
| B | 0.759075000 | -1.513039000 | -0.458399000 |
| H | -1.344337000 | 2.537917000 | 0.719198000 |
| H | 1.303727000 | -1.506779000 | 2.141932000 |
| H | -1.343494000 | -2.546301000 | 0.691470000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -1.303700000 | -1.483414000 | -2.158060000 |
| H | 1.343494000 | 2.546301000 | -0.691470000 |
| Mn | -2.079793000 | -0.000420000 | 0.087932000 |
| Mn | 2.079793000 | 0.000420000 | -0.087932000 |

Icosahedral Mn₂B₁₀H₈ (quintet)

Total thermal enthalpies: -2555.641376 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | 0.751383000 | 0.007695000 | -1.381268000 |
| B | -0.748203000 | 1.511086000 | 0.463548000 |
| B | 0.719819000 | -0.895703000 | 1.276602000 |
| B | -0.719892000 | -0.881651000 | -1.285769000 |
| B | -0.751383000 | -0.007695000 | 1.381268000 |
| B | -0.748386000 | -1.516364000 | 0.447275000 |
| H | -1.305413000 | 1.524859000 | -2.123037000 |
| H | 1.305418000 | 1.501494000 | 2.139133000 |
| H | 1.349184000 | -2.524302000 | -0.735237000 |
| B | 0.719892000 | 0.881651000 | 1.285769000 |
| B | 0.748386000 | 1.516364000 | -0.447275000 |
| B | -0.719819000 | 0.895703000 | -1.276602000 |
| B | 0.748203000 | -1.511086000 | -0.463548000 |
| H | -1.349184000 | 2.524302000 | 0.735237000 |
| H | 1.305413000 | -1.524859000 | 2.123037000 |
| H | -1.348185000 | -2.533168000 | 0.707655000 |
| H | -1.305418000 | -1.501494000 | -2.139133000 |
| H | 1.348185000 | 2.533168000 | -0.707655000 |
| Mn | -2.140302000 | -0.000210000 | 0.081368000 |
| Mn | 2.140302000 | 0.000210000 | -0.081368000 |

Icosahedral Mn₂B₁₀H₈ (septet)

Total thermal enthalpies: -2555.642856 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | 0.706669000 | -0.000124000 | -1.378246000 |
| B | -0.708837000 | 1.564547000 | 0.458403000 |
| B | 0.705403000 | -0.890229000 | 1.305310000 |
| B | -0.724275000 | -0.930428000 | -1.255123000 |
| B | -0.764471000 | -0.000120000 | 1.332931000 |
| B | -0.708827000 | -1.564513000 | 0.458977000 |
| H | -1.183856000 | 1.522287000 | -2.199688000 |
| H | 1.275424000 | 1.482476000 | 2.186208000 |
| H | 1.523394000 | -2.422495000 | -0.712626000 |
| B | 0.705403000 | 0.890678000 | 1.300492000 |
| B | 0.780300000 | 1.484597000 | -0.442323000 |
| B | -0.724385000 | 0.930532000 | -1.250380000 |
| B | 0.780324000 | -1.484465000 | -0.442627000 |
| H | -1.132980000 | 2.643060000 | 0.821408000 |
| H | 1.275693000 | -1.482370000 | 2.185924000 |
| H | -1.132629000 | -2.642714000 | 0.822811000 |
| H | -1.183595000 | -1.522558000 | -2.199534000 |
| H | 1.523004000 | 2.423286000 | -0.711615000 |
| Mn | -2.249009000 | -0.000071000 | 0.062579000 |
| Mn | 2.200970000 | -0.000063000 | -0.087777000 |

Icosahedral Mn₂B₁₀H₈ (-) (doublet)

Total thermal enthalpies: -2555.708075 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Mn | 0.000000000 | 0.000000000 | 1.229978000 |
| B | 0.000000000 | 0.871104000 | 2.973996000 |
| B | 0.000000000 | -0.871104000 | 2.973996000 |
| B | 0.000000000 | -1.935563000 | 1.625198000 |
| B | 0.000000000 | 1.935563000 | 1.625198000 |
| Mn | 0.000000000 | 0.000000000 | -1.229978000 |
| B | 0.000000000 | -0.871104000 | -2.973996000 |
| B | 0.000000000 | 0.871104000 | -2.973996000 |
| B | 0.000000000 | 1.935563000 | -1.625198000 |
| B | 0.000000000 | -1.935563000 | -1.625198000 |
| B | 0.000000000 | 1.524829000 | 0.000000000 |
| B | 0.000000000 | -1.524829000 | 0.000000000 |
| H | 0.000000000 | 3.107789000 | -1.895414000 |
| H | 0.000000000 | 1.373066000 | -4.069590000 |
| H | 0.000000000 | -1.373066000 | -4.069590000 |
| H | 0.000000000 | -3.107789000 | -1.895414000 |
| H | 0.000000000 | -3.107789000 | 1.895414000 |
| H | 0.000000000 | -1.373066000 | 4.069590000 |
| H | 0.000000000 | 1.373066000 | 4.069590000 |
| H | 0.000000000 | 3.107789000 | 1.895414000 |

Icosahedral $\text{Mn}_2\text{B}_{10}\text{H}_8$ (-) (quartet)

Total thermal enthalpies: -2555.713328 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | -0.747404000 | -0.000290000 | 1.397013000 |
| B | 0.744325000 | 1.514705000 | -0.484218000 |
| B | -0.756729000 | -0.902346000 | -1.252939000 |
| B | 0.756729000 | -0.902346000 | 1.252939000 |
| B | 0.747404000 | -0.000290000 | -1.397012000 |
| B | 0.743781000 | -1.515304000 | -0.483723000 |
| H | 1.335693000 | 1.528780000 | 2.118441000 |
| H | -1.335693000 | 1.528780000 | -2.118441000 |
| H | -1.329872000 | -2.542615000 | 0.773452000 |
| B | -0.756910000 | 0.901115000 | -1.252719000 |
| B | -0.744324000 | 1.514704000 | 0.484218000 |
| B | 0.756910000 | 0.901115000 | 1.252719000 |
| B | -0.743781000 | -1.515303000 | 0.483723000 |
| H | 1.327687000 | 2.543597000 | -0.773861000 |
| H | -1.334050000 | -1.530356000 | -2.119284000 |
| H | 1.329870000 | -2.542616000 | -0.773452000 |
| H | 1.334050000 | -1.530356000 | 2.119284000 |
| H | -1.327688000 | 2.543596000 | 0.773860000 |
| Mn | 2.086149000 | 0.000448000 | -0.081697000 |
| Mn | -2.086149000 | 0.000448000 | 0.081696000 |

Icosahedral $\text{Mn}_2\text{B}_{10}\text{H}_8$ (-) (sextet)

Total thermal enthalpies: -2555.715129 a. u.

| | | | |
|---|--------------|--------------|--------------|
| B | -0.757296000 | 0.000008000 | 1.350958000 |
| B | 0.720287000 | 1.572206000 | -0.447754000 |
| B | -0.716697000 | -0.903525000 | -1.266342000 |
| B | 0.705774000 | -0.927137000 | 1.247657000 |
| B | 0.768706000 | 0.000073000 | -1.353477000 |

| | | | |
|----|--------------|--------------|--------------|
| B | 0.720351000 | -1.572203000 | -0.447724000 |
| H | 1.189853000 | 1.499566000 | 2.202556000 |
| H | -1.285434000 | 1.468002000 | -2.180285000 |
| H | -1.368727000 | -2.575666000 | 0.728208000 |
| B | -0.716822000 | 0.903588000 | -1.266218000 |
| B | -0.793918000 | 1.542784000 | 0.434163000 |
| B | 0.705814000 | 0.926976000 | 1.247595000 |
| B | -0.793894000 | -1.542711000 | 0.434056000 |
| H | 1.189293000 | 2.631880000 | -0.803237000 |
| H | -1.285291000 | -1.468019000 | -2.180359000 |
| H | 1.189325000 | -2.631822000 | -0.803416000 |
| H | 1.189534000 | -1.499724000 | 2.202744000 |
| H | -1.368382000 | 2.575867000 | 0.728516000 |
| Mn | 2.197356000 | 0.000004000 | -0.063481000 |
| Mn | -2.143823000 | -0.000019000 | 0.081109000 |

Twisted Fe₂B₁₀H₁₀ (singlet)

Total thermal enthalpies: -2782.293849 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 1.182955000 | -0.000200000 | 0.000075000 |
| Fe | -1.182957000 | 0.000038000 | 0.000305000 |
| B | 1.548106000 | 1.619652000 | 0.918849000 |
| B | 2.933320000 | -0.705560000 | -0.412599000 |
| B | 0.000579000 | 1.595823000 | 0.000345000 |
| B | 2.933570000 | 0.705226000 | 0.411246000 |
| B | 1.547530000 | -1.620210000 | -0.918400000 |
| B | -1.548789000 | -1.620210000 | 0.917941000 |
| B | -0.000045000 | -1.595962000 | 0.000829000 |
| B | -2.932975000 | 0.706226000 | -0.412524000 |
| B | -1.546954000 | 1.620745000 | -0.917889000 |
| B | -2.933867000 | -0.705103000 | 0.410527000 |
| H | 1.612324000 | 2.515082000 | 1.706518000 |
| H | 3.841357000 | 1.379955000 | 0.814782000 |
| H | -0.000167000 | 2.811141000 | -0.000092000 |
| H | 1.610502000 | -2.516002000 | -1.705761000 |
| H | 3.841294000 | -1.379647000 | -0.816767000 |
| H | -3.842260000 | -1.379273000 | 0.813591000 |
| H | -1.610572000 | 2.516278000 | -1.705515000 |
| H | -3.840962000 | 1.380349000 | -0.816576000 |
| H | -0.000174000 | -2.811251000 | 0.002641000 |
| H | -1.613655000 | -2.515541000 | 1.705667000 |

Twisted Fe₂B₁₀H₁₀ (triplet)

Total thermal enthalpies: -2782.285092 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 1.134782000 | -0.072795000 | 0.004011000 |
| Fe | -1.230623000 | 0.252329000 | 0.365181000 |
| B | 1.797765000 | 1.495383000 | 0.866837000 |
| B | 2.589669000 | -1.157523000 | -0.681983000 |
| B | 0.263517000 | 1.673196000 | 0.199155000 |
| B | 2.950454000 | 0.408361000 | -0.183880000 |
| B | 1.150321000 | -1.976225000 | -0.564150000 |
| B | -1.882220000 | -1.591143000 | 0.861993000 |
| B | -0.291889000 | -1.463034000 | 0.269548000 |

| | | | |
|---|--------------|--------------|--------------|
| B | -2.539613000 | 0.902742000 | -0.935412000 |
| B | -1.003137000 | 1.724647000 | -0.909632000 |
| B | -2.700322000 | -0.723823000 | -0.410995000 |
| H | 2.505102000 | 2.103543000 | 1.615330000 |
| H | 3.972548000 | 1.029584000 | -0.167613000 |
| H | 0.823180000 | 2.689811000 | 0.670329000 |
| H | 0.913134000 | -3.074820000 | -0.986765000 |
| H | 3.586575000 | -1.682776000 | -1.099371000 |
| H | -3.412251000 | -1.409240000 | -1.092209000 |
| H | -0.804184000 | 2.478724000 | -1.821352000 |
| H | -3.436484000 | 1.449053000 | -1.518077000 |
| H | -0.977257000 | -2.558639000 | 0.432065000 |
| H | -2.351214000 | -2.156048000 | 1.811263000 |

Twisted Fe₂B₁₀H₁₀ (quintet)

Total thermal enthalpies: -2782.255475 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | 1.133355000 | -0.068872000 | 0.319833000 |
| Fe | -1.137483000 | -0.074871000 | -0.324371000 |
| B | 1.565318000 | 1.695770000 | 0.950998000 |
| B | 2.803414000 | -0.666371000 | -0.571733000 |
| B | -0.005047000 | 1.508013000 | -0.007847000 |
| B | 2.831372000 | 0.840488000 | 0.127478000 |
| B | 1.311539000 | -1.458232000 | -1.040878000 |
| B | -1.292760000 | -1.468631000 | 1.035128000 |
| B | 0.006466000 | -1.863503000 | -0.007284000 |
| B | -2.832015000 | 0.830895000 | -0.103783000 |
| B | -1.578768000 | 1.686827000 | -0.955521000 |
| B | -2.790887000 | -0.674521000 | 0.597210000 |
| H | 1.632419000 | 2.664241000 | 1.647104000 |
| H | 3.697423000 | 1.662086000 | -0.002859000 |
| H | -0.016101000 | 2.725407000 | -0.018389000 |
| H | 1.343788000 | -2.042493000 | -2.088138000 |
| H | 3.754622000 | -1.296350000 | -0.948585000 |
| H | -3.738404000 | -1.300358000 | 0.990070000 |
| H | -1.667468000 | 2.645923000 | -1.661986000 |
| H | -3.695357000 | 1.656558000 | 0.018582000 |
| H | 0.013408000 | -3.073361000 | -0.016879000 |
| H | -1.310158000 | -2.058006000 | 2.080204000 |

Twisted Fe₂B₁₀H₁₀ (septet)

Total thermal enthalpies: -2782.251178 a. u.

| | | | |
|----|--------------|--------------|--------------|
| Fe | -1.246280000 | -0.070471000 | -0.153126000 |
| Fe | 1.246851000 | 0.071009000 | -0.157068000 |
| B | -1.675862000 | 1.892377000 | -0.432248000 |
| B | -2.920876000 | -0.904554000 | 0.414838000 |
| B | -0.039848000 | 1.642451000 | -0.074133000 |
| B | -2.874980000 | 0.870260000 | 0.311499000 |
| B | -1.565330000 | -1.956647000 | 0.356062000 |
| B | 1.675946000 | -1.893070000 | -0.432035000 |
| B | 0.040483000 | -1.641756000 | -0.073536000 |
| B | 2.920314000 | 0.903997000 | 0.416430000 |
| B | 1.565076000 | 1.956047000 | 0.358155000 |
| B | 2.873011000 | -0.870406000 | 0.314283000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.121352000 | 2.691905000 | -1.214959000 |
| H | -3.901745000 | 1.349280000 | 0.700662000 |
| H | -0.737271000 | 2.696617000 | 0.203080000 |
| H | -1.829284000 | -3.048668000 | 0.777608000 |
| H | -4.020041000 | -1.315244000 | 0.656607000 |
| H | 3.897816000 | -1.350325000 | 0.707576000 |
| H | 1.827537000 | 3.046393000 | 0.784973000 |
| H | 4.019620000 | 1.313829000 | 0.659142000 |
| H | 0.736745000 | -2.695965000 | 0.204473000 |
| H | 2.123474000 | -2.695290000 | -1.210695000 |

Planar Fe₂B₁₀H₈ (singlet)

Total thermal enthalpies: -2781.134637 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Fe | 0.000000000 | 0.000000000 | 1.246847000 |
| B | 0.000000000 | 0.867509000 | 2.959718000 |
| B | 0.000000000 | -0.867509000 | 2.959718000 |
| B | 0.000000000 | -1.917561000 | 1.608629000 |
| B | 0.000000000 | 1.917561000 | 1.608629000 |
| Fe | 0.000000000 | 0.000000000 | -1.246847000 |
| B | 0.000000000 | -0.867509000 | -2.959718000 |
| B | 0.000000000 | 0.867509000 | -2.959718000 |
| B | 0.000000000 | 1.917561000 | -1.608629000 |
| B | 0.000000000 | -1.917561000 | -1.608629000 |
| B | 0.000000000 | 1.477389000 | 0.000000000 |
| B | 0.000000000 | -1.477389000 | 0.000000000 |
| H | 0.000000000 | 3.090899000 | -1.849817000 |
| H | 0.000000000 | 1.362957000 | -4.051482000 |
| H | 0.000000000 | -1.362957000 | -4.051482000 |
| H | 0.000000000 | -3.090899000 | -1.849817000 |
| H | 0.000000000 | -3.090899000 | 1.849817000 |
| H | 0.000000000 | -1.362957000 | 4.051482000 |
| H | 0.000000000 | 1.362957000 | 4.051482000 |
| H | 0.000000000 | 3.090899000 | 1.849817000 |

Planar Fe₂B₁₀H₈ (triplet)

Total thermal enthalpies: -2781.121260 a. u.

| | | | |
|----|-------------|--------------|--------------|
| Fe | 0.000000000 | 0.000000000 | 1.254073000 |
| B | 0.000000000 | 0.872415000 | 2.974184000 |
| B | 0.000000000 | -0.872415000 | 2.974184000 |
| B | 0.000000000 | -1.917569000 | 1.618078000 |
| B | 0.000000000 | 1.917569000 | 1.618078000 |
| Fe | 0.000000000 | 0.000000000 | -1.254073000 |
| B | 0.000000000 | -0.872415000 | -2.974184000 |
| B | 0.000000000 | 0.872415000 | -2.974184000 |
| B | 0.000000000 | 1.917569000 | -1.618078000 |
| B | 0.000000000 | -1.917569000 | -1.618078000 |
| B | 0.000000000 | 1.478605000 | 0.000000000 |
| B | 0.000000000 | -1.478605000 | 0.000000000 |
| H | 0.000000000 | 3.090771000 | -1.858732000 |
| H | 0.000000000 | 1.357882000 | -4.069424000 |
| H | 0.000000000 | -1.357882000 | -4.069424000 |
| H | 0.000000000 | -3.090771000 | -1.858732000 |
| H | 0.000000000 | -3.090771000 | 1.858732000 |

| | | | |
|---|------------|-------------|------------|
| H | 0.00000000 | -1.35788200 | 4.06942400 |
| H | 0.00000000 | 1.35788200 | 4.06942400 |
| H | 0.00000000 | 3.09077100 | 1.85873200 |

Planar Fe₂B₁₀H₈ (quintet)

Total thermal enthalpies: -2781.099381 a. u.

(One imaginary frequency)

| | | | |
|----|------------|-------------|-------------|
| Fe | 0.00000000 | 0.00000000 | 1.24738200 |
| B | 0.00000000 | 0.90937400 | 2.98894700 |
| B | 0.00000000 | -0.90937400 | 2.98894700 |
| B | 0.00000000 | -1.93369900 | 1.63633400 |
| B | 0.00000000 | 1.93369900 | 1.63633400 |
| Fe | 0.00000000 | 0.00000000 | -1.24738200 |
| B | 0.00000000 | -0.90937400 | -2.98894700 |
| B | 0.00000000 | 0.90937400 | -2.98894700 |
| B | 0.00000000 | 1.93369900 | -1.63633400 |
| B | 0.00000000 | -1.93369900 | -1.63633400 |
| B | 0.00000000 | 1.54628900 | 0.00000000 |
| B | 0.00000000 | -1.54628900 | 0.00000000 |
| H | 0.00000000 | 3.11141000 | -1.86232300 |
| H | 0.00000000 | 1.29337400 | -4.12333300 |
| H | 0.00000000 | -1.29337400 | -4.12333300 |
| H | 0.00000000 | -3.11141000 | -1.86232300 |
| H | 0.00000000 | -3.11141000 | 1.86232300 |
| H | 0.00000000 | -1.29337400 | 4.12333300 |
| H | 0.00000000 | 1.29337400 | 4.12333300 |
| H | 0.00000000 | 3.11141000 | 1.86232300 |

Planar Fe₂B₁₀H₈ (septet)

Total thermal enthalpies: -2781.048865 a. u.

(Three imaginary frequencies)

| | | | |
|----|------------|-------------|-------------|
| Fe | 0.00000000 | 0.00000000 | 1.27631100 |
| B | 0.00000000 | 0.90332400 | 2.99981000 |
| B | 0.00000000 | -0.90332400 | 2.99981000 |
| B | 0.00000000 | -1.92708300 | 1.63874400 |
| B | 0.00000000 | 1.92708300 | 1.63874400 |
| Fe | 0.00000000 | 0.00000000 | -1.27631100 |
| B | 0.00000000 | -0.90332400 | -2.99981000 |
| B | 0.00000000 | 0.90332400 | -2.99981000 |
| B | 0.00000000 | 1.92708300 | -1.63874400 |
| B | 0.00000000 | -1.92708300 | -1.63874400 |
| B | 0.00000000 | 1.61000600 | 0.00000000 |
| B | 0.00000000 | -1.61000600 | 0.00000000 |
| H | 0.00000000 | 3.12484200 | -1.74930700 |
| H | 0.00000000 | 1.34122200 | -4.11603300 |
| H | 0.00000000 | -1.34122200 | -4.11603300 |
| H | 0.00000000 | -3.12484200 | -1.74930700 |
| H | 0.00000000 | -3.12484200 | 1.74930700 |
| H | 0.00000000 | -1.34122200 | 4.11603300 |
| H | 0.00000000 | 1.34122200 | 4.11603300 |
| H | 0.00000000 | 3.12484200 | 1.74930700 |

Planar Fe₂B₁₀H₈ (-) (doublet)

Total thermal enthalpies: -2781.235876 a. u.

| | | | |
|----|------------|-------------|-------------|
| Fe | 0.00000000 | 0.00000000 | 1.27237800 |
| B | 0.00000000 | 0.87153200 | 2.97856300 |
| B | 0.00000000 | -0.87153200 | 2.97856300 |
| B | 0.00000000 | -1.91196400 | 1.61851500 |
| B | 0.00000000 | 1.91196400 | 1.61851500 |
| Fe | 0.00000000 | 0.00000000 | -1.27237800 |
| B | 0.00000000 | -0.87153200 | -2.97856300 |
| B | 0.00000000 | 0.87153200 | -2.97856300 |
| B | 0.00000000 | 1.91196400 | -1.61851500 |
| B | 0.00000000 | -1.91196400 | -1.61851500 |
| B | 0.00000000 | 1.45462200 | 0.00000000 |
| B | 0.00000000 | -1.45462200 | 0.00000000 |
| H | 0.00000000 | 3.09037500 | -1.85482700 |
| H | 0.00000000 | 1.36977000 | -4.07473500 |
| H | 0.00000000 | -1.36977000 | -4.07473500 |
| H | 0.00000000 | -3.09037500 | -1.85482700 |
| H | 0.00000000 | -3.09037500 | 1.85482700 |
| H | 0.00000000 | -1.36977000 | 4.07473500 |
| H | 0.00000000 | 1.36977000 | 4.07473500 |
| H | 0.00000000 | 3.09037500 | 1.85482700 |

Planar Fe₂B₁₀H₈ (-) (quartet)

Total thermal enthalpies: -2781.221930 a. u.

| | | | |
|----|------------|-------------|-------------|
| Fe | 0.00000000 | 0.00000000 | 1.23207600 |
| B | 0.00000000 | 0.89726600 | 2.97936700 |
| B | 0.00000000 | -0.89726600 | 2.97936700 |
| B | 0.00000000 | -1.92440500 | 1.63900600 |
| B | 0.00000000 | 1.92440500 | 1.63900600 |
| Fe | 0.00000000 | 0.00000000 | -1.23207600 |
| B | 0.00000000 | -0.89726600 | -2.97936700 |
| B | 0.00000000 | 0.89726600 | -2.97936700 |
| B | 0.00000000 | 1.92440500 | -1.63900600 |
| B | 0.00000000 | -1.92440500 | -1.63900600 |
| B | 0.00000000 | 1.51804900 | 0.00000000 |
| B | 0.00000000 | -1.51804900 | 0.00000000 |
| H | 0.00000000 | 3.11495300 | -1.81471600 |
| H | 0.00000000 | 1.30142300 | -4.11543300 |
| H | 0.00000000 | -1.30142300 | -4.11543300 |
| H | 0.00000000 | -3.11495300 | -1.81471600 |
| H | 0.00000000 | -3.11495300 | 1.81471600 |
| H | 0.00000000 | -1.30142300 | 4.11543300 |
| H | 0.00000000 | 1.30142300 | 4.11543300 |
| H | 0.00000000 | 3.11495300 | 1.81471600 |

Planar Fe₂B₁₀H₈ (-) (sextet)

Total thermal enthalpies: -2781.193783 a. u.

(Two imaginary frequencies)

| | | | |
|----|------------|-------------|------------|
| Fe | 0.00000000 | 0.00000000 | 1.23593300 |
| B | 0.00000000 | 0.91782800 | 2.97121900 |
| B | 0.00000000 | -0.91782800 | 2.97121900 |
| B | 0.00000000 | -1.95420500 | 1.62807800 |

| | | | |
|----|------------|-------------|-------------|
| B | 0.00000000 | 1.95420500 | 1.62807800 |
| Fe | 0.00000000 | 0.00000000 | -1.23593300 |
| B | 0.00000000 | -0.91782800 | -2.97121900 |
| B | 0.00000000 | 0.91782800 | -2.97121900 |
| B | 0.00000000 | 1.95420500 | -1.62807800 |
| B | 0.00000000 | -1.95420500 | -1.62807800 |
| B | 0.00000000 | 1.59831300 | 0.00000000 |
| B | 0.00000000 | -1.59831300 | 0.00000000 |
| H | 0.00000000 | 3.13400900 | -1.86318700 |
| H | 0.00000000 | 1.30234600 | -4.11230300 |
| H | 0.00000000 | -1.30234600 | -4.11230300 |
| H | 0.00000000 | -3.13400900 | -1.86318700 |
| H | 0.00000000 | -3.13400900 | 1.86318700 |
| H | 0.00000000 | -1.30234600 | 4.11230300 |
| H | 0.00000000 | 1.30234600 | 4.11230300 |
| H | 0.00000000 | 3.13400900 | 1.86318700 |

Icosahedral Fe₂B₁₀H₁₀ (triplet)

Total thermal enthalpies: -2782.390227 a. u.

| | | | |
|----|-------------|-------------|-------------|
| B | 0.75344100 | 0.33041800 | 1.50341900 |
| B | -0.75343000 | -1.53196100 | -0.15036000 |
| B | 0.75348800 | 0.61641500 | -1.41053800 |
| B | -0.75360300 | 1.15109900 | 1.02206000 |
| B | -0.75344100 | -0.33041800 | -1.50341900 |
| B | -0.75352700 | 1.32772600 | -0.77884800 |
| H | -1.37675000 | -1.03147600 | 2.36016800 |
| H | 1.37681700 | -1.92605000 | -1.71023300 |
| H | 1.37668500 | 2.56339100 | 0.25156900 |
| B | 0.75360300 | -1.15109900 | -1.02206000 |
| B | 0.75352700 | -1.32772600 | 0.77884800 |
| B | -0.75348800 | -0.61641500 | 1.41053800 |
| B | 0.75343000 | 1.53196100 | 0.15036000 |
| H | -1.37668500 | -2.56339100 | -0.25157000 |
| H | 1.37675000 | 1.03147600 | -2.36016800 |
| H | -1.37670900 | 2.22167600 | -1.30329600 |
| H | -1.37681600 | 1.92605000 | 1.71023300 |
| H | 1.37662300 | 0.55292600 | 2.51568500 |
| H | 1.37671000 | -2.22167600 | 1.30329600 |
| H | -1.37662300 | -0.55292600 | -2.51568500 |
| Fe | -2.05073500 | -0.00003300 | -0.00001900 |
| Fe | 2.05073500 | 0.00003300 | 0.00001900 |

Icosahedral Fe₂B₁₀H₁₀ (quintet)

Total thermal enthalpies: -2782.369493 a. u.

| | | | |
|---|-------------|-------------|-------------|
| B | 0.74577600 | 0.31091500 | -1.45431900 |
| B | -0.74708700 | 1.40847500 | 0.74356700 |
| B | 0.74994600 | -1.17974600 | 1.02438500 |
| B | -0.74812100 | -0.66878600 | -1.35298100 |
| B | -0.74577600 | -0.31091500 | 1.45431900 |
| B | -0.73993400 | -1.61320100 | 0.18081100 |
| H | -1.33618900 | 1.86653300 | -1.82498300 |
| H | 1.38924400 | 1.00916000 | 2.32121900 |
| H | 1.30907800 | -2.28430300 | -1.35192100 |

| | | | |
|----|--------------|--------------|--------------|
| B | 0.748121000 | 0.668786000 | 1.352980000 |
| B | 0.739933000 | 1.613201000 | -0.180811000 |
| B | -0.749946000 | 1.179747000 | -1.024386000 |
| B | 0.747087000 | -1.408474000 | -0.743567000 |
| H | -1.309081000 | 2.284303000 | 1.351921000 |
| H | 1.336186000 | -1.866533000 | 1.824982000 |
| H | -1.279727000 | -2.678712000 | 0.334607000 |
| H | -1.389247000 | -1.009159000 | -2.321219000 |
| H | 1.415218000 | 0.459267000 | -2.453611000 |
| H | 1.279725000 | 2.678712000 | -0.334607000 |
| H | -1.415221000 | -0.459267000 | 2.453610000 |
| Fe | -2.081859000 | -0.001110000 | 0.000472000 |
| Fe | 2.081859000 | 0.001110000 | -0.000472000 |

Icosahedral Fe₂B₁₀H₁₀ (septet)

Total thermal enthalpies: -2782.364947 a. u.

(Five imaginary frequencies)

| | | | |
|----|--------------|--------------|--------------|
| B | 0.737783000 | 1.551168000 | 0.175849000 |
| B | -0.737890000 | -0.646555000 | 1.420721000 |
| B | 0.738016000 | -1.151649000 | -1.053900000 |
| B | -0.737897000 | 1.358214000 | -0.769573000 |
| B | -0.737776000 | -1.551173000 | -0.175850000 |
| B | -0.737787000 | -0.312103000 | -1.529592000 |
| H | -1.307443000 | 1.936958000 | 1.772797000 |
| H | 1.307264000 | -2.284580000 | 1.294378000 |
| H | 1.307445000 | 1.087532000 | -2.389711000 |
| B | 0.737899000 | -1.358211000 | 0.769576000 |
| B | 0.737782000 | 0.312101000 | 1.529596000 |
| B | -0.738013000 | 1.151652000 | 1.053900000 |
| B | 0.737885000 | 0.646555000 | -1.420726000 |
| H | -1.307461000 | -1.087529000 | 2.389702000 |
| H | 1.307452000 | -1.936952000 | -1.772795000 |
| H | -1.307162000 | -0.524909000 | -2.572783000 |
| H | -1.307258000 | 2.284585000 | -1.294378000 |
| H | 1.307268000 | 2.609033000 | 0.295649000 |
| H | 1.307149000 | 0.524909000 | 2.572791000 |
| H | -1.307248000 | -2.609047000 | -0.295650000 |
| Fe | -2.130382000 | -0.000040000 | -0.000013000 |
| Fe | 2.130382000 | 0.000040000 | 0.000013000 |

Icosahedral Fe₂B₁₀H₈ (triplet)

Total thermal enthalpies: -2781.155510 a. u.

| | | | |
|---|--------------|--------------|--------------|
| B | 0.696299000 | -0.000297000 | 1.357288000 |
| B | -0.751087000 | -1.528411000 | -0.471709000 |
| B | 0.752367000 | 0.908382000 | -1.261644000 |
| B | -0.752387000 | 0.907819000 | 1.261928000 |
| B | -0.696299000 | 0.000297000 | -1.357288000 |
| B | -0.751207000 | 1.528665000 | -0.471189000 |
| H | -1.346427000 | -1.532180000 | 2.104132000 |
| H | 1.346517000 | -1.531230000 | -2.104661000 |
| H | 1.344050000 | 2.545507000 | 0.740864000 |
| B | 0.752387000 | -0.907819000 | -1.261928000 |

| | | | |
|----|--------------|--------------|--------------|
| B | 0.751206000 | -1.528665000 | 0.471189000 |
| B | -0.752366000 | -0.908382000 | 1.261644000 |
| B | 0.751087000 | 1.528411000 | 0.471709000 |
| H | -1.344051000 | -2.545507000 | -0.740864000 |
| H | 1.346427000 | 1.532180000 | -2.104132000 |
| H | -1.344051000 | 2.545927000 | -0.739927000 |
| H | -1.346517000 | 1.531230000 | 2.104661000 |
| H | 1.344052000 | -2.545927000 | 0.739926000 |
| Fe | -2.048954000 | -0.000006000 | -0.092045000 |
| Fe | 2.048954000 | 0.000006000 | 0.092045000 |

Icosahedral Fe₂B₁₀H₈ (quintet)

Total thermal enthalpies: -2781.152501 a. u.

(Two imaginary frequencies)

| | | | |
|----|--------------|--------------|--------------|
| B | 0.685326000 | -0.000120000 | 1.303652000 |
| B | -0.728088000 | -1.572847000 | -0.491137000 |
| B | 0.776722000 | 0.927468000 | -1.221952000 |
| B | -0.776748000 | 0.927204000 | 1.222067000 |
| B | -0.685328000 | 0.000119000 | -1.303652000 |
| B | -0.728116000 | 1.572927000 | -0.490941000 |
| H | -1.328114000 | -1.463810000 | 2.149850000 |
| H | 1.328233000 | -1.463472000 | -2.149959000 |
| H | 1.250752000 | 2.593151000 | 0.859213000 |
| B | 0.776747000 | -0.927204000 | -1.222069000 |
| B | 0.728120000 | -1.572926000 | 0.490939000 |
| B | -0.776722000 | -0.927471000 | 1.221950000 |
| B | 0.728093000 | 1.572844000 | 0.491136000 |
| H | -1.250742000 | -2.593155000 | -0.859219000 |
| H | 1.328121000 | 1.463805000 | -2.149850000 |
| H | -1.251006000 | 2.593192000 | -0.858802000 |
| H | -1.328229000 | 1.463473000 | 2.149959000 |
| H | 1.251020000 | -2.593187000 | 0.858795000 |
| Fe | -2.100189000 | -0.000008000 | -0.091771000 |
| Fe | 2.100186000 | 0.000009000 | 0.091774000 |

Icosahedral Fe₂B₁₀H₈ (septet)

Total thermal enthalpies: -2781.127730 a. u.

| | | | |
|---|--------------|--------------|--------------|
| B | 0.655989000 | 0.000066000 | 1.275452000 |
| B | -0.735503000 | -1.592080000 | -0.487295000 |
| B | 0.775075000 | 0.970381000 | -1.205195000 |
| B | -0.775117000 | 0.970418000 | 1.205161000 |
| B | -0.655989000 | -0.000066000 | -1.275452000 |
| B | -0.735562000 | 1.592031000 | -0.487343000 |
| H | -1.310669000 | -1.474876000 | 2.158016000 |
| H | 1.310727000 | -1.474886000 | -2.157988000 |
| H | 1.282621000 | 2.588638000 | 0.878685000 |
| B | 0.775117000 | -0.970418000 | -1.205161000 |
| B | 0.735562000 | -1.592031000 | 0.487343000 |
| B | -0.775075000 | -0.970381000 | 1.205195000 |
| B | 0.735504000 | 1.592080000 | 0.487295000 |
| H | -1.282621000 | -2.588638000 | -0.878685000 |
| H | 1.310669000 | 1.474876000 | -2.158016000 |
| H | -1.282664000 | 2.588574000 | -0.878792000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -1.310727000 | 1.474886000 | 2.157988000 |
| H | 1.282664000 | -2.588574000 | 0.878792000 |
| Fe | -2.151493000 | -0.000010000 | -0.088959000 |
| Fe | 2.151493000 | 0.000010000 | 0.088959000 |

Icosahedral Fe₂B₁₀H₈ (-) (doublet)

Total thermal enthalpies: -2781.230009 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | -0.741027000 | 0.000144000 | 1.399012000 |
| B | 0.758628000 | 1.514789000 | -0.464133000 |
| B | -0.736330000 | -0.894596000 | -1.276162000 |
| B | 0.736330000 | -0.894595000 | 1.276162000 |
| B | 0.741028000 | 0.000144000 | -1.399012000 |
| B | 0.758565000 | -1.514610000 | -0.463915000 |
| H | 1.303217000 | 1.553106000 | 2.123245000 |
| H | -1.303217000 | 1.553106000 | -2.123246000 |
| H | -1.335559000 | -2.557280000 | 0.709369000 |
| B | -0.736573000 | 0.894491000 | -1.275850000 |
| B | -0.758628000 | 1.514789000 | 0.464132000 |
| B | 0.736573000 | 0.894491000 | 1.275850000 |
| B | -0.758565000 | -1.514609000 | 0.463915000 |
| H | 1.334162000 | 2.558208000 | -0.709635000 |
| H | -1.302540000 | -1.553347000 | -2.123703000 |
| H | 1.335559000 | -2.557281000 | -0.709368000 |
| H | 1.302540000 | -1.553346000 | 2.123703000 |
| H | -1.334163000 | 2.558208000 | 0.709634000 |
| Fe | 2.037008000 | -0.000069000 | -0.081807000 |
| Fe | -2.037008000 | -0.000069000 | 0.081807000 |

Icosahedral Fe₂B₁₀H₈ (-) (quartet)

Total thermal enthalpies: -2781.232213 a. u.

| | | | |
|----|--------------|--------------|--------------|
| B | -0.689955000 | 0.000046000 | 1.354446000 |
| B | 0.732875000 | 1.607244000 | -0.464972000 |
| B | -0.747309000 | -0.917119000 | -1.242247000 |
| B | 0.747422000 | -0.955778000 | 1.234943000 |
| B | 0.726414000 | 0.000573000 | -1.323448000 |
| B | 0.733297000 | -1.607017000 | -0.464448000 |
| H | 1.266678000 | 1.511864000 | 2.178017000 |
| H | -1.324613000 | 1.493279000 | -2.141260000 |
| H | -1.409662000 | -2.525641000 | 0.777034000 |
| B | -0.748073000 | 0.917359000 | -1.241252000 |
| B | -0.772729000 | 1.536675000 | 0.460941000 |
| B | 0.747692000 | 0.954968000 | 1.234540000 |
| B | -0.772587000 | -1.536116000 | 0.460062000 |
| H | 1.156213000 | 2.690029000 | -0.807072000 |
| H | -1.322357000 | -1.493373000 | -2.142905000 |
| H | 1.157353000 | -2.689232000 | -0.807575000 |
| H | 1.264172000 | -1.512830000 | 2.179487000 |
| H | -1.407253000 | 2.527471000 | 0.778599000 |
| Fe | 2.077501000 | -0.000023000 | -0.086877000 |
| Fe | -2.045415000 | -0.000199000 | 0.084678000 |

Icosahedral Fe₂B₁₀H₈ (-) (sextet)

Total thermal enthalpies: -2781.228951 a. u.

(One negative frequency)

| | | | |
|----|--------------|--------------|--------------|
| B | -0.683386000 | -0.002192000 | 1.288708000 |
| B | 0.744317000 | 1.607742000 | -0.484649000 |
| B | -0.776097000 | -0.970806000 | -1.195991000 |
| B | 0.775576000 | -0.970261000 | 1.196170000 |
| B | 0.683369000 | -0.002346000 | -1.288742000 |
| B | 0.741234000 | -1.612294000 | -0.483722000 |
| H | 1.314280000 | 1.468826000 | 2.159929000 |
| H | -1.314748000 | 1.468434000 | -2.159472000 |
| H | -1.226123000 | -2.647264000 | 0.882942000 |
| B | -0.775746000 | 0.964802000 | -1.197058000 |
| B | -0.743440000 | 1.607758000 | 0.484443000 |
| B | 0.776241000 | 0.965369000 | 1.196887000 |
| B | -0.742091000 | -1.612287000 | 0.483930000 |
| H | 1.221218000 | 2.645885000 | -0.884297000 |
| H | -1.314225000 | -1.474330000 | -2.158859000 |
| H | 1.226563000 | -2.647025000 | -0.881805000 |
| H | 1.314597000 | -1.473962000 | 2.158445000 |
| H | -1.221643000 | 2.645672000 | 0.883144000 |
| Fe | 2.090946000 | 0.002432000 | -0.088273000 |
| Fe | -2.090939000 | 0.002812000 | 0.088277000 |