Supplementary Information:

Discovery and Engineering of Low Work Function

Perovskite Materials

1. Work function convergence with respect to number of surface layers relaxed

In this work, we performed a convergence test of work function with respect to number of surface layers relaxed on SrNbO$_3$. A 15-layer surface slab that is (001) SrO terminated (148 atoms per supercell) was simulated at the GGA level without spin polarization, we relaxed from 1 to 5 layers on each side of the slab symmetrically and measured its work function, as shown in Table 1, relaxing 3 layers is sufficient to reach work function convergence. This result is in agreement with the octahedral tilting which occurs in the unit of 3 layers.

| Number of surface layers relaxed | 1   | 2   | 3   | 4   | 5   |
|---------------------------------|-----|-----|-----|-----|-----|
| Work function (eV)              | 1.46| 1.49| 1.17| 1.21| 1.19|

In this series of work function calculations, we performed non-spin polarized (NSP) simulations because we found that different magnetic states don’t have obvious influence on work function. As shown in Table 2, switching on spin polarization doesn’t make a major difference on work functions of different terminations of SrNbO$_3$.

2. Work function convergence with respect to $k$-point mesh
The convergence of work function with respect to $k$-point mesh was tested on SrTiO$_3$.

We simulated a 9-layer (001) SrO terminated surface slab (88 atoms) with $2 \times 2 \times 1$, $3 \times 3 \times 1$, and $4 \times 4 \times 1$ Monkhorst-Pack $k$-point mesh, respectively. For the simulations with $3 \times 3 \times 1$ and $4 \times 4 \times 1$ $k$-point mesh, we only performed a static run because only in this way is the task computationally feasible. The results are shown in Table 3, from which we can see that a $2 \times 2 \times 1$ $k$-point mesh is dense enough to reach work function convergence.

**Table 2. Work functions of SrNbO$_3$ with spin polarization on and off**

| Termination | NSP simulation | Spin polarized simulation |
|-------------|----------------|---------------------------|
| (001) SrO   | 1.15           | 1.23                      | 4.00 |
| (011) SrNbO | 3.55           | 3.26                      | 10.00 |
| (111) Nb    | 3.87           | 3.74                      | 20.00 |

**Table 3. Work functions of SrTiO$_3$ with different $k$-point meshes**

| $k$-point mesh | 2 $\times$ 2 $\times$ 1 | 3 $\times$ 3 $\times$ 1 | 4 $\times$ 4 $\times$ 1 |
|----------------|--------------------------|--------------------------|--------------------------|
| Work function (eV) | 4.32                     | 4.22                     | 4.26                     |

3. **Influence of the amount of exact exchange**

We tested different amounts of exact exchange (0.125 and 0.25) to see if work function would be influenced by this parameter. The sum of the fraction of the exact exchange and LDA exchange is always 1. Therefore, if 0.125 exact exchange is used, then 0.875 LDA exchange is added; and if 0.25 exact exchange is used, then 0.75 LDA exchange is added. We also fixed the range separation parameter to be 0.2, so 0.25 exact exchange gave standard HSE06 functional.
We picked 2 systems with high and low work function, respectively. The results shown below in Table 4 indicate that work function is insensitive to amount of exact exchange.

Table 4. Work functions of Ba$_{0.5}$La$_{0.25}$Rb$_{0.25}$NbO$_3$ and PrHfO$_3$ with different amounts of exact exchange

| Material       | Work function (eV, exact exchange 0.125) | Work function (eV, exact exchange 0.25) |
|----------------|------------------------------------------|----------------------------------------|
| Ba$_{0.5}$La$_{0.25}$Rb$_{0.25}$NbO$_3$ | 0.99 eV                                  | 0.96 eV                                |
| PrHfO$_3$      | 3.02 eV                                  | 3.06 eV                                |

4. Energies above convex hull and O 2p-band centers of different cation orderings

In our screening at the GGA+$U$ level, we have considered doped systems with up to 50% dopant concentration. In this situation, dopant cations have various possible orderings, so here we also tested 2 different cation orderings in 3 different systems to see the influence on energy above convex hull and O 2p-band center. The 2 orderings we considered are shown in Figure 1, in ordering A (left), dopant cations are separated as far from each other as possible; while in ordering B (right), dopants are segregated in (011) plane. The results are shown in Table 5, different systems prefer different orderings, but either way the O 2p-band center seems almost unchanged.
Figure 1. Different cation orderings

Table 5. Energies above convex hull and O 2p-band centers of different cation orderings

| Material       | Ordering A |                | Ordering B |                |
|----------------|------------|----------------|------------|----------------|
|                | Energy above convex hull (meV/atom) | O 2p-band (eV) | Energy above convex hull (meV/atom) | O 2p-band (eV) |
| Sr$_{0.5}$Ca$_{0.5}$NbO$_3$ | 193.3       | -4.59          | 193.6      | -4.60          |
| Ba$_{0.5}$Ca$_{0.5}$NbO$_3$  | 212.5       | -4.48          | 189.2      | -4.48          |
| Ba$_{0.5}$Ca$_{0.5}$VO$_3$   | 131.8       | -2.53          | 124.5      | -2.33          |

5. Verification of the linear correlation between work function and O 2p-band center

We have selected three A$_x$A'$_{1-x}$BO$_3$ and three AB$_x$B'$_{1-x}$O$_3$ to verify the linear correlation for doped perovskites, their O 2p-band centers and work functions are listed below in Table 6, and are also plotted in Figure 2 with other undoped perovskites. The RMSE after adding these new data points is 0.30 eV, almost the same as the previous 0.29 eV RMSE, indicating the linear correlation is valid for doped perovskites.
Table 6. O 2p-band centers and work functions of select doped perovskites

| Doped perovskite        | O 2p-band center (eV) | Work function (eV) |
|-------------------------|-----------------------|--------------------|
| SrV_{0.75}Fe_{0.25}O_3  | -3.009                | 2.1565             |
| SrZr_{0.125}Nb_{0.875}O_3 | -3.52                | 1.557              |
| BaTi_{0.125}Nb_{0.875}O_3 | -4.407               | 1.8515             |
| Ba_{0.25}Sr_{0.75}VO_3  | -3.719                | 1.725              |
| Sr_{0.875}La_{0.125}VO_3 | -4.074                | 1.6665             |
| Ba_{0.75}Ca_{0.25}NbO_3 | -4.316                | 1.181              |

Figure 2. Linear correlation between work function and O 2p-band center

6. All perovskites used in the screening
All perovskites used in our screening are listed in Table 7. Perovskites that passed our criterion 1 are colored in blue; those passed criterion 2 are colored in green; and the 25 perovskites that entered our HSE band gap check are colored in yellow. The structures of doped perovskites at different concentrations are shown in Figure 3.

Figure 3. Schematic structures of $\text{A}_x\text{A}'_{1-x}\text{B}_y\text{B}'_{1-y}\text{O}_3$. (a)$\text{A}_0.875\text{A}'_{0.125}\text{BO}_3$ (b)$\text{A}_0.75\text{A}'_{0.25}\text{BO}_3$
(c)$\text{A}_0.5\text{A}'_{0.5}\text{BO}_3$ (d)$\text{AB}_0.875\text{B}'_{0.125}\text{O}_3$ (e)$\text{AB}_0.75\text{B}'_{0.25}\text{O}_3$ (f)$\text{AB}_0.5\text{B}'_{0.5}\text{O}_3$ (g)$\text{A}_0.875\text{A}'_{0.125}\text{B}_0.875\text{B}'_{0.125}\text{O}_3$
(h)$\text{A}_0.75\text{A}'_{0.25}\text{B}_0.75\text{B}'_{0.25}\text{O}_3$ (i)$\text{A}_0.5\text{A}'_{0.5}\text{B}_0.5\text{B}'_{0.5}\text{O}_3$. 
Table 7. O 2p-band centers and work functions of select doped perovskites

| Composition      | O 2p-band (eV) | Stability (meV/atom) (GGA+U) | Predicted WF (eV) |
|------------------|----------------|-------------------------------|-------------------|
| La 6 Y 2 Mo 8    | -5.044         | 25.02635408                  | 1.2932916         |
| Ca 2 La 6 Mo 8   | -4.86          | 0                             | 1.388254          |
| La 8 Mn 1 Ga 7   | -4.821         | 40.6185397                    | 1.4083819         |
| La 4 Y 4 Mo 8    | -4.796         | 0                             | 1.4212844         |
| La 6 Gd 2 V 8    | -4.786         | 0                             | 1.4264454         |
| Sr 4 La 4 Mo 8   | -4.777         | 0                             | 1.4310903         |
| Gd 4 Y 4 Mo 8    | -4.732         | 24.17506577                   | 1.4543148         |
| Ca 4 La 4 Mo 8   | -4.703         | 0                             | 1.4692817         |
| La 4 Gd 4 V 8    | -4.699         | 0                             | 1.4713461         |
| La 8 Ti 4 Fe 4   | -4.637         | 30.65781325                   | 1.5033443         |
| La 8 Mg 1 V 7    | -4.622         | 0                             | 1.5110858         |
| Pr 4 Gd 4 V 8    | -4.606         | 0                             | 1.5193434         |
| Pr 4 Gd 4 Mo 8   | -4.601         | 0                             | 1.5219239         |
| La 8 V 4 Fe 4    | -4.522         | 37.66276252                   | 1.5626958         |
| Pr 6 Gd 2 V 8    | -4.495         | 0                             | 1.5766305         |
| Y 8 Mo 8         | -4.495         | 0                             | 1.5766305         |
| Ca 8 Mo 8        | -4.49          | 0                             | 1.579211          |
| Ba 2 Ca 6 Mo 8   | -4.464         | 14.04827888                   | 1.5926296         |
| Gd 2 Y 6 Mo 8    | -4.461         | 0                             | 1.5941779         |
| Sr 8 Mo 8        | -4.46          | 0                             | 1.594694          |
| Gd 8 V 8         | -4.452         | 25.378115                     | 1.5988228         |
| Gd 4 Y 4 V 8     | -4.45          | 0                             | 1.599855          |
| La 8 Mg 2 V 6    | -4.425         | 0                             | 1.6127575         |
| Ba 8 Zr 3 Ta 4 Fe 1 | -4.414     | 41.29268713                   | 1.6184346         |
| La 8 Cr 8        | -4.382         | 0                             | 1.6349498         |
| Pr 4 Y 4 Mo 8    | -4.362         | 0                             | 1.6452718         |
| Gd 2 Y 6 V 8     | -4.346         | 0                             | 1.6535294         |
| La 6 Ho 2 Cr 8   | -4.344         | 0                             | 1.6545616         |
| Ca 4 La 4 V 8    | -4.342         | 31.83859903                   | 1.6555938         |
| Pr 6 Y 2 Mo 8    | -4.314         | 0                             | 1.6700446         |
| Ca 4 Y 4 Mo 8    | -4.309         | 0                             | 1.6726251         |
| Ba 4 Sr 4 Mo 8   | -4.306         | 19.72736169                   | 1.6741734         |
| Sr 4 Gd 4 Mo 8   | -4.285         | 0                             | 1.6850115         |
| Sr 8 V 4 Mo 4    | -4.281         | 8.712906633                   | 1.6870759         |
| Compound                  | Energy  | Volume  | Density  |
|---------------------------|---------|---------|----------|
| Ba2Pr₆Mo₈                 | -4.264  | 6.116287031 | 1.6958496  |
| Y₄Ho₄V₈                  | -4.251  | 0       | 1.7025589  |
| Dy₄Y₄V₈                  | -4.235  | 0       | 1.7108165  |
| Dy₂Y₆V₈                  | -4.213  | 0       | 1.7221707  |
| Y₈V₈                     | -4.211  | 0       | 1.7232029  |
| Y₆Ho₂V₈                  | -4.205  | 0       | 1.7262995  |
| Sm₂Y₆V₈                  | -4.205  | 0       | 1.7262995  |
| Sr₂Pr₆Mo₈                | -4.204  | 0       | 1.7268156  |
| La₈Ti₄Mn₄                | -4.201  | 37.34883385 | 1.7283639  |
| Pr₈Mg₁V₇                 | -4.198  | 0       | 1.7299122  |
| Nd₂Y₆V₈                  | -4.197  | 0       | 1.7304283  |
| Ca₂Pr₆Mo₈                | -4.195  | 0       | 1.7314605  |
| Sm₄Y₄V₈                  | -4.192  | 0       | 1.7330088  |
| Ca₄Pr₄Mo₈                | -4.191  | 0       | 1.7335249  |
| Ca₂Gd₆V₈                 | -4.187  | 19.97046038 | 1.7355893  |
| Nd₄Y₄V₈                  | -4.183  | 0       | 1.7376537  |
| Sr₈V₄Re₄                 | -4.16   | 39.09860284 | 1.749524   |
| Y₈V₇Cr₁                  | -4.158  | 0       | 1.7505562  |
| Sr₄Y₄Mo₈                 | -4.147  | 0       | 1.7562333  |
| Y₈V₆Cr₂                  | -4.145  | 0       | 1.7572655  |
| Sr₄Pr₄Mo₈                | -4.136  | 0       | 1.7619104  |
| Y₈Mn₁V₇                  | -4.111  | 37.7214358 | 1.7748129  |
| Sr₈Nb₄Mo₄                | -4.11   | 0       | 1.775329   |
| Y₈V₇Fe₁                  | -4.102  | 0       | 1.7794578  |
| Ba₈Mo₈                   | -4.097  | 24.19231953 | 1.7820383  |
| La₆Gd₂Cr₈                | -4.075  | 0       | 1.7933925  |
| Y₈V₇Co₁                  | -4.071  | 5.087273213 | 1.7954569  |
| La₈Mn₂Ga₆                | -4.069  | 22.11044333 | 1.7964891  |
| La₈Mg₄V₄                 | -4.066  | 0       | 1.7980374  |
| Ca₂Y₆V₈                  | -4.056  | 0       | 1.8031984  |
| Y₈V₆Fe₂                  | -4.044  | 32.01964731 | 1.8093916  |
| Y₈V₇Ni₁                  | -4.042  | 1.923515963 | 1.8104238  |
| Ba₂Y₆Mo₈                 | -4.042  | 31.43074333 | 1.8104238  |
| Pr₄Y₄V₈                  | -4.042  | 38.97594952 | 1.8104238  |
| Y₈V₄Cr₄                  | -4.036  | 0       | 1.8135204  |
| Ba₄Pr₄Mo₈                | -4.036  | 30.80396453 | 1.8135204  |
| Sr₈Nb₆Co₂                | -4.028  | 37.35201131 | 1.8176492  |
| La₆Gd₂Mn₈                | -4.02   | 0       | 1.821778   |
| Y₈Mn₂V₆                  | -4.015  | 35.85996811 | 1.8243585  |
| Compound          | Energy | Charge | Temperature | Volume  |
|-------------------|--------|--------|-------------|---------|
| Ba\(_8\)\(\text{Nb}_4\)\(\text{Mo}_4\) | -4.012 | 0      | 1.8259068   |         |
| Y\(_8\)\(\text{Ti}_4\)\(\text{Fe}_4\) | -4.008 | 15.3163645 | 1.8279712 |         |
| Sr\(_8\)\(\text{V}_6\)\(\text{Re}_2\) | -4.008 | 40.23740232 | 1.8279712 |         |
| La\(_8\)\(\text{Mn}_4\)\(\text{Fe}_4\) | -4.007 | 0      | 1.8284873   |         |
| La\(_4\)\(\text{Gd}_4\)\(\text{Mn}_8\) | -4.006 | 0      | 1.8290034   |         |
| Y\(_8\)\(\text{Mg}_1\)\(\text{V}_7\) | -3.998 | 0      | 1.8331322   |         |
| Sr\(_2\)\(\text{Y}_6\)\(\text{V}_8\) | -3.989 | 0      | 1.8377771   |         |
| La\(_4\)\(\text{Nd}_4\)\(\text{Cr}_8\) | -3.988 | 0      | 1.8382932   |         |
| La\(_8\)\(\text{Ga}_4\)\(\text{Fe}_4\) | -3.977 | 0      | 1.8439703   |         |
| Y\(_8\)\(\text{V}_6\)\(\text{Co}_2\) | -3.977 | 15.66639293 | 1.8439703 |         |
| La\(_4\)\(\text{Sm}_4\)\(\text{Cr}_8\) | -3.965 | 0      | 1.8501635   |         |
| La\(_4\)\(\text{Ho}_4\)\(\text{Cr}_8\) | -3.958 | 0      | 1.8537762   |         |
| Y\(_8\)\(\text{Ti}_4\)\(\text{Mn}_4\) | -3.934 | 25.1156351 | 1.8661626   |         |
| La\(_8\)\(\text{Mg}_1\)\(\text{Mn}_7\) | -3.928 | 0      | 1.8692592   |         |
| La\(_8\)\(\text{Mg}_2\)\(\text{Mn}_6\) | -3.921 | 0      | 1.8728719   |         |
| La\(_8\)\(\text{Fe}_8\) | -3.918 | 0      | 1.8744202   |         |
| Sr\(_8\)\(\text{Nb}_4\)\(\text{V}_4\) | -3.913 | 0      | 1.8770007   |         |
| La\(_8\)\(\text{Sc}_4\)\(\text{Fe}_4\) | -3.913 | 0      | 1.8770007   |         |
| La\(_6\)\(\text{Nd}_2\)\(\text{Fe}_8\) | -3.904 | 0      | 1.8816456   |         |
| Sr\(_8\)\(\text{Ta}_4\)\(\text{V}_4\) | -3.902 | 0      | 1.8826778   |         |
| La\(_8\)\(\text{Cr}_7\)\(\text{Fe}_1\) | -3.893 | 0      | 1.8873227   |         |
| La\(_8\)\(\text{Mn}_4\)\(\text{Ga}_4\) | -3.882 | 0      | 1.8929998   |         |
| La\(_6\)\(\text{Dy}_2\)\(\text{Fe}_8\) | -3.881 | 0      | 1.8935159   |         |
| La\(_8\)\(\text{Mn}_2\)\(\text{Fe}_6\) | -3.877 | 32.61975717 | 1.8955803 |         |
| Ba\(_8\)\(\text{Zr}_5\)\(\text{Ta}_2\)\(\text{Fe}_1\) | -3.876 | 7.10543E-13 | 1.8960964 |         |
| La\(_8\)\(\text{Mn}_4\)\(\text{Cr}_4\) | -3.875 | 0      | 1.8966125   |         |
| La\(_6\)\(\text{Sm}_2\)\(\text{Fe}_8\) | -3.874 | 0      | 1.8971286   |         |
| Ba\(_8\)\(\text{Zr}_3\)\(\text{Nb}_4\)\(\text{Fe}_1\) | -3.873 | 21.41356744 | 1.8976447 |         |
| La\(_6\)\(\text{Gd}_2\)\(\text{Fe}_8\) | -3.87 | 0      | 1.899193    |         |
| Ca\(_4\)\(\text{Gd}_4\)\(\text{V}_8\) | -3.86 | 15.86530577 | 1.904354   |         |
| La\(_6\)\(\text{Ho}_2\)\(\text{Fe}_8\) | -3.857 | 0      | 1.9059023   |         |
| Ca\(_8\)\(\text{V}_8\) | -3.851 | 0      | 1.9089989   |         |
| Sr\(_8\)\(\text{V}_6\)\(\text{Mo}_2\) | -3.848 | 31.14049421 | 1.9105472 |         |
| Ca\(_4\)\(\text{Y}_4\)\(\text{V}_8\) | -3.84 | 0      | 1.914676    |         |
| Y\(_8\)\(\text{V}_4\)\(\text{Fe}_4\) | -3.836 | 0      | 1.9167404   |         |
| La\(_4\)\(\text{Gd}_4\)\(\text{Fe}_8\) | -3.832 | 0      | 1.9188048   |         |
| Sr\(_4\)\(\text{Ca}_4\)\(\text{Nb}_4\)\(\text{V}_4\) | -3.821 | 16.98337637 | 1.9244819 |         |
| Gd\(_4\)\(\text{Y}_4\)\(\text{Mn}_8\) | -3.818 | 0      | 1.9260302   |         |
| La\(_8\)\(\text{Cr}_6\)\(\text{Co}_2\) | -3.818 | 30.02468793 | 1.9260302 |         |
| Compound                  | E (eV) | Relative Intensity | bandgap (eV) |
|---------------------------|--------|-------------------|--------------|
| La$_8$Cr$_2$Ga$_6$        | -3.815 | 0                 | 1.9275785    |
| Pr$_8$Mg$_2$V$_6$         | -3.809 | 0                 | 1.9306751    |
| La$_4$Nd$_4$Fe$_8$        | -3.794 | 0                 | 1.9384166    |
| Y$_8$Mg$_2$V$_6$          | -3.793 | 0                 | 1.9389327    |
| Y$_8$Mn$_4$V$_4$          | -3.79  | 26.31509721       | 1.940481     |
| La$_8$Fe$_7$Co$_1$        | -3.784 | 0                 | 1.9435776    |
| La$_4$Sm$_4$Fe$_8$        | -3.781 | 0                 | 1.9451259    |
| Ba$_2$Sr$_6$Nb$_4$V$_4$   | -3.773 | 26.95458893       | 1.9492547    |
| Gd$_4$Y$_4$Cr$_8$         | -3.769 | 0                 | 1.9513191    |
| La$_8$Sc$_4$Cr$_4$        | -3.764 | 0                 | 1.9538996    |
| La$_4$Ho$_4$Fe$_8$        | -3.761 | 0                 | 1.9554479    |
| La$_4$Dy$_4$Fe$_8$        | -3.758 | 0                 | 1.9569962    |
| Sr$_8$Ta$_2$V$_6$         | -3.751 | 0                 | 1.9606089    |
| Gd$_2$Y$_6$Mn$_8$         | -3.745 | 0                 | 1.9637055    |
| La$_8$Fe$_7$Ni$_1$        | -3.738 | 22.01071324       | 1.9673182    |
| Pr$_4$Gd$_4$Cr$_8$        | -3.735 | 0                 | 1.9688665    |
| Ca$_4$Pr$_4$V$_8$         | -3.734 | 39.48324603       | 1.9693826    |
| Sr$_4$Y$_4$V$_8$          | -3.73  | 5.738521398       | 1.971447     |
| La$_8$Sc$_6$Mn$_2$        | -3.721 | 0                 | 1.9760919    |
| Pr$_4$Gd$_4$Mn$_8$        | -3.716 | 0                 | 1.9786724    |
| La$_8$Mn$_1$Fe$_7$        | -3.715 | 0                 | 1.9791885    |
| Sr$_8$V$_7$Re$_1$         | -3.709 | 38.96777081       | 1.9822851    |
| Sr$_8$Nb$_2$V$_6$         | -3.703 | 0                 | 1.9853817    |
| Sr$_1$La$_7$Fe$_8$        | -3.702 | 0                 | 1.9858978    |
| La$_8$Cr$_1$Ga$_7$        | -3.702 | 1.747132          | 1.9858978    |
| Ca$_1$La$_7$Fe$_8$        | -3.697 | 0.310343248       | 1.9884783    |
| Sr$_8$V$_7$Mo$_1$         | -3.688 | 35.97619175       | 1.9931232    |
| La$_8$Sc$_6$Fe$_2$        | -3.685 | 0                 | 1.9946715    |
| Ba$_4$Sr$_4$Nb$_4$V$_4$   | -3.668 | 32.73468826       | 2.0034452    |
| La$_8$Cr$_2$Fe$_6$        | -3.665 | 25.80506          | 2.0049935    |
| Y$_8$Mn$_1$Cr$_7$         | -3.665 | 30.87097007       | 2.0049935    |
| Ba$_4$Sr$_4$Ta$_4$V$_4$   | -3.661 | 36.2432757        | 2.0070579    |
| Sr$_8$V$_8$               | -3.657 | 41.8718893        | 2.0091223    |
| Ba$_2$Y$_6$V$_8$          | -3.931 | 42.79143678       | 1.8677109    |
| La$_4$Y$_4$V$_8$          | -4.507 | 43.80730252       | 1.5704373    |
| Sr$_4$Ca$_4$Nb$_2$V$_6$   | -3.741 | 44.4696198        | 1.9657699    |
| La$_8$V$_4$Co$_4$         | -4.144 | 44.51707137       | 1.7577816    |
| Sr$_7$La$_1$V$_8$         | -3.719 | 44.96170958       | 1.9771241    |
| Sr$_6$Pr$_2$V$_8$         | -3.829 | 45.08272836       | 1.9203531    |
| Formula                  | Energy  | Volume  | Pressure |
|--------------------------|---------|---------|----------|
| Sr 7 La 1 Ta 1 V 7      | -3.836  | 45.105 | 1.91674  |
| Sr 4 La 4 V 8           | -4.377  | 45.208 | 1.63753  |
| La 8 Mn 2 V 6           | -4.456  | 45.712 | 1.59675  |
| Sr 2 Gd 6 V 8           | -4.153  | 45.736 | 1.75313  |
| Ca 2 Pr 6 V 8           | -3.918  | 46.711 | 1.87442  |
| Sr 6 Nd 2 V 8           | -3.841  | 47.476 | 1.91415  |
| Pr 4 Ba 4 Ta 4 Fe 4     | -4.33    | 47.556 | 1.66178  |
| Ca 2 La 6 V 8           | -4.584  | 47.712 | 1.53069  |
| La 6 Pr 2 Mo 8          | -5.108  | 48.208 | 1.26026  |
| Sr 7 Ca 1 V 8           | -4.947  | 49.155 | 1.92801  |
| La 8 V 6 Fe 2           | -4.643  | 49.409 | 1.50024  |
| Sr 2 La 6 V 8           | -4.598  | 49.428 | 1.52347  |
| Sr 7 Gd 1 V 8           | -3.674  | 49.557 | 2.00348  |
| Sr 6 La 2 V 8           | -4.031  | 49.918 | 1.81610  |
| La 8 Ti 4 Co 4          | -3.668  | 50.227 | 2.00345  |
| Pr 6 Y 2 V 8            | -4.037  | 50.433 | 1.81300  |
| La 4 Sm 4 V 8           | -4.662  | 50.497 | 1.49044  |
| Pr 8 Ti 4 Fe 4          | -4.294  | 50.937 | 1.68036  |
| Sr 6 Sm 2 V 8           | -3.829  | 50.973 | 1.92035  |
| Ba 4 Ca 4 Mo 8          | -4.392  | 51.512 | 1.62978  |
| Sr 6 Ca 2 Ta 2 V 6      | -3.87   | 51.616 | 1.89919  |
| Pr 8 V 8                | -4.051  | 51.671 | 1.80578  |
| Pr 4 Dy 4 V 8           | -4.255  | 51.690 | 1.70049  |
| La 8 V 7 Fe 1           | -4.692  | 51.781 | 1.47495  |
| Pr 4 Ho 4 V 8           | -4.252  | 52.267 | 1.70204  |
| Ba 2 Ca 6 Nb 4 V 4      | -3.84   | 52.884 | 1.91467  |
| La 8 V 7 Cr 1           | -4.752  | 53.367 | 1.44399  |
| Ba 8 Zr 4 Nb 4          | -4.167  | 53.891 | 1.74591  |
| La 6 Nd 2 V 8           | -4.722  | 53.925 | 1.45947  |
| La 8 Mn 8               | -4.046  | 53.977 | 1.80835  |
| Sr 6 Gd 2 V 8           | -3.923  | 54.221 | 1.87183  |
| La 6 Sm 2 V 8           | -4.725  | 54.255 | 1.45792  |
| Y 8 V 6 Ni 2            | -3.859  | 54.406 | 1.90487  |
| La 4 Dy 4 V 8           | -4.667  | 54.555 | 1.48786  |
| La 4 Pr 4 V 8           | -4.52   | 54.612 | 1.56372  |
| La 6 Nd 2 Mn 8          | -4.025  | 54.638 | 1.81919  |
| La 4 Nd 4 Mn 8          | -3.921  | 54.852 | 1.87281  |
| Pr 6 Dy 2 V 8           | -4.209  | 54.933 | 1.72423  |
| La 8 V 8               | -4.601  | 54.948 | 1.52192  |
| Formula          | E    | χ   | ρ   |
|------------------|------|-----|-----|
| La₈Mn₇Fe₁        | -4.034 | 55.19317994 | 1.8145526 |
| Ba₈Nb₆Mo₂        | -4.004 | 55.28567158 | 1.8300356 |
| Sr₆Y₂V₈          | -3.818 | 55.34170535 | 1.9260302 |
| La₆Y₂V₈          | -4.567 | 55.83737702 | 1.5394713 |
| La₈Mn₇Cr₁        | -4.036 | 56.03238787 | 1.8135204 |
| Rb₂Ba₆Nb₆Cr₂     | -3.659 | 56.21313698 | 2.0080901 |
| Pr₆Ho₂V₈         | -4.189 | 56.22736552 | 1.7345571 |
| Sr₆Ca₂V₈         | -3.77  | 56.51132962 | 1.950803  |
| La₄Ho₄V₈         | -4.678 | 56.80208852 | 1.4821842 |
| Pr₈Mn₄V₄         | -3.806 | 57.12295448 | 1.9322234 |
| Sr₄Gd₄V₈         | -3.846 | 57.60337715 | 1.9115794 |
| La₈V₄Cr₄         | -4.6   | 58.69015252 | 1.52244   |
| Ba₈Nb₆V₂         | -3.838 | 58.73852368 | 1.9157082 |
| Sr₆La₂Ta₂V₆      | -4.14  | 58.77874872 | 1.759846  |
| La₆Dy₂V₈         | -4.717 | 58.95033327 | 1.4620563 |
| La₈Mn₆Fe₂        | -3.366 | 59.10169994 | 1.9012574 |
| Sr₄Ca₄Ta₄V₄      | -4.167 | 60.22745447 | 1.7459113 |
| Ba₄Gd₄Mo₈        | -4.209 | 60.7756999 | 1.7242351 |
| La₈Mn₆Cr₂        | -4.002 | 60.91102582 | 1.8310678 |
| Ba₆Sr₂Nb₆Fe₂     | -3.763 | 60.9854941 | 1.9544157 |
| La₆Sm₂Mn₈        | -4.016 | 60.9868669 | 1.8238424 |
| Ba₈Mn₂Nb₆        | -3.786 | 61.70016795 | 1.9425454 |
| Rb₁Ba₇Nb₇Fe₁     | -3.784 | 61.80598226 | 1.9435776 |
| La₆Ho₂V₈         | -4.695 | 61.91852002 | 1.4734105 |
| Sr₆La₂V₆Cr₂      | -3.725 | 61.99285407 | 1.9740275 |
| Sr₆Dy₂V₈         | -3.814 | 61.9954116 | 1.9280946 |
| Pr₈V₄Fe₄         | -3.949 | 62.241837 | 1.8584211 |
| Ba₈Ti₄Nb₄        | -3.88  | 62.29706988 | 1.894032  |
| Sr₆La₂Nb₂V₆      | -4.179 | 62.8541661 | 1.7397181 |
| La₈V₆Cr₂         | -4.693 | 62.87042702 | 1.4744427 |
| Sr₂La₆Mn₈        | -3.74  | 63.07105696 | 1.966286 |
| La₈Mn₇Co₁        | -3.973 | 63.29718009 | 1.8460347 |
| Pr₈V₄Cr₄         | -4.15  | 63.86570852 | 1.754685  |
| Ba₄Y₄Mo₈         | -3.9   | 64.1844354 | 1.88371   |
| Sr₆Ho₂V₈         | -3.66  | 64.93634835 | 2.007574  |
| Pr₈Ti₄Mn₄        | -4.027 | 65.01144835 | 1.8181653 |
| La₄Sm₄Mn₈        | -3.934 | 65.09673386 | 1.8661626 |
| Sr₂Pr₂V₈         | -4.156 | 65.52165647 | 1.7515884 |
| Y₈Mn₄Fe₄         | -3.679 | 66.18414933 | 1.9977681 |
| Composition       | Energy (eV) | Impedance (Ω) | Conductivity (S/cm) |
|-------------------|-------------|---------------|---------------------|
| Pr 8 V 6 Fe 2     | -4.217      | 67.50141627   | 1.7201063           |
| La 8 V 6 Co 2     | -4.482      | 68.35951145   | 1.5833398           |
| Pr 8 V 6 Cr 2     | -4.144      | 69.12585202   | 1.7577816           |
| Sr 8 Nb 6 Fe 2    | -3.86       | 69.45791595   | 1.904354            |
| Rb 1 Ba 7 Nb 7 V 1| -3.895      | 69.75085376   | 1.8862905           |
| Y 8 Mn 6 Fe 2     | -3.664      | 69.81278463   | 2.0055096           |
| La 8 V 7 Co 1     | -4.634      | 70.60523149   | 1.5048926           |
| Pr 8 V 7 Cr 1     | -4.323      | 71.14642378   | 1.6653997           |
| Pr 8 V 7 Fe 1     | -4.243      | 72.3704559    | 1.7066877           |
| Ba 6 Sr 2 Nb 6 V 2| -3.934      | 72.40780726   | 1.8661626           |
| La 6 Dy 2 Mn 8    | -4.019      | 72.68491143   | 1.822941            |
| Sr 6 Ca 2 Mn 2 Nb 6| -3.961    | 72.84192851   | 1.852279            |
| Rb 2 Sr 6 Nb 6 Cr 2| -3.91      | 72.9959526    | 1.878549            |
| Ba 2 Ca 6 Nb 2 V 6| -3.658      | 73.11999462   | 2.0086062           |
| Pr 8 Mn 1 V 7     | -4.094      | 73.36379777   | 1.7835866           |
| La 8 Mn 4 V 4     | -4.253      | 73.3952221    | 1.7015267           |
| Pr 8 V 7 Co 1     | -4.215      | 73.44172793   | 1.7211385           |
| Ba 2 Sr 6 Mn 2 Nb 6| -3.889     | 73.68424024   | 1.8893871           |
| Ba 2 La 6 V 8     | -4.538      | 74.06224296   | 1.5544382           |
| Y 8 Mn 8          | -3.664      | 74.22941993   | 2.0055096           |
| Pr 6 Nd 2 V 8     | -4.387      | 75.67911628   | 1.6323693           |
| La 6 Ho 2 Mn 8    | -4.001      | 75.79915399   | 1.8315839           |
| Pr 4 Nd 4 V 8     | -4.39       | 76.75098703   | 1.630821            |
| Pr 8 Mn 2 V 6     | -3.965      | 76.8666       | 1.8501635           |
| Ba 2 Gd 6 Mo 8    | -4.622      | 77.39264008   | 1.5110858           |
| Ba 8 Nb 7 Fe 1    | -3.879      | 77.43944879   | 1.8945481           |
| Sr 4 La 4 Ti 4 V 4| -4.478      | 78.24449527   | 1.5854042           |
| Ba 6 Sr 2 Mn 2 Nb 6| -3.872     | 78.95620152   | 1.8981608           |
| Ba 2 La 6 Mn 8    | -3.667      | 79.10546449   | 2.0039613           |
| Cs 1 Ba 7 Nb 7 Fe 1| -3.748     | 79.68245826   | 1.9621572           |
| Pr 6 Sm 2 V 8     | -4.392      | 80.27434353   | 1.6297888           |
| Ba 8 Zr 6 Fe 1 W 1| -3.734      | 80.62302869   | 1.9693826           |
| Ba 4 Sr 4 Ti 4 Nb 4| -4.045     | 80.7791329    | 1.8088755           |
| Sr 8 Ti 4 Nb 4    | -4.201      | 81.12931445   | 1.7283639           |
| La 8 Cr 4 Co 4    | -3.719      | 81.32277235   | 1.9771241           |
| Pr 8 V 4 Co 4     | -3.669      | 82.14642512   | 2.0029291           |
| Pr 4 Sm 4 V 8     | -4.401      | 82.15069153   | 1.6251439           |
| Rb 2 Ba 6 Nb 8    | -3.886      | 82.25343383   | 1.8909354           |
| Sr 4 La 4 V 4 Cr 4| -4.004      | 82.53993722   | 1.8300356           |
| Compound                      | Enthalpy | Entropy  | Temperature |
|-------------------------------|----------|----------|-------------|
| La 4 Dy 4 Mn 8                | -3.928   | 83.4555293 | 1.8692592  |
| Rb 1 Ba 7 Nb 7 Cr 1           | -3.912   | 83.52408223 | 1.8775168  |
| Rb 4 Ba 4 Ta 4 Nb 4           | -3.925   | 83.79187363 | 1.8708075  |
| Ca 2 La 6 Mn 8                | -3.765   | 84.39626436 | 1.9533835  |
| Ba 8 Nb 6 Cr 2                | -3.875   | 84.43142859 | 1.8966125  |
| Ba 8 Mn 1 Nb 7                | -3.899   | 84.56681177 | 1.8842261  |
| Ba 2 Pr 6 V 8                 | -3.858   | 85.39825581 | 1.9053862  |
| Ba 8 Nb 7 V 1                 | -3.984   | 85.41936464 | 1.8403576  |
| Ba 4 Sr 4 Nb 6 V 2            | -4.035   | 85.46809083 | 1.8140365  |
| Dy 4 Y 4 Mn 8                 | -3.681   | 85.60736883 | 1.9967359  |
| La 8 V 7 Ni 1                 | -4.614   | 86.20772424 | 1.5152146  |
| Sr 8 Nb 7 Co 1                | -4.423   | 86.31640921 | 1.6137897  |
| Ba 8 Nb 7 Mo 1                | -4.079   | 86.58206359 | 1.7913281  |
| Sr 8 Nb 6 V 2                 | -4.236   | 86.85803974 | 1.7103004  |
| La 6 Gd 2 Mo 8                | -5.123   | 87.26848633 | 1.2525197  |
| Rb 1 Sr 7 Mn 1 Nb 7           | -4.029   | 87.54292313 | 1.8171331  |
| Cs 1 Ba 7 Nb 7 V 1            | -3.861   | 87.72137411 | 1.9038379  |
| La 8 Mn 6 Co 2                | -3.875   | 87.82261025 | 1.8966125  |
| Sr 8 Zr 4 Nb 4                | -4.443   | 87.85366645 | 1.6034677  |
| Pr 8 V 6 Co 2                 | -4.119   | 87.96546032 | 1.7706841  |
| Sr 8 V 7 Os 1                 | -3.678   | 88.44990912 | 1.9982842  |
| Y 4 Ho 4 Mn 8                 | -3.694   | 88.81101082 | 1.9900266  |
| Rb 4 Sr 4 Nb 8                | -3.873   | 90.2516162  | 1.8976447  |
| La 8 Mn 7 Ni 1                | -4.029   | 90.85467284 | 1.8171331  |
| Sr 8 Nb 6 Mo 2                | -4.315   | 91.43620605 | 1.6695285  |
| Ba 2 Sr 6 Nb 6 V 2            | -4.12    | 92.57113908 | 1.770168   |
| Ba 7 Sr 1 Mn 1 Nb 7           | -3.942   | 92.60407856 | 1.8620338  |
| Ba 7 Sr 1 Nb 7 V 1            | -4.033   | 92.61213143 | 1.8150687  |
| Ba 8 Nb 6 Fe 2                | -3.689   | 92.76895126 | 1.9926071  |
| Ba 8 Nb 8                     | -4.29    | 92.8362056  | 1.682431   |
| Ba 6 Ca 2 Nb 6 Fe 2           | -3.868   | 92.89156791 | 1.9002252  |
| Ba 8 Zr 2 Nb 6                | -4.111   | 93.32919564 | 1.7748129  |
| Ba 6 Sr 2 Nb 6 Cr 2           | -3.949   | 94.56054079 | 1.8584211  |
| Sr 4 La 4 Nb 4 V 4            | -4.705   | 95.25269391 | 1.4682495  |
| Ba 8 Hf 4 Nb 4                | -4.272   | 95.9841047  | 1.6917208  |
| Rb 2 Ba 6 Ta 2 Nb 6           | -4.033   | 96.33430982 | 1.8150687  |
| Ba 8 Ti 2 Nb 6                | -4.001   | 96.57627128 | 1.8315839  |
| Sr 6 Ca 2 Nb 6 V 2            | -4.292   | 96.97098313 | 1.6813988  |
| Ba 6 Ca 2 Nb 6 V 2            | -4.052   | 97.04525166 | 1.8052628  |
| Compound | ΔG (J/mol) | E (eV) | T (K) |
|----------|------------|--------|-------|
| Sr 4 La 4 Ti 8 | -4.984 | 98.41497463 | 1.3242576 |
| Sr 4 Ca 4 Nb 6 V 2 | -4.349 | 99.30542754 | 1.6519811 |
| Rb 1 Ba 7 Nb 8 | -4.042 | 99.40944472 | 1.8104238 |
| La 7 Zn 1 Fe 8 | -3.661 | 99.85916922 | 2.0070579 |
| Ca 4 La 4 Ti 8 | -5.013 | 99.98824376 | 1.3092907 |
| La 7 Mn 8 Zn 1 | -3.932 | 100.3018875 | 1.8671948 |
| Ba 4 La 4 V 8 | -4.233 | 101.0012844 | 1.7118487 |
| La 8 Mn 1 V 7 | -4.63 | 101.188942 | 1.506957 |
| Ba 8 Nb 7 Cr 1 | -3.747 | 101.7316221 | 1.9626733 |
| Y 6 Ta 2 Mn 6 Zn 2 | -3.657 | 102.3783285 | 2.0091223 |
| Cs 1 Ba 7 Nb 7 Cr 1 | -3.883 | 102.5813082 | 1.8924837 |
| Rb 1 Sr 7 Nb 7 V 1 | -4.178 | 103.8201523 | 1.7402342 |
| Y 8 Ti 4 Cr 4 | -4.854 | 103.9255144 | 1.3913506 |
| Ba 7 Ca 1 Mn 1 Nb 7 | -4.011 | 104.1808008 | 1.8264229 |
| Cs 1 Sr 7 Mn 1 Nb 7 | -4.001 | 104.2189359 | 1.8315839 |
| La 4 Gd 4 Mo 8 | -5.085 | 104.2822676 | 1.2721315 |
| Ba 7 Ca 1 Nb 7 V 1 | -4.088 | 104.4118536 | 1.7866832 |
| Sr 4 La 4 Sc 4 V 4 | -3.833 | 105.734136 | 1.9182887 |
| Pr 8 V 7 Ni 1 | -4.183 | 106.8107207 | 1.7376537 |
| Ba 8 Zr 1 Nb 7 | -4.141 | 107.0650191 | 1.7593299 |
| Sr 4 Nd 4 V 8 | -4.255 | 107.4705589 | 1.7004945 |
| Ba 8 Ti 1 Nb 7 | -4.074 | 107.5219884 | 1.7939086 |
| Pr 8 V 6 Ni 2 | -3.834 | 107.8589458 | 1.9177726 |
| Rb 1 Ba 7 Ta 1 Nb 7 | -4.112 | 107.9375884 | 1.7742968 |
| Ba 7 Sr 1 Nb 7 Cr 1 | -4.074 | 107.9588155 | 1.7939086 |
| Sr 8 Mn 1 Nb 7 | -4.162 | 108.200729 | 1.7484918 |
| Ba 6 Sr 2 Ti 2 Nb 6 | -4.084 | 108.2213049 | 1.7887476 |
| Sr 4 Pr 4 Ti 8 | -4.887 | 108.6171835 | 1.3743193 |
| Ca 4 Pr 4 Ti 8 | -4.985 | 108.6235318 | 1.3237415 |
| Ba 8 Hf 2 Nb 6 | -4.117 | 108.74556 | 1.7717163 |
| Ba 4 Pr 4 V 8 | -3.7 | 109.0354314 | 1.98693 |
| Sr 8 Nb 6 Cr 2 | -4.143 | 109.1473144 | 1.7582977 |
| Ba 6 Sr 2 Nb 8 | -4.371 | 109.4369892 | 1.6406269 |
| Ba 8 Nb 6 Ni 2 | -3.727 | 109.6104509 | 1.9729953 |
| Ba 2 Sr 6 Nb 6 Cr 2 | -4.168 | 110.1099732 | 1.7453952 |
| Ba 6 Ca 2 Mn 2 Nb 6 | -3.965 | 110.3838959 | 1.8501635 |
| Chemical Formula       | Energy  | Mass      | Density  |
|------------------------|---------|-----------|----------|
| La$_6$Ta$_2$Zn$_2$Fe$_6$ | -3.827  | 110.8397137 | 1.9213853 |
| Ba$_8$Nb$_7$Ni$_1$     | -3.934  | 111.1476894 | 1.8661626 |
| Cs$_2$Sr$_6$Nb$_6$Cr$_2$ | -3.825  | 111.4916375 | 1.9224175 |
| La$_6$Nb$_2$Zn$_2$Fe$_6$ | -3.889  | 111.6681212 | 1.8893871 |
| Sr$_8$Nb$_7$Fe$_1$     | -4.112  | 111.9032529 | 1.7742968 |
| Ba$_8$Nb$_6$Ru$_2$     | -4.171  | 112.4818777 | 1.7438469 |
| Ba$_8$Nb$_7$Ru$_1$     | -4.307  | 113.1301527 | 1.6736573 |
| La$_8$Ti$_4$Cr$_4$     | -5.227  | 113.2446319 | 1.9988453 |
| Ba$_8$Nb$_6$Sb$_2$     | -4.11   | 113.6720837 | 1.775329  |
| Ba$_1$Sr$_7$Nb$_7$Fe$_1$ | -4.105  | 113.7265332 | 1.7779095 |
| Sr$_6$Ca$_2$Nb$_6$Fe$_2$ | -3.945  | 113.7900629 | 1.8604855 |
| Ba$_1$Sr$_7$Mn$_1$Nb$_7$ | -4.129  | 113.8010346 | 1.7655231 |
| Ba$_8$Hf$_1$Nb$_7$     | -4.157  | 113.877484  | 1.7510723 |
| Ba$_7$Sr$_1$Ti$_1$Nb$_7$ | -4.118  | 113.9875052 | 1.7712002 |
| Ba$_8$Ta$_2$Nb$_6$     | -4.436  | 114.4247429 | 1.6070804 |
| Rb$_1$Sr$_7$Nb$_7$Cr$_1$ | -4.157  | 114.6805212 | 1.7510723 |
| Rb$_4$Sr$_4$Ta$_4$Nb$_4$ | -4.167  | 115.4294536 | 1.7459113 |
| Rb$_2$Sr$_6$Nb$_8$     | -4.156  | 115.706478  | 1.7515884 |
| Sr$_4$Y$_4$Ti$_8$      | -4.775  | 116.8075373 | 1.4321225 |
| Ba$_2$Sr$_6$Nb$_6$Fe$_2$ | -3.845  | 117.2367264 | 1.9120955 |
| Cs$_1$Ba$_7$Nb$_8$     | -4.009  | 117.5977151 | 1.8274551 |
| Sr$_7$Ca$_1$Mn$_1$Nb$_7$ | -4.213  | 117.7231342 | 1.7221707 |
| Ba$_7$Sr$_1$Nb$_7$Ni$_1$ | -3.997  | 118.3492061 | 1.8336483 |
| La$_6$Zr$_2$Mn$_6$Zn$_2$ | -3.873  | 118.8020681 | 1.8976447 |
| Ba$_4$Ca$_4$Nb$_6$V$_2$ | -4.174  | 118.8467296 | 1.7422986 |
| Cs$_1$Sr$_7$Nb$_7$V$_1$ | -4.136  | 118.8671168 | 1.7619104 |
| Cs$_2$Ba$_6$Nb$_8$     | -3.823  | 119.7417245 | 1.9234497 |
| La$_6$Ta$_2$Mn$_6$Zn$_2$ | -4.012  | 119.7743548 | 1.8259068 |
| Ba$_6$Sr$_2$Nb$_6$Ni$_2$ | -3.797  | 119.8289521 | 1.9368683 |
| Ba$_7$Ca$_1$Nb$_7$Cr$_1$ | -4.131  | 119.9530378 | 1.7644909 |
| Sr$_7$Ca$_1$Nb$_7$Fe$_1$ | -4.153  | 120.5504514 | 1.7531367 |
| Ba$_7$Sr$_1$Nb$_7$Fe$_1$ | -3.914  | 120.7834656 | 1.8764846 |
| Ba$_4$La$_4$Ti$_8$     | -4.87   | 122.138953  | 1.383093  |
| Sr$_8$Nb$_6$Ni$_2$     | -3.827  | 122.1667468 | 1.9213853 |
| Sr$_8$Nb$_7$V$_1$      | -4.298  | 122.9574398 | 1.6783022 |
| La$_8$Mn$_6$Ni$_2$     | -3.894  | 123.4763457 | 1.8868066 |
| Ba$_2$Ca$_6$Nb$_6$V$_2$ | -4.352  | 124.3592223 | 1.6504328 |
| Ba$_4$Sr$_4$Nb$_8$     | -4.451  | 124.5207727 | 1.5993389 |
| Ba$_4$La$_4$Nb$_4$Fe$_4$ | -4.109  | 124.768635  | 1.7758451 |
| Compound          | Energy  | Density  | Hardness  |
|-------------------|---------|----------|-----------|
| Ba$_6$Ca$_2$Nb$_6$Cr$_2$ | -4.064  | 125.0486292 | 1.7990696 |
| La$_8$V$_6$Ni$_2$   | -4.407  | 125.0609969  | 1.6220473  |
| Y$_8$Ti$_6$Co$_2$    | -4.558  | 125.2411956  | 1.5441162  |
| Y$_8$Mg$_2$Ti$_6$    | -4.968  | 125.5389292  | 1.3325152  |
| La$_6$Mn$_6$Nb$_2$Zn$_2$ | -3.997  | 125.8759223  | 1.8336483  |
| Rb$_1$Sr$_7$Nb$_7$Fe$_1$ | -4.041  | 126.153447   | 1.8109399  |
| Ba$_4$La$_4$Nb$_4$Co$_4$ | -3.982  | 126.2774742  | 1.8413898  |
| Cs$_1$Ba$_7$Ta$_1$Nb$_7$ | -4.079  | 126.4006087  | 1.7913281  |
| Sr$_4$Gd$_4$Zr$_8$   | -5.4    | 126.9589288  | 1.10956    |
| Y$_8$Ti$_6$Fe$_2$    | -4.663  | 126.9939811  | 1.4899257  |
| Ba$_7$Sr$_1$Nb$_8$   | -4.175  | 127.2309724  | 1.7417825  |
| Ba$_7$La$_1$Nb$_7$Fe$_1$ | -4.244  | 127.6355792  | 1.7061716  |
| Ba$_1$Sr$_7$Nb$_7$V$_1$ | -4.284  | 127.8759895  | 1.6855276  |
| Ba$_2$Sr$_6$Ti$_2$Nb$_6$ | -4.235  | 127.9937364  | 1.7108165  |
| Ba$_7$Ca$_1$Ti$_1$Nb$_7$ | -4.17   | 128.1577274  | 1.744363   |
| Sr$_8$V$_6$Os$_2$    | -3.817  | 128.3424289  | 1.9265463  |
| Rb$_1$Ba$_7$Mn$_1$Nb$_7$ | -3.787  | 129.0050509  | 1.9420293  |
| Ba$_6$Sr$_2$Nb$_6$Sb$_2$ | -4.142  | 129.1017287  | 1.7588138  |
| Sr$_8$Hf$_4$Nb$_4$   | -4.556  | 129.5792807  | 1.5451484  |
| Ba$_8$Ta$_1$Nb$_7$   | -4.207  | 129.7480992  | 1.7252673  |
| Sr$_8$Nb$_6$Ru$_2$   | -4.375  | 129.8941736  | 1.6385625  |
| Sr$_7$Ca$_1$Nb$_7$V$_1$ | -4.348  | 130.1232865  | 1.6524972  |
| Sr$_6$La$_2$Mn$_2$Nb$_6$ | -4.343  | 130.3553437  | 1.6550777  |
| Ba$_2$Sr$_6$Nb$_6$Ni$_2$ | -3.823  | 130.3704819  | 1.9234497  |
| Sr$_8$Ta$_2$Nb$_6$   | -4.284  | 130.4905772  | 1.6855276  |
| Ba$_4$Pr$_4$Ti$_8$   | -4.726  | 130.6399198  | 1.4574114  |
| Sr$_8$Nb$_7$Mo$_1$   | -4.38   | 130.824398   | 1.635982   |
| Ba$_7$La$_1$Nb$_7$Co$_1$ | -4.292  | 131.339327   | 1.6813988  |
| Rb$_2$Sr$_6$Ta$_2$Nb$_6$ | -4.304  | 131.7398968  | 1.6752056  |
| Sr$_8$Zr$_2$Nb$_6$   | -4.385  | 131.7731282  | 1.6334015  |
| La$_6$Ti$_2$Mn$_6$Zn$_2$ | -3.848  | 131.8015671  | 1.9105472  |
| Pr$_8$Mg$_2$Ti$_6$   | -4.894  | 131.8979286  | 1.3707066  |
| Ba$_8$Nb$_4$Sn$_4$   | -3.735  | 132.0197634  | 1.9688665  |
| La$_8$Mg$_2$Ti$_6$   | -5.085  | 132.282592   | 1.2721315  |
| Cs$_1$Sr$_7$Nb$_7$Cr$_1$ | -4.116  | 132.511284   | 1.7722324  |
| Ba$_4$Gd$_4$V$_8$    | -3.713  | 132.5185758  | 1.9802207  |
| Ba$_4$Ca$_4$Ti$_4$Nb$_4$ | -4.276  | 132.6341919  | 1.6896564  |
| Ba$_7$Ca$_1$Nb$_7$Ni$_1$ | -4.002  | 133.2219283  | 1.8310678  |
| Ba$_2$Sr$_6$Nb$_8$   | -4.523  | 133.2485563  | 1.5621797  |
| Chemical Composition | Lattice Energy (eV) | Atomic Volume (Å³) | Density (g/cm³) |
|----------------------|---------------------|--------------------|-----------------|
| Ba$_8$Nb$_7$Sn$_1$   | -4.156              | 133.678531         | 1.7515884       |
| Sr$_6$La$_2$Nb$_6$Fe$_2$ | -4.447              | 133.8151431        | 1.6014033       |
| Ba$_7$La$_1$Mn$_1$Nb$_7$ | -4.273              | 134.3741921        | 1.6912047       |
| Ba$_4$Sr$_4$Nb$_6$Sb$_2$ | -4.223              | 134.7995068        | 1.7170097       |
| Sr$_4$Sm$_4$V$_8$     | -4.29               | 134.8922634        | 1.682431        |
| Cs$_2$Ba$_6$Ta$_2$Nb$_6$ | -3.938              | 134.9710118        | 1.8640982       |
| Ba$_7$Ca$_1$Nb$_7$Fe$_1$ | -3.985              | 135.4704378        | 1.8398415       |
| Ba$_7$La$_1$Nb$_7$V$_1$ | -4.319              | 135.663245         | 1.6674641       |
| Ba$_6$Ca$_2$Ti$_2$Nb$_6$ | -4.194              | 136.3212493        | 1.7319766       |
| Ba$_6$Sr$_2$Ta$_2$Nb$_6$ | -4.525              | 136.9831031        | 1.5611475       |
| Pr$_8$Ti$_4$Cr$_4$    | -4.857              | 137.1960703        | 1.3898023       |
| Sr$_8$Nb$_7$Cr$_1$    | -4.347              | 137.3003272        | 1.6530133       |
| Ba$_8$Nb$_7$Ge$_1$    | -3.998              | 137.4416548        | 1.8331322       |
| Ba$_1$Sr$_7$Nb$_7$Cr$_1$ | -4.338              | 137.4557816        | 1.6576582       |
| Sr$_6$La$_2$Nb$_6$Co$_2$ | -4.344              | 137.998882         | 1.6545616       |
| Y$_8$Ti$_6$Mn$_2$     | -4.755              | 138.1171915        | 1.4424445       |
| Sr$_6$Ca$_2$Nb$_6$Ni$_2$ | -3.872              | 138.6295243        | 1.8981608       |
| Sr$_4$La$_4$Zr$_8$    | -5.609              | 139.1075824        | 1.0016951       |
| Sr$_8$Nb$_7$Ni$_1$    | -4.097              | 139.236152         | 1.7820383       |
| La$_8$Ti$_6$Fe$_2$    | -5.118              | 140.1937368        | 1.2551002       |
| Ba$_8$Ta$_4$Nb$_4$    | -4.583              | 140.3577802        | 1.5312137       |
| Ba$_7$Sr$_1$Ta$_1$Nb$_7$ | -4.255              | 140.6810293        | 1.7004945       |
| Ba$_7$Sr$_1$Nb$_7$Sn$_1$ | -4.202              | 141.2707978        | 1.7278478       |
| La$_8$Ti$_6$Co$_2$    | -5.006              | 141.4667324        | 1.3129034       |
| Ba$_1$Sr$_7$Nb$_7$Ni$_1$ | -4.07               | 141.5827695        | 1.795973        |
| Pr$_8$Ti$_6$Fe$_2$    | -4.624              | 141.7348234        | 1.5100536       |
| Ba$_7$Ca$_1$Nb$_8$    | -4.228              | 141.9786946        | 1.7144292       |
| Sr$_4$Pr$_4$Zr$_8$    | -5.191              | 142.1303761        | 1.2174249       |
| Sr$_8$Nb$_8$          | -4.58               | 142.8025899        | 1.532762        |
| Rb$_1$Sr$_7$Nb$_8$    | -3.24               | 143.133534         | 1.6648836       |
| Sr$_8$Nb$_7$Ru$_1$    | -4.545              | 144.6556153        | 1.5508255       |
| Sr$_6$Ca$_2$Ti$_2$Nb$_6$ | -4.388              | 145.0724617        | 1.6318532       |
| Ba$_8$Nb$_6$Sn$_2$    | -4.167              | 145.2705241        | 1.7459113       |
| Ba$_2$Sr$_6$Nb$_6$Sb$_2$ | -4.215              | 145.5695349        | 1.7211385       |
| Ba$_6$La$_2$Nb$_6$Fe$_2$ | -4.36               | 145.7022213        | 1.646304        |
| Sr$_7$Ca$_1$Nb$_7$Cr$_1$ | -4.374              | 145.9772331        | 1.6390786       |
| Ba$_4$La$_4$Mn$_4$Nb$_4$ | -4.411              | 146.5706758        | 1.6199829       |
| Ba$_7$La$_1$Sc$_1$Nb$_7$ | -4.363              | 146.7503668        | 1.6447557       |
| Cs$_1$Ba$_7$Mn$_1$Nb$_7$ | -3.752              | 147.1383212        | 1.9600928       |
| Formula            | Energy (eV) | Atomic Number | Density (g/cm³) |
|--------------------|-------------|---------------|-----------------|
| Sr 6 La 2 Mn 2 V 6 | -3.785      | 147.2405394   | 1.9430615       |
| Sr 6 Ca 2 Nb 6 Cr 2| -4.224      | 148.5901263   | 1.7164936       |
| Ba 1 Sr 7 Ti 1 Nb 7| -4.345      | 148.6084131   | 1.6540455       |
| Pr 8 Ti 6 Mn 2     | -4.652      | 149.2209587   | 1.4956028       |
| La 8 Ti 6 Mn 2     | -5.082      | 149.4103721   | 1.2736798       |
| Sr 8 Ti 1 Nb 7     | -4.376      | 149.6959585   | 1.6380464       |
| Sr 7 Ca 1 Nb 7 Ni 1| -4.13       | 149.8238071   | 1.765007        |
| Cs 2 Sr 6 Nb 8     | -4.07       | 149.8317536   | 1.795973        |
| Sr 8 Hf 2 Nb 6     | -4.401      | 149.9625603   | 1.6251439       |
| Ba 7 La 1 Nb 7 Cr 1| -4.383      | 150.2556791   | 1.6344337       |
| Sr 8 Zr 1 Nb 7     | -4.407      | 150.973109    | 1.6220473       |
| Sr 7 La 1 Mn 1 Nb 7| -4.441      | 151.2040918   | 1.6044999       |
| Sr 4 Y 4 Zr 8      | -4.78       | 152.2380974   | 1.429542        |
| Sr 7 La 1 Nb 7 Fe 1| -4.442      | 152.4041165   | 1.6039838       |
| Sr 7 La 1 Nb 7 Co 1| -4.514      | 152.413236    | 1.5668246       |
| Pr 8 Ti 6 Co 2     | -4.571      | 152.519819    | 1.5374069       |
| Ba 4 Sr 4 Ta 2 Nb 6| -4.612      | 152.6708866   | 1.5162468       |
| Ba 6 La 2 Nb 6 Co 2| -4.313      | 152.7252806   | 1.6705607       |
| Rb 1 Sr 7 Ta 1 Nb 7| -4.397      | 152.9063683   | 1.6272083       |
| La 6 Hf 2 Mn 6 Zn 2| -3.949      | 153.1355143   | 1.8584211       |
| Ba 7 Ca 1 Ta 1 Nb 7| -4.303      | 153.4225603   | 1.6757217       |
| Ba 4 Gd 4 Zr 8     | -5.301      | 154.1937904   | 1.1606539       |
| Ba 7 Ca 1 Nb 7 Sn 1| -4.269      | 156.3078651   | 1.6932691       |
| Ba 7 Nb 8 Zn 1     | -3.932      | 156.6375691   | 1.8671948       |
| Sr 4 La 4 Sc 4 Nb 4| -4.912      | 156.8194441   | 1.3614168       |
| Ba 7 La 1 Ti 1 Nb 7| -4.337      | 156.8668688   | 1.6581743       |
| Ba 6 Ca 2 Nb 6 Ni 2| -3.903      | 157.0816779   | 1.8821617       |
| Sr 6 La 2 Nb 6 V 2 | -4.62       | 157.5785169   | 1.512118        |
| La 8 V 4 Ni 4      | -4.093      | 157.6627924   | 1.7841027       |
| Ba 7 La 1 Nb 7 Ni 1| -4.295      | 157.9908197   | 1.6798505       |
| Sr 7 Ca 1 Ti 1 Nb 7| -4.429      | 158.0520258   | 1.6106931       |
| Ba 8 Re 8          | -4.541      | 158.4976702   | 1.5528899       |
| Ba 6 Sr 2 Nb 6 Sn 2| -4.27       | 159.1173424   | 1.692753        |
| Ba 8 Nb 6 Ge 2     | -3.726      | 159.9208541   | 1.9735114       |
| Cs 1 Sr 7 Nb 8     | -4.288      | 160.1022967   | 1.6834632       |
| Sr 8 Hf 1 Nb 7     | -4.425      | 160.1740751   | 1.6127575       |
| Ba 6 Mg 2 Nb 6 V 2 | -3.95       | 161.2835403   | 1.857905        |
| Ba 6 La 2 Nb 6 V 2 | -4.45       | 161.3837844   | 1.599855        |
| Ba 4 Pr 4 Zr 8     | -5.067      | 161.5726406   | 1.2814213       |
| Compound              | ΔG  (kcal/mol) | ΔG  (kJ/mol)  | ΔG  (kcal/mol) |
|-----------------------|----------------|---------------|---------------|
| Ca₂Y₆Ti₈              | -5.161         | 161.8546761   | 1.2329079     |
| Ba₂Sr₆Ta₂Nb₆          | -4.682         | 163.6286702   | 1.4801198     |
| Sr₇La₁Nb₇V₁           | -4.576         | 164.0020534   | 1.5348264     |
| Sr₄Mg₄Nb₆V₂           | -4.039         | 164.677457    | 1.8119721     |
| Ba₆Ca₂Nb₈             | -4.316         | 164.8729336   | 1.6690124     |
| Ba₆La₂Mn₂Nb₆          | -4.271         | 165.515678    | 1.6922369     |
| Pr₄Ba₄Zr₇Co₁          | -4.73          | 165.7765276   | 1.455347      |
| Sr₂La₆Ti₈             | -5.269         | 166.0585674   | 1.1771691     |
| Cs₂Sr₆Ta₂Nb₆          | -4.213         | 166.9359223   | 1.7221707     |
| Y₈Ti₆Cr₂              | -4.963         | 167.1873999   | 1.3350957     |
| Ca₂La₆Ti₈             | -5.289         | 168.678952    | 1.1668471     |
| Ba₁Sr₇Nb₈             | -4.386         | 168.7040731   | 1.632854      |
| Ba₆Sr₂Ta₄Nb₄          | -4.677         | 168.9304669   | 1.4827003     |
| Cs₁Sr₇Ta₁Nb₇          | -4.362         | 169.4388811   | 1.6452718     |
| Ca₄Pr₄Zr₈             | -5.031         | 170.3802659   | 1.3000009     |
| Cs₄Ba₄Ta₄Nb₄          | -3.79          | 171.3573521   | 1.940481      |
| Ba₆Ca₂Nb₆Sb₂           | -4.101         | 172.2961946   | 1.7799739     |
| Ba₇La₁Nb₈             | -4.47          | 173.036586    | 1.589533      |
| Ba₈Ta₆Nb₂              | -4.8           | 173.1993175   | 1.41922       |
| Y₈Ti₆Ni₂              | -4.544         | 173.3099311   | 1.5513416     |
| Sr₈Nb₇Sn₁              | -4.408         | 173.4892934   | 1.6215312     |
| Ba₁Sr₇Nb₇Sn₁          | -4.374         | 173.512851    | 1.6390786     |
| Y₈Ti₇Co₁              | -4.798         | 173.5137406   | 1.4202522     |
| Ca₄Mg₄Nb₆V₂           | -4.29          | 174.1080157   | 1.682431      |
| Sr₂Y₆Ti₈              | -5.138         | 174.3510364   | 1.2447782     |
| Ca₄La₄Zr₈             | -5.49          | 174.7474721   | 1.063111      |
| Y₈Mg₁Ti₇              | -5.144         | 176.1174308   | 1.2416816     |
| Sr₇La₁Sc₁Nb₇          | -4.591         | 176.2440936   | 1.5270849     |
| Y₈Ti₇Fe₁              | -4.845         | 176.9695083   | 1.3959955     |
| Ba₂La₆Ti₈             | -5.215         | 177.1955181   | 1.2050385     |
| Ba₄Y₄Ti₈              | -4.602         | 177.2536036   | 1.5214078     |
| Ba₂Sr₆Nb₆Sn₂           | -4.367         | 177.7833621   | 1.6426913     |
| Sr₇La₁Nb₇Cr₁           | -4.586         | 178.1126907   | 1.5296654     |
| Sr₇La₁Nb₇Ni₁           | -4.451         | 178.4692287   | 1.5993389     |
| Sr₇Ca₁Nb₈              | -4.47          | 179.0340621   | 1.589533      |
| Ba₆La₂Nb₆Cr₂           | -4.573         | 179.124476    | 1.5363747     |
| Sr₆La₂Sc₂Nb₆           | -4.609         | 179.6545974   | 1.5177951     |
| Cs₄Sr₄Nb₈              | -3.732         | 179.9492361   | 1.9704148     |
| Ba₆Be₂Nb₆V₂            | -3.824         | 180.0773535   | 1.9229336     |
| Compound                  | a (Å)   | b (Å)   | c (Å)   |
|---------------------------|---------|---------|---------|
| Ba 6 La 2 Sc 2 Nb 6       | -4.458  | 180.436028 | 1.5957262 |
| Ba 1 Sr 7 Ta 1 Nb 7       | -4.477  | 181.21138 | 1.5859203 |
| Y 8 Ti 7 Mn 1             | -4.869  | 181.3437385 | 1.3836091 |
| Sr 4 La 4 Ta 4 V 4        | -5.252  | 181.6821081 | 1.1859428 |
| Sr 4 Ca 4 Nb 6 Sb 2       | -4.17   | 182.1919315 | 1.744363 |
| Sr 8 Ta 1 Nb 7            | -4.498  | 182.244243 | 1.5750822 |
| Ba 4 Sr 4 Ta 4 Nb 4       | -4.769  | 182.7925005 | 1.4352191 |
| Ba 4 Ca 4 Nb 6 Sb 2       | -4.163  | 182.8972813 | 1.7479757 |
| Sr 6 La 2 Nb 6 Cr 2       | -4.636  | 183.3087916 | 1.5038604 |
| Ba 4 La 1 Ta 1 Nb 7       | -4.54   | 184.0934796 | 1.553406 |
| Sr 2 Pr 6 Ti 8            | -5.212  | 184.7008263 | 1.2065868 |
| Sr 7 Ca 1 Nb 7 Sn 1       | -4.424  | 184.7586605 | 1.6132736 |
| Pr 4 Ba 4 Hf 7 Co 1       | -4.996  | 185.5226367 | 1.3180644 |
| Sr 6 Ca 2 Nb 8            | -5.14   | 185.9151343 | 1.5668246 |
| Ca 2 Pr 6 Ti 8            | -5.27   | 186.3098754 | 1.176653 |
| Ba 6 Ca 2 Ta 2 Nb 6       | -4.476  | 187.806165 | 1.5864364 |
| Sr 6 La 2 Nb 6 Ni 2       | -5.299  | 187.9458761 | 1.1616861 |
| Sr 7 Nb 8 Ge 1            | -4.243  | 188.1939615 | 1.7066877 |
| Pr 8 Ti 6 Cr 2            | -4.873  | 188.965196 | 1.3815447 |
| Ba 4 Ca 4 Nb 8            | -4.87   | 189.2466616 | 1.584372 |
| Ba 4 La 4 Nb 4 V 4        | -4.79   | 189.4766426 | 1.424381 |
| Sr 6 La 2 Nb 6 Ni 2       | -4.264  | 189.7526175 | 1.6958496 |
| Sr 7 Nb 8 Zn 1            | -4.199  | 190.387132 | 1.7293961 |
| Sr 7 Ca 1 Ta 1 Nb 7       | -4.554  | 190.6766465 | 1.5461806 |
| Sr 7 La 1 Ti 1 Nb 7       | -5.94   | 191.3690721 | 1.5255366 |
| Sr 8 Ti 7 Co 1            | -5.244  | 191.8731963 | 1.1900716 |
| Ca 4 Be 4 Nb 4 V 4        | -3.731  | 192.3522954 | 1.9709309 |
| Sr 8 Ti 6 Cr 2            | -3.759  | 192.6977276 | 1.9564801 |
| Sr 8 V 4 Os 4             | -3.759  | 192.763961 | 1.1059473 |
| Pr 8 Ti 6 Ni 2            | -5.09   | 192.763045 | 1.5694051 |
| La 8 Ti 7 Fe 1            | -5.296  | 193.0661985 | 1.1632344 |
| Sr 4 Ca 4 Nb 8            | -4.585  | 193.3264787 | 1.5301815 |
| Ba 2 Ca 6 Nb 6 Sb 2       | -4.243  | 193.7218681 | 1.7066877 |
| Ca 8 Nb 8                 | -4.733  | 193.9518675 | 1.4537987 |
| Ba 6 Ca 2 Nb 6 Sn 2       | -4.38   | 194.3555246 | 1.635982 |
| Ba 2 Pr 6 Ti 8            | -5.125  | 194.55434 | 1.2514875 |
| Sr 8 Ta 2 Nb 6            | -4.581  | 194.6155086 | 1.5322459 |
| Sr 4 Dy 4 V 8             | -4.394  | 195.0776839 | 1.6287566 |
| Ba 2 Sr 6 Ta 4 Nb 4       | -4.848  | 195.1987841 | 1.3944472 |
| Formula                  | Enthalpy | Atom Mass   | Density  |
|--------------------------|----------|-------------|----------|
| Ba$_6$La$_2$Ti$_2$Nb$_6$ | -4.516   | 195.413032  | 1.5657924 |
| Sr$_6$Ca$_2$Nb$_6$Sn$_2$ | -4.446   | 195.5441312 | 1.6019194 |
| La$_8$Ti$_7$Mn$_1$       | -5.294   | 197.1410162 | 1.1642666 |
| Y$_8$Ti$_7$Ni$_1$        | -4.782   | 198.1717333 | 1.4285098 |
| Sr$_2$Ca$_6$Nb$_8$       | -4.684   | 198.1816731 | 1.4790876 |
| Ba$_6$Sr$_2$Ta$_6$Nb$_2$ | -4.892   | 200.0925042 | 1.3717388 |
| Y$_8$Ti$_7$Cr$_1$        | -5.002   | 202.1130927 | 1.3149678 |
| Ba$_6$Be$_2$Nb$_6$Sb$_2$ | -4.074   | 202.4587806 | 1.7939086 |
| Ba$_2$Ca$_6$Nb$_8$       | -4.644   | 202.4973895 | 1.4997316 |
| Ca$_4$Y$_4$Zr$_8$        | -5.43    | 203.2794871 | 1.094077  |
| Ba$_6$La$_2$Nb$_6$Ni$_2$ | -4.222   | 203.9261023 | 1.7175258 |
| Ba$_4$La$_4$Nb$_4$Cr$_4$ | -4.746   | 205.1821121 | 1.4470894 |
| Ba$_6$Nb$_8$Zn$_2$       | -3.713   | 206.3831827 | 1.9802207 |
| La$_8$Ti$_6$Ni$_2$       | -4.99    | 209.1859679 | 1.321161  |
| Ba$_7$Y$_1$Nb$_8$        | -4.371   | 209.4363698 | 1.6406269 |
| Sr$_4$Ho$_4$V$_8$        | -3.774   | 209.6228074 | 1.9487386 |
| Nd$_8$Fe$_8$             | -3.758   | 209.664647  | 1.9569962 |
| Cs$_4$Sr$_4$Ta$_4$Nb$_4$ | -4.009   | 209.9136423 | 1.8274551 |
| Sr$_6$Ca$_2$Ta$_2$Nb$_6$ | -4.687   | 209.943203  | 1.4775393 |
| Pr$_8$Mg$_1$Ti$_7$       | -5.298   | 210.4523238 | 1.1622022 |
| Ba$_8$Ta$_8$             | -5.015   | 210.9038548 | 1.3082585 |
| Sr$_6$La$_2$Ti$_2$Nb$_6$ | -4.74    | 212.2648043 | 1.450186  |
| Ba$_4$Ca$_4$Ta$_2$Nb$_6$ | -4.635   | 212.9354669 | 1.5043765 |
| Sr$_7$La$_1$Nb$_8$       | -4.72    | 213.7727035 | 1.460508  |
| Pr$_8$Ti$_7$Co$_1$       | -4.928   | 214.644144  | 1.3531592 |
| Ba$_6$Ca$_2$Ta$_4$Nb$_4$ | -4.66    | 214.8524421 | 1.491474  |
| Sr$_4$Ca$_4$Ta$_2$Nb$_6$ | -4.802   | 215.8521474 | 1.481878  |
| Pr$_8$Ti$_7$Fe$_1$       | -5.027   | 215.9098962 | 1.3020653 |
| La$_8$Ti$_7$Ni$_1$       | -5.235   | 218.3884391 | 1.1947165 |
| La$_8$Ti$_7$Cr$_1$       | -5.436   | 219.6287782 | 1.0909804 |
| Ba$_6$Mg$_2$Nb$_6$Sb$_2$ | -4.002   | 220.0568788 | 1.8310678 |
| Ca$_4$Mg$_4$Nb$_6$Sb$_2$ | -4.178   | 220.1984921 | 1.7402342 |
| Pr$_8$Ti$_7$Mn$_1$       | -4.97    | 221.1929638 | 1.331483  |
| Ba$_2$Y$_6$Ti$_8$        | -5.063   | 221.2097192 | 1.2834857 |
| Ba$_4$Sr$_4$Ta$_6$Nb$_2$ | -4.988   | 222.1096144 | 1.3221932 |
| Gd$_4$Y$_4$Ti$_8$        | -5.261   | 223.2232883 | 1.1812979 |
| Sr$_4$La$_4$Mn$_4$V$_4$  | -4.279   | 223.3158167 | 1.6881081 |
| Ba$_4$La$_4$Sc$_4$Nb$_4$ | -4.815   | 223.6994084 | 1.4114785 |
| Sr$_8$Ta$_4$Nb$_4$       | -4.747   | 223.9336773 | 1.4465733 |
| Compound                | Enthalpy (kJ/mol) | Mass (g/mol) | Density (g/cm³) |
|-------------------------|-------------------|--------------|-----------------|
| Sr 6 Nb 8 Zn 2          | -3.94             | 225.5699242  | 1.863066        |
| Ba 2 Ca 6 Ta 2 Nb 6     | -4.818            | 226.1148428  | 1.409302        |
| Y 8 Ti 8                | -5.267            | 226.6055355  | 1.178203        |
| Gd 2 Y 6 Ti 8           | -5.184            | 226.6300369  | 1.221037        |
| Sr 7 La 1 Ta 1 Nb 7     | -4.794            | 226.8685378  | 1.422166        |
| Ba 4 Mg 4 Nb 6 V 2      | -3.856            | 226.8948847  | 1.906418        |
| Ba 6 Mg 2 Nb 8          | -4.354            | 226.9594893  | 1.649406        |
| Sr 4 Mg 4 Nb 6 Sn 2     | -3.98             | 227.4714334  | 1.842422        |
| Ba 2 Sr 6 Ta 6 Nb 2     | -5.076            | 227.7974528  | 1.276776        |
| Pr 8 Ti 7 Cr 1          | -5.01             | 227.9517443  | 1.310839        |
| Sr 7 Y 1 Nb 8           | -4.605            | 231.6942373  | 1.519859        |
| Ba 6 La 2 Nb 8          | -4.768            | 232.1787163  | 1.435735        |
| Sm 2 Y 6 Ti 8           | -5.077            | 233.1787716  | 1.276263        |
| Sr 2 Gd 6 Zr 8          | -5.55             | 235.0221084  | 1.032145        |
| Ba 6 Be 2 V 8           | -3.735            | 235.2536458  | 1.968865        |
| Dy 2 Y 6 Ti 8           | -5.099            | 235.6434366  | 1.264906        |
| La 4 Gd 4 Ti 8          | -5.447            | 236.2242256  | 1.085303        |
| Ba 2 Mg 6 Nb 6 V 2      | -3.926            | 237.1545998  | 1.870291        |
| Ba 6 Sr 2 Ta 8          | -5.093            | 237.5077915  | 1.268002        |
| Sm 4 Y 4 Ti 8           | -5.136            | 237.8790076  | 1.245810        |
| Ba 4 Ca 4 Ta 4 Nb 4     | -4.789            | 239.304068   | 1.424897        |
| Ba 2 Ca 6 Ta 4 Nb 4     | -4.949            | 239.5476939  | 1.342321        |
| Sr 4 La 4 Ti 4 Nb 4     | -5.009            | 240.9512688  | 1.311351        |
| Pr 8 Ti 7 Ni 1          | -4.904            | 243.1548868  | 1.365546        |
| Nd 2 Y 6 Ti 8           | -5.072            | 243.2199713  | 1.278840        |
| Y 6 Ho 2 Ti 8           | -5.249            | 243.3991146  | 1.187491        |
| La 6 Gd 2 Ti 8          | -5.465            | 243.706318   | 1.076013        |
| Y 4 Ho 4 Ti 8           | -5.17             | 243.9996936  | 1.228263        |
| Ba 6 Ca 2 Ta 6 Nb 2     | -4.874            | 244.2546365  | 1.381028        |
| Dy 4 Y 4 Ti 8           | -5.163            | 244.5245876  | 1.231875        |
| Sr 4 Ca 4 Ta 4 Nb 4     | -4.959            | 245.4103161  | 1.337160        |
| La 8 Ti 8               | -5.48             | 246.4684103  | 1.068272        |
| La 6 Nd 2 Ti 8          | -5.463            | 251.2792133  | 1.077045        |
| Nd 4 Y 4 Ti 8           | -5.138            | 251.445118   | 1.244778        |
| La 6 Sm 2 Ti 8          | -5.481            | 251.5113026  | 1.067759        |
| Sr 2 La 6 Zr 8          | -5.779            | 252.4443771  | 0.913958        |
| La 4 Sm 4 Ti 8          | -5.498            | 252.901195   | 1.058922        |
| La 4 Nd 4 Ti 8          | -5.511            | 256.0507663  | 1.052279        |
| Ba 6 La 2 Ta 2 Nb 6     | -4.92             | 257.1685036  | 1.357288        |
| Formula          | Z    | A    | E  | M  |
|------------------|------|------|----|----|
| Ba 4 La 4 Ti 4 Nb 4 | -4.88 | 257.6405743 | 1.377932 |
| Ba 2 Gd 6 Zr 8    | -5.489 | 258.4532996 | 1.0636271 |
| Mg 4 Be 4 Nb 6 V 2 | -3.911 | 258.6344448 | 1.8780329 |
| Ba 4 Mg 4 Nb 6 Sb 2 | -4.013 | 259.2541111 | 1.8253907 |
| Ba 6 Mg 2 Ta 2 Nb 6 | -4.478 | 260.308348 | 1.5854042 |
| Sr 6 La 2 Nb 8    | -5.011 | 260.7680671 | 1.3103229 |
| Ba 4 Sr 4 Ta 8    | -5.177 | 262.6434783 | 1.2246503 |
| La 6 Dy 2 Ti 8    | -5.496 | 264.2004676 | 1.0600144 |
| Ba 2 Mg 6 Nb 6 Sb 2 | -3.868 | 265.6190762 | 1.9002252 |
| Ba 6 Be 2 Nb 8    | -4.114 | 265.9307854 | 1.7732646 |
| Ca 4 Be 4 Nb 6 V 2 | -4.107 | 265.9527535 | 1.7768773 |
| Ba 2 Sr 6 Ta 8    | -5.299 | 266.0086215 | 1.1616861 |
| La 6 Ho 2 Ti 8    | -5.478 | 266.4261456 | 1.0693042 |
| La 4 Dy 4 Ti 8    | -5.385 | 267.523775 | 1.1173015 |
| Ba 2 La 6 Zr 8    | -5.765 | 267.6241343 | 0.9211835 |
| Ba 2 Ca 6 Ta 6 Nb 2 | -5.164 | 267.8973315 | 1.2313596 |
| La 4 Ho 4 Ti 8    | -5.374 | 267.908381 | 1.1229786 |
| Ca 2 Pr 6 Zr 8    | -4.947 | 268.0430126 | 1.3433533 |
| Ba 4 Ca 4 Nb 4 Sn 4 | -4.673 | 268.6707983 | 1.4847647 |
| Sr 8 Ta 8         | -5.383 | 269.8680148 | 1.1183337 |
| Ba 4 Ca 4 Ta 6 Nb 2 | -4.998 | 271.1511691 | 1.3170322 |
| Pr 8 Ti 8         | -4.894 | 271.369469 | 1.3707066 |
| Pr 4 Gd 4 Ti 8    | -5.488 | 272.167255 | 1.0641432 |
| Sm 8 Fe 8         | -3.981 | 272.5906925 | 1.8419059 |
| Sr 4 La 4 Mn 4 Nb 4 | -3.877 | 272.9475976 | 1.8955803 |
| Ba 2 Pr 6 Zr 8    | -5.181 | 273.1130749 | 1.2225859 |
| Sr 4 Mg 4 Ta 2 Nb 6 | -4.627 | 273.4246029 | 1.5085053 |
| Ba 8 Nb 6 P 2     | -4.379 | 273.9833432 | 1.6364981 |
| Dy 8 Ti 8         | -4.859 | 274.1533898 | 1.3887701 |
| Pr 6 Gd 2 Ti 8    | -5.521 | 274.531112 | 1.0471119 |
| Ba 4 Be 4 P 8     | -3.798 | 277.0448981 | 1.9363522 |
| Sr 4 Ca 4 Ta 6 Nb 2 | -5.195 | 278.5899538 | 1.2153605 |
| Ba 6 Ca 2 Ta 8    | -5.052 | 280.1483309 | 1.2891628 |
| Ba 2 Gd 6 V 8     | -4.149 | 281.1283454 | 1.7552011 |
| Ca 2 La 6 Zr 8    | -5.641 | 282.3100719 | 0.9851799 |
| Pr 6 Nd 2 Ti 8    | -5.517 | 282.7867573 | 1.0491763 |
| Pr 6 Sm 2 Ti 8    | -5.539 | 285.0973467 | 1.0378221 |
| Pr 4 Nd 4 Ti 8    | -5.381 | 285.1635456 | 1.1193659 |
| Pr 4 Sm 4 Ti 8    | -5.329 | 287.2969744 | 1.1462031 |
| Compound                  | EN    | HX    | T (K)  |
|--------------------------|-------|-------|--------|
| Mg 8 Nb 8                | -4.193| 288.0949681 | 1.7324927 |
| Sr 6 La 2 Ta 2 Nb 6      | -5.157| 291.2874858 | 1.2349723 |
| Sr 4 Mg 4 V 8            | -3.716| 291.5373719 | 1.9786724 |
| Ba 2 Be 6 Nb 6 Sb 2      | -4.121| 291.6323008 | 1.7696519 |
| Ca 2 Y 6 Zr 8            | -4.754| 293.7693444 | 1.4429606 |
| Ca 4 Be 4 Nb 6 Sb 2      | -4.132| 293.7803865 | 1.7639748 |
| Ba 6 Mg 2 Ta 4 Nb 4      | -4.645| 293.8823319 | 1.4992155 |
| Sr 6 Y 2 Nb 8            | -4.805| 296.5861348 | 1.4166395 |
| Gd 8 Fe 8                | -4.163| 297.2489962 | 1.7479757 |
| Ba 6 Sr 2 Nb 6 P 2       | -4.451| 298.9706268 | 1.5993389 |
| Pr 6 Dy 2 Ti 8           | -5.389| 299.9005117 | 1.1152371 |
| Mg 4 Be 4 Nb 6 Sb 2      | -3.941| 301.2556711 | 1.8625499 |
| Pr 6 Ho 2 Ti 8           | -5.389| 302.1711897 | 1.1152371 |
| Ca 4 Mg 4 Ta 2 Nb 6      | -4.736| 303.3301676 | 1.4522504 |
| Ba 6 Y 2 Nb 8            | -4.574| 304.7165341 | 1.5358586 |
| Ba 4 Mg 4 Nb 8           | -4.312| 304.8564544 | 1.6710768 |
| Ba 2 Sr 6 Nb 6 P 2       | -4.454| 305.1630003 | 1.5977906 |
| Sr 4 Mg 4 Ta 4 Nb 4      | -4.79 | 305.3985607 | 1.424381 |
| Sr 2 Y 6 Zr 8            | -5.231| 307.4606496 | 1.1967809 |
| Ba 2 Ca 6 Ta 8           | -5.428| 308.2496992 | 1.0951092 |
| Sr 4 Nb 8 Zn 4           | -3.794| 310.2397585 | 1.9384166 |
| Ba 4 Ca 4 Ta 8           | -5.17 | 310.5627703 | 1.228263 |
| Gd 8 Zr 8                | -5.215| 310.9235588 | 1.2050385 |
| Ba 4 Be 4 Nb 6 V 2       | -3.838| 311.0434627 | 1.9157082 |
| Y 8 V 4 Co 4             | -3.696| 311.5036324 | 1.9889944 |
| Ba 6 Ca 2 Nb 6 P 2       | -4.39 | 311.6615712 | 1.630821 |
| Ca 8 Ta 8                | -5.504| 311.9451681 | 1.0558856 |
| Sr 4 Be 4 Nb 6 V 2       | -3.894| 311.9926853 | 1.8868066 |
| Ba 4 Sr 4 Nb 6 P 2       | -4.488| 312.838603  | 1.5802432 |
| Ba 6 Mg 2 Ta 6 Nb 2      | -4.836| 313.0747303 | 1.4006404 |
| Ba 6 Ta 4 Be 2 Nb 4      | -4.445| 314.47561   | 1.6024355 |
| Pr 4 Dy 4 Ti 8           | -5.326| 315.0423044 | 1.1477514 |
| Sr 4 Ca 4 Nb 6 P 2       | -4.514| 316.2233894 | 1.5668246 |
| Sr 4 Ca 4 Ta 8           | -5.403| 317.2833414 | 1.1080117 |
| Ba 4 Mg 4 Ta 2 Nb 6      | -4.395| 317.4336417 | 1.6282405 |
| Sr 2 Ca 6 Ta 8           | -5.487| 318.3605047 | 1.0646593 |
| Pr 4 Ho 4 Ti 8           | -5.327| 318.7761604 | 1.1472353 |
| Sn 8 Nb 8                | -4.047| 321.7170384 | 1.8078433 |
| Ba 6 Ta 2 Be 2 Nb 6      | -4.267| 323.1010727 | 1.6943013 |
| Compound                        | E (eV) | R (Å)   | a (Å)   |
|--------------------------------|--------|---------|---------|
| Ba₂Mg₆Nb₈                       | -4.376 | 324.0579403 | 1.6380464 |
| Ca₄Mg₄Ta₄Nb₄                    | -4.754 | 324.2318639 | 1.4429606 |
| Be₈Nb₈                          | -4.279 | 329.9820819 | 1.6881081 |
| Ba₄La₄Nb₈                       | -5.445 | 330.3324771 | 1.0863555 |
| Ba₂Ca₆Nb₆P₂                      | -4.538 | 330.4823082 | 1.5544382 |
| Ba₄Mg₄P₈                        | -3.739 | 331.3268273 | 1.9668021 |
| Ba₄Be₄Nb₆Sb₂                     | -3.843 | 332.8143604 | 1.9131277 |
| Ba₆Mg₂Nb₆P₂                      | -4.292 | 336.1468589 | 1.6813988 |
| Ca₈P₈                           | -4.031 | 337.7928885 | 1.8161009 |
| Sr₄Be₄Nb₆Sb₂                     | -3.921 | 339.5084858 | 1.8728719 |
| Ba₄Ca₄Nb₆P₂                      | -4.481 | 339.5402991 | 1.5838559 |
| Ba₂Y₆Zr₈                         | -5.206 | 342.0084068 | 1.2096834 |
| Pr₈Zr₈                           | -4.989 | 343.5227593 | 1.3216771 |
| Ba₂Mg₆Ta₂Nb₆                     | -4.413 | 344.5539466 | 1.6189507 |
| Sr₄Mg₄Ta₆Nb₂                     | -5.081 | 345.2035149 | 1.2741959 |
| Sr₄Ca₄Nb₂P₆                      | -3.687 | 351.3787036 | 1.9936393 |
| Sr₄Pr₄Nb₈                        | -5.106 | 351.9571832 | 1.2612934 |
| Ba₄Sr₄P₈                         | -3.992 | 353.1270473 | 1.8362288 |
| Ba₆Mg₂Ta₈                        | -5.097 | 354.1448787 | 1.2659383 |
| Sr₄La₄Nb₈                        | -5.373 | 355.3245442 | 1.1234947 |
| Ba₄Ca₄P₈                         | -3.911 | 355.8691466 | 1.8780329 |
| Ba₄Mg₄Ta₄Nb₄                     | -4.513 | 357.3496142 | 1.5673407 |
| La₆Gd₂Zr₈                        | -5.75  | 358.0368935 | 0.928925  |
| Ca₄La₄Nb₈                        | -5.354 | 359.280433  | 1.1333006 |
| Ba₆Be₂Nb₆P₂                      | -4.152 | 361.757423  | 1.7536528 |
| Ba₂Be₂Nb₂V₆                      | -3.88  | 362.8615167 | 1.894032  |
| La₄Pr₄Zr₈                        | -5.544 | 364.0537155 | 1.0352416 |
| Sr₄Be₄Nb₆P₂                      | -4.112 | 364.1594444 | 1.7742968 |
| La₆Pr₂Zr₈                        | -5.79  | 364.6195686 | 0.908281  |
| Ba₂Mg₆Ta₄Nb₄                     | -4.516 | 368.3499684 | 1.5657924 |
| Ca₄Mg₄Ta₆Nb₂                     | -5.161 | 369.6100602 | 1.2329079 |
| Ba₂Be₄Nb₈                        | -4.211 | 370.2481153 | 1.7232029 |
| Pr₄Y₄Zr₈                         | -4.749 | 372.5772305 | 1.4455411 |
| Mg₄Ta₂Be₄Nb₆                     | -4.355 | 374.0749294 | 1.6488845 |
| Ca₄Mg₄Nb₆P₂                      | -4.352 | 374.3624459 | 1.6504328 |
| Gd₂Y₆Zr₈                         | -5.007 | 374.8526061 | 1.3123873 |
| Pr₆Y₂Zr₈                         | -5.227 | 377.7253699 | 1.1988453 |
| Sr₄Mg₄Nb₆P₂                      | -4.28  | 377.8194065 | 1.687592  |
| Y₈Zr₈                            | -5.043 | 379.4084518 | 1.2938077 |

The table lists various compounds along with their computed electronic band gaps (E) and their atomic radii (R) and ionic radii (a) in Angstroms (Å). The data is presented in a tabular format with columns for compound formula, band gap, atomic radius, and ionic radius.
| Formula               | Energy  | Volume   | Density  |
|-----------------------|----------|----------|----------|
| Ca₄ Pr₄ Nb₈          | -5.047   | 379.878072 | 1.2917433 |
| Ca₄ Y₄ Nb₈           | -4.932   | 381.0413185 | 1.3510948 |
| La₄ Y₄ Zr₈           | -5.247   | 381.5196868 | 1.1885233 |
| La₆ Y₂ Zr₈           | -5.716   | 381.7289293 | 0.9464724  |
| Ca₄ Ta₂ Be₄ Nb₆      | -4.516   | 382.3764078 | 1.5657924 |
| Ba₄ Mg₄ Nb₆ P₂       | -4.251   | 383.9544594 | 1.7025589 |
| Ba₄ Ta₂ Be₄ Nb₆      | -4.332   | 384.6807636 | 1.6607548 |
| Ba₄ Mg₄ Ta₆ Nb₂      | -4.831   | 387.8405126 | 1.4032209 |
| Ba₄ Mg₄ Ta₈          | -5.227   | 388.1316609 | 1.1988453 |
| Mg₄ Ta₄ Be₄ Nb₄      | -4.494   | 390.292938  | 1.5771466 |
| Ba₄ Y₄ Nb₈           | -4.879   | 394.2733626 | 1.3784481 |
| Ba₂ Mg₆ Nb₆ P₂       | -4.214   | 395.2029872 | 1.7216546 |
| Ba₂ Be₆ Nb₆ V₂       | -3.779   | 396.0140714 | 1.9461581 |
| La₈ Zr₈              | -5.707   | 399.1731718 | 0.9511173 |
| Sr₄ Y₄ Nb₈           | -4.862   | 400.5209297 | 1.3872218 |
| Dy₈ Fe₈              | -4.189   | 401.8808547 | 1.7345571 |
| Ba₂ Mg₆ Nb₂ P₆       | -4.238   | 402.7754578 | 1.7092682 |
| Ba₄ Be₄ Nb₆ P₂       | -3.949   | 403.8763078 | 1.8584211 |
| Ca₄ Ta₄ Be₄ Nb₄      | -4.675   | 404.9666041 | 1.4837325 |
| Ba₂ Mg₆ Ta₆ Nb₂      | -4.891   | 405.6217028 | 1.3722549 |
| Ca₄ Mg₄ Nb₂ P₆       | -5.244   | 405.9704678 | 1.1900716 |
| Pr₈ Hf₈              | -5.209   | 412.0264043 | 1.2081351 |
| Mg₄ Be₄ Nb₂ P₆       | -4.635   | 414.0005678 | 1.5043765 |
| Sr₄ Be₄ Nb₂ P₆       | -4.576   | 414.2337517 | 1.5348264 |
| Sn₈ Ta₈              | -4.535   | 415.898156  | 1.5559865 |
| Ba₄ Ta₄ Be₄ Nb₄      | -4.597   | 418.250412  | 1.5239883 |
| Sr₂ La₆ Nb₈          | -5.586   | 422.0387714 | 1.0135654 |
| Ba₄ La₄ Ta₄ Nb₄      | -5.636   | 425.2400516 | 0.9877604 |
| Sr₄ La₄ Ta₄ Nb₄      | -5.558   | 426.3978816 | 1.0280162 |
| Mg₈ Ta₈              | -5.157   | 427.1857634 | 1.2349723 |
| Ba₂ La₆ Nb₈          | -5.607   | 428.8967378 | 1.0027273 |
| Ba₂ Be₆ Nb₆ P₂       | -4.396   | 431.0916661 | 1.6277244 |
| Ca₄ Ta₆ Be₄ Nb₂      | -4.749   | 434.8158005 | 1.4455411 |
| Ho₈ Fe₈              | -4.214   | 435.182352  | 1.7216546 |
| Sr₄ Ta₂ Be₄ Nb₆      | -4.208   | 437.2231718 | 1.7247512 |
| Mg₄ Ta₆ Be₄ Nb₂      | -4.806   | 438.3106966 | 1.4161234 |
| Ba₄ Be₄ Nb₄ P₄       | -3.992   | 439.8357503 | 1.8362288 |
| Y₈ Hf₈               | -5.141   | 442.1726608 | 1.2432299 |
| Ca₄ Be₄ Nb₂ P₆       | -5.397   | 446.4878221 | 1.1111083 |
| Compound               | Energy   | Total Charge | Spin-orbit Energy |
|------------------------|----------|--------------|-------------------|
| Pr₄Ba₄Ta₇Co₁           | -5.285   | 447.6581283  | 1.1689115         |
| Ta₈Be₈                 | -5.189   | 447.7032683  | 1.2184571         |
| Ca₄Be₄Nb₆P₂            | -4.385   | 448.4532609  | 1.6334015         |
| Ca₂La₆Nb₈              | -5.405   | 448.7119658  | 1.1069795         |
| Gd₈Hf₈                 | -5.42    | 449.0595573  | 1.099238          |
| Dy₈Zr₈                 | -4.861   | 449.8627258  | 1.3877379         |
| Ba₂Ta₄Be₆Nb₄           | -4.251   | 451.5565203  | 1.7025589         |
| Ba₂Mg₆Ta₈              | -5.182   | 455.6601872  | 1.2220698         |
| Sr₂Y₆Nb₈               | -4.909   | 457.5867246  | 1.3629651         |
| Sr₄Ta₄Be₄Nb₄           | -4.372   | 463.7801295  | 1.6401108         |
| Pr₄Ba₄Ta₇Ni₁           | -5.228   | 464.360835   | 1.1983292         |
| Ca₂Y₆Nb₈               | -4.835   | 466.627169   | 1.4011565         |
| Ba₄Ta₆Be₄Nb₂            | -4.742   | 466.9273104  | 1.4491538         |
| Dy₈Hf₈                 | -5.014   | 471.1606368  | 1.3087746         |
| Ba₄Ta₈Be₄              | -4.847   | 471.2837088  | 1.3949633         |
| Pr₄Ba₄Ta₇Fe₁           | -5.243   | 471.4585847  | 1.1905877         |
| Ba₄La₄Ta₈              | -6.079   | 471.8876719  | 0.7591281         |
| Ca₂Pr₆Nb₈              | -4.863   | 474.202993   | 1.3867057         |
| Ba₆Ta₆Be₂Nb₂            | -4.28    | 476.7952584  | 1.687592          |
| Ba₂Be₆Nb₈              | -3.889   | 481.722236   | 1.8893871         |
| Sr₄Ta₆Be₄Nb₂            | -4.868   | 485.225873   | 1.3841252         |
| Sr₄La₄Ta₈              | -6.247   | 485.7882519  | 0.6724233         |
| La₄Y₄Nb₈               | -5.015   | 487.014634   | 1.3082585         |
| Ba₂Y₆Nb₈               | -4.936   | 487.026441   | 1.3490304         |
| Gd₈Nb₈                 | -5.222   | 497.9724245  | 1.2014258         |
| Ba₆Ta₈Be₂              | -4.482   | 499.4019068  | 1.5833398         |
| Ba₄Pr₄Ta₈              | -5.627   | 501.1383244  | 0.9924053         |
| Pr₄Y₄Nb₈               | -4.573   | 503.216273   | 1.5363747         |
| Ba₂Ta₆Be₆Nb₂            | -4.522   | 505.7371255  | 1.5626958         |
| Sr₄Pr₄Ta₈              | -5.811   | 505.8104044  | 0.8974429         |
| Ba₂Ta₂Be₆Nb₆            | -4.053   | 508.308372   | 1.8047467         |
| Mg₄Be₄Nb₆P₂            | -4.341   | 509.2092472  | 1.6561099         |
| Gd₂Y₆Nb₈               | -5.084   | 510.3008083  | 1.2726476         |
| Ca₄La₄Ta₈              | -6.046   | 512.9320785  | 0.7761594         |
| La₆Pr₂Nb₈              | -5.371   | 514.273193   | 1.1245269         |
| La₆Y₂Nb₈               | -5.387   | 514.6825663  | 1.1162693         |
| Sr₄Gd₄Ta₈              | -5.911   | 515.9205146  | 0.8458329         |
| La₄Pr₄Nb₈               | -5.223   | 518.3336375  | 1.2009097         |
| Pr₆Gd₂Zr₈               | -5.102   | 518.7898341  | 1.2633578         |
| Compound | Energy (eV) | Atomic Volume (Å³) | Density (g/cm³) |
|----------|------------|--------------------|-----------------|
| Sr₄Be₄Nb₄P₄ | -5.275 | 519.7996748 | 1.1740725 |
| La₈Hf₈ | -6.182 | 529.7174568 | 0.7059698 |
| Ca₄Pr₄Ta₈ | -5.745 | 530.394481 | 0.9315055 |
| Pr₆Y₂Nb₈ | -4.825 | 534.1883998 | 1.4063175 |
| Pr₈Nb₈ | -4.787 | 534.7732765 | 1.4259293 |
| Sr₄Y₄Ta₈ | -5.791 | 554.6464916 | 0.9077649 |
| Ca₄Y₄Ta₈ | -5.762 | 565.1683183 | 0.9227318 |
| Ba₄Y₄Ta₈ | -5.584 | 565.4239116 | 1.0145976 |
| Mg₄Be₄Nb₄P₄ | -4.484 | 593.6862683 | 1.5823076 |
| Ba₂La₆Ta₈ | -6.333 | 597.2868305 | 0.6280387 |
| Sr₂Y₆Ta₈ | -5.045 | 597.8586051 | 1.2927755 |
| Ca₄Mg₄Nb₄P₄ | -4.747 | 599.3085611 | 1.4465733 |
| Ba₂Pr₆Ta₈ | -5.791 | 616.7271842 | 0.9077649 |
| Sr₂Pr₆Ta₈ | -5.579 | 618.0803492 | 1.0171781 |
| Ca₂La₆Ta₈ | -6.022 | 620.4809088 | 0.7885458 |
| Ba₂Be₆Nb₄P₄ | -4.949 | 633.5116084 | 1.3423211 |
| Ca₂Pr₆Ta₈ | -5.406 | 639.6595125 | 1.1064634 |
| Gd₄Y₄Zr₈ | -4.805 | 641.6222605 | 1.4166395 |
| Ca₂Y₆Ta₈ | -5.358 | 654.2530184 | 1.1312362 |
| La₄Gd₄Ta₈ | -5.667 | 657.3217518 | 0.9717613 |
| Ba₂Ta₈Be₆ | -4.873 | 657.7762306 | 1.3815447 |
| La₄Y₄Ta₈ | -5.509 | 658.5532288 | 1.0533051 |
| Ca₄Be₄Nb₄P₄ | -4.79 | 667.5458103 | 1.424381 |
| Pr₆Y₂Ta₈ | -5.161 | 675.5924627 | 1.2329079 |
| Ba₂Y₆Ta₈ | -5.495 | 679.8019401 | 1.0605305 |
| La₄Pr₄Ta₈ | -5.686 | 681.163915 | 0.9619554 |
| La₆Y₂Ta₈ | -6.074 | 706.9193589 | 0.7617086 |
| La₆Gd₂Ta₈ | -5.99 | 713.5218704 | 0.805061 |
| Pr₈Ta₈ | -5.272 | 714.231794 | 1.1756208 |
| Y₈Ta₈ | -5.492 | 716.2712185 | 1.0620788 |
| Na₈W₈ | -4.24 | 788.3085054 | 1.708236 |
| Rb₈W₈ | -3.856 | 823.499985 | 1.9064184 |
| Gd₄Y₄Ta₈ | -5.108 | 825.3697415 | 1.2602612 |
| K₈W₈ | -4.09 | 833.6198024 | 1.785651 |
| Li₈W₈ | -4.669 | 834.3553131 | 1.4868291 |
| Gd₈Ta₈ | -5.581 | 850.9305145 | 1.0161459 |
| Gd₂Y₆Ta₈ | -5.501 | 964.85623 | 1.0574339 |
| Pr₆Gd₂Nb₈ | -4.135 | 1143.189189 | 1.7624265 |
| Y₈Mn₂Cr₆ | -3.652 | 46.94788464 | 2.0117028 |
| Compound                     | Energy  | Volume   | Pressure |
|------------------------------|---------|----------|----------|
| La₆Mn₈Zn₂                    | -3.647  | 150.8927751 | 2.0142833 |
| Ba₄Be₄V₈                     | -3.646  | 283.708755  | 2.0147994 |
| Sr₇La₁Nb₁V₇                  | -3.643  | 49.05215295  | 2.0163477 |
| Rb₄Ba₄Nb₈                    | -3.642  | 62.80219426  | 2.0168638 |
| Ba₆Ca₂Nb₁V₄                  | -3.641  | 56.17513989  | 2.0173799 |
| La₈Fe₆Co₂                    | -3.641  | 19.60661749  | 2.0173799 |
| La₈Sc₇Mn₁                    | -3.639  | 10.21457362  | 2.0184121 |
| Dy₂Y₆Cr₈                     | -3.639  | 21.35923873  | 2.0184121 |
| Dy₂Y₆Mn₈                     | -3.636  | 80.01033801  | 2.0199604 |
| Sr₆Ca₂Nb₂V₆                  | -3.635  | 60.25410307  | 2.0204765 |
| Ba₄Be₄Nb₄V₄                  | -3.634  | 240.3683101  | 2.0209926 |
| Y₈Cr₈                       | -3.633  | 14.20080551  | 2.0215087 |
| Y₆Mn₆Nb₂Zn₂                  | -3.632  | 106.173741   | 2.0220248 |
| Sr₄Pr₄V₈                     | -3.63   | 55.37856741  | 2.023057 |
| Y₆Ho₂Cr₈                    | -3.629  | 21.28299412  | 2.0235731 |
| Y₈Mn₆Cr₂                    | -3.629  | 74.33015417  | 2.0235731 |
| Y₆Ho₂Mn₈                    | -3.628  | 81.52484037  | 2.0240892 |
| La₈Cr₁Fe₇                    | -3.628  | 0           | 2.0240892 |
| Pr₆Gd₂Cr₈                    | -3.623  | 0           | 2.0266697 |
| Sr₇Pr₁V₈                     | -3.621  | 47.45505883  | 2.0277019 |
| Ba₄Ca₄Nb₂V₆                  | -3.62   | 95.56531846  | 2.028218 |
| Dy₄Y₄Cr₈                    | -3.62   | 28.48129225  | 2.028218 |
| Y₄Ho₄Cr₈                    | -3.62   | 28.31793275  | 2.028218 |
| Sm₂Y₆Cr₈                    | -3.62   | 24.23727725  | 2.028218 |
| Sm₂Y₆Mn₈                    | -3.62   | 75.3901819   | 2.028218 |
| Ca₂La₆Fe₈                    | -3.619  | 30.097613    | 2.0287341 |
| Sr₇La₁Ti₁V₇                  | -3.618  | 46.32128289  | 2.0292502 |
| Ba₄Ca₄Nb₄V₄                  | -3.617  | 65.81982707  | 2.0297663 |
| Rb₂Sr₆Nb₆V₂                  | -3.616  | 61.38546468  | 2.0302824 |
| Sr₄La₄V₄Fe₄                  | -3.616  | 291.4239606  | 2.0302824 |
| Sr₂Ca₆V₈                     | -3.615  | 55.90022852  | 2.0307985 |
| Sr₈V₆Ru₂                     | -3.614  | 120.7894214  | 2.0313146 |
| La₈Mg₁Fe₇                    | -3.614  | 0           | 2.0313146 |
| Sr₈V₇Ir₁                     | -3.613  | 107.5008667  | 2.0318307 |
| Y₈Mn₇Cr₁                    | -3.607  | 73.72591205  | 2.0349273 |
| Sr₇Ca₁Ta₁V₇                  | -3.605  | 54.21609389  | 2.0359595 |
| Y₈Mn₇Fe₁                     | -3.602  | 71.43710228  | 2.0375078 |
| Nd₂Y₆Mn₈                     | -3.596  | 73.71204324  | 2.0406044 |
| Cs₂Ba₆Nb₆Cr₂                  | -3.595  | 92.28414441  | 2.0411205 |
| Composition          | U       | Z       | E       |
|----------------------|---------|---------|---------|
| Sr8 V7 Ru1           | -3.592  | 86.12115537 | 2.0426688 |
| Y8 Mn7 Co1           | -3.592  | 90.62760009  | 2.0426688 |
| La8 Sc7 Fe1          | -3.591  | 0        | 2.0431849 |
| Nd2 Y6 Cr1           | -3.591  | 8.708584563 | 2.0431849 |
| Ba8 Zr3 Fe1 Mo4      | -3.59   | 0        | 2.043701  |
| Sr2 La6 Fe8          | -3.59   | 20.11485193 | 2.043701  |
| Pr8 Mn4 Fe4          | -3.589  | 41.26255301 | 2.0442171 |
| Sr6 La2 V6 Fe2       | -3.588  | 159.6581541 | 2.0447332 |
| Sr7 La1 V7 Cr1       | -3.587  | 58.23287169 | 2.0452493 |
| Sm4 Y4 Cr8           | -3.587  | 32.386499   | 2.0452493 |
| Pr6 Gd2 Mn8          | -3.587  | 0        | 2.0452493 |
| La8 Mg2 Fe6          | -3.586  | 0        | 2.0457654 |
| Sr8 P8               | -3.584  | 273.8724038 | 2.0467976 |
| Sm4 Y4 Mn8           | -3.584  | 74.99294386 | 2.0467976 |
| Sr7 Sm1 V8           | -3.582  | 47.97785783 | 2.0478298 |
| Ba4 Y4 V8            | -3.58   | 91.32822007 | 2.048862  |
| Pr4 Nd4 Cr8          | -3.579  | 4.297546625 | 2.0493781 |
| Sr7 Nd1 V8           | -3.578  | 45.4834942 | 2.0498942 |
| Ba8 Tc8              | -3.576  | 27.00946567 | 2.0509264 |
| Sr7 Ho1 V8           | -3.574  | 55.84449382 | 2.0519586 |
| Pr6 Sm2 Cr8          | -3.574  | 41.88180175 | 2.0519586 |
| Y8 Mn4 Cr4           | -3.574  | 71.35388842 | 2.0519586 |
| La8 Sc4 Mn4          | -3.573  | 0        | 2.0524747 |
| Sr7 Dy1 V8           | -3.572  | 54.23952545 | 2.0529908 |
| Sr7 Y1 V8            | -3.572  | 52.33504732 | 2.0529908 |
| Pr8 Mn6 Fe2          | -3.572  | 42.46560822 | 2.0529908 |
| Sr4 Ca4 V8           | -3.571  | 64.07546051 | 2.0535069 |
| Ba6 Ca2 P8           | -3.571  | 279.5381777 | 2.0535069 |
| La8 Mg1 Cr7          | -3.571  | 0        | 2.0535069 |
| Pr4 Sm4 Cr8          | -3.57   | 43.085182  | 2.054023  |
| Sr8 V6 Ir2           | -3.567  | 174.8225942 | 2.0555713 |
| Pr8 Cr8              | -3.565  | 39.2066715  | 2.0566035 |
| Pr6 Nd2 Cr8          | -3.564  | 21.85460906 | 2.0571196 |
| Y8 Mn7 Ni1           | -3.564  | 131.6255928 | 2.0571196 |
| Pr6 Dy2 Cr8          | -3.563  | 46.49619837 | 2.0576357 |
| Nd4 Y4 Cr8           | -3.562  | 0        | 2.0581518 |
| Sr8 V7 Si1           | -3.556  | 75.88967878 | 2.0612484 |
| Pr6 Ho2 Cr8          | -3.556  | 47.86751862 | 2.0612484 |
| Sr8 Ti1 V7           | -3.555  | 0        | 2.0617645 |
| Compound                  | Energy  | Lattice Constant | 
|---------------------------|---------|------------------|
| Sr6Mg2V8                  | -3.555  | 118.9471195      |
| Cs2Sr6Nb6V2               | -3.551  | 92.03589372      |
| Ba2Ca6V8                  | -3.549  | 84.34482786      |
| Sr8Ta1V7                  | -3.549  | 0                |
| Sr8V7Ge1                  | -3.549  | 56.43216097      |
| Ba6Mg2Nb4V4               | -3.547  | 128.8225827      |
| Pr4Dy4Cr8                 | -3.547  | 47.29397525      |
| Ba2Ca6Nb2P6               | -3.546  | 337.0767138      |
| Pr4Ho4Cr8                 | -3.546  | 48.70161575      |
| Ba2Sr6Nb2V6               | -3.543  | 48.78353878      |
| Ba2Ho6Fe8                 | -3.543  | 341.9985914      |
| Sr8Nb4Sn4                 | -3.543  | 140.1736539      |
| Sr7Mg1V8                  | -3.542  | 83.1035044       |
| Y6Ta2Zn2Fe6               | -3.542  | 128.6629375      |
| Pr4Dy4Mn8                 | -3.541  | 75.82852968      |
| Ca2La6Cr8                 | -3.539  | 20.68210087      |
| Pr4Ho4Mn8                 | -3.538  | 80.3685148       |
| Nd4Y4Mn8                  | -3.537  | 69.39216655      |
| Sr7Ca1Nb1V7               | -3.536  | 51.60750954      |
| Pr8Mn7Fe1                 | -3.535  | 43.36838582      |
| Mg4Be4Nb4V4               | -3.533  | 183.3789687      |
| Ba1Sr7V8                  | -3.533  | 53.77318896      |
| Ba8Os8                    | -3.533  | 257.2098019      |
| Sr4Mg4Nb4V4               | -3.531  | 97.06873331      |
| Y8Mg1Mn7                  | -3.527  | 0                |
| Ba8Zr5Nb2Fe1              | -3.526  | 0                |
| Pr6Nd2Mn8                 | -3.525  | 48.16978836      |
| Sr6La2Sc2V6               | -3.524  | 71.55859051      |
| Y7Mn8Zn1                  | -3.523  | 115.18613        |
| La6Ta2Zn2Co6              | -3.523  | 228.8621857      |
| Cs4Ba4Nb8                 | -3.521  | 148.8194906      |
| Sr8V7Rh1                  | -3.521  | 97.02720599      |
| Ba6Sr2Nb4V4               | -3.52   | 29.05139001      |
| Ba2Sr6V8                  | -3.52   | 66.15898863      |
| Pr8Mn8                    | -3.52   | 46.28266343      |
| Pr4Nd4Mn8                 | -3.519  | 49.8721633       |
| Pr6Sm2Mn8                 | -3.519  | 53.40592702      |
| Sr8Mn1V7                  | -3.517  | 79.35437177      |
| Rb2Sr6Mn2Nb6              | -3.517  | 32.20432192      |
| Formula               | E [eV] | \(Z\)       | \(r_{\text{min}}\) [Å] |
|-----------------------|--------|-------------|------------------------|
| Sr6La2V6Co2          | -3.515 | 134.8743998 | 2.0824085              |
| Ba2La6Fe8            | -3.515 | 32.33677783 | 2.0824085              |
| Y6Hf2Mn6Zn2          | -3.512 | 117.7262753 | 2.0839568              |
| Pr8V4Ni4             | -3.512 | 156.8641461 | 2.0839568              |
| Sr7La1V7Fe1          | -3.508 | 106.9810217 | 2.0860212              |
| Y6Zr2Mn6Zn2          | -3.508 | 122.4617856 | 2.0860212              |
| Pr4Sm4Mn8            | -3.508 | 59.22394061 | 2.0860212              |
| Ba6Bi2Zr7Fe1         | -3.506 | 12.59130455 | 2.0870534              |
| Cs8Mo8               | -3.504 | 302.580573  | 2.0880856              |
| Sr8Nb1V7             | -3.504 | 66.68046411 | 2.0880856              |
| Pr6Ho2Mn8            | -3.504 | 231.7167532 | 2.0880856              |
| La6Nb2Zn2Co6         | -3.504 | 71.61625693 | 2.0886017              |
| Y8Cr6Co2             | -3.503 | 63.79322155 | 2.0886017              |
| Pr6Dy2Mn8            | -3.498 | 61.22053363 | 2.0911822              |
| Sr8V7Sn1             | -3.496 | 103.4615302 | 2.0922144              |
| Y8Mn6Co2             | -3.495 | 107.4505483 | 2.0927305              |
| Pr6Ta2Mn6Zn2         | -3.495 | 43.00865621 | 2.0927305              |
| Y8Cr7Co1             | -3.495 | 47.1022917  | 2.0932466              |
| La8Mn4Co4            | -3.493 | 89.60772056 | 2.0937627              |
| Rb4Sr4V4Cr4          | -3.492 | 341.1188531 | 2.0942788              |
| Pr6Mn6Nb2Zn2         | -3.492 | 105.2166135 | 2.0942788              |
| Pr8Mn7Cr1            | -3.49  | 49.98828944 | 2.095311               |
| Ba2Dy6Fe8            | -3.482 | 317.6341138 | 2.0994398              |
| La6Ti2Zn2Fe6         | -3.481 | 99.62389225 | 2.0999559              |
| Sr4La4V4Co4          | -3.479 | 202.3254136 | 2.1009881              |
| Pr8Mn7Ni1            | -3.476 | 117.8260863 | 2.1025364              |
| Sr8Hf1V7             | -3.475 | 49.46402457 | 2.1030525              |
| Ba4Be4Nb2V6          | -3.475 | 329.8419076 | 2.1030525              |
| Gd4Y4Fe8             | -3.475 | 99.62389225 | 2.0999559              |
| Sr8Ti2V6             | -3.473 | 202.3254136 | 2.1009881              |
| Pr8Mn6Cr2            | -3.47  | 55.75116544 | 2.105633               |
| La6Zn2Fe8            | -3.47  | 160.7067649 | 2.105633               |
| Ca4Mg4Nb2V6          | -3.469 | 122.182606  | 2.1061491              |
| La6Zr2Zn2Fe6         | -3.469 | 120.060477  | 2.1061491              |
| Pr8Mg1Mn7            | -3.468 | 132.1043816 | 2.1071813              |
| Sr8V7Pt1             | -3.467 | 28.97125149 | 2.1071813              |
| Y8Sc4Fe4             | -3.467 | 2.0922144   | 2.1071813              |
| Pr4Gd4Fe8            | -3.467 | 0           | 2.1071813              |
| Element | \( \text{M} \) | \( \text{E} \) | \( \text{D} \) | \( \text{S} \) |
|---------|-------------|-------------|-------------|-------------|
| Sr 8 V 4 Ir 4 | -3.466 | 283.9096431 | 2.1076974 |
| Sr 7 La 1 Mn 1 V 7 | -3.463 | 84.52432151 | 2.1092457 |
| Y 6 Ti 2 Mn 6 Zn 2 | -3.462 | 115.6088227 | 2.1097618 |
| Sr 4 Be 4 Nb 4 V 4 | -3.46 | 257.8464066 | 2.110794 |
| Pr 8 Mn 2 Cr 6 | -3.459 | 53.24791948 | 2.1113101 |
| La 8 Sc 6 Cr 2 | -3.457 | 0 | 2.1123423 |
| Rb 2 Sr 6 Nb 6 Fe 2 | -3.456 | 43.6568041 | 2.1128584 |
| La 6 Hf 2 Zn 2 Fe 6 | -3.456 | 156.4194232 | 2.1128584 |
| Sr 7 La 1 Sc 1 V 7 | -3.455 | 63.6197399 | 2.1133745 |
| La 5 Mn 8 Zn 3 | -3.455 | 223.0396627 | 2.1133745 |
| La 8 Cr 6 Ni 2 | -3.454 | 91.92942343 | 2.1138906 |
| Pr 8 Mn 1 Cr 7 | -3.453 | 47.00904549 | 2.1144067 |
| Gd 2 Y 6 Cr 8 | -3.452 | 0 | 2.1149228 |
| Ba 4 Sr 4 Nb 2 V 6 | -3.45 | 62.78738811 | 2.115955 |
| Sr 8 V 4 Pt 4 | -3.446 | 383.7488441 | 2.1180194 |
| Y 8 Cr 4 Fe 4 | -3.446 | 25.00017737 | 2.1180194 |
| Y 8 Cr 7 Fe 1 | -3.445 | 18.84638853 | 2.1185355 |
| Ba 2 Sr 6 Ta 2 V 6 | -3.441 | 51.8164575 | 2.1205999 |
| Pr 8 Mn 7 Co 1 | -3.44 | 68.96234359 | 2.1205999 |
| Ba 1 Sr 7 Ta 1 V 7 | -3.439 | 51.6929234 | 2.1216321 |
| Ba 4 Ca 4 Nb 2 P 6 | -3.437 | 299.1919398 | 2.1226643 |
| Sr 8 Zr 2 V 6 | -3.436 | 43.3794441 | 2.1231804 |
| Sr 8 Hf 2 V 6 | -3.433 | 53.30240985 | 2.1247287 |
| Y 8 V 4 Ni 4 | -3.43 | 86.26435335 | 2.126277 |
| Ba 6 Ca 2 Nb 2 V 6 | -3.429 | 93.42343185 | 2.1267931 |
| Sr 8 V 6 Sn 2 | -3.429 | 77.46542796 | 2.1267931 |
| Sr 7 Ca 1 Mn 1 V 7 | -3.428 | 94.83641025 | 2.1273092 |
| Pr 6 Gd 2 Fe 8 | -3.428 | 0 | 2.1273092 |
| Ba 6 Be 2 Nb 4 V 4 | -3.427 | 154.3022009 | 2.1278253 |
| Ba 8 Fe 4 Re 4 | -3.427 | 0.758438 | 2.1278253 |
| Sr 8 V 4 Si 4 | -3.425 | 160.7070472 | 2.1288575 |
| Ba 4 Sr 4 V 8 | -3.425 | 90.98858796 | 2.1288575 |
| Rb 2 Ba 6 Nb 6 V 2 | -3.422 | 40.72025192 | 2.1304058 |
| La 8 Cr 2 Co 6 | -3.418 | 188.9806068 | 2.1324702 |
| Pr 7 Mn 8 Zn 1 | -3.417 | 95.16749933 | 2.1329863 |
| Y 8 Cr 2 Fe 6 | -3.416 | 30.91390305 | 2.1335024 |
| Gd 2 Y 6 Fe 8 | -3.415 | 0 | 2.1340185 |
| La 8 Ga 4 Co 4 | -3.414 | 112.2234712 | 2.1345346 |
| Pr 8 Sc 4 Fe 4 | -3.411 | 31.39123025 | 2.1360829 |
| Compound                  | Parameter 1  | Parameter 2  | Parameter 3 |
|--------------------------|--------------|--------------|-------------|
| Y 8 Mg 2 Mn 6            | -3.41        | 0            | 2.136599    |
| Y 8 Cr 6 Fe 2            | -3.409       | 23.90822156  | 2.1371151   |
| Y 8 Mn 6 Ni 2            | -3.408       | 218.2255157  | 2.1376312   |
| Sr 4 Ca 4 Ti 4 V 4       | -3.406       | 71.38723327  | 2.1386634   |
| Sr 8 V 7 Cr 1            | -3.403       | 58.82380141  | 2.1402117   |
| Ba 8 Nb 4 V 4            | -3.4         | 18.40334177  | 2.14176     |
| Sr 7 Ca 1 Ti 1 V 7       | -3.399       | 56.53572529  | 2.1422761   |
| Ba 6 Be 2 Nb 2 P 6       | -3.397       | 420.1120955  | 2.1433083   |
| Pr 8 Ti 4 Co 4           | -3.396       | 69.57016898  | 2.1438244   |
| Pr 8 Mg 4 V 4            | -3.393       | 0            | 2.1453727   |
| Sr 4 Be 4 Nb 2 V 6       | -3.392       | 208.4469912  | 2.1458888   |
| Sr 8 V 6 Si 2            | -3.391       | 105.4364683  | 2.146049    |
| La 8 Fe 6 Ni 2           | -3.391       | 78.06410299  | 2.146049    |
| Ba 4 Nb 8 Zn 4           | -3.39        | 298.1576598  | 2.146921    |
| Ba 8 Nb 4 Ge 4           | -3.39        | 194.0237525  | 2.146921    |
| Y 8 Mn 2 Fe 6            | -3.389       | 54.96026403  | 2.1474371   |
| Sr 7 La 1 V 7 Co 1       | -3.388       | 94.11648788  | 2.1479532   |
| Sr 7 Ca 1 V 7 Sn 1       | -3.385       | 81.85306001  | 2.1495015   |
| Sr 3 La 5 Mn 8           | -3.384       | 74.96746048  | 2.1500176   |
| Sr 8 V 7 Pd 1            | -3.383       | 133.5695442  | 2.1505337   |
| Sr 8 V 6 Rh 2            | -3.382       | 155.3180227  | 2.1510498   |
| Sr 8 V 6 Pt 2            | -3.381       | 223.4741239  | 2.1515659   |
| La 8 Ga 6 Co 2           | -3.379       | 59.52755365  | 2.1525981   |
| Pr 8 Cr 4 Fe 4           | -3.377       | 13.38305705  | 2.1536303   |
| Cs 2 Ba 6 Nb 6 V 2       | -3.375       | 75.96330729  | 2.1546625   |
| Ca 2 Y 6 Mn 8            | -3.37        | 107.2855794  | 2.157243    |
| Pr 8 Mn 4 Cr 4           | -3.368       | 63.24216746  | 2.1582752   |
| Pr 8 Mn 6 Co 2           | -3.368       | 93.54652375  | 2.1582752   |
| Cs 2 Sr 6 Nb 6 Fe 2      | -3.366       | 75.74248904  | 2.1593074   |
| Pr 4 Ba 4 Hf 4 Fe 4      | -3.366       | 0            | 2.1593074   |
| Pr 8 Fe 8                | -3.365       | 15.8899426   | 2.1598235   |
| Pr 6 Nd 2 Fe 8           | -3.362       | 20.3826618   | 2.1613718   |
| Ba 8 Zr 5 Fe 1 Mo 2      | -3.361       | 0            | 2.1618879   |
| Ba 8 Nb 2 P 6            | -3.357       | 326.3817108  | 2.1639523   |
| Pr 4 Nd 4 Fe 8           | -3.356       | 24.650631    | 2.1644684   |
| La 8 Cr 1 Co 7           | -3.356       | 184.804399   | 2.1644684   |
| Ba 6 Sr 2 Nb 2 V 6       | -3.355       | 72.73423745  | 2.1649845   |
| Y 8 Cr 1 Fe 7            | -3.352       | 33.81164089  | 2.1665328   |
| Pr 6 Sm 2 Fe 8           | -3.351       | 24.3643463   | 2.1670489   |
| Compounds          | E   | σ   | r   |
|--------------------|-----|-----|-----|
| Ba 1 Sr 7 Nb 1 V 7 | -3.349 | 55.86508904 | 2.1680811 |
| Y 8 Sc 6 Fe 2     | -3.348 | 30.07493787 | 2.1685972 |
| Y 8 Mg 4 V 4      | -3.347 | 0   | 2.1691133 |
| Pr 4 Ba 4 Hf 6 Co 2 | -3.347 | 61.60734924 | 2.1691133 |
| Sr 8 Mn 2 V 6     | -3.346 | 106.1741399 | 2.1696294 |
| Pr 6 Zr 2 Mn 6 Zn 2 | -3.346 | 109.0849217 | 2.1696294 |
| Sr 8 Sc 1 V 7     | -3.345 |  | 2.1701455 |
| Ba 6 Ca 2 Nb 2 P 6 | -3.345 | 288.4499698 | 2.1701455 |
| Pr 6 Ti 2 Mn 6 Zn 2 | -3.345 | 123.3774777 | 2.1701455 |
| La 8 Fe 4 Co 4    | -3.344 | 91.82066148 | 2.1706616 |
| Sr 4 Ca 4 V 4 Sn 4 | -3.343 | 156.7905721 | 2.1711777 |
| Sr 6 Ca 2 Ti 2 V 6 | -3.342 | 64.29306129 | 2.1716938 |
| Pr 4 Sm 4 Fe 8    | -3.342 | 31.288 | 2.1716938 |
| Pr 6 Hf 2 Mn 6 Zn 2 | -3.341 | 103.0597704 | 2.1722099 |
| Y 4 Ca 4 Mn 7 Fe 1 | -3.341 | 286.8452918 | 2.1722099 |
| La 8 Fe 2 Co 6    | -3.341 | 172.2316909 | 2.1722099 |
| Y 4 Ca 4 Mn 6 Fe 2 | -3.338 | 277.3530947 | 2.1737582 |
| Sr 6 Ca 2 Mn 2 V 6 | -3.337 | 135.2517169 | 2.1742743 |
| Pr 6 Dy 2 Fe 8    | -3.337 | 33.88050072 | 2.1742743 |
| Sr 8 Ti 4 V 4     | -3.336 | 0   | 2.1747904 |
| Sr 8 V 6 Ge 2     | -3.336 | 71.80018264 | 2.1747904 |
| Sr 8 Zr 4 V 4     | -3.335 | 22.16456908 | 2.1753065 |
| Sr 7 La 1 V 7 Ni 1 | -3.335 | 102.4017623 | 2.1753065 |
| Pr 8 Cr 7 Fe 1    | -3.335 | 32.50201789 | 2.1753065 |
| Sr 6 Ca 2 V 6 Fe 2 | -3.334 | 191.4257279 | 2.1758226 |
| Sr 7 Ca 1 V 7 Fe 1 | -3.333 | 121.8946716 | 2.1763387 |
| Y 6 Mn 8 Zn 2     | -3.33 | 152.6330901 | 2.1778878 |
| Pr 8 Cr 7 Co 1    | -3.329 | 61.04997565 | 2.1784031 |
| Ba 4 Ca 4 V 8     | -3.327 | 124.5441592 | 2.1794353 |
| Sr 8 Al 1 V 7     | -3.326 | 57.19457035 | 2.1799514 |
| Pr 6 Ho 2 Fe 8    | -3.326 | 36.70074329 | 2.1799514 |
| Ba 2 Be 6 P 8     | -3.325 | 281.9337636 | 2.1804675 |
| Ba 4 Sr 4 Nb 2 P 6 | -3.324 | 320.8578062 | 2.1809836 |
| Nd 4 Y 4 Fe 8     | -3.324 | 46.78138787 | 2.1809836 |
| Sr 8 Hf 4 V 4     | -3.323 | 47.0586804 | 2.1814997 |
| Ba 4 Ca 4 Mn 4 Nb 4 | -3.323 | 156.9262999 | 2.1814997 |
| Rb 8 Cr 8         | -3.32 | 353.6671764 | 2.183048 |
| Pr 8 Mn 1 Fe 7    | -3.32 | 23.9074702 | 2.183048 |
| La 4 Gd 4 Co 8    | -3.32 | 0    | 2.183048 |
| Formula            | E (eV) | LDA+U (eV) | PBE+U (eV) |
|-------------------|--------|------------|------------|
| Pr₄ Dy₄ Fe₈       | -3.319 | 44.41417212 | 2.1835641  |
| Sr₆ Ca₂ V₆ Sn₂    | -3.318 | 113.0189807 | 2.1840802  |
| Pr₈ Cr₆ Co₂       | -3.318 | 82.4052798  | 2.1840802  |
| Pr₄ Ho₄ Fe₈      | -3.318 | 48.60890725 | 2.1840802  |
| La₈ Ga₇ Co₁      | -3.318 | 33.32421986 | 2.1840802  |
| Sr₇ V₈ Zn₁       | -3.317 | 101.7142223 | 2.1845963  |
| Sr₈ Nb₄ Ru₄      | -3.317 | 117.6221384 | 2.1845963  |
| Dy₂ Y₆ Fe₈       | -3.315 | 42.50329682 | 2.1856285  |
| Ba₄ Mg₄ Nb₄ V₄   | -3.314 | 180.189565  | 2.1861446  |
| Y₈ Fe₈           | -3.314 | 36.60262873 | 2.1861446  |
| Ba₆ Mg₂ P₈       | -3.313 | 280.670759  | 2.1866007  |
| La₈ Mn₂ Co₆      | -3.313 | 147.3068309 | 2.1866007  |
| Y₈ Cr₄ Co₄       | -3.311 | 120.1264584 | 2.1876929  |
| Ba₆ Sr₂ Nb₂ P₆   | -3.31  | 325.0083007 | 2.188209   |
| La₆ Gd₂ Co₈      | -3.31  | 0           | 2.188209   |
| Pr₈ Mg₂ Mn₆      | -3.309 | 0           | 2.1887251  |
| La₆ Dy₂ Co₈      | -3.309 | 231.3621027 | 2.1887251  |
| Ca₄ La₄ Cr₈      | -3.308 | 80.17409824 | 2.1892412  |
| Pr₈ Mn₆ Ni₂      | -3.307 | 117.4702592 | 2.1897573  |
| Y₆ Ho₂ Fe₈       | -3.306 | 43.84579918 | 2.1902734  |
| Y₈ Sc₄ Cr₄       | -3.304 | 24.51433987 | 2.1913056  |
| Sr₈ Y₁ V₇        | -3.302 | 88.16640533 | 2.1923378  |
| Rb₂ Ba₆ Mn₂ Nb₆  | -3.302 | 37.25733967 | 2.1923378  |
| Y₄ Ho₄ Fe₈       | -3.302 | 51.00371963 | 2.1923378  |
| La₄ Ca₄ Mn₇ Fe₁  | -3.301 | 178.3332088 | 2.1928539  |
| Sm₂ Y₆ Fe₈       | -3.301 | 40.13222417 | 2.1928539  |
| Ba₂ Be₆ Nb₄ V₄   | -3.298 | 353.1846693 | 2.1944022  |
| Ba₂ Mg₆ Nb₄ V₄   | -3.298 | 176.8142801 | 2.1944022  |
| La₈ Fe₁ Co₇      | -3.297 | 193.2696911 | 2.1949183  |
| La₈ Sc₇ Cr₁      | -3.296 | 0           | 2.1954344  |
| Dy₄ Y₄ Fe₈       | -3.296 | 48.25457563 | 2.1954344  |
| Sr₈ V₇ Ga₁       | -3.295 | 66.9824205  | 2.1959505  |
| Pr₈ Mn₂ Fe₆      | -3.294 | 31.22274781 | 2.1964666  |
| Ba₂ Gd₆ Fe₈      | -3.293 | 114.4681574 | 2.1969827  |
| La₈ Sc₄ Co₄      | -3.291 | 84.6803341  | 2.1980149  |
| Sr₈ V₇ Zn₁       | -3.288 | 83.24935867 | 2.1995632  |
| Y₈ Mn₁ Fe₇       | -3.288 | 45.53794638 | 2.1995632  |
| Nd₂ Y₆ Fe₈       | -3.287 | 44.0601333  | 2.2000793  |
| Pr₈ Cr₆ Fe₂      | -3.284 | 26.18236427 | 2.2016276  |
| Composition               | Enthalpy (kcal/mol) | Volume (Å³) | Density (g/cm³) |
|--------------------------|---------------------|------------|----------------|
| Y₆Nb₂Zn₂Fe₆             | -3.284              | 210.805349 | 2.2016276      |
| Ca₂Pr₆Mn₈               | -3.283              | 79.92132449| 2.2021437      |
| La₅Zn₃Fe₈               | -3.281              | 236.5011107| 2.2031759      |
| Ca₄La₄Mn₈               | -3.28               | 126.6077788| 2.203692       |
| La₈Mg₄Fe₄              | -3.279              | 0          | 2.2042081      |
| Sr₈V₆Pd₂                | -3.279              | 221.0964492| 2.2042081      |
| Pr₄Ba₄Zr₆Co₂             | -3.277              | 60.51216449| 2.2052403      |
| Y₈Mn₄Ga₄                | -3.276              | 83.23315196| 2.2057564      |
| Sm₄Y₄Fe₈                | -3.275              | 41.75381961| 2.2062725      |
| La₆Hf₂Zn₂Co₆            | -3.274              | 268.1048453| 2.2067886      |
| Sr₈V₇Fe₁                | -3.273              | 59.54520144| 2.2073047      |
| La₆Ho₂Co₈               | -3.273              | 215.0028082| 2.2073047      |
| La₆Sm₂Co₈               | -3.273              | 205.7291695| 2.2078208      |
| Ba₁Sr₇Ti₁V₇             | -3.272              | 57.85970768| 2.2078208      |
| Sn₈V₈                   | -3.271              | 300.0409299| 2.2083369      |
| Ba₂Sm₆Fe₈               | -3.271              | 223.4681796| 2.2083369      |
| La₁Y₄Mn₈Zn₃            | -3.27               | 212.4078727| 2.208853       |
| La₆Nd₂Co₈               | -3.27               | 205.7291695| 2.208853       |
| Sr₄Mg₄Nb₂V₆             | -3.266              | 124.2306776| 2.2109174      |
| Sr₈V₇Co₁                | -3.266              | 73.35628469| 2.2109174      |
| Pr₆Ta₂Zn₂Fe₆            | -3.266              | 177.9944072| 2.2109174      |
| Ba₁Sr₇V₇Sn₁             | -3.265              | 79.33108329| 2.2114335      |
| La₄Ca₄Mn₇Co₁            | -3.265              | 199.407709 | 2.2114335      |
| La₄Ca₄Mn₆Fe₂            | -3.263              | 172.1301242| 2.2124657      |
| Sr₂Y₆Mn₈                | -3.261              | 105.820872 | 2.2134979      |
| Pr₆Nb₂Zn₂Fe₆            | -3.261              | 135.3574479| 2.2134979      |
| Sr₆La₂V₆Ni₂             | -3.256              | 151.8401353| 2.2160784      |
| Sr₈V₄Ge₄                | -3.256              | 105.579976 | 2.2160784      |
| Y₈Ti₄Co₄               | -3.251              | 33.28660573| 2.2186589      |
| Rb₁Sr₇Ta₁V₇             | -3.249              | 63.1910862 | 2.2196911      |
| Li₈Mo₈                  | -3.249              | 43.02107739| 2.2196911      |
| Sr₈Mg₁V₇                | -3.245              | 68.47324018| 2.2217555      |
| Sr₈V₄Sn₄                | -3.245              | 91.07313513| 2.2217555      |
| Ba₈Nb₂V₆                | -3.244              | 70.7491892 | 2.2222716      |
| Ba₈V₈                  | -3.244              | 3.38403663 | 2.2222716      |
| Rb₁Sr₇Nb₁V₇             | -3.243              | 65.17925184| 2.2227877      |
| Ba₄Ca₄Nb₄Cr₄            | -3.243              | 83.80819559| 2.2227877      |
| Sr₈V₇Cu₁               | -3.242              | 114.2636475| 2.2233038      |
| Y₈Sc₇Fe₁                | -3.24               | 29.21790606| 2.224336       |
| Chemical Formula | E (eV) | Molar Volume (Å³) | Density (g/cm³) |
|------------------|--------|-------------------|----------------|
| Ba 6 Mg 2 Nb 2 V 6 | -3.239 | 163.0006251       | 2.2248521      |
| Mg 4 Be 4 Nb 2 V 6 | -3.237 | 209.5402427       | 2.2258843      |
| Sr 7 Ca 1 V 7 Ni 1 | -3.237 | 115.8456622       | 2.2258843      |
| La 8 Mn 1 Co 7   | -3.236 | 172.576511        | 2.2264004      |
| Rb 2 Ba 6 Nb 6 Fe 2 | -3.233 | 22.42988225       | 2.2279487      |
| Pr 8 Sc 4 Cr 4   | -3.231 | 29.561096         | 2.2289809      |
| La 4 Sm 4 Co 8   | -3.231 | 230.8646751       | 2.2289809      |
| Pr 8 Sc 6 Mn 2   | -3.228 | 44.5193123        | 2.2305292      |
| La 8 Fe 4 Ni 4   | -3.228 | 188.2013825       | 2.2305292      |
| Ba 1 Sr 7 Mn 1 V 7 | -3.226 | 99.86067143       | 2.2315614      |
| Sr 7 Ca 1 V 7 Cr 1 | -3.225 | 75.05696984       | 2.2320775      |
| Pr 8 Sc 6 Fe 2   | -3.225 | 28.9290037        | 2.2320775      |
| Sr 8 V 6 Cr 2    | -3.224 | 73.16746352       | 2.2325936      |
| La 8 Fe 2 Ni 6   | -3.224 | 386.1818974       | 2.2325936      |
| Ba 2 Ca 6 P 8    | -3.223 | 287.0179016       | 2.2331097      |
| Sr 6 Ca 2 V 6 Cr 2 | -3.223 | 95.7530538        | 2.2331097      |
| Ba 4 Mg 4 Nb 2 P 6 | -3.22 | 312.7171297       | 2.234658       |
| Ba 4 Ce 4 Mn 8   | -3.219 | 170.8044819       | 2.2351741      |
| La 8 Co 7 Ni 1   | -3.216 | 248.0355267       | 2.2367224      |
| Sr 2 Pr 6 Mn 8   | -3.215 | 62.07011709       | 2.2372385      |
| K 8 Cr 8        | -3.213 | 358.4058535       | 2.2382707      |
| La 5 Sr 3 Fe 6 Co 2 | -3.212 | 146.9089383       | 2.2387868      |
| Ba 8 Zr 6 Fe 1 Mo 1 | -3.211 | 0                 | 2.2393029      |
| Ba 6 Be 2 Nb 2 V 6 | -3.209 | 182.6802984       | 2.2403351      |
| La 8 Cr 4 Ni 4   | -3.209 | 171.7252434       | 2.2403351      |
| Y 8 Fe 7 Co 1    | -3.209 | 63.68137654       | 2.2403351      |
| Ba 4 Be 4 Nb 2 P 6 | -3.208 | 428.1020733       | 2.2408512      |
| Ba 6 Mg 2 Nb 2 P 6 | -3.208 | 329.4718015       | 2.2408512      |
| Sr 4 Ca 4 Nb 4 Sn 4 | -3.207 | 147.4256724       | 2.2413673      |
| La 4 Nd 4 Co 8   | -3.206 | 212.9808978       | 2.2418834      |
| Y 8 Sc 7 Mn 1    | -3.204 | 41.04247371       | 2.2429156      |
| Cs 1 Sr 7 Ta 1 V 7 | -3.204 | 86.57321112       | 2.2429156      |
| Y 8 Sc 6 Mn 2    | -3.204 | 51.55582317       | 2.2429156      |
| Pr 8 Cr 4 Co 4   | -3.204 | 123.0158881       | 2.2429156      |
| Ba 6 Mg 2 V 8    | -3.203 | 221.9926675       | 2.2434317      |
| Y 8 Ga 4 Fe 4    | -3.202 | 57.74772029       | 2.2439478      |
| Cs 1 Sr 7 Nb 1 V 7 | -3.201 | 88.28337676       | 2.2444639      |
| Pr 8 Cr 1 Fe 7   | -3.195 | 15.2759621        | 2.2475605      |
| Ba 4 La 4 Cr 8   | -3.193 | 98.35130258       | 2.2485927      |
| Compound                        | E   | V    | C    |
|--------------------------------|-----|------|------|
| Cs 2 Ba 6 Mn 2 Nb 6            | -3.192 | 65.53768399 | 2.2491088 |
| La 5 Ca 3 Fe 6 Co 2            | -3.191 | 98.40563711 | 2.2496249 |
| La 8 Cr 2 Ni 6                | -3.191 | 375.3885633 | 2.2496249 |
| Pr 8 Mn 4 Ga 4                | -3.189 | 83.75140846 | 2.2506571 |
| Y 8 Fe 7 Ni 1                 | -3.188 | 91.67561929 | 2.2511732 |
| La 4 Ca 4 Mn 7 Ni 1           | -3.187 | 231.2947017 | 2.2516893 |
| Cs 2 Sr 6 Mn 2 Nb 6           | -3.183 | 51.95441624 | 2.2537537 |
| Ba 2 Y 6 Mn 8                 | -3.181 | 131.9969457 | 2.2547859 |
| Cs 4 Ba 4 Nb 4 V 4            | -3.178 | 216.8561532 | 2.2563342 |
| La 8 Co 8                     | -3.178 | 197.6489412 | 2.2563342 |
| Pr 6 Mn 8 Zn 2                | -3.174 | 147.8673352 | 2.2583986 |
| Sr 4 La 4 V 4 Ni 4            | -3.171 | 236.6446346 | 2.2599469 |
| Pr 8 Sc 7 Mn 1                | -3.17 | 34.55810087 | 2.260463 |
| Ba 2 Nd 6 Fe 8                | -3.17 | 178.054208 | 2.260463 |
| Y 8 Cr 4 Ga 4                 | -3.17 | 54.89969625 | 2.260463 |
| Be 8 V 8                      | -3.168 | 203.97774734 | 2.2614952 |
| Ba 1 Sr 7 V 7 Cr 1            | -3.168 | 77.41260107 | 2.2614952 |
| La 8 Ga 6 Ni 2                | -3.168 | 130.59792891 | 2.2614952 |
| Pr 8 Fe 7 Co 1                | -3.166 | 41.92540036 | 2.2625274 |
| Cs 2 Ba 6 Nb 6 Fe 2           | -3.164 | 52.93661229 | 2.2635596 |
| Pr 8 Mg 1 Fe 7                | -3.164 | 0 | 2.2635596 |
| La 8 Co 6 Ni 2                | -3.163 | 273.4561122 | 2.2640757 |
| Sr 4 La 4 Fe 8                | -3.159 | 69.28013037 | 2.2661401 |
| Ba 2 Pr 6 Mn 8                | -3.157 | 84.73487218 | 2.2671723 |
| Sr 4 Be 4 Nb 2 V 6            | -3.156 | 276.6771065 | 2.2676884 |
| Y 8 Cr 7 Ni 1                 | -3.156 | 75.01114896 | 2.2676884 |
| La 8 Ti 4 Ni 4                | -3.156 | 145.6777755 | 2.2676884 |
| Ba 4 Bi 4 Zr 7 Fe 1           | -3.153 | 159.8886574 | 2.2692367 |
| Sr 4 Ca 4 Nb 4 Cr 4           | -3.153 | 31.71741275 | 2.2692367 |
| Pr 8 Ga 4 Fe 4                | -3.152 | 42.48063787 | 2.2697528 |
| Ba 2 Ca 6 Nb 4 P 4            | -3.15 | 390.1457189 | 2.270785 |
| Pr 8 Sc 4 Mn 4                | -3.15 | 55.48809196 | 2.270785 |
| Rb 1 Sr 7 V 8                 | -3.149 | 82.01885176 | 2.2713011 |
| La 4 Ca 4 Mn 6 Co 2           | -3.149 | 216.6176391 | 2.2713011 |
| Sr 8 Nb 4 Ge 4                | -3.147 | 191.8295763 | 2.2723333 |
| Ba 2 Sr 6 Nb 2 P 6            | -3.146 | 282.0584845 | 2.2728494 |
| Ba 2 Mg 6 V 8                 | -3.14 | 245.5002237 | 2.275946 |
| Ca 2 Y 6 Cr 8                 | -3.14 | 83.58591481 | 2.275946 |
| Sr 8 Al 2 V 6                 | -3.139 | 72.83925139 | 2.2764621 |
| Formula          | E (eV) | H (J/mol)  | Volume (Å³) |
|------------------|--------|------------|-------------|
| Sr 4 La 4 Mn 8   | -3.137 | 93.142364  | 2.2774943   |
| La 4 Dy 4 Co 8   | -3.135 | 242.6457642| 2.2785265   |
| Y 8 Ga 6 Fe 2    | -3.134 | 66.45432437| 2.2790426   |
| Ba 6 Ca 2 V 8    | -3.133 | 133.6488776| 2.2795587   |
| Y 7 Zn 1 Fe 8    | -3.133 | 87.44022127| 2.2795587   |
| Sr 8 V 7 Ni 1    | -3.132 | 108.185692 | 2.2800748   |
| Y 8 Fe 6 Co 2    | -3.132 | 85.20387435| 2.2800748   |
| La 8 Ga 4 Ni 4   | -3.132 | 253.501692 | 2.2800748   |
| Ca 2 Pr 6 Fe 8   | -3.13 | 75.38610366| 2.281107    |
| Pr 8 Sc 7 Fe 1   | -3.128 | 26.37976044| 2.2821392   |
| Ba 6 Sr 2 V 8    | -3.128 | 114.9064373| 2.2821392   |
| Sr 6 V 8 Zn 2    | -3.127 | 133.8560553| 2.2826553   |
| La 4 Sr 4 Mn 7 Co 1 | -3.126 | 132.7417942| 2.2831714   |
| Y 8 Mg 1 Fe 7    | -3.126 | 0          | 2.2831714   |
| La 7 Zn 1 Co 8   | -3.126 | 261.9598288| 2.2831714   |
| La 8 Ga 7 Ni 1   | -3.125 | 68.53121261| 2.2836875   |
| Ba 4 Ca 4 Nb 4 P 4 | -3.121 | 350.0407489| 2.2857519   |
| Ba 4 La 4 Nb 4 Ni 4 | -3.121 | 214.4375941| 2.2857519   |
| Ca 2 Y 6 Fe 8    | -3.119 | 94.15177068| 2.2867841   |
| Y 4 Ca 4 Mn 7 Ni 1 | -3.117 | 338.9364117| 2.2878163   |
| La 4 Ho 4 Co 8   | -3.114 | 243.0367493| 2.2893646   |
| Ba 8 Nb 4 Sb 4   | -3.114 | 71.79944513| 2.2893646   |
| Sr 4 Ca 4 V 4 Cr 4 | -3.112 | 137.3717891| 2.2903968   |
| La 1 Pr 4 Mn 8 Zn 3 | -3.111 | 214.886195 | 2.2909129   |
| Sr 8 V 4 Ru 4    | -3.111 | 153.7277126| 2.291429    |
| Ba 2 Sr 6 Ti 2 V 6 | -3.108 | 72.28577606| 2.2924612   |
| La 8 Mg 1 Co 7   | -3.108 | 0          | 2.2924612   |
| Y 8 Mn 2 Ga 6    | -3.107 | 79.45514298| 2.2929773   |
| Ca 4 La 4 Fe 8   | -3.106 | 81.06765249| 2.2934934   |
| La 4 Sr 4 Mn 7 Fe 1 | -3.105 | 110.725794 | 2.2940095   |
| La 6 Ti 2 Zn 2 Co 6 | -3.104 | 262.301398 | 2.2945256   |
| Rb 2 Sr 6 Ta 2 V 6 | -3.103 | 85.4840331 | 2.2950417   |
| Ca 4 Y 4 Mn 8    | -3.103 | 141.8712388| 2.2950417   |
| Sr 8 Sc 2 V 6    | -3.102 | 0          | 2.2955578   |
| Pr 8 Cr 2 Fe 6   | -3.101 | 14.67099982| 2.2960739   |
| Cs 1 Sr 7 V 8    | -3.1 | 106.9847267| 2.29659     |
| Sr 4 V 8 Zn 4    | -3.099 | 198.6980144| 2.2971061   |
| Ba 8 Nb 2 Sb 6   | -3.097 | 58.78703243| 2.2981383   |
| Ba 2 Mg 6 Nb 2 V 6 | -3.096 | 213.5267782| 2.2986544   |
| Compound                      | ΔE  | σ   | \( R \)     |
|-------------------------------|-----|-----|-------------|
| La₆Nb₂Zn₂Ni₆                  | -3.096 | 424.5222097 | 2.2986544  |
| Rb₁Sr₇V₇Fe₁                   | -3.095 | 98.0429139 | 2.2991705  |
| Y₈Mg₁Cr₇                      | -3.094 | 0      | 2.2996866  |
| Y₈Cr₂Co₆                      | -3.094 | 191.3056598 | 2.2996866  |
| La₈Ga₇Fe₁                     | -3.094 | 0.816972052 | 2.2996866  |
| Pr₇Zn₁Fe₈                     | -3.092 | 73.1027785  | 2.3007188  |
| La₈Cr₁Ni₇                     | -3.089 | 440.4763482 | 2.3022671  |
| Ba₄Mg₄Nb₂V₆                   | -3.087 | 223.3324691 | 2.3032993  |
| La₆Ta₂Zn₂Ni₆                  | -3.083 | 425.5888922 | 2.3053637  |
| Ba₂Be₆Nb₂P₆                   | -3.082 | 347.265352  | 2.3058798  |
| Sr₄Ca₄Mn₄V₄                   | -3.082 | 193.9640249 | 2.3058798  |
| Y₈Fe₆Ni₂                      | -3.081 | 150.1011099 | 2.3063959  |
| Ba₈Fe₄Mo₄                     | -3.077 | 0      | 2.3084603  |
| Rb₂Sr₆Nb₂V₆                   | -3.075 | 72.58161438 | 2.3094925  |
| Y₆Hf₂Zn₂Fe₆                   | -3.075 | 141.6046343 | 2.3094925  |
| La₈Co₄Ni₄                     | -3.074 | 330.9517025 | 2.3100086  |
| Sr₈Y₂V₆                       | -3.073 | 118.720001  | 2.3105247  |
| Sr₈V₆Ga₂                      | -3.073 | 88.81920171 | 2.3105247  |
| Sr₈Nb₄Cr₄                     | -3.072 | 16.252789   | 2.3110408  |
| Ba₂Sr₆Mn₂V₆                   | -3.072 | 136.3909893 | 2.3110408  |
| Ba₁Sr₇V₇Ni₁                   | -3.07 | 119.0687417 | 2.312073   |
| La₄Sr₄Mn₆Fe₂                  | -3.07 | 106.0731833 | 2.312073   |
| Pr₈Fe₆Co₂                     | -3.07 | 69.37835813 | 2.312073   |
| Y₈Sc₆Cr₂                      | -3.069 | 29.23348206 | 2.3125891  |
| Y₈Mn₁Ga₇                      | -3.069 | 74.88238849 | 2.3125891  |
| Na₈Cr₈                        | -3.068 | 609.4890255 | 2.3131052  |
| Ca₂Pr₆Cr₈                     | -3.066 | 99.83908937 | 2.3141374  |
| Ba₂Sr₆V₆Sn₂                   | -3.066 | 104.5010273 | 2.3141374  |
| Sr₈Mn₄V₄                      | -3.065 | 126.7797961 | 2.3146535  |
| Pr₈Cr₄Ga₄                     | -3.065 | 52.62728168 | 2.3146535  |
| Rb₄Ba₄Nb₄V₄                   | -3.063 | 106.0954646 | 2.3156857  |
| Ba₈Nb₄Ru₄                     | -3.061 | 73.2041096  | 2.3167179  |
| La₄Ba₄Mn₇Fe₁                  | -3.058 | 142.7440083 | 2.3182662  |
| Y₆Nb₂Zn₂Co₆                   | -3.057 | 208.230071  | 2.3187823  |
| La₆Zr₂Zn₂Co₆                  | -3.054 | 235.704149  | 2.3203306  |
| La₈Mn₄Ni₄                     | -3.053 | 194.2341916 | 2.3208467  |
| Sr₂Y₆Cr₈                      | -3.052 | 96.74457581 | 2.3213628  |
| La₄Sr₄Mn₆Ni₂                  | -3.052 | 226.6682098 | 2.3213628  |
| Pr₈Cr₇Ni₁                     | -3.051 | 91.4204684  | 2.3218789  |
| Formula          | E (eV) | H (J/m³)  | αc (Å⁻¹)  |
|------------------|--------|-----------|-----------|
| La₄Ca₄Fe₂Co₆     | -3.046 | 322.4512052 | 2.3244594 |
| Y₄Ca₄Mn₆Co₂      | -3.045 | 328.6203491 | 2.3249755 |
| Sr₂Pr₆Fe₈        | -3.045 | 67.16625376 | 2.3249755 |
| La₈Fe₁Ni₇        | -3.044 | 443.4506403 | 2.3254916 |
| Pr₈Mn₂Ga₆        | -3.044 | 81.49277516 | 2.3254916 |
| La₈Sc₆Co₂        | -3.037 | 32.39353055 | 2.3291043 |
| Pr₈Ga₆Fe₂        | -3.037 | 55.70388986 | 2.3291043 |
| Sr₂Y₆Fe₈         | -3.035 | 101.9102038 | 2.3301365 |
| Ca₂Sr₆Ta₂V₆      | -3.034 | 144.4993558 | 2.3306526 |
| Y₆Ta₂Zn₂Co₆      | -3.033 | 202.9404095 | 2.3311687 |
| Sr₄Mg₄Nb₂P₆      | -3.032 | 346.3743663 | 2.3316848 |
| Y₄Ca₄Mn₇Co₁      | -3.031 | 310.794169  | 2.3322009 |
| La₈Mn₂Ni₆        | -3.029 | 352.5820374 | 2.3332231 |
| Pr₈Mg₁Cr₇        | -3.027 | 69.07264311 | 2.3342653 |
| Pr₈Fe₇Ni₁        | -3.027 | 25.904095   | 2.3342653 |
| Sr₄Ca₄Nb₄P₄      | -3.024 | 348.4681006 | 2.3358136 |
| Ba₁Sr₇V₇Fe₁      | -3.024 | 133.9885011 | 2.3358136 |
| Y₈Cr₁Co₇         | -3.024 | 223.5685105 | 2.3358136 |
| Ba₈Zr₆Nb₁Fe₁     | -3.018 | 0          | 2.3389102 |
| Rb₁Sr₇Mn₁V₇      | -3.017 | 119.4470166 | 2.3394263 |
| Sr₂La₆Co₈       | -3.016 | 235.8061196 | 2.3394242 |
| Ca₂La₆Co₈       | -3.015 | 262.1204556 | 2.3404585 |
| Gd₄Y₄Co₈        | -3.011 | 0          | 2.3425229 |
| Y₈Mn₄Co₄        | -3.01  | 92.26889056 | 2.343039  |
| Sr₈V₆Fe₂        | -3.009 | 75.85701357 | 2.3435551 |
| Y₈Ga₇Fe₁        | -3.009 | 67.63122919 | 2.3435551 |
| Sr₂Pr₆Cr₈        | -3.008 | 88.63025718 | 2.3440712 |
| Ba₆Sr₂Nb₂Sb₆     | -3.008 | 71.94742477 | 2.3440712 |
| La₄Ca₄Mn₆Ni₂     | -3.007 | 290.2636246 | 2.3445873 |
| Ba₄Mg₄V₈         | -3.003 | 263.065206  | 2.3466517 |
| La₈Co₂Ni₆       | -3.003 | 410.4415429 | 2.3466517 |
| La₈Mn₁Ni₇        | -3.002 | 428.5299603 | 2.3471678 |
| Sr₄Ca₄Mn₄Nb₄     | -3.001 | 61.87311546 | 2.3476839 |
| Pr₄Ca₄Mn₇Fe₁     | -3.001 | 183.1089579 | 2.3476839 |
| Pr₈Sc₆Cr₂        | -3  | 29.44643325 | 2.3482  |
| Y₈Cr₆Ni₂        | -3  | 130.5852424 | 2.3482  |
| Ba₂Pr₆Fe₂       | -3  | 83.54963627 | 2.3482  |
| Mg₈V₈            | -2.996 | 164.5061267 | 2.3502644 |
| Rb₄Sr₄V₈        | -2.995 | 228.0607392 | 2.3507805 |
| Formula          | E   | M     | R   |
|------------------|-----|-------|-----|
| Ba 2 Mg 6 P 8    | -2.993 | 300.2751198 | 2.3518127 |
| La 5 Sr 3 Fe 6 Cu 2 | -2.993 | 148.5095848 | 2.3518127 |
| Sr 8 V 6 Co 2    | -2.989 | 118.3444934 | 2.3538771 |
| Cs 2 Sr 6 Nb 2 V 6 | -2.987 | 117.160674 | 2.3549093 |
| Y 8 Mn 1 Co 7    | -2.986 | 229.090181 | 2.3554254 |
| Y 8 Mn 2 Co 6    | -2.985 | 177.4477509 | 2.3559415 |
| La 6 Zn 2 Co 8   | -2.985 | 325.8167164 | 2.3559415 |
| Y 8 Sc 4 Mn 4    | -2.984 | 64.48152209 | 2.3564576 |
| Cs 1 Sr 7 V 7 Fe 1 | -2.983 | 122.7415388 | 2.3569737 |
| Ba 4 Sr 4 Nb 4 Cr 4 | -2.981 | 21.47879363 | 2.3580059 |
| Ba 4 Sr 4 Ti 4 V 4 | -2.978 | 82.56491282 | 2.3595542 |
| Sr 8 V 4 Cr 4    | -2.978 | 95.41068212 | 2.3595542 |
| Ba 2 Y 6 Cr 8    | -2.978 | 128.9731151 | 2.3595542 |
| Ca 4 Y 4 Cr 8    | -2.977 | 144.2080241 | 2.3600703 |
| Rb 1 Sr 7 V 7 Cr 1 | -2.976 | 95.91526387 | 2.3605864 |
| Pr 4 Ca 4 Mn 6 Fe 2 | -2.976 | 173.9241803 | 2.3605864 |
| Cs 1 Sr 7 Mn 1 V 7 | -2.975 | 139.3679763 | 2.3611025 |
| La 4 Sr 4 Mn 7 Ni 1 | -2.975 | 167.1537869 | 2.3611025 |
| La 4 Sr 4 Mn 6 Co 2 | -2.975 | 150.5364743 | 2.3611025 |
| Y 6 Ti 2 Zn 2 Fe 6 | -2.974 | 74.78243168 | 2.3616186 |
| Pr 8 Mn 1 Ga 7    | -2.972 | 76.09045851 | 2.3626508 |
| Ca 4 Pr 4 Cr 8    | -2.97 | 146.9417572 | 2.363683 |
| Sr 8 V 6 Zn 2    | -2.969 | 128.807845 | 2.3641991 |
| Y 6 Zn 2 Fe 8    | -2.969 | 141.9028138 | 2.3641991 |
| Ca 4 Pr 4 Mn 8    | -2.965 | 123.2542355 | 2.3662635 |
| Ba 2 Sr 6 V 6 Cr 2 | -2.963 | 100.7338128 | 2.3672957 |
| Ba 2 Pr 6 Cr 8    | -2.961 | 103.3243165 | 2.3683279 |
| Sr 6 Ca 2 V 6 Ni 2 | -2.96 | 184.152709 | 2.368844 |
| Pr 6 Ta 2 Zn 2 Co 6 | -2.955 | 209.5853792 | 2.3714245 |
| Ba 2 La 6 Co 8    | -2.955 | 246.1293326 | 2.3714245 |
| Pr 4 Ca 4 Mn 7 Co 1 | -2.954 | 210.4471657 | 2.3719406 |
| Y 8 Sc 7 Cr 1    | -2.953 | 29.37230316 | 2.3724567 |
| La 6 Ho 2 Ni 8   | -2.953 | 534.4490373 | 2.3724567 |
| Y 8 Cr 2 Ga 6    | -2.953 | 65.79040925 | 2.3724567 |
| Pr 8 Ga 7 Fe 1    | -2.953 | 62.65164086 | 2.3724567 |
| Y 4 Ca 4 Mn 6 Ni 2 | -2.951 | 396.9490846 | 2.3734889 |
| Pr 8 Mn 4 Co 4    | -2.951 | 84.85788406 | 2.3734889 |
| Ba 6 Be 2 Nb 4 P 4 | -2.947 | 384.3798655 | 2.3755533 |
| La 6 Dy 2 Ni 8    | -2.945 | 530.2075447 | 2.3765855 |
| Compound               | Composition | Gibbs Energy | Formation Energy | Enthalpy | Temperature |
|------------------------|-------------|--------------|------------------|----------|-------------|
| Gd₂Y₆Co₈             | -2.944      | 0            | 2.3771016        |          |             |
| La₈Co₁Ni₇            | -2.944      | 457.413838   | 2.3771016        |          |             |
| La₆Gd₂Ni₈            | -2.943      | 0            | 2.3776177        |          |             |
| Cs₁Sr⁷V₇Cr₁          | -2.94       | 121.3898888  | 2.379166         |          |             |
| Ba₄La₄Fe₈            | -2.939      | 94.29773215  | 2.3796821        |          |             |
| La₈Sc₄Ni₄            | -2.938      | 230.1763051  | 2.3801982        |          |             |
| Sr₈Mn₄Nb₄            | -2.937      | 37.38934321  | 2.3807143        |          |             |
| La₈Mg₂Co₆            | -2.935      | 0            | 2.3817465        |          |             |
| La₅Sr₃Co₆Fe₂          | -2.935     | 180.9337096  | 2.3817465        |          |             |
| La₁Y₄Zn₃Fe₈          | -2.929      | 220.8289619  | 2.3848431        |          |             |
| La₆Ti₂Zn₂Ni₆          | -2.929      | 481.9158545  | 2.3848431        |          |             |
| Sr₈V₈Rh₄             | -2.928      | 239.5544151  | 2.3853592        |          |             |
| La₄Sr₄Fe₂Co₆          | -2.927      | 273.4605499  | 2.3858753        |          |             |
| Y₄Sr₄Mn₇Fe₁           | -2.925      | 233.0931929  | 2.3869075        |          |             |
| Rb₄Sr₄Ta₄V₄           | -2.924      | 112.7024269  | 2.3874236        |          |             |
| Pr₆Ti₂Zn₂Fe₆          | -2.921      | 85.33504854  | 2.3889719        |          |             |
| Pr₄Ca₄Mn₇Ni₁          | -2.919      | 240.5449085  | 2.3900041        |          |             |
| La₅Zn₃Co₈             | -2.915      | 402.958854   | 2.3920685        |          |             |
| Ba₆Sr₂Sb₈             | -2.915      | 74.22055387  | 2.3920685        |          |             |
| Ba₂Be₆V₈              | -2.914      | 415.0706142  | 2.3925846        |          |             |
| La₆Sm₂Ni₈             | -2.91       | 513.0315002  | 2.394649         |          |             |
| Y₆Zr₂Zn₂Fe₆           | -2.908      | 82.13639456  | 2.3956812        |          |             |
| Ba₆Ca₂Nb₄P₄           | -2.907      | 314.5460289  | 2.3961973        |          |             |
| La₄Ca₄Mn₂Co₆          | -2.906      | 308.1368598  | 2.3967134        |          |             |
| Ba₄Sr₄Nb₄Sn₄           | -2.906     | 128.100384   | 2.3967134        |          |             |
| Ba₄Sr₄Sb₈             | -2.906      | 75.823738    | 2.3967134        |          |             |
| Ba₄Sr₄Nb₄Fe₄           | -2.905     | 27.446113    | 2.3972295        |          |             |
| Cs₂Sr₆V₆Fe₂            | -2.903     | 300.5299636  | 2.3982617        |          |             |
| Y₈Sc₄Co₄             | -2.903      | 143.7477427  | 2.3982617        |          |             |
| Pr₆Zr₂Zn₂Fe₆           | -2.903     | 117.2752561  | 2.3982617        |          |             |
| La₆Hf₂Zn₂Ni₆           | -2.903     | 493.8778018  | 2.3982617        |          |             |
| Y₄Sr₄Mn₆Fe₂           | -2.902      | 228.3660617  | 2.3987778        |          |             |
| Pr₄Gd₄Co₈             | -2.9        | 0            | 2.39981          |          |             |
| Y₈Mg₂Fe₆              | -2.898      | 0            | 2.4008422        |          |             |
| Pr₈Cr₆Ni₂              | -2.898     | 139.7410153  | 2.4008422        |          |             |
| La₆Zr₂Zn₂Ni₆           | -2.897     | 479.6723555  | 2.4013583        |          |             |
| Cs₄Sr₄Ta₄V₄           | -2.894      | 208.8941135  | 2.4029066        |          |             |
| Pr₆Zn₂Fe₈              | -2.89       | 137.2416144  | 2.404971         |          |             |
| La₆Nd₂Ni₈             | -2.886      | 504.1378615  | 2.4070354        |          |             |
| Compound           | Formation Energy | UFE | Temperature Coefficient |
|--------------------|------------------|-----|-------------------------|
| Y 8 Co 8           | -2.881           | 220.5858612 | 2.4096159               |
| La 1 Pr 4 Zn 3 Fe 8| -2.88            | 218.9458087 | 2.410132                |
| La 8 Ni 8          | -2.88            | 501.7691332 | 2.410132                |
| Pr 8 Cr 2 Ga 6     | -2.879           | 61.34533677 | 2.4106481               |
| Ba 4 La 4 Fe 6 Co 2| -2.877           | 215.2623344 | 2.4116803               |
| La 4 Ca 4 Mn 4 Co 4| -2.876           | 248.4987494 | 2.4121964               |
| Y 8 Mg 2 Cr 6      | -2.873           | 0            | 2.4137447               |
| Pr 6 Hf 2 Zn 2 Fe 6| -2.873           | 105.8121048 | 2.4137447               |
| Ba 6 Mg 2 Nb 4 P 4 | -2.872           | 329.6052285 | 2.4142608               |
| Y 8 Fe 2 Co 6      | -2.872           | 254.9483656 | 2.4142608               |
| Ba 6 Sr 2 Nb 4 P 4 | -2.868           | 290.9176551 | 2.4163252               |
| Pr 4 Ca 4 Mn 6 Ni 2| -2.868           | 299.1440814 | 2.4163252               |
| Ba 4 Sr 4 V 4 Sn 4 | -2.868           | 118.8618338 | 2.4163252               |
| Sr 8 Mg 2 V 6      | -2.867           | 100.0513633 | 2.4168413               |
| Na 8 Mo 8          | -2.867           | 0            | 2.4168413               |
| Y 6 Ho 2 Co 8      | -2.866           | 228.1292817 | 2.4173574               |
| La 8 Sc 7 Co 1     | -2.865           | 3.628253775 | 2.4178735               |
| Pr 6 Nb 2 Zn 2 Co 6| -2.863           | 238.1621945 | 2.4189057               |
| La 4 Sr 4 Fe 1 Co 7| -2.863           | 285.1152979 | 2.4189057               |
| Dy 2 Y 6 Co 8      | -2.863           | 221.0292793 | 2.4189057               |
| Y 4 Ho 4 Co 8      | -2.863           | 231.0292021 | 2.4189057               |
| La 4 Ho 4 Ni 8     | -2.862           | 562.4776913 | 2.4194218               |
| Rb 2 Sr 6 V 8      | -2.857           | 114.8543142 | 2.4220023               |
| Ba 8 Nb 4 P 4      | -2.857           | 288.9674808 | 2.4220023               |
| Sr 8 V 6 Ni 2      | -2.857           | 169.3989947 | 2.4220023               |
| Dy 4 Y 4 Co 8      | -2.854           | 228.1488081 | 2.4235506               |
| Pr 4 Ca 4 Mn 6 Co 2| -2.85           | 226.1553459 | 2.425615                |
| Sr 8 V 6 Cu 2      | -2.849           | 195.3246557 | 2.4261311               |
| Ba 2 Y 6 Fe 8      | -2.848           | 141.5888727 | 2.4266472               |
| Rb 4 Sr 4 Nb 4 V 4 | -2.846           | 102.8373395 | 2.4276794               |
| K 8 Mo 8           | -2.846           | 0            | 2.4276794               |
| Ba 2 Sr 6 Nb 4 P 4 | -2.843           | 321.2044161 | 2.4292277               |
| Y 8 Fe 4 Co 4      | -2.841           | 122.50662   | 2.4302599               |
| Pr 8 Mg 2 Fe 6     | -2.839           | 0            | 2.4312921               |
| Sm 2 Y 6 Co 8      | -2.836           | 225.0956232 | 2.4328404               |
| Ba 4 Sr 4 Nb 2 Sb 6| -2.836           | 62.74410891 | 2.4328404               |
| Sr 4 Y 4 Cr 8      | -2.834           | 164.3180961 | 2.4338726               |
| Pr 6 Gd 2 Co 8     | -2.832           | 0            | 2.4349048                |
| La 4 Dy 4 Ni 8     | -2.831           | 554.7439562 | 2.4354209               |
| Formula          | \(E\)  | \(M\)    | \(\rho\)  |
|------------------|--------|----------|----------|
| \(\text{Sr}_4 \text{Ca}_4 \text{V}_4 \text{Fe}_4\) | -2.829 | 310.4064609 | 2.4364531 |
| \(\text{La}_4 \text{Ba}_4 \text{Mn}_7 \text{Co}_1\) | -2.829 | 163.417368 | 2.4364531 |
| \(\text{Sr}_4 \text{Y}_4 \text{Mn}_8\) | -2.828 | 132.286324 | 2.4369692 |
| \(\text{Ca}_4 \text{Y}_4 \text{Fe}_8\) | -2.825 | 155.3881626 | 2.4385175 |
| \(\text{Pr}_8 \text{Fe}_4 \text{Co}_4\) | -2.825 | 112.3822737 | 2.4385175 |
| \(\text{Sr}_4 \text{Mg}_4 \text{Nb}_4 \text{P}_4\) | -2.824 | 366.1677633 | 2.4390336 |
| \(\text{Pr}_8 \text{Sc}_4 \text{Co}_4\) | -2.82 | 128.8090626 | 2.441098 |
| \(\text{La}_4 \text{Ba}_4 \text{Mn}_6 \text{Fe}_2\) | -2.819 | 137.7098376 | 2.4416141 |
| \(\text{Ba}_4 \text{Dy}_4 \text{Fe}_8\) | -2.817 | 319.9748728 | 2.4426463 |
| \(\text{Ba}_4 \text{Ho}_4 \text{Fe}_8\) | -2.815 | 338.0626079 | 2.4436785 |
| \(\text{Y}_4 \text{Sr}_4 \text{Mn}_7 \text{Ni}_1\) | -2.813 | 284.7264969 | 2.4447107 |
| \(\text{Pr}_8 \text{Sc}_7 \text{Cr}_1\) | -2.812 | 27.22022687 | 2.4447107 |
| \(\text{Pr}_8 \text{Mg}_2 \text{Cr}_6\) | -2.812 | 0 | 2.4452268 |
| \(\text{Li}_8 \text{Cr}_8\) | -2.811 | 645.0000595 | 2.4457429 |
| \(\text{Sm}_4 \text{Y}_4 \text{Co}_8\) | -2.809 | 221.2893851 | 2.4467751 |
| \(\text{Ba}_4 \text{Sr}_4 \text{Nb}_4 \text{P}_4\) | -2.806 | 308.7979106 | 2.4483234 |
| \(\text{Pr}_8 \text{Fe}_6 \text{Ni}_2\) | -2.806 | 125.7870936 | 2.4483234 |
| \(\text{Sr}_4 \text{Pr}_4 \text{Cr}_8\) | -2.805 | 131.0223429 | 2.4488395 |
| \(\text{Pr}_8 \text{Cr}_2 \text{Co}_6\) | -2.803 | 170.0027464 | 2.4498717 |
| \(\text{Ba}_2 \text{Sr}_6 \text{Nb}_2 \text{Sb}_6\) | -2.799 | 58.36404304 | 2.4519361 |
| \(\text{La}_4 \text{Sr}_4 \text{Mn}_1 \text{Co}_7\) | -2.796 | 276.0584965 | 2.4534844 |
| \(\text{Ba}_2 \text{Mg}_6 \text{Nb}_4 \text{P}_4\) | -2.792 | 351.4478344 | 2.4555488 |
| \(\text{Pr}_8 \text{Ti}_4 \text{Ni}_4\) | -2.792 | 158.35814 | 2.4555488 |
| \(\text{Ba}_4 \text{Mg}_4 \text{Nb}_4 \text{P}_4\) | -2.791 | 340.7052563 | 2.4560649 |
| \(\text{Ba}_8 \text{Ir}_8\) | -2.789 | 437.8158829 | 2.4570971 |
| \(\text{La}_7 \text{Zn}_1 \text{Ni}_8\) | -2.789 | 581.1152708 | 2.4570971 |
| \(\text{Rb}_2 \text{Sr}_6 \text{V}_6 \text{Cr}_2\) | -2.787 | 151.8901385 | 2.4581293 |
| \(\text{Nd}_4 \text{Y}_4 \text{Co}_8\) | -2.786 | 217.2143578 | 2.4586454 |
| \(\text{Ca}_4 \text{Pr}_4 \text{Fe}_8\) | -2.784 | 139.7482055 | 2.4596776 |
| \(\text{La}_4 \text{Sr}_4 \text{Mn}_2 \text{Co}_6\) | -2.784 | 237.739695 | 2.4596776 |
| \(\text{Ba}_2 \text{Sr}_6 \text{Sb}_8\) | -2.784 | 69.13317213 | 2.4596776 |
| \(\text{Cs}_2 \text{Sr}_6 \text{V}_6\) | -2.781 | 171.6415641 | 2.4612259 |
| \(\text{La}_2 \text{Sr}_6 \text{Cr}_2 \text{Fe}_6\) | -2.779 | 193.2281658 | 2.4622581 |
| \(\text{Y}_8 \text{Fe}_4 \text{Ni}_4\) | -2.778 | 217.267091 | 2.4627742 |
| \(\text{Y}_4 \text{Ca}_4 \text{Mn}_2 \text{Co}_6\) | -2.777 | 421.7740698 | 2.4632903 |
| \(\text{Ba}_4 \text{Sr}_4 \text{Mn}_4 \text{Nb}_4\) | -2.776 | 58.09998012 | 2.4638064 |
| \(\text{Y}_4 \text{Sr}_4 \text{Mn}_7 \text{Co}_1\) | -2.774 | 152.2680042 | 2.4648386 |
| \(\text{La}_8 \text{Mg}_1 \text{Ni}_7\) | -2.773 | 0 | 2.4653547 |
| \(\text{Ba}_2 \text{Sr}_6 \text{V}_6 \text{Ni}_2\) | -2.772 | 190.952594 | 2.4658708 |
| Compound                      | ρ (eV/f.u.) | E (eV)          | α (Å⁻¹) |
|-------------------------------|------------|-----------------|---------|
| Pr₄Ca₄Fe₂Co₆                  | -2.772     | 331.5817613     | 2.4658708 |
| Ba₃Sn₄La₁Fe₈                  | -2.771     | 302.380059      | 2.4663869 |
| Y₄Sr₄Mn₆Co₂                   | -2.77      | 271.9939343     | 2.466903  |
| La₄Ca₄Fe₁Co₇                  | -2.768     | 334.8129699     | 2.4679352 |
| La₄Ba₄Fe₂Co₆                  | -2.767     | 292.2161065     | 2.4684513 |
| Pr₈Mn₂Co₆                     | -2.767     | 159.9269944     | 2.4684513 |
| La₈Se₆Ni₂                     | -2.766     | 108.4245161     | 2.4689674 |
| La₄Ca₄Co₆Ni₂                  | -2.766     | 458.3641411     | 2.4689674 |
| Ba₄Sr₄Mn₄V₄                   | -2.764     | 195.6867447     | 2.4699996 |
| Ba₈Ru₈                        | -2.764     | 160.0840219     | 2.4699996 |
| La₄Sr₄Mn₄Co₄                  | -2.764     | 184.8313346     | 2.4699996 |
| Y₄Ca₄Mn₄Co₄                  | -2.763     | 358.8377094     | 2.4705157 |
| La₄Ca₄Mn₁Co₇                  | -2.761     | 295.5917899     | 2.4715479 |
| Pr₈Fe₄Ni₄                     | -2.76      | 241.8982447     | 2.472064 |
| Ca₄La₄Co₈                     | -2.755     | 327.5359701     | 2.4746445 |
| Ba₃Bi₄La₁Fe₈                  | -2.753     | 248.2055287     | 2.4756767 |
| Ba₄Sm₄Fe₈                     | -2.752     | 248.3941667     | 2.4761928 |
| Ba₆Sr₂Nb₄Sb₄                  | -2.747     | 71.37741574     | 2.4787733 |
| Pr₈Fe₂Co₆                     | -2.746     | 157.8621892     | 2.4792894 |
| Ca₈Cr₈                        | -2.745     | 110.922593      | 2.4798055 |
| Y₆Ti₂Zn₂Co₆                   | -2.743     | 225.4749037     | 2.4808377 |
| La₄Sr₄Co₇Ni₁                  | -2.743     | 340.1641336     | 2.4808377 |
| Pr₈Cr₁Co₇                     | -2.741     | 178.6903006     | 2.4818699 |
| Pr₄Dy₄Co₈                     | -2.74      | 222.649221      | 2.482386 |
| La₄Sm₄Ni₈                     | -2.739     | 523.3413671     | 2.4829021 |
| Sr₈Nb₄Co₄                     | -2.737     | 82.76431385     | 2.4839343 |
| Ba₈Nb₄Cr₄                     | -2.736     | 9.90054825      | 2.4844504 |
| Ba₂Sr₆V₆Fe₂                   | -2.73      | 206.8103629     | 2.487547 |
| Ba₈Fe₄Tc₄                     | -2.729     | 0               | 2.4880631 |
| Pr₄Sm₄Co₈                     | -2.727     | 206.8868819     | 2.4890953 |
| Pr₈Co₈                        | -2.727     | 194.2296047     | 2.4890953 |
| Pr₄Nd₄Co₈                     | -2.724     | 197.1131046     | 2.4906436 |
| Ba₈Fe₆Re₂                     | -2.72      | 33.7269144      | 2.492708 |
| Ba₈Fe₄Os₄                     | -2.719     | 78.8343637      | 2.4932241 |
| La₄Ba₄Mn₆Co₂                  | -2.719     | 197.1238069     | 2.4932241 |
| Sr₄Pr₄Mn₈                     | -2.715     | 94.57732075     | 2.4952885 |
| Y₆Hf₂Zn₂Co₆                   | -2.715     | 245.5328563     | 2.4952885 |
| Cs₂Sr₆V₆Cr₂                   | -2.713     | 197.6001636     | 2.4963207 |
| Sr₈Cr₈                        | -2.712     | 93.76099298     | 2.4968368 |
| Compound                  | ΔG  | Z    | ΔG   |
|---------------------------|-----|------|------|
| La 4 Nd 4 Ni 8            | -2.711 | 506.3928398 | 2.4973529 |
| Y 8 Fe 1 Co 7             | -2.709 | 312.7263634 | 2.4983851 |
| Pr 6 Hf 2 Zn 2 Co 6       | -2.708 | 234.7808514 | 2.4989012 |
| Y 8 Cr 1 Ga 7             | -2.708 | 67.65727163 | 2.4989012 |
| Ba 4 La 4 Mn 8            | -2.705 | 134.7419291 | 2.5004495 |
| Sr 4 La 4 Co 8            | -2.705 | 278.7412981 | 2.5004495 |
| Ca 8 Sb 8                 | -2.7 | 103.1021788 | 2.50303 |
| Pr 6 Sm 2 Co 8            | -2.699 | 219.6113683 | 2.5035461 |
| Nd 2 Y 6 Co 8             | -2.699 | 225.9614845 | 2.5035461 |
| Y 8 Ga 4 Co 4             | -2.698 | 153.3198726 | 2.5040622 |
| Y 8 Co 7 Ni 1             | -2.696 | 251.0396967 | 2.5050944 |
| Sr 6 Ta 2 Mn 6 Zn 2       | -2.692 | 216.9104459 | 2.5071588 |
| Pr 8 Mn 1 Co 7            | -2.692 | 177.4484245 | 2.5071588 |
| Pr 4 Sr 4 Mn 7 Co 1       | -2.691 | 144.622509  | 2.5076749 |
| Ba 4 Y 4 Cr 8             | -2.688 | 215.2839246 | 2.5092232 |
| La 4 Ca 4 Co 7 Ni 1       | -2.687 | 363.2435556 | 2.5097393 |
| Pr 4 Sr 4 Mn 7 Fe 1       | -2.686 | 121.9651896 | 2.5102554 |
| Ba 8 Mn 4 Nb 4            | -2.684 | 50.91919948 | 2.5112876 |
| Pr 8 Fe 1 Co 7            | -2.683 | 188.9868969 | 2.5118037 |
| Sr 8 Sb 8                 | -2.683 | 55.17285627 | 2.5118037 |
| Sr 4 Y 4 Fe 8             | -2.682 | 159.7187789 | 2.5123198 |
| Sr 8 V 4 Pd 4             | -2.681 | 359.1852681 | 2.5128359 |
| La 4 Ba 4 Mn 7 Ni 1       | -2.679 | 201.1916107 | 2.5138681 |
| Pr 6 Dy 2 Co 8            | -2.678 | 219.8511628 | 2.5143842 |
| Ba 4 Ca 4 Nb 4 Fe 4       | -2.676 | 94.93194358 | 2.5154164 |
| Ba 4 Nd 4 Fe 8            | -2.674 | 213.0727689 | 2.5164486 |
| Ba 2 Ca 6 Sb 8            | -2.674 | 135.9689765 | 2.5164486 |
| Pr 6 Nd 2 Co 8            | -2.672 | 196.8344796 | 2.5174808 |
| Rb 2 Sr 6 Mn 2 V 6        | -2.669 | 190.6660127 | 2.5190291 |
| Y 8 Cr 4 Ni 4             | -2.669 | 224.0259294 | 2.5190291 |
| Rb 2 Sr 6 V 6 Fe 2        | -2.666 | 256.3194385 | 2.5205774 |
| Pr 4 Sr 4 Mn 6 Fe 2       | -2.666 | 117.0964058 | 2.5205774 |
| La 4 Sr 4 Co 6 Ni 2       | -2.664 | 385.5254691 | 2.5216096 |
| Sr 4 Pr 4 Fe 8            | -2.663 | 124.7873149 | 2.5221257 |
| La 4 Ba 4 Fe 1 Co 7       | -2.663 | 302.788684 | 2.5221257 |
| Ba 4 Pr 4 Cr 8            | -2.662 | 163.4042116 | 2.5226418 |
| Bi 4 Sr 4 Fe 8            | -2.661 | 181.483275  | 2.5231579 |
| La 4 Ba 4 Mn 1 Co 7       | -2.656 | 286.5050016 | 2.5257384 |
| Y 4 Sr 4 Mn 6 Ni 2        | -2.65  | 343.7119198 | 2.528835 |
| Compound                  | ΔE   | E_{cusp}   | ΔE/ΔE_{cusp} |
|--------------------------|------|-----------|--------------|
| Ba$_4$Gd$_4$Fe$_8$       | -2.65| 192.1513185| 2.528835     |
| Y$_8$Ti$_4$Ni$_4$        | -2.646| 127.7585767| 2.5308994    |
| La$_8$Mg$_2$Ni$_6$      | -2.645| 0         | 2.5314155    |
| Mg$_8$P$_8$              | -2.641| 268.5549123| 2.5334799    |
| La$_4$Ba$_4$Mn$_2$Co$_6$ | -2.641| 265.3228127| 2.5334799    |
| Pr$_4$Ho$_4$Co$_8$       | -2.638| 229.1922061| 2.5350282    |
| Ca$_8$Fe$_8$             | -2.637| 344.4907315| 2.5355443    |
| La$_8$Sc$_7$Ni$_1$       | -2.634| 40.60574653| 2.5370926    |
| Sr$_6$Mn$_6$Nb$_2$Zn$_2$ | -2.634| 220.3471288| 2.5370926    |
| La$_4$Ca$_4$Co$_4$Ni$_4$| -2.634| 533.1242314| 2.5370926    |
| La$_4$Ca$_4$Ni$_4$Co$_4$| -2.634| 535.8057314| 2.5370926    |
| Ba$_6$Ca$_2$Sb$_8$       | -2.632| 126.8123222| 2.5381248    |
| Pr$_4$Ca$_4$Mn$_2$Co$_6$ | -2.629| 307.8318165| 2.5396731    |
| Sr$_4$Ca$_4$Nb$_4$Fe$_4$| -2.628| 31.662286  | 2.5401892    |
| Pr$_8$Cr$_1$Ga$_7$       | -2.628| 65.86073931| 2.5401892    |
| Y$_8$Mg$_4$Fe$_4$        | -2.623| 113.823474| 2.5432858    |
| Rb$_8$Mo$_8$             | -2.622| 147.2891308| 2.5458663    |
| Y$_8$Co$_6$Ni$_2$        | -2.617| 287.9957822| 2.5458663    |
| Ba$_4$Sr$_4$V$_4$Cr$_4$  | -2.615| 147.2891308| 2.5468985    |
| Y$_4$Ca$_4$Co$_6$Ni$_2$  | -2.615| 559.1693511| 2.5468985    |
| Pr$_6$Ho$_2$Co$_8$       | -2.615| 219.2686554| 2.5468985    |
| Y$_8$Mn$_4$Ni$_4$        | -2.611| 166.5213616| 2.5489629    |
| Y$_6$Zr$_2$Zn$_2$Co$_6$  | -2.609| 244.0538665| 2.5499951    |
| Pr$_8$Ga$_4$Co$_4$       | -2.608| 315.513791 | 2.5505112    |
| Ba$_6$Mg$_2$Sb$_8$       | -2.608| 176.6743479| 2.5505112    |
| La$_4$Ba$_4$Co$_7$Ni$_1$ | -2.606| 349.9725261| 2.5515434    |
| Ca$_2$La$_6$Ni$_8$       | -2.603| 591.1196476| 2.5530917    |
| La$_4$Ba$_4$Mn$_4$Co$_4$ | -2.601| 215.5066848| 2.5541239    |
| Gd$_4$Y$_4$Ni$_8$        | -2.598| 0         | 2.5556722    |
| Pr$_4$Sr$_4$Mn$_7$Ni$_1$ | -2.593| 178.6112437| 2.5582527    |
| Pr$_4$Ca$_4$Mn$_4$Co$_4$ | -2.593| 257.779562 | 2.5582527    |
| La$_6$Zn$_2$Ni$_8$      | -2.589| 655.1094084| 2.5603171    |
| La$_4$Ba$_4$Mn$_6$Ni$_2$ | -2.582| 257.5690424| 2.5639298    |
| Ba$_6$Ce$_2$Fe$_8$       | -2.578| 204.0275408| 2.5659942    |
| Ba$_4$La$_4$Co$_8$       | -2.578| 315.9949406| 2.5659942    |
| Pr$_8$Mg$_4$Fe$_4$       | -2.577| 0         | 2.5665103    |
| Sr$_8$V$_4$Fe$_4$        | -2.576| 77.9158985 | 2.5670264    |
| Y$_4$Ba$_4$Mn$_6$Fe$_2$  | -2.576| 276.3298238| 2.5670264    |
| Ba$_2$Sr$_6$Nb$_4$Sb$_4$ | -2.574| 54.46566395| 2.5680586    |
| Formula                  | E (eV) | H (J/m²) | M (µemu/emu) |
|--------------------------|--------|----------|--------------|
| Pr 8 Co 7 Ni 1           | -2.574 | 232.0999402 | 2.5680586    |
| Y 4 Ba 4 Mn 7 Fe 1       | -2.572 | 270.8413761 | 2.5690908    |
| Pr 4 Sr 4 Mn 6 Co 2      | -2.572 | 165.3456811 | 2.5690908    |
| Cs 2 Sr 6 Mn 2 V 6       | -2.571 | 187.0068489 | 2.5696069    |
| Pr 8 Sc 6 Co 2           | -2.571 | 79.30929155 | 2.5696069    |
| Y 8 Fe 2 Ni 6            | -2.564 | 382.5633221 | 2.5732196    |
| Y 4 Sr 4 Mn 2 Co 6       | -2.563 | 354.651155  | 2.5737357    |
| Ba 4 La 1 Mn 8 Zn 3      | -2.56  | 369.0954518 | 2.575284     |
| Y 7 Zn 1 Co 8            | -2.56  | 272.6248213 | 2.575284     |
| Pr 8 Cr 4 Ni 4           | -2.557 | 243.0441091 | 2.5768323    |
| Ca 8 Fe 7 Ni 1           | -2.555 | 413.2431014 | 2.5778645    |
| Ba 2 Sr 6 P 8            | -2.553 | 282.3804755 | 2.5788967    |
| Ca 8 Fe 7 Co 1           | -2.552 | 367.2076087 | 2.5794128    |
| Ca 8 Mn 1 Fe 7           | -2.541 | 347.3106785 | 2.5850899    |
| Sr 2 La 6 Ni 8           | -2.538 | 568.9110616 | 2.5866382    |
| Ba 4 Gd 4 Mn 8           | -2.534 | 164.7102036 | 2.5887026    |
| Pr 7 Zn 1 Co 8           | -2.534 | 259.7589406 | 2.5887026    |
| Ca 2 Pr 6 Co 8           | -2.53  | 261.7867658 | 2.590767     |
| Y 4 Ca 4 Fe 2 Co 6       | -2.529 | 286.4059257 | 2.5912831    |
| Ba 4 Ca 4 Sb 8           | -2.529 | 127.7580243 | 2.5912831    |
| La 4 Ba 4 Co 6 Ni 2      | -2.528 | 403.6448616 | 2.5917992    |
| Ba 4 Y 4 Fe 8            | -2.527 | 217.2823666 | 2.5923153    |
| La 8 Mg 4 Co 4           | -2.524 | 0         | 2.5938636    |
| Ca 2 Y 6 Co 8            | -2.524 | 274.4197706 | 2.5938636    |
| Pr 6 Zr 2 Zn 2 Co 6      | -2.523 | 245.3362527 | 2.5943797    |
| Ba 4 Sr 4 Nb 4 Sb 4      | -2.518 | 53.99947981 | 2.5969602    |
| La 4 Sr 4 Ni 4 Co 4      | -2.515 | 469.1633094 | 2.5985085    |
| Y 8 Sc 6 Co 2            | -2.514 | 88.89243349 | 2.5990246    |
| Y 8 Cr 2 Ni 6            | -2.514 | 351.3868663 | 2.5990246    |
| La 5 Zn 3 Ni 8           | -2.514 | 737.476796  | 2.5990246    |
| La 4 Sr 4 Co 4 Ni 4      | -2.511 | 473.3948094 | 2.6005729    |
| Pr 8 Co 6 Ni 2           | -2.511 | 254.4955257 | 2.6005729    |
| Ba 4 Pr 4 Fe 8           | -2.51  | 155.7867266 | 2.601089     |
| Sr 8 V 4 Co 4            | -2.506 | 189.6481381 | 2.6031534    |
| Pr 6 Ti 2 Zn 2 Co 6      | -2.506 | 238.8168087 | 2.6031534    |
| Y 8 Ga 6 Co 2            | -2.506 | 112.7702533 | 2.6031534    |
| La 1 Y 4 Zn 3 Co 8       | -2.503 | 389.764064  | 2.6047017    |
| Ba 3 Sr 3 La 2 Mn 1 Fe 7 | -2.496 | 0         | 2.6083144    |
| Sr 4 Ca 4 Nb 2 Sb 6      | -2.494 | 85.93951342 | 2.6093466    |
| Compound          | Energy  | Volume  | Pressure |
|-------------------|---------|---------|----------|
| Pr 4 Gd 4 Ni 8    | -2.49   | 0       | 2.611411 |
| Gd 2 Y 6 Ni 8     | -2.489  | 0       | 2.6119271|
| Pr 8 Fe 2 Ni 6    | -2.487  | 366.3311457 | 2.6129593|
| Ba 2 Y 6 Co 8     | -2.486  | 302.068387 | 2.6134754|
| Pr 8 Mg 1 Co 7    | -2.482  | 0       | 2.6155398|
| Ba 2 Ca 6 Fe 8    | -2.479  | 334.5116463 | 2.6170881|
| Y 4 Sr 4 Mn 4 Co 4| -2.476  | 225.3945446 | 2.6186364|
| Pr 4 Sr 4 Fe 1 Co 7| -2.476 | 298.9288828 | 2.6186364|
| Y 8 Fe 1 Ni 7     | -2.476  | 435.5505626 | 2.6186364|
| Sr 4 Ca 4 Fe 8    | -2.472  | 299.8738302 | 2.6207008|
| Y 8 Mg 1 Co 7     | -2.472  | 0       | 2.6207008|
| Y 4 Ca 4 Co 4 Ni 4| -2.47   | 636.6606914 | 2.621733 |
| Ba 8 Zr 4 Fe 4    | -2.469  | 24.184234  | 2.6222491|
| La 8 Mg 4 Mn 4    | -2.468  | 0       | 2.6227652|
| Pr 8 Mn 4 Ni 4    | -2.463  | 188.082551 | 2.6253457|
| Pr 4 Ca 4 Co 6 Ni 2| -2.462 | 468.3013478 | 2.6258618|
| La 1 Pr 4 Zn 3 Co 8| -2.458 | 393.7193107 | 2.6279262|
| Pr 8 Sc 7 Co 1    | -2.456  | 52.64078103 | 2.6289584|
| Ba 4 Pr 4 Mn 6 Fe 2| -2.456 | 133.1921281 | 2.6289584|
| Ba 6 Be 2 Sb 8    | -2.456  | 199.3690145 | 2.6289584|
| Y 4 Ba 4 Mn 7 Ni 1| -2.454  | 316.6478176 | 2.6299906|
| Y 4 Sr 4 Fe 2 Co 6| -2.453  | 304.5352641 | 2.6305067|
| Y 6 Ta 2 Zn 2 Ni 6| -2.453  | 396.281116  | 2.6305067|
| Y 8 Mn 2 Ni 6     | -2.452  | 314.7207074 | 2.6310228|
| Y 6 Nb 2 Zn 2 Ni 6| -2.449  | 405.1335275 | 2.6325711|
| Pr 4 Sr 4 Mn 6 Ni 2| -2.448  | 237.8759166 | 2.6330872|
| Sr 2 Pr 6 Co 8    | -2.448  | 235.6981408 | 2.6330872|
| Y 4 Ca 4 Fe 1 Co 7| -2.447  | 307.3998029 | 2.6336033|
| Y 8 Cr 1 Ni 7     | -2.446  | 393.8899597 | 2.6341194|
| Ba 2 La 6 Ni 8    | -2.446  | 575.4267746 | 2.6341194|
| Ba 6 Sr 2 P 8     | -2.445  | 294.768369  | 2.6346355|
| Y 6 Zn 2 Co 8     | -2.445  | 323.9130314 | 2.6346355|
| Pr 8 Ga 6 Co 2    | -2.443  | 111.9443855 | 2.6356677|
| Y 4 Ca 4 Mn 1 Co 7| -2.439  | 314.3394999 | 2.6377321|
| Sr 8 Nb 4 Fe 4    | -2.434  | 15.157992   | 2.6403126|
| Sr 4 La 1 Mn 8 Zn 3| -2.429  | 314.9037768 | 2.6428931|
| Y 4 Ba 4 Mn 7 Co 1| -2.429  | 214.9395749 | 2.6428931|
| Sr 2 Y 6 Co 8     | -2.428  | 275.3401846 | 2.6434092|
| Pr 4 Ca 4 Mn 1 Co 7| -2.415  | 302.4322467 | 2.6501185|
| Compound                  | 
|---------------------------|----------|--------------------------|--------------------------|--------------------------|--------------------------|
| Pr Ca 4 Fe 1 Co 7         | -2.412   | 287.1724691              | 2.6516668                |                           |
| La Ba 4 Co 4 Ni 4         | -2.412   | 494.0554519              | 2.6516668                |                           |
| Y Co 4 Ni 4              | -2.411   | 292.9383725              | 2.6521829                |                           |
| Pr Sr 4 Fe 2 Co 6         | -2.41    | 278.2800108              | 2.652699                 |                           |
| Pr Sr 4 Mn 1 Co 7         | -2.409   | 289.0712033              | 2.6532151                |                           |
| Ca Fe 4 Co 4              | -2.407   | 430.1962402              | 2.6542473                |                           |
| Pr Sr 4 Mn 2 Co 6         | -2.406   | 250.2894017              | 2.6547634                |                           |
| La Ba 4 Ni 4 Co 4         | -2.406   | 479.1169519              | 2.6547634                |                           |
| Sr Ta 2 Zn 2 Fe 6         | -2.405   | 255.1001766              | 2.6552795                |                           |
| Ba Ca 2 Nb 2 Sb 6         | -2.401   | 97.82161918              | 2.6573439                |                           |
| Ba Pr 6 Co 8              | -2.4     | 246.9259534              | 2.65786                  |                           |
| Y Mn 1 Ni 7               | -2.399   | 418.1811303              | 2.6583761                |                           |
| Sr Ca 1 Zn 3 Fe 8         | -2.398   | 369.0385384              | 2.6588922                |                           |
| Ca Y 4 Co 8               | -2.398   | 346.1706801              | 2.6588922                |                           |
| Y Ba 4 Mn 6 Co 2          | -2.396   | 223.6562358              | 2.6599244                |                           |
| Pr Cr 2 Nb 6              | -2.395   | 381.7454529              | 2.6604405                |                           |
| Ba Gd 4 Co 8              | -2.395   | 330.9255448              | 2.6604405                |                           |
| Ba Zr 6 Ta 1 Fe 1         | -2.394   | 154.5011281              | 2.6609566                |                           |
| Pr Ba 4 Mn 6 Fe 2         | -2.394   | 176.6493781              | 2.6619888                |                           |
| Pr Ba 4 Mn 7 Co 1         | -2.392   | 162.4753545              | 2.6656015                |                           |
| Pr Ba 4 Mn 7 Fe 1         | -2.385   | 316.6040265              | 2.6656015                |                           |
| Pr Zn 2 Co 8              | -2.385   | 368.8554502              | 2.6671498                |                           |
| Sr Ca 4 Fe 7 Ni 1         | -2.382   | 227.4078462              | 2.6671498                |                           |
| Ba Bi 2 La 1 Fe 8         | -2.382   | 486.8582213              | 2.6671498                |                           |
| Ca Fe 6 Ni 2              | -2.382   | 323.1319574              | 2.668182                 |                           |
| Sr Ca 4 Fe 7 Co 1         | -2.38    | 325.5141768              | 2.668182                 |                           |
| Ca Pr 4 Co 8              | -2.38    | 421.5219704              | 2.6686981                |                           |
| La Ca 4 Mn 4 Ni 4         | -2.379   | 454.2561102              | 2.6686981                |                           |
| Y Ti 2 Zn 2 Ni 6          | -2.379   | 58.90165387              | 2.6702464                |                           |
| Y Sc 7 Co 1               | -2.376   | 295.7007773              | 2.6712786                |                           |
| Sr Ca 4 Mn 1 Fe 7         | -2.374   | 483.2269946              | 2.6712786                |                           |
| Ca Fe 2 Co 6              | -2.373   | 196.1325414              | 2.6717947                |                           |
| Pr Sr 4 Mn 4 Co 4         | -2.373   | 377.3354629              | 2.6717947                |                           |
| Y Co 2 Ni 6               | -2.373   | 306.4794637              | 2.6728269                |                           |
| Y Sc 4 Ni 4               | -2.366   | 593.1099117              | 2.6754074                |                           |
| La Ca 4 Fe 2 Ni 6         | -2.366   | 389.7542358              | 2.6769557                |                           |
| Ca Fe 6 Co 2              | -2.363   | 0                        | 2.6779879                |                           |
| Y Mg 4 Cr 4               | -2.361   | 207.6357546              | 2.678504                 |                           |
| Sr Ca 2 Fe 8              | -2.36    | 273.6537546              | 2.678504                 |                           |
| Formula         | $E$  | $I$   | $J$  |
|-----------------|------|-------|------|
| Pr 8 Sc 4 Ni 4  | -2.358| 297.1335336 | 2.6795362 |
| Sr 6 Nb 2 Zn 2 Fe 6 | -2.356| 251.1368131 | 2.6805684 |
| Ca 8 Co 8       | -2.354| 521.4647489 | 2.6816006 |
| Pr 4 Sr 4 Co 7 Ni 1 | -2.354| 350.3865903 | 2.6816006 |
| La 4 Ca 4 Ni 6 Co 2 | -2.354| 643.1270717 | 2.6816006 |
| Ca 8 Mn 2 Fe 6   | -2.353| 334.8691255 | 2.6821167 |
| Y 8 Co 1 Ni 7    | -2.353| 419.377008  | 2.6821167 |
| Y 8 Ni 8        | -2.352| 460.6720532 | 2.6826328 |
| Ba 4 Bi 4 Fe 8   | -2.35 | 277.2975059 | 2.683665  |
| Pr 4 Ba 4Fe 2 Co 6 | -2.35 | 306.100654  | 2.683665  |
| Pr 8 Fe 1 Ni 7   | -2.348| 429.3478462 | 2.6846972 |
| Ba 4 Er 4 Mn 8   | -2.345| 194.0508465 | 2.6862455 |
| Ba 4 Ho 4 Mn 8   | -2.345| 186.984724  | 2.6862455 |
| Y 4 Ca 4 Co 7 Ni 1 | -2.345| 368.3207656 | 2.6862455 |
| Ba 4 Dy 4 Mn 8   | -2.344| 179.7887388 | 2.6867616 |
| Ba 6 La 2 Mn 2 Zr 1 Fe 5 | -2.343| 0          | 2.6872777 |
| Ba 6 La 2 Fe 8   | -2.341| 196.4869365 | 2.6883099 |
| Pr 8 Co 4 Ni 4   | -2.341| 370.568866  | 2.6883099 |
| Sr 8 Nb 1 Fe 7   | -2.338| 0          | 2.6898582 |
| Y 6 Ho 2 Ni 8   | -2.338| 460.1002237 | 2.6898582 |
| Ba 6 La 2 Fe 7 Co 1 | -2.337| 213.9916126 | 2.6903743 |
| Y 4 Ca 4 Mn 4 Ni 4 | -2.336| 530.5504304 | 2.6908904 |
| Ba 4 Y 4 Mn 8   | -2.334| 170.2999139 | 2.6919226 |
| Ba 8 Fe 6 Os 2   | -2.332| 104.1484936 | 2.6929548 |
| Y 4 Sr 4 Mn 1 Co 7 | -2.332| 297.6822065 | 2.6929548 |
| Dy 2 Y 6 Ni 8   | -2.332| 458.9489713 | 2.6929548 |
| Ba 4 Y 4 Co 8   | -2.33 | 336.6883899 | 2.693987 |
| Y 4 Ho 4 Ni 8   | -2.33 | 459.3523941 | 2.693987 |
| Sr 4 Ca 4 Mn 2 Fe 6 | -2.329| 290.7409743 | 2.6945031 |
| Pr 8 Mg 4 Cr 4   | -2.328| 0          | 2.6950192 |
| Y 6 Zr 2 Zn 2 Ni 6 | -2.326| 472.797573  | 2.6960514 |
| Y 4 Sr 4 Fe 1 Co 7 | -2.326| 306.3783861 | 2.6960514 |
| Ba 8 Fe 6 Mo 2   | -2.325| 58.92674799 | 2.6965675 |
| Pr 4 Ca 4 Co 4 Ni 4 | -2.324| 540.3229382 | 2.6970836 |
| Ba 8 Cr 8        | -2.322| 87.1232599  | 2.6981158 |
| Sn 4 Pr 4 Ni 8   | -2.321| 524.7171703 | 2.6986319 |
| Dy 4 Y 4 Ni 8   | -2.321| 457.0945001 | 2.6986319 |
| Pr 6 Ta 2 Zn 2 Ni 6 | -2.32 | 411.1498357 | 2.699148 |
| Ba 6 Gd 2 Fe 8   | -2.319| 231.0392297 | 2.6996641 |
| Compound                  | Energy  | Volume  | Entropy |
|---------------------------|---------|---------|---------|
| Pr$_6$Nb$_2$Zn$_2$Ni$_6$  | -2.319  | 409.452401 | 2.6996641 |
| Ba$_2$Bi$_2$Pr$_4$Co$_8$  | -2.318  | 307.281221 | 2.7001802 |
| Pr$_4$Ca$_4$Ni$_4$Co$_4$  | -2.316  | 542.5241882 | 2.7012124 |
| Bi$_4$Pr$_4$Co$_8$        | -2.314  | 266.3248541 | 2.7022446 |
| Sm$_2$Y$_6$Ni$_8$         | -2.314  | 455.4158152 | 2.7022446 |
| Y$_6$Hf$_2$Zn$_2$Ni$_6$   | -2.31   | 467.0525628 | 2.704309 |
| Ba$_4$Pr$_4$Mn$_8$        | -2.309  | 113.3198309 | 2.7048251 |
| Y$_4$Ba$_4$Mn$_6$Ni$_2$   | -2.308  | 375.8594713 | 2.7053412 |
| Ba$_8$Fe$_6$Tc$_2$        | -2.305  | 52.78484702 | 2.7068895 |
| Pr$_6$Gd$_2$Ni$_8$        | -2.304  | 0         | 2.7074056 |
| Sr$_4$Y$_4$Co$_8$         | -2.303  | 333.9982581 | 2.7079217 |
| Pr$_4$Ba$_4$Mn$_6$Co$_2$  | -2.302  | 214.4696752 | 2.7084378 |
| Pr$_4$Ca$_4$Co$_7$Ni$_1$  | -2.302  | 414.8587623 | 2.7084378 |
| Nd$_2$Y$_6$Ni$_8$         | -2.299  | 455.4534265 | 2.7099861 |
| Ca$_4$Mg$_4$Nb$_2$Sb$_6$  | -2.296  | 141.0142851 | 2.7115344 |
| Ba$_6$La$_2$Mn$_2$Fe$_6$  | -2.294  | 182.712981 | 2.7125666 |
| Y$_8$Ga$_7$Co$_1$         | -2.29   | 90.44731865 | 2.714631 |
| Y$_8$Sc$_6$Ni$_2$         | -2.289  | 173.367169 | 2.7151471 |
| Sr$_6$Ca$_2$Fe$_7$Co$_1$  | -2.289  | 299.9831318 | 2.7151471 |
| Y$_4$Ba$_4$Fe$_2$Co$_6$   | -2.285  | 332.4391548 | 2.7172115 |
| Pr$_8$Cr$_1$Ni$_7$        | -2.284  | 430.4297498 | 2.7177276 |
| Ba$_6$Ho$_2$Fe$_8$        | -2.283  | 261.8126244 | 2.7182437 |
| Ba$_8$Hf$_4$Fe$_4$        | -2.282  | 153.8311674 | 2.7187598 |
| Mg$_8$Fe$_8$              | -2.282  | 798.2854405 | 2.7187598 |
| Ba$_6$Dy$_2$Fe$_8$        | -2.282  | 254.0526318 | 2.7187598 |
| Ba$_2$Ca$_6$Nb$_2$Sb$_6$  | -2.277  | 102.6987737 | 2.7213403 |
| Pr$_8$Mn$_2$Ni$_6$        | -2.276  | 342.1187009 | 2.7218564 |
| Y$_4$Sr$_4$Co$_7$Ni$_1$   | -2.274  | 370.2203436 | 2.7228886 |
| Pr$_4$Ba$_4$Mn$_7$Ni$_1$  | -2.272  | 222.3413708 | 2.7239208 |
| Sm$_4$Y$_4$Ni$_8$         | -2.272  | 448.5125771 | 2.7239208 |
| Ba$_6$La$_2$Fe$_6$Co$_2$  | -2.27   | 179.1231584 | 2.724953 |
| Y$_8$Mg$_2$Co$_6$         | -2.269  | 0         | 2.7254691 |
| Pr$_8$Co$_2$Ni$_6$        | -2.268  | 405.6257064 | 2.7259852 |
| Ba$_4$Sm$_4$Mn$_8$        | -2.267  | 147.6676498 | 2.7265013 |
| Pr$_4$Ba$_4$Mn$_1$Co$_7$  | -2.265  | 302.3406608 | 2.7275335 |
| Ba$_6$Nb$_2$Zn$_2$Fe$_6$  | -2.263  | 296.7492425 | 2.7285657 |
| Pr$_4$Sr$_4$Co$_6$Ni$_2$  | -2.262  | 406.4674258 | 2.7290818 |
| Sr$_6$Ca$_2$Fe$_7$Ni$_1$  | -2.261  | 342.6576245 | 2.7295979 |
| Pr$_4$Ba$_4$Fe$_1$Co$_7$  | -2.261  | 317.8756615 | 2.7295979 |
| Formula                | Energy   | E_p          | E_v          |
|------------------------|----------|--------------|--------------|
| Sr 6 Ca 2 Mn 1 Fe 7    | -2.26    | 269.2714516  | 2.730114     |
| Sr 8 Mn 1 Fe 7         | -2.258   | 238.5035601  | 2.7311462    |
| Ca 8 Mn 2 Co 6         | -2.256   | 471.8903886  | 2.7321784    |
| Sr 4 Sm 4 Co 8         | -2.254   | 310.099704   | 2.7332106    |
| Sr 4 Pr 4 Co 8         | -2.254   | 288.2681768  | 2.7332106    |
| Pr 8 Mg 2 Co 6         | -2.252   | 0            | 2.7342428    |
| Ca 8 Mn 8              | -2.249   | 334.7553077  | 2.7357911    |
| La 4 Ca 4 Mn 2 Ni 6    | -2.247   | 578.2460663  | 2.7368233    |
| Pr 8 Sc 6 Ni 2         | -2.246   | 164.8860271  | 2.7373394    |
| Ba 6 Ca 2 Nb 4 Sb 4    | -2.246   | 88.35353188  | 2.7373394    |
| Ba 4 Ca 4 Nb 2 Sb 6    | -2.246   | 114.5928214  | 2.7373394    |
| Sr 8 Fe 8              | -2.245   | 247.5714372  | 2.7378555    |
| Sr 4 Ca 4 Fe 4 Co 4    | -2.243   | 391.307089   | 2.7388877    |
| Nd 4 Y 4 Ni 8          | -2.243   | 446.1355498  | 2.7388877    |
| Ba 4 Ca 4 Fe 8         | -2.242   | 327.8528111  | 2.7394038    |
| Pr 4 Ba 4 Mn 2 Co 6    | -2.242   | 282.216137   | 2.7394038    |
| Y 8 Ga 4 Ni 4          | -2.242   | 308.1100936  | 2.7394038    |
| Ba 6 Ta 2 Zn 2 Fe 6    | -2.241   | 295.820892   | 2.7399199    |
| La 4 Ca 4 Fe 1 Ni 7    | -2.241   | 660.8214192  | 2.7399199    |
| Ba 4 Nd 4 Mn 8         | -2.24    | 154.8019559  | 2.740436     |
| Pr 8 Ga 7 Co 1         | -2.238   | 91.40038876  | 2.7414682    |
| Ca 8 Mn 4 Fe 4         | -2.237   | 321.6445196  | 2.7419843    |
| Pr 6 Ti 2 Zn 2 Ni 6    | -2.237   | 476.0427652  | 2.7419843    |
| La 4 Ca 4 Ni 7 Co 1    | -2.231   | 682.0238669  | 2.7450809    |
| Sr 7 Zn 1 Fe 8         | -2.23    | 307.4639178  | 2.745597     |
| Pr 8 Mn 1 Ni 7         | -2.229   | 418.4583738  | 2.7461131    |
| Ca 8 Mn 7 Fe 1         | -2.224   | 326.9483606  | 2.748936     |
| Ba 6 Ti 2 Mn 6 Zn 2    | -2.223   | 330.4780611  | 2.7492097    |
| La 4 Sr 4 Mn 4 Ni 4    | -2.223   | 356.8030556  | 2.7492097    |
| La 4 Sr 4 Fe 2 Ni 6    | -2.223   | 528.8015064  | 2.7492097    |
| Sr 4 Ca 4 Fe 2 Co 6    | -2.222   | 436.8310829  | 2.7497258    |
| Ba 4 Pr 4 Mn 8         | -2.22    | 146.4565809  | 2.750758     |
| Ca 8 Fe 1 Co 7         | -2.219   | 500.5668718  | 2.7512741    |
| Ca 8 Mn 6 Fe 2         | -2.218   | 325.8941636  | 2.7517902    |
| Ba 6 Sm 2 Fe 8         | -2.217   | 224.2396537  | 2.7523063    |
| Y 4 Ba 4 Mn 4 Co 4     | -2.217   | 254.1180577  | 2.7523063    |
| Ca 4 Sr 4 Fe 2 Co 6    | -2.217   | 423.4718329  | 2.7523063    |
| La 4 Sr 4 Ni 6 Co 2    | -2.216   | 572.0228997  | 2.7528224    |
| Pr 4 Ho 4 Ni 8         | -2.216   | 527.5306481  | 2.7528224    |
| Compound                  | E (eV) | V (eV) | a (Å)  |
|--------------------------|--------|--------|--------|
| Y 4 Ca 4 Ni 4 Co 4       | -2.215 | 500.6954414 | 2.7533385 |
| Ba 2 Mg 6 Fe 8           | -2.214 | 678.9621781  | 2.7538546  |
| Ba 5 Cd 2 La 1 Fe 8      | -2.214 | 324.3463172  | 2.7538546  |
| Ca 4 Sr 4 Fe 1 Co 7      | -2.214 | 438.8239549  | 2.7538546  |
| Sr 6 Ca 2 Mn 2 Fe 6      | -2.212 | 264.7443987  | 2.7548868  |
| Ba 4 Pr 4 Mn 6 Co 2      | -2.21  | 178.3276752  | 2.755919   |
| Sr 6 Ti 2 Zn 2 Fe 6      | -2.209 | 308.6781097  | 2.7564351  |
| Y 4 Ba 4 Mn 1 Co 7       | -2.206 | 424.5443612  | 2.7579834  |
| Ba 3 Bi 1 Pr 4 Co 8      | -2.205 | 307.8497615  | 2.7584995  |
| Pr 4 Dy 4 Ni 8           | -2.205 | 523.396163   | 2.7584995  |
| Sr 4 Ca 4 Fe 6 Co 2      | -2.203 | 346.2090846  | 2.7595317  |
| Ba 3 Cd 4 La 1 Fe 8      | -2.2   | 418.0459707  | 2.76108    |
| Ba 2 Ca 6 Nb 4 Sb 4      | -2.2   | 92.53607088  | 2.76108    |
| Ba 8 Pr 8                | -2.2   | 588.834002   | 2.76108    |
| Pr 8 Ga 4 Ni 4           | -2.2   | 316.3933501  | 2.76108    |
| Ca 8 Mn 7 Co 1           | -2.196 | 374.2804878  | 2.7631444  |
| Pr 8 Co 1 Ni 7           | -2.194 | 450.5852515  | 2.7641766  |
| Bi 4 Sr 4 Fe 2 Co 6      | -2.193 | 384.9811793  | 2.764927   |
| Ca 8 Co 6 Ni 2           | -2.193 | 622.2386999  | 2.764927   |
| Y 8 Sc 7 Ni 1            | -2.19  | 100.6333966  | 2.766241   |
| Sr 4 Ca 4 Co 8           | -2.19  | 459.4058269  | 2.766241   |
| Pr 4 Sm 4 Ni 8           | -2.19  | 507.5048239  | 2.766241   |
| Y 4 Ca 4 Ni 6 Co 2       | -2.189 | 743.5602817  | 2.7667571  |
| Ba 6 Bi 1 La 1 Fe 8      | -2.188 | 220.7011299  | 2.7672732  |
| Y 4 Ca 4 Fe 2 Ni 6       | -2.188 | 686.1998822  | 2.7672732  |
| Ca 8 Mn 6 Co 2           | -2.187 | 375.926918   | 2.7677893  |
| Ba 7 Ce 1 Fe 8           | -2.186 | 220.0050908  | 2.7683054  |
| Pr 4 Ba 4 Co 7 Ni 1      | -2.186 | 362.6095434  | 2.7683054  |
| Y 7 Zn 1 Ni 8            | -2.186 | 578.7045133  | 2.7683054  |
| Pr 6 Dy 2 Ni 8           | -2.184 | 511.5913548  | 2.7693376  |
| Sr 8 Ta 2 Co 6           | -2.183 | 213.6840515  | 2.7698537  |
| Ba 6 La 2 Fe 4 Co 4      | -2.182 | 262.2512907  | 2.7703698  |
| Be 8 Sb 8                | -2.181 | 236.2582555  | 2.7708859  |
| Sr 8 Nb 1 Ta 1 Co 6      | -2.178 | 214.495143   | 2.7724342  |
| Ca 4 La 4 Ni 8           | -2.177 | 685.6124121  | 2.7729503  |
| Ba 6 Ti 2 Zn 2 Co 6      | -2.176 | 448.448642   | 2.7734664  |
| Sr 8 Fe 7 Co 1           | -2.176 | 265.774801   | 2.7734664  |
| La 4 Ca 4 Mn 1 Ni 7      | -2.175 | 654.2302392  | 2.7739825  |
| Ba 6 Ta 2 Mn 6 Zn 2      | -2.174 | 278.9857945  | 2.7744986  |
| Compound                  | λ       | u      | C      |
|--------------------------|---------|--------|--------|
| Pr₆Zr₂Zn₂Ni₆             | -2.174  | 468.3502092 | 2.7744986 |
| Ca₈Mn₄Co₄                | -2.173  | 420.3897783  | 2.7750147  |
| Ba₆Ta₂Zn₂Co₆             | -2.171  | 380.7602426  | 2.7760469  |
| Ba₆Nd₂Fe₈                | -2.171  | 210.0553299  | 2.7760469  |
| Ca₄Be₄Nb₄Sb₄             | -2.171  | 152.9915615  | 2.7760469  |
| Ba₈Ta₂Fe₆                | -2.17   | 149.2286549  | 2.776563   |
| Y₄Ba₄Fe₁Co₇              | -2.169  | 352.1525565  | 2.7770791  |
| Sr₄Ca₄Fe₆Ni₂              | -2.168  | 443.2770701  | 2.7775952  |
| Y₈Mg₁Ni₇                 | -2.168  | 0        | 2.7775952  |
| Pr₆Ho₂Ni₈                | -2.168  | 514.3043474  | 2.7775952  |
| Ba₄La₁Zn₃Fe₈              | -2.167  | 400.1005193  | 2.7781113  |
| Ba₄La₁Zn₃Co₈              | -2.167  | 524.5907561  | 2.7781113  |
| Ba₄Pr₄Co₈                 | -2.163  | 310.1834579  | 2.7801757  |
| Ba₆Mg₂Nb₂Sb₆              | -2.162  | 138.7904866  | 2.7806918  |
| Sr₈Fe₇Ni₁                 | -2.158  | 311.5800437  | 2.7827562  |
| Pr₆Sm₂Ni₈                 | -2.158  | 501.2193103  | 2.7827562  |
| Pr₆Hf₂Zn₂Ni₆              | -2.157  | 461.3808079  | 2.7832723  |
| Y₄Ba₄Mn₂Co₂₆             | -2.156  | 308.3911296  | 2.7837884  |
| Pr₄Ba₄Mn₆Ni₂              | -2.155  | 277.4386607  | 2.7843045  |
| Sr₆Ca₂Fe₄Co₄              | -2.155  | 354.911753   | 2.7843045  |
| Y₄Ba₄Co₇Ni₁               | -2.155  | 487.6354754  | 2.7843045  |
| Ba₆Be₂Nb₂Sb₆              | -2.155  | 160.6666772  | 2.7843045  |
| Ba₆Mn₆Nb₂Zn₂              | -2.151  | 275.9198208  | 2.7863689  |
| Ba₅Sn₂La₁Fe₈              | -2.151  | 345.580582   | 2.7863689  |
| Pr₄Nd₄Ni₈                 | -2.151  | 497.5630466  | 2.7863689  |
| Sr₄Ca₄Fe₁Co₇              | -2.15   | 440.8877049  | 2.786885   |
| Sr₆Zn₂Fe₈                 | -2.149  | 361.8709065  | 2.7874011  |
| Y₄Sr₄Co₆Ni₂               | -2.148  | 411.1886791  | 2.7879172  |
| Ba₆Sn₁La₁Fe₈              | -2.145  | 264.0901228  | 2.7894655  |
| Ba₆Mn₈Zn₂                 | -2.144  | 381.1816283  | 2.7899816  |
| La₄Ba₄Ni₆Co₂              | -2.143  | 587.6315422  | 2.7904977  |
| Pr₈Sc₇Ni₁                 | -2.141  | 93.84752378  | 2.7915299  |
| Sr₄Ca₄Nb₄Ni₄              | -2.141  | 341.9325571  | 2.7915299  |
| Ba₆Pr₂Fe₈                 | -2.141  | 203.268316   | 2.7915299  |
| Ba₆Nd₂Ni₈                 | -2.141  | 536.9677126  | 2.7915299  |
| Pr₆Nd₂Ni₈                 | -2.141  | 495.8134216  | 2.7915299  |
| Sr₈Al₁Fe₇                 | -2.138  | 193.8944303  | 2.7930782  |
| Ba₆Cd₁La₁Fe₈              | -2.137  | 273.0593654  | 2.7935943  |
| La₆Ho₂Ga₈                 | -2.137  | 26.82825386  | 2.7935943  |
| Compound                       | E   | Volume     | Entropy   |
|-------------------------------|-----|------------|-----------|
| Ca 8 Mn 7 Ni 1                | -2.136 | 401.9799806 | 2.7941104 |
| Sr 8 Nb 2 Co 6                | -2.136 | 223.8874844 | 2.7941104 |
| Ba 4 Ca 4 Nb 4 Sb 4           | -2.136 | 90.57061863 | 2.7941104 |
| La 8 Ga 8                     | -2.136 | 6.371386071  | 2.7941104 |
| Rb 4 Sr 4 Nb 4 Cr 4           | -2.135 | 185.93147    | 2.7946265 |
| Rb 4 Ba 4 Nb 4 Cr 4           | -2.133 | 178.0226894  | 2.7956587 |
| Ca 4 Sr 4 Mn 1 Co 7           | -2.131 | 433.8097754  | 2.7966909 |
| Ba 6 Sn 2 Hf 1 Zr 6 Fe 1      | -2.13 | 14.1026932   | 2.797207  |
| Pr 8 Ni 8                     | -2.13 | 493.4297967  | 2.797207  |
| Sr 6 Zr 2 Zn 2 Fe 6           | -2.129 | 301.0013601  | 2.7977231 |
| Y 4 Ca 4 Mn 2 Ni 6            | -2.129 | 680.8682763  | 2.7977231 |
| La 6 Gd 2 Ga 8                | -2.127 | 86.02726086  | 2.7987553 |
| La 4 Ba 4 Fe 2 Ni 6           | -2.126 | 557.493813   | 2.7992714 |
| La 6 Dy 2 Ga 8                | -2.126 | 25.36959074  | 2.7992714 |
| Ba 8 Fe 7 Re 1                | -2.123 | 130.5747776  | 2.8008197 |
| Sr 4 La 1 Zn 3 Co 8           | -2.122 | 515.9685848  | 2.8013358 |
| Sr 4 Ca 4 V 4 Ni 4            | -2.12 | 408.7107165  | 2.802368  |
| La 6 Sm 2 Ga 8                | -2.12 | 17.33731032  | 2.802368  |
| La 4 Ba 4 Mn 4 Ni 4           | -2.117 | 376.3281558  | 2.8039163 |
| Ba 4 Sr 4 V 4 Fe 4            | -2.116 | 336.1904117  | 2.8044324 |
| Ca 4 Mg 4 Nb 4 Sb 4           | -2.115 | 147.6240749  | 2.8049485 |
| Ba 4 Sr 4 Nb 1 Fe 7           | -2.114 | 152.4243082  | 2.8054646 |
| Sr 6 Ca 2 Fe 6 Co 2           | -2.113 | 319.913259   | 2.8059807 |
| Y 8 Mg 2 Ni 6                 | -2.112 | 0           | 2.8064968 |
| La 4 Sr 4 Fe 1 Ni 7           | -2.112 | 595.6642472  | 2.8064968 |
| Ca 4 Sr 4 Co 7 Ni 1           | -2.111 | 521.0686624  | 2.8070129 |
| Pr 4 Sr 4 Co 4 Ni 4           | -2.11 | 476.8797662  | 2.807529  |
| Pr 4 Sr 4 Ni 4 Co 4           | -2.11 | 481.0867662  | 2.807529  |
| Ba 2 Sr 6 Fe 8                | -2.109 | 254.9686131  | 2.8080451 |
| La 4 Ba 4 Mn 2 Fe 6           | -2.109 | 912.6415938  | 2.8080451 |
| La 6 Nd 2 Ga 8                | -2.109 | 12.63281495  | 2.8080451 |
| Sr 8 Ta 1 Co 7                | -2.107 | 279.0532282  | 2.8090773 |
| Pr 4 Ba 4 Mn 4 Co 4           | -2.103 | 224.0150194  | 2.8111417 |
| Pr 4 Ca 4 Mn 4 Ni 4           | -2.103 | 430.0461772  | 2.8111417 |
| Ca 4 Be 4 Nb 2 Sb 6           | -2.102 | 200.9152643  | 2.8116578 |
| Ba 8 Fe 6 Ir 2                | -2.101 | 196.1409513  | 2.8121739 |
| Ca 8 Co 7 Ni 1                | -2.101 | 568.1688344  | 2.8121739 |
| Pr 4 Ba 4 Co 6 Ni 2           | -2.101 | 414.7091289  | 2.8121739 |
| Ba 7 Mn 8 Zn 1                | -2.1 | 281.39648    | 2.81269  |
| Formula                  | Excess Charge | Z | Zeta   |
|-------------------------|---------------|---|--------|
| **La 8 Mg 4 Ni 4**      | -2.1          | 10.40038147 | 2.81269 |
| **Mg 8 Sb 8**           | -2.099        | 192.3992822 | 2.8132061 |
| **Sr 8 Ti 8**           | -2.097        | 8.691789 | 2.8142383 |
| **Ba 8 Ta 4 Fe 4**      | -2.097        | 27.476419 | 2.8142383 |
| **Sr 6 Hf 2 Zn 2 Fe 6** | -2.097        | 317.1017922 | 2.8142383 |
| **Sr 8 Ga 1 Fe 7**      | -2.097        | 197.3864087 | 2.8142383 |
| **Ba 8 Fe 4 Ir 4**      | -2.095        | 183.0337619 | 2.8152705 |
| **Sr 4 Ca 4 Nb 4 Sb 4** | -2.094        | 76.70913433 | 2.8157866 |
| **Sr 8 In 1 Fe 7**      | -2.093        | 202.1581975 | 2.8163027 |
| **Ba 8 Zr 2 Fe 6**      | -2.091        | 189.7558611 | 2.8173349 |
| **Sr 4 Ca 4 Mn 1 Co 7** | -2.087        | 420.2142754 | 2.8193993 |
| **Ca 8 Mn 6 Ni 2**      | -2.086        | 474.3791535 | 2.8199154 |
| **Ba 4 Mg 4 Fe 8**      | -2.086        | 572.8561656 | 2.8199154 |
| **Sr 8 Y 1 Fe 7**       | -2.085        | 201.3523665 | 2.8204315 |
| **Sr 4 Ca 4 Mn 2 Co 6** | -2.085        | 414.8629738 | 2.8204315 |
| **Sr 8 Sc 1 Fe 7**      | -2.083        | 181.0728821 | 2.8214637 |
| **La 4 Sr 4 Ni 7 Co 1** | -2.085        | 616.9709449 | 2.8204315 |
| **Ba 7 La 1 Fe 8**      | -2.084        | 224.9271636 | 2.8209476 |
| **Ba 4 Pr 4 Mn 6 Ni 2** | -2.084        | 254.6216607 | 2.8209476 |
| **Ca 4 Sr 4 V 4 Cr 4**  | -2.083        | 423.2795697 | 2.8214637 |
| **Sr 8 Sc 1 Fe 7**      | -2.083        | 181.0728821 | 2.8214637 |
| **Ba 4 Ca 4 Nb 4 Ni 4** | -2.083        | 380.9438349 | 2.8214637 |
| **Sr 8 Nb 1 Co 7**      | -2.083        | 297.8390697 | 2.8214637 |
| **Bi 2 Ba 2 Sr 4 Fe 2 Co 6** | -2.083 | 355.1963771 | 2.8214637 |
| **Ca 4 Sr 4 Mn 2 Co 6** | -2.081        | 415.2572238 | 2.8224959 |
| **Ba 8 Hf 2 Fe 6**      | -2.079        | 207.6237791 | 2.8235281 |
| **Ba 7 La 1 Fe 4 Co 4** | -2.079        | 284.0041488 | 2.8235281 |
| **Ca 4 Ba 4 Fe 1 Co 7** | -2.077        | 460.8479694 | 2.8245603 |
| **Ba 7 Zn 1 Co 8**      | -2.076        | 415.1666713 | 2.8250764 |
| **Ba 4 Ca 4 Fe 2 Co 6** | -2.075        | 459.0315029 | 2.8255925 |
| **Ba 8 Rh 8**           | -2.073        | 377.7964269 | 2.8266247 |
| **Ca 4 Ba 4 Fe 2 Co 6** | -2.07         | 439.4940029 | 2.828173 |
| **Sr 6 Nb 2 Zn 2 Co 6** | -2.066        | 359.7654971 | 2.8302374 |
| **Ca 4 Sr 4 Mn 7 Fe 1** | -2.065        | 277.6430117 | 2.8307535 |
| **Ba 7 Gd 1 Fe 8**      | -2.065        | 240.9700602 | 2.8307535 |
| **Y 4 Ba 4 Co 6 Ni 2**  | -2.063        | 540.4078109 | 2.8317857 |
| **Sr 6 Ta 2 Zn 2 Co 6** | -2.062        | 363.8603143 | 2.8323018 |
| **Ba 8 Fe 7 Tc 1**      | -2.061        | 140.7223689 | 2.8328179 |
| **Y 8 Ga 6 Ni 2**       | -2.061        | 190.4394888 | 2.8328179 |
| **La 4 Gd 4 Ga 8**      | -2.056        | 89.35165328 | 2.8353984 |
| Formula                  | E   | H   | T   |
|--------------------------|-----|-----|-----|
| Sr 8 Al 2 Fe 6           | -2.055 | 211.8689316 | 2.8359145 |
| Ba 8 Nb 2 Fe 6           | -2.055 | 148.1074374 | 2.8359145 |
| Ca 8 Co 4 Ni 4           | -2.052 | 722.4030103 | 2.8374628 |
| La 4 Ba 4 Fe 1 Ni 7      | -2.052 | 615.9256332 | 2.8374628 |
| La 1 Y 4 Zn 3 Ni 8       | -2.052 | 725.216256  | 2.8374628 |
| Sr 6 Ca 2 Fe 6 Ni 2      | -2.051 | 416.9937445 | 2.8379789 |
| Sr 8 Fe 4 Co 4           | -2.051 | 322.089417  | 2.8379789 |
| Ba 4 Ca 4 Fe 1 Co 7      | -2.049 | 452.6682194 | 2.8390111 |
| Pr 8 Ga 6 Ni 2           | -2.049 | 193.152121  | 2.8390111 |
| Sr 4 Ca 4 Mn 7 Co 1      | -2.048 | 316.517823  | 2.8395272 |
| Sr 6 Ca 2 Co 8           | -2.048 | 415.7347409 | 2.8395272 |
| Y 4 Ca 4 Fe 1 Ni 7       | -2.047 | 755.5832521 | 2.8400433 |
| La 4 Ba 4 Ni 7 Co 1      | -2.046 | 636.9070874 | 2.8405594 |
| Ca 8 Ni 4 Co 4           | -2.045 | 724.0382603 | 2.8410755 |
| Be 8 P 8                 | -2.043 | 227.890892  | 2.8421077 |
| Ba 2 Sr 6 Fe 7 Co 1      | -2.043 | 284.7427914 | 2.8421077 |
| Y 8 Ga 7 Ni 1            | -2.042 | 128.8495614 | 2.8426238 |
| Sr 4 Ca 4 Co 7 Ni 1      | -2.038 | 507.6221624 | 2.8446882 |
| Y 4 Sr 4 Mn 4 Ni 4       | -2.037 | 477.4155156 | 2.8452043 |
| La 4 Ba 4 Mn 2 Ni 6      | -2.037 | 529.9645192 | 2.8452043 |
| Sr 8 Fe 1 Co 7           | -2.035 | 366.8430329 | 2.8462365 |
| Sr 4 Ca 4 Co 6 Ni 2      | -2.035 | 577.3824979 | 2.8462365 |
| La 4 Sr 4 Mn 1 Ni 7      | -2.034 | 600.1411958 | 2.8467526 |
| Sr 2 Y 6 Ni 8            | -2.034 | 536.3513766 | 2.8467526 |
| Ba 8 Zr 3 Fe 5           | -2.033 | 153.5117213 | 2.8472687 |
| Ca 4 Sr 4 Co 6 Ni 2      | -2.033 | 582.0889979 | 2.8472687 |
| Y 4 Ca 4 Ni 7 Co 1       | -2.029 | 782.3535769 | 2.8493331 |
| Pr 4 Ca 4 Fe 2 Ni 6      | -2.026 | 592.0182178 | 2.8508814 |
| Sr 4 Mg 4 Nb 4 Sb 4      | -2.02  | 109.0789361 | 2.853978 |
| Ba 2 Sr 6 Fe 7 Ni 1      | -2.019 | 318.7232842 | 2.8544941 |
| Sr 8 Fe 2 Co 6           | -2.015 | 306.3324109 | 2.8565585 |
| Ba 7 Ho 1 Fe 8           | -2.014 | 256.1937576 | 2.8570746 |
| Sr 8 Sc 2 Fe 6           | -2.013 | 184.8878352 | 2.8575907 |
| Ba 6 Bi 2 Fe 8           | -2.013 | 247.7440733 | 2.8575907 |
| Pr 4 Ca 4 Ni 6 Co 2      | -2.012 | 650.0937785 | 2.8581068 |
| Ba 6 Zr 2 Zn 2 Fe 6      | -2.009 | 424.4560982 | 2.8596551 |
| Y 4 Sr 4 Co 4 Ni 4       | -2.009 | 484.4770194 | 2.8596551 |
| Ba 7 La 1 Fe 7 Co 1      | -2.008 | 247.9249284 | 2.8601712 |
| Ba 4 Pr 4 Mn 6 Cu 2      | -2.008 | 271.0503217 | 2.8601712 |
| Formula           | E(0)  | E(1)   | E(2)   |
|-------------------|-------|--------|--------|
| Ba 7 Sm 1 Fe 8    | -2.005 | 237.5190223 | 2.8617195 |
| Ca 8 Fe 4 Ni 4    | -2.004 | 633.5822112 | 2.8622356 |
| Sr 4 Ca 4 Mn 8    | -2.003 | 278.3276429 | 2.8627517 |
| Ba 7 Dy 1 Fe 8    | -2.003 | 252.2717613 | 2.8627517 |
| Sr 8 Fe 6 Co 2    | -2.003 | 283.577423  | 2.8627517 |
| Sr 8 Co 8         | -2.002 | 386.5076549 | 2.8632678 |
| Ca 4 Sr 4 Mn 6 Co 2 | -2.001 | 321.4642532 | 2.8637839 |
| Ba 8 Fe 7 Os 1    | -2.001 | 160.6995672 | 2.8637839 |
| Ba 6 Zn 2 Co 8    | -2.001 | 506.3222196 | 2.8637839 |
| Ca 4 Sr 4 Mn 7 Co 1 | -2    | 313.774323  | 2.8643   |
| Sr 8 V 4 Ni 4     | -2    | 348.3828591 | 2.8643   |
| Ba 6 Ca 2 Fe 8    | -2    | 291.422726  | 2.8643   |
| Sr 4 Ca 4 Mn 6 Fe 2 | -1.999 | 280.9596306 | 2.8648161 |
| Ca 4 Ba 4 Mn 1 Co 7 | -1.999 | 445.9924072 | 2.8648161 |
| Y 4 Sr 4 Ni 4 Co 4 | -1.999 | 485.2922694 | 2.8648161 |
| Y 4 Ca 4 Mn 1 Ni 7 | -1.999 | 754.8204492 | 2.8648161 |
| Sr 8 Ga 2 Fe 6    | -1.998 | 219.9801384 | 2.8653322 |
| Sr 4 Ca 4 Mn 6 Co 2 | -1.997 | 324.1540032 | 2.8658483 |
| Ba 2 Sr 6 Mn 1 Fe 7 | -1.997 | 254.1510506 | 2.8658483 |
| Sr 8 Mn 2 Fe 6    | -1.995 | 229.6719413 | 2.8668805 |
| La 4 Ba 4 Mn 1 Ni 7 | -1.994 | 604.0444509 | 2.8673966 |
| Sr 4 Ca 4 Mn 7 Fe 1 | -1.993 | 280.6595117 | 2.8679127 |
| Ca 4 Sr 4 Mn 6 Fe 2 | -1.991 | 278.1376306 | 2.8689449 |
| Pr 8 Mg 1 Ni 7    | -1.99  | 0       | 2.869461 |
| Ba 4 Sr 4 Mn 7 Co 1 | -1.985 | 268.7477101 | 2.8720415 |
| Pr 7 Zn 1 Ni 8    | -1.985 | 571.5666326 | 2.8720415 |
| Ba 7 Nd 1 Fe 8    | -1.984 | 230.7494853 | 2.8725576 |
| Ca 2 Pr 6 Ni 8    | -1.982 | 582.8379578 | 2.8735898 |
| Ba 4 Sr 4 Fe 8    | -1.981 | 263.377789  | 2.8741059 |
| Sr 4 Ca 4 Mn 4 Fe 4 | -1.98  | 278.1373683 | 2.874622 |
| Pr 8 Ga 7 Ni 1    | -1.98  | 131.3143814 | 2.874622 |
| Ba 4 Be 4 Sb 8    | -1.98  | 254.2526593 | 2.874622 |
| Ba 6 Mg 2 Nb 4 Sb 4 | -1.974 | 101.9765834 | 2.8777186 |
| Ca 4 Ba 4 Co 7 Ni 1 | -1.973 | 523.3975214 | 2.8782347 |
| Ba 7 La 1 Fe 6 Co 2 | -1.972 | 256.0614657 | 2.8787508 |
| Sr 4 Ca 4 Mn 4 Co 4 | -1.97  | 363.2118635 | 2.879783 |
| Ca 4 Sr 4 Mn 4 Co 4 | -1.97  | 361.5226135 | 2.879783 |
| Ba 4 Ca 4 Mn 1 Co 7 | -1.97  | 436.7011572 | 2.879783 |
| Sr 4 Ba 4 Sc 1 Fe 7 | -1.969 | 193.8227154 | 2.8802991 |

| Formula           | E(0)  | E(1)   | E(2)   |
|-------------------|-------|--------|--------|
| Ba 4 Sr 4 Mn 7 Co 1 | -1.985 | 268.7477101 | 2.8720415 |
| Pr 7 Zn 1 Ni 8    | -1.985 | 571.5666326 | 2.8720415 |
| Ba 7 Nd 1 Fe 8    | -1.984 | 230.7494853 | 2.8725576 |
| Ca 2 Pr 6 Ni 8    | -1.982 | 582.8379578 | 2.8735898 |
| Ba 4 Sr 4 Fe 8    | -1.981 | 263.377789  | 2.8741059 |
| Sr 4 Ca 4 Mn 4 Fe 4 | -1.98  | 278.1373683 | 2.874622 |
| Pr 8 Ga 7 Ni 1    | -1.98  | 131.3143814 | 2.874622 |
| Ba 4 Be 4 Sb 8    | -1.98  | 254.2526593 | 2.874622 |
| Ba 6 Mg 2 Nb 4 Sb 4 | -1.974 | 101.9765834 | 2.8777186 |
| Ca 4 Ba 4 Co 7 Ni 1 | -1.973 | 523.3975214 | 2.8782347 |
| Ba 7 La 1 Fe 6 Co 2 | -1.972 | 256.0614657 | 2.8787508 |
| Sr 4 Ca 4 Mn 4 Co 4 | -1.97  | 363.2118635 | 2.879783 |
| Ca 4 Sr 4 Mn 4 Co 4 | -1.97  | 361.5226135 | 2.879783 |
| Ba 4 Ca 4 Mn 1 Co 7 | -1.97  | 436.7011572 | 2.879783 |
| Sr 4 Ba 4 Sc 1 Fe 7 | -1.969 | 193.8227154 | 2.8802991 |
| Formula                  | log(j)  | Enthalpy (J/mol)        | Tc (K)   |
|-------------------------|---------|-------------------------|----------|
| Ba 7 Pr 1 Fe 8          | -1.969  | 227.5288534             | 2.8802991|
| Ca 8 Mn 4 Ni 4          | -1.967  | 627.6902493             | 2.8813313|
| Ba 4 Sr 4 Fe 2 Co 5 Nb 1| -1.963  | 261.6518439             | 2.8833957|
| Bi 1 Ba 3 Sr 4 Fe 2 Co 6| -1.963  | 360.6171345             | 2.8833957|
| Sr 8 Mn 1 Co 7          | -1.962  | 362.3346034             | 2.8839118|
| Sr 8 Nb 4 Ni 4          | -1.961  | 317.9647849             | 2.8844279|
| Ba 4 Mg 4 Nb 4 Sb 4     | -1.961  | 122.7012678             | 2.8844279|
| Ba 2 Sr 6 Fe 4 Co 4     | -1.96   | 328.1024074             | 2.8849444|
| Ba 4 Sr 4 Fe 7 Co 1     | -1.958  | 289.4332819             | 2.8859762|
| Ba 8 Fe 2 Nb 1 Co 5     | -1.958  | 288.5363584             | 2.8859762|
| Ba 8 Fe 7 Mo 1          | -1.955  | 157.9973194             | 2.8875245|
| Ca 8 Ni 6 Co 2          | -1.955  | 846.7546006             | 2.8875245|
| Pr 4 Ba 4 Ni 4 Co 4     | -1.954  | 491.2207193             | 2.8880406|
| Ba 4 Ca 4 Co 7 Ni 1     | -1.95   | 516.1507714             | 2.890105 |
| Sr 4 La 4 Ni 8          | -1.95   | 637.4396621             | 2.890105 |
| Ca 4 Sr 4 Mn 7 Ni 1     | -1.944  | 345.4173158             | 2.8932016|
| Y 4 Sr 4 Ni 6 Co 2      | -1.943  | 692.6156097             | 2.8937177|
| Sr 4 Ca 4 Mn 7 Ni 1     | -1.942  | 346.4053158             | 2.8942338|
| Ba 6 Sn 2 Fe 8          | -1.94   | 371.853592              | 2.895266 |
| Ba 8 Nb 4 Fe 4          | -1.939  | 20.142234               | 2.8957821|
| Ba 4 Ca 4 Mn 2 Co 6     | -1.939  | 433.1243785             | 2.8957821|
| Sr 7 Zn 1 Co 8          | -1.939  | 441.3655363             | 2.8957821|
| Ba 6 Nb 2 Zn 2 Co 6     | -1.936  | 381.6042986             | 2.8973304|
| Sr 6 Ti 2 Mn 6 Zn 2     | -1.935  | 264.0562236             | 2.8978465|
| Ba 2 Sr 6 Co 8          | -1.935  | 382.9788344             | 2.8978465|
| Pr 4 Ca 4 Mn 2 Ni 6     | -1.935  | 584.915523              | 2.8978465|
| Ba 7 Bi 1 Fe 8          | -1.934  | 250.9448571             | 2.8983626|
| Ba 2 Y 6 Ni 8           | -1.933  | 565.689079              | 2.8988787|
| Ca 4 Ba 4 Mn 2 Co 6     | -1.931  | 425.8248785             | 2.8999109|
| Y 4 Sr 4 Fe 2 Ni 6      | -1.93   | 642.6879706             | 2.900427 |
| Ba 4 La 4 Ni 8          | -1.93   | 664.2121326             | 2.900427 |
| Sr 8 Al 4 V 4           | -1.929  | 95.04900638             | 2.9009431|
| Ca 8 Fe 2 Ni 6          | -1.929  | 780.2682011             | 2.9009431|
| Ba 6 Mg 2 Fe 8          | -1.927  | 409.6339032             | 2.9019753|
| Ba 2 Sr 6 Fe 6 Co 2     | -1.927  | 290.8859134             | 2.9019753|
| Ba 4 Mg 4 Sb 8          | -1.926  | 192.493076              | 2.9024914|
| Ba 8 Fe 4 Ru 4          | -1.923  | 87.89333137             | 2.9040397|
| Sr 8 Fe 6 Ni 2          | -1.921  | 380.5064085             | 2.9050719|
| Ca 4 Y 4 Ni 8           | -1.92   | 619.7508721             | 2.905588 |
| Compound                  | Potential | Volume   | Density   |
|---------------------------|-----------|----------|-----------|
| Sr 8 Co 7 Ni 1            | -1.916    | 439.2632404 | 2.9076524 |
| Ba 4 Ca 4 Co 6 Ni 2       | -1.915    | 578.3931069 | 2.9081685 |
| Ca 4 Ba 4 Co 6 Ni 2       | -1.914    | 566.1173569 | 2.9086846 |
| Ca 8 Mn 1 Co 7            | -1.913    | 445.4650688 | 2.9092007 |
| Ba 8 Co 8                 | -1.913    | 343.7523729 | 2.9092007 |
| Y 6 Zn 2 Ni 8             | -1.913    | 642.0327234 | 2.9092007 |
| Ba 4 Sn 4 Fe 8            | -1.912    | 488.6953807 | 2.9097168 |
| Sr 6 Ca 2 Mn 8            | -1.911    | 245.8214355 | 2.9102329 |
| Ba 2 Be 6 Nb 2 Sb 6       | -1.911    | 175.9001805 | 2.9102329 |
| Ba 4 Cd 4 Fe 8            | -1.909    | 459.1721979 | 2.9112651 |
| La 1 Pr 4 Zn 3 Ni 8       | -1.908    | 29.72225273 | 2.9117812 |
| Ba 4 Sr 4 Al 1 Fe 7       | -1.906    | 297.5784426 | 2.9128134 |
| Ba 2 Sn 2 Pr 4 Ni 8       | -1.906    | 649.17345   | 2.9128134 |
| Sr 2 Ba 6 Sc 1 Fe 7       | -1.905    | 190.1769559 | 2.9133295 |
| Sr 4 Ba 4 Y 1 Fe 7        | -1.904    | 221.3729766 | 2.9138456 |
| Y 4 Ba 4 Ni 4 Co 4        | -1.904    | 530.3694013 | 2.9138456 |
| Sr 8 Mn 2 Co 6            | -1.902    | 352.8753018 | 2.9148778 |
| Sr 8 In 2 Fe 6            | -1.901    | 225.170716  | 2.9153939 |
| Sr 4 Ba 4 Al 1 Fe 7       | -1.9      | 216.8881685 | 2.91591  |
| Sr 4 Ca 4 Mn 6 Ni 2       | -1.9      | 418.2957387 | 2.91591  |
| Ca 8 Ni 7 Co 1            | -1.9      | 888.0273958 | 2.91591  |
| Pr 4 Ca 4 Fe 1 Ni 7       | -1.9      | 661.8566683 | 2.91591  |
| Ca 4 Sr 4 Mn 6 Ni 2       | -1.899    | 416.8194887 | 2.9164261 |
| Sr 8 Al 1 Co 7            | -1.898    | 330.6150969 | 2.9169422 |
| Sr 8 Sc 1 Co 7            | -1.895    | 313.4383495 | 2.9189605 |
| Y 4 Ba 4 Co 4 Ni 4        | -1.892    | 522.3044013 | 2.9200388 |
| Sr 6 Ti 2 Zn 2 Co 6       | -1.891    | 428.263592  | 2.9205549 |
| Ba 4 Sr 4 Fe 7 Ni 1       | -1.891    | 326.8227746 | 2.9205549 |
| Ba 7 Zn 1 Fe 8            | -1.889    | 327.8302594 | 2.9215871 |
| La 4 Dy 4 Ga 8            | -1.889    | 32.0782685  | 2.9215871 |
| Ba 6 Ti 2 Zn 2 Fe 6       | -1.887    | 364.3848861 | 2.9226193 |
| Ca 8 Mn 2 Ni 6            | -1.887    | 779.2283451 | 2.9226193 |
| Ba 4 Sn 4 Hf 1 Zr 6 Fe 1  | -1.886    | 103.0740965 | 2.9231354 |
| Ba 6 Hf 2 Zn 2 Fe 6       | -1.884    | 357.7450162 | 2.9241676 |
| Ba 4 Ca 4 Mn 7 Co 1       | -1.884    | 338.8363749 | 2.9241676 |
| Ba 7 Sn 1 Fe 8            | -1.884    | 313.7876    | 2.9241676 |
| Pr 8 Mg 2 Ni 6            | -1.884    | 0          | 2.9241676 |
| Ba 2 Sr 6 Mn 2 Fe 6       | -1.883    | 237.1519317 | 2.9246837 |
| Ba 8 Fe 1 Co 7            | -1.882    | 343.3989064 | 2.9251998 |
| Compound | Form | Value 1 | Value 2 | Value 3 |
|----------|------|---------|---------|---------|
| Ca 4 Ba 4 Mn 7 Co 1 | -1.881 | 328.6353749 | 2.9257159 |
| Ba 8 Zr 3 Fe 1 Co 4 | -1.88 | 215.6610583 | 2.926232 |
| Ca 4 Sr 4 Co 4 Ni 4 | -1.88 | 662.3220883 | 2.926232 |
| Ba 2 La 6 Ga 8 | -1.88 | 144.1748072 | 2.926232 |
| Pr 4 Ca 4 Ni 7 Co 1 | -1.879 | 688.2205737 | 2.9267481 |
| La 4 Ho 4 Ga 8 | -1.879 | 33.56831065 | 2.9267481 |
| Ba 8 Ti 8 | -1.876 | 19.43465 | 2.9282964 |
| Ba 6 Cd 2 Hf 1 Zr 6 Fe 1 | -1.876 | 25.85285955 | 2.9282964 |
| Sr 4 Ca 4 Co 4 Ni 4 | -1.876 | 664.5268383 | 2.9282964 |
| Sr 4 Ca 4 Ni 4 Co 4 | -1.874 | 668.5175883 | 2.9293286 |
| Ba 7 Ca 1 Fe 8 | -1.872 | 275.2111834 | 2.9303608 |
| Ba 6 Sr 2 Fe 8 | -1.872 | 260.4049649 | 2.9303608 |
| Sr 4 Ba 4 Fe 1 Co 7 | -1.872 | 374.7482974 | 2.9303608 |
| Sr 4 Sr 4 Fe 1 Co 7 | -1.872 | 365.5440474 | 2.9303608 |
| Ca 4 Ba 4 Mn 6 Co 2 | -1.869 | 344.419805 | 2.9319091 |
| Ba 4 Ca 4 Mn 6 Co 2 | -1.869 | 351.175805 | 2.9319091 |
| Ca 4 Sr 4 Ni 4 Co 4 | -1.869 | 665.4313383 | 2.9319091 |
| Sr 4 Ba 4 Al 2 Fe 6 | -1.868 | 241.4586771 | 2.9324252 |
| Ba 4 Sr 4 Mn 1 Fe 7 | -1.868 | 253.935041 | 2.9324252 |
| Y 4 Ba 4 Mn 2 Fe 6 | -1.868 | 1038.720502 | 2.9324252 |
| Sr 6 Ca 2 Mn 4 Fe 4 | -1.866 | 242.7919109 | 2.9334574 |
| Ba 4 Sr 4 Fe 6 Co 2 | -1.866 | 299.1716539 | 2.9334574 |
| La 8 Mg 4 Ti 4 | -1.865 | 22.18427375 | 2.9397375 |
| Ba 4 Sn 4 Zr 7 Fe 1 | -1.865 | 156.5083604 | 2.9397375 |
| Ca 8 Mn 1 Ni 7 | -1.865 | 854.991518 | 2.9397375 |
| Sr 7 Mn 8 Zn 1 | -1.864 | 259.2114621 | 2.9344896 |
| Ba 8 Nb 1 Fe 7 | -1.864 | 205.6142891 | 2.9344896 |
| Sr 6 Zn 2 Co 8 | -1.864 | 491.5344177 | 2.9344896 |
| Ca 8 Ni 8 | -1.86 | 931.2131909 | 2.936554 |
| Ba 7 Mg 1 Fe 8 | -1.859 | 333.499772 | 2.9370701 |
| Ba 8 Zr 1 Fe 7 | -1.857 | 223.537251 | 2.9381023 |
| Ba 4 Sr 4 Co 8 | -1.857 | 379.5415139 | 2.9381023 |
| Ba 7 Bi 1 Zr 7 Fe 1 | -1.856 | 0 | 2.9386184 |
| Ba 4 Sr 4 Al 2 Fe 6 | -1.855 | 318.5213462 | 2.9391345 |
| Ba 4 Be 4 Nb 4 Sb 4 | -1.855 | 151.2613555 | 2.9391345 |
| Sr 2 La 6 Ga 8 | -1.855 | 124.9590582 | 2.9391345 |
| Sr 2 Pr 6 Ni 8 | -1.854 | 560.4315828 | 2.9396506 |
| Sr 8 Ga 1 Co 7 | -1.853 | 342.0909155 | 2.9401667 |
| Ca 4 Ba 4 Mn 7 Fe 1 | -1.852 | 308.9878583 | 2.9406828 |
| Compound | Energy | lattice parameter | Unit cell volume |
|----------|--------|-------------------|------------------|
| Ba₄Ca₄Mn₇Fe₁ | -1.852 | 311.623583 | 2.9406828 |
| Ba₈Fe₆Ru₂ | -1.852 | 152.5277361 | 2.9406828 |
| Sr₈Y₁Co₇ | -1.852 | 327.9648339 | 2.9406828 |
| Ba₈Zr₆Fe₂ | -1.851 | 37.3593017 | 2.9411989 |
| Sr₂Ba₆Y₁Fe₇ | -1.851 | 214.115717 | 2.9411989 |
| Sr₈Mn₈ | -1.85 | 214.7947281 | 2.941715 |
| Ba₆Cd₂Fe₈ | -1.849 | 356.4587943 | 2.9422311 |
| Ba₄Sr₄Fe₂Co₆ | -1.849 | 356.8095809 | 2.9422311 |
| Pr₄Ba₄Co₄Ni₄ | -1.847 | 469.3334693 | 2.9432633 |
| Sr₄Mg₄Nb₂Sb₆ | -1.847 | 127.8698152 | 2.9432633 |
| La₄Nd₄Ga₈ | -1.847 | 15.44290641 | 2.9432633 |
| Sr₈Y₂Fe₆ | -1.846 | 215.3808039 | 2.9437794 |
| Sr₆Hf₂Mn₆Zn₂ | -1.845 | 260.8748196 | 2.9442955 |
| Sr₄Ba₄In₁Fe₇ | -1.845 | 209.2171784 | 2.9442955 |
| Ca₄Ba₄Mn₆Fe₂ | -1.843 | 317.966272 | 2.9453277 |
| Ca₄Ba₄Mn₆Fe₂ | -1.842 | 304.542022 | 2.9458438 |
| Sr₂Ba₆Y₁Co₇ | -1.842 | 307.2482385 | 2.9458438 |
| Ba₈Fe₄Rh₄ | -1.842 | 223.5185339 | 2.9458438 |
| Ba₈Ta₁Fe₇ | -1.84 | 206.0350229 | 2.946876 |
| Sr₆Zr₂Mn₆Zn₂ | -1.839 | 244.1643875 | 2.9473921 |
| Ca₄Ba₄Mn₇Ni₁ | -1.839 | 367.6898676 | 2.9473921 |
| Ba₈Fe₇Ir₁ | -1.839 | 221.7974211 | 2.9473921 |
| Sr₄Ba₄Y₁Co₇ | -1.839 | 328.96552 | 2.9473921 |
| Sr₈Co₆Ni₂ | -1.838 | 488.9458259 | 2.9479082 |
| Pr₄Ca₄Mn₁Ni₇ | -1.838 | 660.1169459 | 2.9479082 |
| La₈Mg₁Ga₇ | -1.838 | 548.0236233 | 2.9479082 |
| Y₈Mg₄Co₄ | -1.837 | 0 | 2.9484243 |
| Y₄Ba₄Mn₄Ni₄ | -1.837 | 506.7597787 | 2.9484243 |
| Sr₆Zr₂Zn₂Co₆ | -1.835 | 417.0961272 | 2.9494565 |
| Pr₄Sr₄Mn₄Ni₄ | -1.835 | 368.0565124 | 2.9494565 |
| Ba₂Be₆Sb₈ | -1.835 | 282.3442074 | 2.9494565 |
| Ba₄Ca₄Mn₇Ni₁ | -1.832 | 370.6873676 | 2.9510048 |
| La₄Sm₄Ga₈ | -1.831 | 22.3715509 | 2.9515209 |
| Y₈Mg₄Mn₄ | -1.83 | 0 | 2.952037 |
| Sr₆Mn₈Zn₂ | -1.83 | 303.3021962 | 2.952037 |
| Ba₄Sr₄Ga₁Fe₇ | -1.829 | 287.3190859 | 2.9525531 |
| Sr₈In₁Co₇ | -1.828 | 335.2259149 | 2.9530692 |
| Ca₂La₆Ga₈ | -1.826 | 114.2591578 | 2.9541014 |
| Formula                          | Enthalpy | E0     | Enthalpy Correction |
|---------------------------------|----------|--------|---------------------|
| Ba 8 Fe 3 Co 3 Zr 2             | -1.825   | 205.1403247 | 2.9546175         |
| Ba 7 Cd 1 Fe 8                 | -1.825   | 308.1113426    | 2.9546175         |
| Ba 4 Sr 4 Fe 4 Co 4            | -1.825   | 335.6841479    | 2.9546175         |
| Sr 6 Hf 2 Zn 2 Co 6            | -1.821   | 416.6373093    | 2.9566819         |
| Ba 8 Zr 5 Fe 1 Co 2            | -1.82    | 140.1926526    | 2.957198          |
| Ba 4 Sr 4 Mn 2 Fe 6             | -1.82    | 245.6824222    | 2.957198          |
| Ba 4 Sr 4 Mn 1 Co 7             | -1.82    | 359.2332352    | 2.957198          |
| Y 4 Sr 4 Fe 1 Ni 7              | -1.82    | 709.0190853    | 2.957198          |
| Ba 4 Mg 4 Nb 2 Sb 6             | -1.82    | 151.3917357    | 2.957198          |
| Sr 8 Al 2 Co 6                 | -1.818   | 333.1396948    | 2.9582302         |
| Ba 2 Sr 6 Fe 6 Ni 2             | -1.818   | 387.1381489    | 2.9582302         |
| Sr 8 Mn 7 Co 1                 | -1.817   | 251.3039082    | 2.9587463         |
| Sr 4 Ba 4 Mn 2 Co 6             | -1.816   | 341.9462065    | 2.9592624         |
| Mg 4 Be 4 Nb 2 Sb 6             | -1.815   | 210.9164219    | 2.9597785         |
| Sr 4 Ba 4 Ga 1 Fe 7             | -1.813   | 216.6057143    | 2.9608107         |
| Sr 4 Be 4 Nb 4 Sb 4             | -1.812   | 168.2472577    | 2.9613268         |
| Ba 4 Sr 4 Zn 1 Fe 7             | -1.81    | 311.1425928    | 2.962359          |
| Ba 8 Fe 2 Co 6                 | -1.81    | 321.9406899    | 2.962359          |
| Sr 4 Ca 4 Fe 4 Ni 4             | -1.81    | 592.42506      | 2.962359          |
| Ba 4 Ca 4 Mn 4 Co 4             | -1.808   | 388.9696653    | 2.9633912         |
| Sr 8 Mn 6 Co 2                 | -1.806   | 256.0735884    | 2.9644234         |
| Ba 7 Sr 1 Fe 8                 | -1.806   | 259.6244279    | 2.9644234         |
| Ca 4 Ba 4 Mn 4 Co 4             | -1.806   | 382.4731653    | 2.9644234         |
| Ba 4 Sr 4 Fe 7 Cu 1             | -1.806   | 329.5698151    | 2.9644234         |
| Pr 4 Sr 4 Fe 2 Ni 6             | -1.803   | 538.5054673    | 2.9659717         |
| Ca 4 Ba 4 Mn 6 Ni 2             | -1.802   | 433.9670405    | 2.9664878         |
| Ba 8 Sc 1 Co 7                 | -1.801   | 309.008462     | 2.9670039         |
| Ba 4 Ca 4 Mn 6 Ni 2             | -1.8     | 437.8077905    | 2.96752           |
| Sr 4 Ba 4 Mn 1 Co 7             | -1.799   | 361.0914852    | 2.9680361         |
| Pr 4 Gd 4 Ta 8                 | -1.798   | 7365.583654    | 2.9685522         |
| Ba 4 Sr 4 Fe 2 Co 5 Zr 1        | -1.798   | 287.9381315    | 2.9685522         |
| Sr 2 Ba 6 Sc 1 Co 7             | -1.798   | 311.4884935    | 2.9685522         |
| Pr 4 Sr 4 Ni 6 Co 2             | -1.798   | 577.9238565    | 2.9685522         |
| Ba 2 Mg 6 Nb 4 Sb 4             | -1.795   | 132.4237329    | 2.9701005         |
| Pr 8 Mg 4 Co 4                 | -1.794   | 0               | 2.9706166         |
| Sr 8 Mn 6 Fe 2                 | -1.793   | 211.9219658    | 2.9711327         |
| Ba 4 Sr 4 Fe 2 Co 5 Y 1         | -1.793   | 328.958681     | 2.9711327         |
| Sr 8 Mn 4 Co 4                 | -1.79    | 297.1616987    | 2.972681          |
| Sr 8 Mn 7 Fe 1                 | -1.789   | 241.4688469    | 2.9731971         |
| Compound                        | Energy  | Mass     | Density  |
|--------------------------------|---------|----------|----------|
| Ca₄Sr₄Mn₄Ni₄                   | -1.789  | 561.9933345 | 2.9731971 |
| Ba₂Mg₆Sb₈                      | -1.789  | 197.5300541 | 2.9731971 |
| Rb₄Sr₄V₄Fe₄                    | -1.788  | 352.5101479 | 2.9737132 |
| Ba₈Sc₁Fe₇                      | -1.788  | 187.7434464 | 2.9737132 |
| Sr₄Ca₄Mn₄Ni₄                   | -1.786  | 564.0348345 | 2.9747454 |
| Sr₄Ba₄Mn₆Co₂                   | -1.783  | 265.7836402 | 2.9762937 |
| Ba₆Zn₂Fe₈                      | -1.783  | 412.5623779 | 2.9762937 |
| Ba₈Fe₇Ru₁                      | -1.783  | 196.9395634 | 2.9762937 |
| Ba₄Sr₄Co₇Ni₁                   | -1.782  | 433.4133494 | 2.9768098 |
| Ba₈Fe₇Co₁                      | -1.78   | 269.4643573 | 2.977842  |
| Sr₄Ba₄Co₇Ni₁                   | -1.779  | 440.2340994 | 2.9783581 |
| Ca₄Pr₄Ni₈                      | -1.778  | 677.8053688 | 2.9788742 |
| Sr₄Ba₄Sc₁Co₇                   | -1.776  | 321.308775  | 2.9799064 |
| Y₄Sr₄Mn₁Ni₇                    | -1.773  | 714.3716558 | 2.9814547 |
| La₈Mg₂Ga₆                      | -1.773  | 100.3646259 | 2.9814547 |
| Ba₆Zr₂Zn₂Co₆                   | -1.771  | 424.576738  | 2.9824869 |
| Sr₂Ba₆Al₁Co₇                   | -1.771  | 334.4732322 | 2.9824869 |
| Ca₈Fe₁Ni₇                      | -1.767  | 853.239071  | 2.9845513 |
| Ba₆Hf₂Zn₂Co₆                   | -1.766  | 451.589048  | 2.9850674 |
| Sr₄Ca₄Ni₆Co₂                   | -1.766  | 789.5879286 | 2.9850674 |
| Ca₄Sr₄Ni₆Co₂                   | -1.766  | 786.1886786 | 2.9850674 |
| Sr₂Ba₆Al₁Fe₇                   | -1.765  | 314.9504189 | 2.9855835 |
| Sr₂Ba₆Al₂Co₆                   | -1.764  | 359.4353101 | 2.9860996 |
| Ba₂Pr₆Ni₈                      | -1.764  | 573.2493954 | 2.9860996 |
| Ba₈Hf₁Fe₇                      | -1.763  | 232.372335  | 2.9866157 |
| Sr₄Ba₄In₁Co₇                   | -1.763  | 337.6858524 | 2.9866157 |
| Ba₂Mg₆Nb₂Sb₆                   | -1.763  | 189.2264573 | 2.9866157 |
| Sr₈Mn₇Ni₁                      | -1.761  | 280.161561  | 2.9876479 |
| Sr₈Sc₂Co₆                      | -1.757  | 0          | 2.9897123 |
| Ca₈Ti₈                         | -1.754  | 12.44807725 | 2.9912606 |
| Ba₂Sr₆Mn₈                      | -1.754  | 220.331629  | 2.9912606 |
| Sr₄Ba₄Sc₂Fe₆                   | -1.752  | 194.999271  | 2.9922928 |
| Ba₄Sr₄Nb₄Ni₄                   | -1.752  | 298.680759  | 2.9922928 |
| Ba₇Sr₁Mn₂Fe₆                   | -1.752  | 239.3482381 | 2.9922928 |
| Sr₄Ba₄Al₁Co₇                   | -1.752  | 365.2542637 | 2.9922928 |
| Ba₄Sr₄Mn₂Co₆                   | -1.751  | 346.1554565 | 2.9928089 |
| Y₄Ba₄Mn₂Ni₆                    | -1.75   | 663.6365861 | 2.993325  |
| Ba₄La₄Ga₈                      | -1.748  | 251.6676226 | 2.9943572 |
| Formula         | Energy  | Formation Energy  | Lattice Parameter |
|-----------------|---------|-------------------|-------------------|
| Sr 4 La 4 Ga 8  | -1.748  | 217.2769291       | 2.9943572         |
| Ca 4 Ba 4 Co 4 Ni 4 | -1.747 | 671.8971973       | 2.9948733         |
| Ca 4 Ba 4 Ni 4 Co 4 | -1.747 | 673.8169473       | 2.9948733         |
| Ba 8 Zr 6 Fe 1 Co 1 | -1.745 | 70.59703222       | 2.9959055         |
| Sr 8 Al 4 Fe 4  | -1.745  | 251.7804341       | 2.9959055         |
| Ba 8 Fe 8       | -1.745  | 258.8621408       | 2.9959055         |
| Ba 4 Sr 4 Ga 2 Fe 6 | -1.745 | 312.3966329       | 2.9959055         |
| Ba 7 Sr 1 Mn 1 Fe 7 | -1.744 | 251.7406517       | 2.9964216         |
| Sr 1 La 7 Mg 2 Ga 6 | -1.744 | 221.9404994       | 2.9964216         |
| Rb 4 Sr 4 Mn 4 V 4 | -1.741 | 372.5957184       | 2.9979699         |
| Y 4 Ba 4 Fe 2 Ni 6 | -1.741 | 695.3448613       | 2.9979699         |
| Ca 4 Sr 4 Fe 2 Ni 6 | -1.74  | 731.0845394       | 2.998486          |
| Sr 8 Mn 4 Fe 4  | -1.738  | 207.9477035       | 2.9995182         |
| Ba 4 Ca 4 Ni 4 Co 4 | -1.738 | 710.4464473       | 2.9995182         |
| Ba 8 Fe 6 Rh 2  | -1.737  | 235.3290873       | 3.0000343         |
| Sr 4 Ca 4 Fe 2 Ni 6 | -1.737 | 734.0282894       | 3.0000343         |
| Ba 8 Fe 7 Rh 1  | -1.733  | 246.3388641       | 3.0020987         |
| Ba 8 Fe 6 Co 2  | -1.733  | 282.9710738       | 3.0020987         |
| Sr 4 Ba 4 Ga 2 Fe 6 | -1.731 | 240.5247687       | 3.0031309         |
| La 6 Ho 2 Sc 8  | -1.73   | 0                 | 3.003647          |
| Sr 4 Ba 4 Sc 2 Co 6 | -1.73  | 297.942614        | 3.003647          |
| Ba 8 Hf 6 Fe 2  | -1.729  | 84.1418057        | 3.0041631         |
| Sr 2 Ba 6 Ga 1 Co 7 | -1.728 | 334.8586335       | 3.0046792         |
| Y 4 Sr 4 Ni 7 Co 1 | -1.728 | 633.7829049       | 3.0046792         |
| La 6 Dy 2 Sc 8  | -1.727  | 0                 | 3.0051953         |
| Ba 8 Fe 6 Pt 2  | -1.726  | 277.5271686       | 3.0057114         |
| Pr 8 Mg 4 Mn 4  | -1.725  | 0                 | 3.0062275         |
| Pr 8 Mg 4 Ti 4  | -1.724  | 34.71888825       | 3.0067436         |
| Ba 8 Mn 2 Co 6  | -1.724  | 321.4643155       | 3.0067436         |
| Ba 4 Be 4 Nb 2 Sb 6 | -1.724 | 200.2107495       | 3.0067436         |
| Ba 8 Mn 1 Co 7  | -1.723  | 328.7718442       | 3.0072597         |
| Sr 2 Ba 6 In 1 Co 7 | -1.722 | 322.7173209       | 3.0077758         |
| Sr 2 Ba 6 Al 2 Fe 6 | -1.721 | 243.2704176       | 3.0082919         |
| Ba 4 Cd 4 Hf 1 Zr 6 Fe 1 | -1.72 | 134.7096834      | 3.008808          |
| Ba 8 Y 1 Co 7   | -1.72   | 300.849207        | 3.008808          |
| Ca 4 Ba 4 Mn 4 Ni 4 | -1.72  | 568.5651363       | 3.008808          |
| Sr 2 Ba 6 In 1 Fe 7 | -1.719 | 203.4596689       | 3.0093241         |
| La 6 Gd 2 Sc 8  | -1.717  | 29.08498069       | 3.0103563         |
| La 8 Sc 8       | -1.716  | 0                 | 3.0108724         |
| Formula          | Energy | EAF Value | Density |
|------------------|--------|-----------|---------|
| Ba 6 Be 2 Nb 4 Sb 4 | -1.715 | 134.3815416 | 3.0113885 |
| Pr 6 Zn 2 Ni 8    | -1.715 | 646.4899685 | 3.0113885 |
| La 4 Gd 4 Sc 8    | -1.714 | 28.6832347 | 3.0119046 |
| Sr 2 Ba 6 Sc 2 Co 6 | -1.713 | 283.6615825 | 3.0124207 |
| Sr 2 Ba 6 Y 2 Co 6 | -1.709 | 288.0390726 | 3.0144851 |
| Pr 4 Ba 4 Mn 2 Fe 6 | -1.708 | 913.8626351 | 3.0150012 |
| Ba 4 Sr 4 Co 6 Ni 2 | -1.708 | 494.0744349 | 3.0150012 |
| Sr 8 In 2 Co 6    | -1.708 | 336.2070809 | 3.0150012 |
| La 6 Sm 2 Sc 8    | -1.706 | 112.084275  | 3.0160334 |
| Ba 8 Zr 6 Fe 1 Ni 1 | -1.706 | 208.0974575 | 3.0160334 |
| Ba 8 Y 1 Fe 7     | -1.706 | 246.8597272 | 3.0160334 |
| Ba 8 Mn 1 Fe 7    | -1.706 | 675.6024473 | 3.0160334 |
| Ba 4 Ca 4 Co 4 Ni 4 | -1.706 | 350.8348239 | 3.0165495 |
| Sr 8 Mn 6 Ni 2    | -1.705 | 405.6149584 | 3.0165495 |
| Ba 8 Co 7 Ni 1    | -1.705 | 482.4809349 | 3.0165495 |
| Sr 4 Ba 4 Co 6 Ni 2 | -1.705 | 271.150301  | 3.0170656 |
| Ba 8 Sc 2 Co 6    | -1.704 | 340.101582  | 3.0175817 |
| La 6 Nd 2 Sc 8    | -1.703 | 767.7522868 | 3.0186139 |
| Sr 8 Ga 2 Co 6    | -1.703 | 752.5685057 | 3.01913 |
| Y 4 Ba 4 Ni 7 Co 1 | -1.701 | 302.9771041 | 3.0201622 |
| Y 4 Ba 4 Fe 1 Ni 7 | -1.7   | 301.4216034 | 3.0212266 |
| Sr 4 Ba 4 Y 2 Co 6 | -1.698 | 1106.613955 | 3.0201622 |
| Ca 4 Ba 4 Mn 2 Fe 6 | -1.698 | 268.5664047 | 3.0201622 |
| Ba 8 Fe 7 Pt 1    | -1.698 | 268.5664047 | 3.0201622 |
| Sr 6 Ca 2 Fe 4 Ni 4 | -1.698 | 555.406474 | 3.0201622 |
| Ba 4 Sr 4 Fe 6 Ni 2 | -1.694 | 394.8663894 | 3.0222266 |
| Ba 8 Sc 4 Fe 4    | -1.694 | 593.5388829 | 3.0222266 |
| Pr 4 Ba 4 Mn 4 Ni 4 | -1.693 | 393.8919904 | 3.0227427 |
| Sr 4 Ca 4 Mn 2 Ni 6 | -1.691 | 198.8709354 | 3.024291 |
| Ba 2 Be 6 Nb 4 Sb 4 | -1.69  | 205.0634914 | 3.0248071 |
| Sr 8 Sc 4 Fe 4    | -1.689 | 723.7539303 | 3.0237749 |
| Sr 2 Ba 6 Ga 1 Fe 7 | -1.689 | 176.0819215 | 3.0248071 |
| Mg 4 Be 4 Nb 4 Sb 4 | -1.689 | 160.4216034 | 3.0253232 |
| Sr 4 Ba 4 Mn 4 Co 4 | -1.688 | 604.9283321 | 3.0253232 |
| Pr 4 Sr 4 Fe 1 Ni 7 | -1.688 | 250.6722101 | 3.0258393 |
| Sr 4 Ba 4 Mn 7 Co 1 | -1.687 | 798.6654042 | 3.0263554 |
| Ca 4 Sr 4 Fe 1 Ni 7 | -1.686 | 607.5313863 | 3.0268715 |
| Ba 4 Ca 4 Mn 4 Ni 4 | -1.685 | 301.4216034 | 3.0253232 |
| Compound                          | free energy (eV) | Total magnetic moment (μB) | spin moment (μB) |
|----------------------------------|------------------|---------------------------|-----------------|
| Ba$_4$Sr$_4$Mn$_6$Co$_2$         | -1.684           | 289.3581402               | 3.0273876       |
| Sr$_4$Be$_4$Nb$_2$Sb$_6$         | -1.684           | 168.5018972               | 3.0273876       |
| Sr$_4$Ba$_4$Ga$_1$Co$_7$         | -1.681           | 364.146665                | 3.0289359       |
| Ca$_4$La$_4$Ga$_8$              | -1.679           | 219.940026                | 3.0299681       |
| Sr$_8$Sc$_4$V$_4$               | -1.676           |                           | 3.0315164       |
| La$_4$Ho$_4$Sc$_8$              | -1.676           | 0.334952917               | 3.0315164       |
| Sr$_4$Ca$_4$Fe$_1$Ni$_7$        | -1.676           | 801.9434042               | 3.0315164       |
| Sr$_4$Ca$_4$Ni$_7$Co$_1$        | -1.676           | 833.0659738               | 3.0315164       |
| Ba$_8$Fe$_7$Ni$_1$              | -1.675           | 335.6406001               | 3.0320325       |
| Y$_4$Ba$_4$Mn$_1$Ni$_7$         | -1.674           | 739.5015605               | 3.0325486       |
| Ca$_4$Sr$_4$Ni$_7$Co$_1$        | -1.673           | 828.9682238               | 3.0330647       |
| La$_8$Mg$_4$Ga$_4$              | -1.671           | 188.7946905               | 3.0340969       |
| Ba$_8$Fe$_7$Pt$_4$              | -1.671           | 294.0624464               | 3.0340969       |
| Pr$_4$Sr$_4$Ni$_7$Co$_1$        | -1.67            | 625.9786517               | 3.034613        |
| Ba$_6$Zr$_2$Mn$_6$Zn$_2$        | -1.668           | 296.6784071               | 3.0356452       |
| Ba$_8$Al$_2$Co$_6$              | -1.667           | 363.4590286               | 3.0361613       |
| Sr$_8$Co$_4$Ni$_4$              | -1.666           | 593.1126663               | 3.0366774       |
| Sr$_4$Ba$_4$Al$_2$Co$_6$        | -1.665           | 360.1730916               | 3.0371935       |
| Pr$_4$Ba$_4$Ni$_6$Co$_2$        | -1.665           | 611.4030596               | 3.0371935       |
| Y$_4$Ba$_4$Ni$_6$Co$_2$         | -1.664           | 715.1212416               | 3.0377096       |
| Sr$_4$Ba$_4$Mn$_7$Fe$_1$        | -1.662           | 224.6499435               | 3.0387418       |
| Ba$_6$Hf$_2$Mn$_6$Zn$_2$        | -1.661           | 314.9117171               | 3.0392579       |
| Sr$_8$Ni$_4$Co$_4$              | -1.661           | 595.4681663               | 3.0392579       |
| Ba$_8$Zr$_6$Fe$_1$Cu$_1$        | -1.66            | 110.0554805               | 3.039774        |
| Sr$_4$Ca$_4$Mn$_1$Ni$_7$        | -1.66            | 799.7904746               | 3.039774        |
| Sr$_8$Al$_4$Co$_4$              | -1.658           | 351.8863906               | 3.0408062       |
| Ba$_8$Fe$_4$Co$_4$              | -1.658           | 307.7795069               | 3.0408062       |
| Ca$_4$Sr$_4$Mn$_1$Ni$_7$        | -1.658           | 823.4522246               | 3.0408062       |
| La$_4$Dy$_4$Sc$_8$              | -1.657           | 0                         | 3.0413223       |
| Sr$_4$Ba$_4$Mn$_7$Ni$_1$        | -1.657           | 287.2274528               | 3.0413223       |
| Sr$_6$Ta$_2$Zn$_2$Ni$_6$        | -1.657           | 663.1807708               | 3.0413223       |
| Ba$_8$Hf$_1$Zr$_6$Fe$_1$        | -1.656           | 3.55271E-12               | 3.0418384       |
| Ba$_4$Sr$_4$Mn$_6$Fe$_2$        | -1.653           | 229.3498572               | 3.0433867       |
| Ba$_4$Sr$_4$Mn$_7$Fe$_1$        | -1.652           | 229.1906935               | 3.0439028       |
| Ba$_7$Cd$_1$Zr$_7$Fe$_1$        | -1.651           | 46.7423636                | 3.0444189       |
| Ba$_8$Fe$_7$Pd$_1$              | -1.651           | 294.1107023               | 3.0444189       |
| Ba$_8$Mn$_2$Fe$_6$              | -1.65            | 235.6203135               | 3.044935        |
| Ba$_8$In$_1$Co$_7$              | -1.65            | 315.6517894               | 3.044935        |
| Ba$_8$Y$_2$Co$_6$               | -1.649           | 274.4990411               | 3.0454511       |
| Formula            | Z      | El      | Rho     |
|--------------------|--------|---------|---------|
| Sr 8 V 4 Ga 4      | -1.645 | 134.2448986 | 3.0475155 |
| Sr 4 Ba 4 Mn 6 Fe 2 | -1.644 | 224.9633572  | 3.0480316 |
| Ba 4 Sr 4 Mn 7 Ni 1 | -1.644 | 291.5262028  | 3.0480316 |
| La 4 Sm 4 Sc 8     | -1.642 | 0        | 3.0490638 |
| Sr 2 Ba 6 Sc 2 Fe 6 | -1.642 | 189.970115  | 3.0490638 |
| Sr 4 Y 4 Ni 8      | -1.641 | 611.0149501 | 3.0495799 |
| Sr 4 Ba 4 In 2 Fe 6 | -1.64  | 222.8274469 | 3.050096  |
| Ba 8 Zr 7 Fe 1     | -1.638 | 0        | 3.0511282 |
| Pr 4 Ba 4 Fe 2 Ni 6 | -1.638 | 571.0231105 | 3.0511282 |
| Sr 4 Ba 4 Ga 2 Co 6 | -1.638 | 352.7093941 | 3.0511282 |
| Ba 8 In 2 Co 6     | -1.637 | 311.3067059 | 3.0516443 |
| La 4 Nd 4 Sc 8     | -1.636 | 0        | 3.0521604 |
| Sr 6 Nb 2 Zn 2 Ni 6 | -1.635 | 666.895936  | 3.0526765 |
| Ba 8 Hf 2 Zr 5 Fe 1 | -1.634 | 8.140079851 | 3.0531926 |
| Ba 4 Sr 4 Mn 4 Co 4 | -1.631 | 305.5581034 | 3.0547409 |
| Ba 2 Sr 6 Mn 4 Fe 4 | -1.63  | 216.180944  | 3.055257  |
| Ba 8 Co 6 Ni 2     | -1.63  | 464.9512939 | 3.055257  |
| Ba 8 Hf 4 Zr 3 Fe 1 | -1.629 | 23.8639785  | 3.0557731 |
| Ba 8 Al 1 Fe 7     | -1.629 | 218.5326494 | 3.0557731 |
| Pr 4 Sr 4 Mn 1 Ni 7 | -1.629 | 600.1284025 | 3.0557731 |
| Ba 8 Ga 2 Co 6     | -1.628 | 334.4053311 | 3.0562892 |
| Sr 4 Ba 4 In 2 Co 6 | -1.628 | 336.7372689 | 3.0562892 |
| Sr 2 Ba 6 In 2 Co 6 | -1.622 | 315.8027374 | 3.0593858 |
| Sr 4 Ca 4 Ni 8     | -1.622 | 869.2945189 | 3.0593858 |
| Ba 7 Cd 1 Hf 1 Zr 6 Fe 1 | -1.62  | 0        | 3.060418  |
| Ba 8 Fe 6 Pd 2     | -1.62  | 324.1810138 | 3.060418  |
| Ca 4 Ba 4 Ni 6 Co 2 | -1.619 | 785.4502876 | 3.0609341 |
| Ba 4 Sr 4 Mn 4 Fe 4 | -1.618 | 225.0341844 | 3.0614502 |
| Sr 4 Ba 4 Y 2 Fe 6 | -1.617  | 227.9474341 | 3.0619663 |
| Sr 2 Ba 6 Ga 2 Co 6 | -1.617  | 348.5878626 | 3.0619663 |
| Ba 4 Ca 4 Ni 6 Co 2 | -1.615  | 793.0120376 | 3.0629985 |
| Ba 3 Sn 1 Pr 4 Ni 8 | -1.615  | 675.5772809 | 3.0629985 |
| Sr 2 Ba 6 Ga 2 Fe 6 | -1.609  | 238.7117591 | 3.0660951 |
| Ba 8 Zn 1 Fe 7     | -1.603  | 300.9575066 | 3.0691917 |
| Ba 4 Sr 4 Al 8     | -1.601  | 373.4425651 | 3.0702239 |
| Sr 4 Ba 4 Mn 6 Ni 2 | -1.6  | 352.2563757 | 3.07074  |
| Ba 4 Sr 4 Mn 6 Ni 2 | -1.6  | 354.5393757 | 3.07074  |
| Y 8 Mg 4 Ti 4      | -1.598  | 5.974325  | 3.0717722 |
| Ba 7 Sn 1 Zr 7 Fe 1 | -1.597  | 24.7171435 | 3.0722883 |
| Sr 4 Ba 4 Sc 4 Fe 4 | -1.596 | 212.6513821 | 3.0728044 |
|--------------------|--------|-------------|-----------|
| Ba 8 Fe 3 Co 3 Y 1 Zr 1 | -1.594 | 240.1843742 | 3.0738366 |
| Ba 8 Mn 6 Co 2 | -1.594 | 274.5580449 | 3.0738366 |
| Ba 8 Al 2 Fe 6 | -1.593 | 246.381408  | 3.0743527 |
| Ba 8 Hf 7 Fe 1 | -1.589 | 46.19749985 | 3.0764171 |
| Ca 4 Ba 4 Fe 2 Ni 6 | -1.587 | 746.2594594 | 3.0774493 |
| Sr 8 Fe 4 Ni 4 | -1.584 | 519.644888  | 3.0789976 |
| Ba 4 Ca 4 Fe 2 Ni 6 | -1.582 | 753.7597094 | 3.0800298 |
| Ba 8 Mn 8 | -1.581 | 213.0473317 | 3.0805459 |
| Ba 8 Mn 7 Co 1 | -1.58 | 242.3113133 | 3.081062 |
| Ba 8 In 1 Fe 7 | -1.58 | 197.8935144 | 3.081062 |
| Pr 4 Ba 4 Mn 2 Ni 6 | -1.58 | 561.0510702 | 3.081062 |
| Ba 7 Sn 1 Hf 1 Zr 6 Fe 1 | -1.575 | 0          | 3.0836425 |
| Pr 4 Ba 4 Fe 1 Ni 7 | -1.575 | 628.1953607 | 3.0836425 |
| Ba 8 Al 1 Co 7 | -1.572 | 361.6709507 | 3.0851908 |
| Sr 8 Mn 4 Ni 4 | -1.571 | 490.5814197 | 3.0857069 |
| Ba 8 Sc 2 Fe 6 | -1.569 | 186.2552519 | 3.0867391 |
| Sr 8 V 4 Cu 4 | -1.569 | 367.6084311 | 3.0867391 |
| Ba 8 Ga 1 Fe 7 | -1.564 | 214.6581952 | 3.0893196 |
| Ca 4 Ba 4 Mn 2 Ni 6 | -1.563 | 725.663085  | 3.0898357 |
| Pr 4 Ba 4 Ni 7 Co 1 | -1.562 | 648.3873548 | 3.0903518 |
| Ba 4 Ca 4 Mn 2 Ni 6 | -1.559 | 753.351085  | 3.0919001 |
| Gd 4 Y 4 Sc 8 | -1.557 | 26.942183   | 3.0929323 |
| Ba 7 Zn 1 Ni 8 | -1.556 | 859.4711133 | 3.0934484 |
| Sr 2 Ba 6 Sc 4 Fe 4 | -1.555 | 203.2618726 | 3.0939645 |
| Sr 2 Ba 6 Y 2 Fe 6 | -1.551 | 227.0050337 | 3.0960289 |
| Sr 8 Y 4 Fe 4 | -1.543 | 241.4806789 | 3.1001577 |
| Sr 8 Ni 6 Co 2 | -1.542 | 715.7380066 | 3.1006738 |
| Ba 8 Ga 1 Co 7 | -1.541 | 354.904352  | 3.1011899 |
| Y 8 Sc 8 | -1.54 | 28.42037425 | 3.101706 |
| Ba 8 Mn 7 Fe 1 | -1.534 | 221.4312454 | 3.1048026 |
| Ca 4 Ba 4 Mn 1 Ni 7 | -1.531 | 811.0558565 | 3.1063509 |
| Sr 4 La 1 Zn 3 Ni 8 | -1.529 | 894.9385268 | 3.1073831 |
| Sr 8 Sc 4 Co 4 | -1.528 | 251.3591513 | 3.1078992 |
| Ba 4 Ca 4 Fe 1 Ni 7 | -1.527 | 817.4001687 | 3.1084153 |
| Ca 4 Ba 4 Fe 1 Ni 7 | -1.526 | 809.0106687 | 3.1089314 |
| Pr 4 Ba 4 Mn 1 Ni 7 | -1.526 | 616.7866101 | 3.1089314 |
| Pr 4 Gd 4 Ga 8 | -1.526 | 78.46623222 | 3.1089314 |
| Ba 4 Sr 4 Ni 4 Co 4 | -1.524 | 596.1225253 | 3.1099636 |
| Formula          | E (eV) | d (Å)  | E (eV) | d (Å)  |
|------------------|--------|--------|--------|--------|
| Sr₂Ba₆In₂Fe₆     | -1.522 | 213.3979374 | 3.1109958 |
| Ba₈Mn₇Ni₁       | -1.521 | 280.9968061 | 3.1115119 |
| Sr₄Ba₄Co₄Ni₄    | -1.521 | 588.5662753 | 3.1115119 |
| Sr₄Ba₄Ni₄Co₄    | -1.521 | 590.6512753 | 3.1115119 |
| Sr₆Ca₂Ni₈       | -1.52 | 832.2189329 | 3.1115119 |
| Sr₈Fe₂Ni₆       | -1.52 | 660.1253674 | 3.112028 |
| Pr₄Gd₄Sc₈       | -1.518 | 16.48859025 | 3.1130602 |
| Ba₈Hf₈          | -1.517 | 8.216444 | 3.1135763 |
| Ca₄Ba₄Ni₇Co₁    | -1.516 | 832.9568828 | 3.1140924 |
| Ba₄Ca₄Ni₇Co₁    | -1.515 | 835.876328 | 3.1146085 |
| Ba₈Mn₆Fe₂       | -1.512 | 212.065769 | 3.1161568 |
| Ba₄Sr₄V₄Ni₄     | -1.509 | 396.068078 | 3.1177051 |
| Ba₂Sr₆Fe₄Ni₄    | -1.509 | 525.3931284 | 3.1177051 |
| Ba₄Ca₄Mn₁Ni₇    | -1.509 | 820.2236065 | 3.1177051 |
| Ba₈Sc₄Fe₄       | -1.506 | 193.686363 | 3.1192534 |
| Ba₈Mn₄Co₄       | -1.504 | 294.713508 | 3.1202856 |
| Ba₈Fe₇Cu₁       | -1.504 | 315.8430565 | 3.1202856 |
| Ba₈Al₈          | -1.503 | 388.6313288 | 3.1208017 |
| Ba₄Sr₄Co₄Ni₄    | -1.502 | 592.0295253 | 3.1213178 |
| Gd₄Y₄Ga₈        | -1.5 | 75.27819525 | 3.12235 |
| Ba₈Y₂Fe₆        | -1.498 | 229.0352741 | 3.1233822 |
| Sr₄Pr₄Ni₈       | -1.497 | 638.6141188 | 3.1238983 |
| Ba₄Sr₄Al₄Fe₄    | -1.491 | 361.407716 | 3.1269949 |
| Sr₈Y₄V₄         | -1.49 | 112.1749515 | 3.127511 |
| Ba₆Cd₂Zr₇Fe₁    | -1.489 | 87.40277555 | 3.1280271 |
| Y₆Ho₂Sc₈        | -1.486 | 37.4386379 | 3.1295754 |
| Sr₄Ba₄Al₄Fe₄    | -1.483 | 292.7046944 | 3.1311237 |
| Sr₄Ba₄Y₄Fe₄     | -1.481 | 241.6149901 | 3.1321559 |
| Ba₆Sn₂Zr₇Fe₁    | -1.474 | 63.07508532 | 3.1357686 |
| Gd₂Y₆Sc₈        | -1.472 | 27.91952863 | 3.1368008 |
| Pr₆Gd₂Ga₈       | -1.467 | 76.1821909 | 3.1393813 |
| Sr₈Mn₂Ni₆       | -1.465 | 648.4577583 | 3.1404135 |
| Y₄Ho₄Sc₈        | -1.463 | 46.36115154 | 3.1414457 |
| Pr₆Gd₂Sc₈       | -1.461 | 21.48093037 | 3.1424779 |
| Ba₄La₁Zn₃Ni₈    | -1.461 | 224.6336981 | 3.1424779 |
| Ba₈Mn₆Ni₂       | -1.46 | 335.2155304 | 3.142994 |
| Sr₈Fe₁Ni₇       | -1.46 | 728.1662322 | 3.142994 |
| Ba₈Nb₄Ni₄       | -1.459 | 248.9902561 | 3.1435101 |
| La₈Mg₂Sc₆       | -1.457 | 73.66589018 | 3.1445423 |
| Formula            | Energy   | Mass      | Density  |
|--------------------|----------|-----------|----------|
| Sr₂Ba₆Y₄Fe₄        | -1.456   | 236.3273407 | 3.1450584 |
| Sr₄Ba₄Al₄Co₄       | -1.456   | 385.998024  | 3.1450584 |
| La₈Mg₁Sc₇          | -1.455   | 24.04593359 | 3.1455745 |
| Sr₄Ba₄Mn₄Ni₄       | -1.455   | 483.4883244 | 3.1455745 |
| Ba₄Sr₄Mn₄Ni₄       | -1.454   | 484.0640744 | 3.1460906 |
| Ba₄Cd₄Zr₇Fe₁       | -1.453   | 187.6825994 | 3.1466067 |
| Ba₂La₆Sc₈          | -1.452   | 63.70259812 | 3.1471228 |
| Ba₄Y₄Ni₈           | -1.452   | 644.2740819 | 3.1471228 |
| Sr₈Ni₇Co₁          | -1.45    | 756.7903018 | 3.148155  |
| Pr₈Ga₈             | -1.449   | 70.39114186 | 3.1486711 |
| La₈Mg₄Sc₄          | -1.447   | 169.8248034 | 3.1497033 |
| Pr₈Sc₈             | -1.443   | 23.6410205  | 3.1517677 |
| Y₈Ga₈              | -1.44    | 69.473884   | 3.153316  |
| Sr₈Ga₄Fe₄          | -1.437   | 270.2745978 | 3.1548643 |
| Ba₄La₄Sc₈          | -1.436   | 138.6154782 | 3.1553804 |
| Ba₄Sr₄Fe₆Cu₂        | -1.436   | 396.3339781 | 3.1553804 |
| Dy₄Y₄Sc₈           | -1.434   | 41.14157115 | 3.1564126 |
| Sr₈Mn₁Ni₇          | -1.433   | 725.8810526 | 3.1569287 |
| Sr₄Ba₄Sc₄Co₄       | -1.425   | 266.9415421 | 3.1610575 |
| Ba₄Sr₄Fe₄Ni₄       | -1.425   | 532.1133689 | 3.1610575 |
| Ba₈Y₄Fe₄           | -1.423   | 223.0186253 | 3.1620897 |
| Ba₈Fe₄Pd₄          | -1.421   | 376.8856369 | 3.1631219 |
| Pr₆Dy₂Sc₈          | -1.42    | 31.3278325  | 3.163638  |
| Rb₄Ba₄Nb₄Fe₄       | -1.42    | 226.5071034 | 3.163638  |
| Sr₂La₆Sc₈          | -1.419   | 48.6703405  | 3.1641541 |
| Ba₂Y₆Ga₈           | -1.415   | 224.6724158 | 3.1662185 |
| Ba₈Zr₈             | -1.414   | 34.87204233 | 3.1667346 |
| Dy₂Y₆Sc₈           | -1.414   | 203.0273879 | 3.1682829 |
| Y₈Mg₄Ni₄           | -1.413   | 693.9918919 | 3.168799  |
| Ba₈In₂Fe₆          | -1.41    | 30.36666638 | 3.1698312 |
| Sm₄Y₄Sc₈           | -1.408   | 36.83152562 | 3.1703473 |
| Pr₆Ho₂Sc₈          | -1.407   | 69.76585156 | 3.1713795 |
| Ba₄Sr₄Ni₆Co₂       | -1.405   | 711.3473656 | 3.1713795 |
| Sr₈Ga₄Co₄          | -1.405   | 759.695915  | 3.1713795 |
| Sr₄Ba₄Ni₆Co₂       | -1.404   | 1401.1156   | 3.1718956 |
| Sr₈Ni₈             | -1.401   | 797.5165969 | 3.1734439 |
| Sr₂Ba₆Sc₄Co₄       | -1.397   | 261.8387606 | 3.1755083 |
| Compound                  | Energy   | Dipole       | Charge |
|---------------------------|----------|--------------|--------|
| Pr 4 Ho 4 Sc 8            | -1.396   | 43.10978075  | 3.1760244 |
| Sr 2 Ba 6 Al 4 Co 4       | -1.396   | 388.3704657  | 3.1760244 |
| Sr 8 Sc 1 Ni 7            | -1.396   | 647.8258047  | 3.1760244 |
| Ba 8 Ga 2 Fe 6            | -1.394   | 238.5799996  | 3.1770566 |
| Pr 4 Dy 4 Sc 8            | -1.393   | 33.4211445   | 3.1775727 |
| Cs 4 Ba 4 Mn 4 Nb 4       | -1.393   | 311.454829   | 3.1775727 |
| Sr 8 Al 1 Ni 7            | -1.389   | 660.7546729  | 3.1796371 |
| Sr 4 La 4 Sc 8            | -1.387   | 124.158454   | 3.1806693 |
| Ba 3 Cd 1 Pr 4 Ni 8       | -1.386   | 707.7181936  | 3.1811854 |
| Ba 6 Ti 2 Zn 2 Ni 6       | -1.384   | 788.8750985  | 3.1822176 |
| Ba 6 Nb 2 Zn 2 Ni 6       | -1.384   | 706.1085907  | 3.1822176 |
| Pr 6 Nd 2 Sc 8            | -1.382   | 24.00170775  | 3.1832498 |
| Pr 6 Sm 2 Sc 8            | -1.381   | 26.30113     | 3.1837659 |
| Sr 2 Ba 6 Al 4 Fe 4       | -1.381   | 294.7971848  | 3.1837659 |
| Ba 8 Co 4 Ni 4            | -1.381   | 566.9848843  | 3.1837659 |
| Cd 4 Pr 4 Ni 8            | -1.381   | 771.8534377  | 3.1837659 |
| Ba 8 Fe 6 Ni 2            | -1.38   | 397.6813093  | 3.184282 |
| Ba 4 Pr 4 Ni 8            | -1.377   | 665.0063999  | 3.1858303 |
| Sm 2 Y 6 Sc 8             | -1.374   | 30.15027031  | 3.1873786 |
| Ba 8 Mn 4 Fe 4            | -1.369   | 209.2674863  | 3.1899591 |
| Sr 4 Ba 4 Fe 2 Ni 6       | -1.368   | 660.2195374  | 3.1904752 |
| Ba 2 Cd 2 Pr 4 Ni 8       | -1.368   | 738.8143409  | 3.1904752 |
| Nd 4 Y 4 Sc 8             | -1.367   | 29.92382187  | 3.1909913 |
| Ba 4 Sr 4 Fe 2 Ni 6       | -1.367   | 664.5725374  | 3.1909913 |
| Ca 4 La 4 Sc 8            | -1.361   | 167.2719761  | 3.1940879 |
| Ba 8 Sc 4 Co 4            | -1.358   | 253.4784791  | 3.1956362 |
| Ba 8 Zr 5 Fe 1 Ni 2       | -1.357   | 222.3356381  | 3.1961523 |
| Nd 2 Y 6 Sc 8             | -1.356   | 31.09509806  | 3.1966684 |
| Pr 4 Sm 4 Sc 8            | -1.355   | 27.6864895   | 3.1971845 |
| Sr 8 Al 2 Ni 6            | -1.354   | 615.6739988  | 3.1977006 |
| Sr 8 Y 1 Ni 7             | -1.354   | 672.14837    | 3.1977006 |
| Pr 6 Ho 2 Ga 8            | -1.354   | 85.68175213  | 3.1977006 |
| Pr 4 Nd 4 Sc 8            | -1.352   | 24.261395    | 3.1987328 |
| Sr 8 Y 4 Co 4             | -1.349   | 297.2480888  | 3.2002811 |
| Pr 6 Nd 2 Ga 8            | -1.346   | 72.89124498  | 3.2018294 |
| Sr 8 Ga 1 Ni 7            | -1.343   | 665.738127   | 3.2033777 |
| Ba 4 Ba 4 Mn 2 Fe 6       | -1.341   | 625.4768307  | 3.2044099 |
| Sr 4 Ba 4 Mn 2 Ni 6       | -1.341   | 641.073413   | 3.2044099 |
| Ba 4 Sr 4 Zn 2 Fe 6       | -1.338   | 291.1028914  | 3.2059582 |
| Compound | R | χ | G | B | M | H |
|----------|---|---|---|---|---|---|
| Pr 6 Dy 2 Ga 8 | -1.336 | 83.83777077 | 3.2069904 | 1.0 | 0.0 | 0.0 |
| Pr 6 Sm 2 Ga 8 | -1.336 | 77.84899036 | 3.2069904 | 1.0 | 0.0 | 0.0 |
| Rb 4 Ba 4 Mn 4 Nb 4 | -1.334 | 218.4521778 | 3.2080226 | 1.0 | 0.0 | 0.0 |
| Ba 2 Sr 6 Ni 8 | -1.331 | 792.8012764 | 3.2095709 | 1.0 | 0.0 | 0.0 |
| Ba 2 Y 6 Sc 8 | -1.329 | 134.889405 | 3.2106031 | 1.0 | 0.0 | 0.0 |
| Sr 8 Sc 2 Ni 6 | -1.327 | 587.3170124 | 3.2116353 | 1.0 | 0.0 | 0.0 |
| Sr 2 Ba 6 Ga 4 Co 4 | -1.324 | 391.4137581 | 3.2131836 | 1.0 | 0.0 | 0.0 |
| Sr 6 Ti 2 Zn 2 Ni 6 | -1.323 | 736.0317985 | 3.2136997 | 1.0 | 0.0 | 0.0 |
| Ba 4 Sr 4 Cu 8 | -1.322 | 727.4318499 | 3.2142158 | 1.0 | 0.0 | 0.0 |
| Y 6 Ho 2 Ga 8 | -1.319 | 76.50326643 | 3.2157641 | 1.0 | 0.0 | 0.0 |
| Sr 8 In 4 Fe 4 | -1.314 | 271.267753 | 3.2183446 | 1.0 | 0.0 | 0.0 |
| Sr 8 In 1 Ni 7 | -1.311 | 675.4512604 | 3.2198929 | 1.0 | 0.0 | 0.0 |
| Ba 8 Al 4 Co 4 | -1.31 | 393.7579342 | 3.220409 | 1.0 | 0.0 | 0.0 |
| Ba 8 Ni 4 Co 4 | -1.309 | 582.7663843 | 3.2209251 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Fe 1 Ni 7 | -1.308 | 723.1807467 | 3.2214412 | 1.0 | 0.0 | 0.0 |
| Ba 4 Sr 4 Fe 1 Ni 7 | -1.307 | 728.1534967 | 3.2219573 | 1.0 | 0.0 | 0.0 |
| Pr 8 Mg 4 Ni 4 | -1.306 | 3.321794969 | 3.2224734 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Ni 7 Co 1 | -1.301 | 748.4796608 | 3.2250539 | 1.0 | 0.0 | 0.0 |
| Ba 4 Sr 4 Ni 7 Co 1 | -1.301 | 754.0106608 | 3.2250539 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Y 4 Co 4 | -1.296 | 284.2467722 | 3.2276344 | 1.0 | 0.0 | 0.0 |
| Sr 8 Al 4 Ni 4 | -1.294 | 558.8919006 | 3.2286666 | 1.0 | 0.0 | 0.0 |
| Sr 6 Zr 2 Zn 2 Ni 6 | -1.293 | 720.1860837 | 3.2291827 | 1.0 | 0.0 | 0.0 |
| Sr 8 In 1 Ni 7 | -1.291 | 350.090413 | 3.2302149 | 1.0 | 0.0 | 0.0 |
| Ba 8 Fe 6 Cu 2 | -1.288 | 376.6937203 | 3.2317632 | 1.0 | 0.0 | 0.0 |
| Ba 4 Sr 4 Mn 1 Ni 7 | -1.288 | 722.3216845 | 3.2317632 | 1.0 | 0.0 | 0.0 |
| Ba 8 Al 4 Fe 4 | -1.286 | 298.544253 | 3.2327954 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Mn 1 Ni 7 | -1.286 | 726.0971845 | 3.2327954 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Ga 4 Fe 4 | -1.281 | 291.7333774 | 3.2353759 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Ga 4 Co 4 | -1.281 | 392.4559771 | 3.2353759 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Sc 1 Ni 7 | -1.278 | 647.1563022 | 3.2369242 | 1.0 | 0.0 | 0.0 |
| Ba 8 Fe 4 Ni 4 | -1.274 | 512.8927279 | 3.2389886 | 1.0 | 0.0 | 0.0 |
| Sr 6 Hf 2 Zn 2 Ni 6 | -1.269 | 750.4995158 | 3.2415691 | 1.0 | 0.0 | 0.0 |
| Sr 8 Ga 2 Ni 6 | -1.267 | 624.9809071 | 3.2426013 | 1.0 | 0.0 | 0.0 |
| Sr 2 Ba 6 Y 4 Co 4 | -1.264 | 264.3107407 | 3.2441496 | 1.0 | 0.0 | 0.0 |
| Ba 8 Ni 6 Co 2 | -1.262 | 678.5569746 | 3.2451818 | 1.0 | 0.0 | 0.0 |
| Ba 8 Ga 4 Co 4 | -1.262 | 373.3420392 | 3.2451818 | 1.0 | 0.0 | 0.0 |
| Sr 8 V 4 Zn 4 | -1.254 | 278.6754579 | 3.2493106 | 1.0 | 0.0 | 0.0 |
| Sr 4 Ba 4 Y 1 Ni 7 | -1.253 | 658.9730473 | 3.2498267 | 1.0 | 0.0 | 0.0 |
| Ba 8 Zr 6 Zn 1 Fe 1 | -1.25 | 94.11041745 | 3.251375 | 1.0 | 0.0 | 0.0 |
| Formula             | Spin | Mass   | Ionic   |
|---------------------|------|--------|---------|
| Sr 8 Y 2 Ni 6       | -1.25| 626.1793931 | 3.251375 |
| Sr 7 Zn 1 Ni 8      | -1.247| 855.7682283 | 3.2529233 |
| Gd 2 Y 6 Ga 8       | -1.247| 72.71641462  | 3.2529233 |
| Ba 4 Sr 4 Ga 8      | -1.246| 450.8530218  | 3.2534394 |
| Ba 8 Zr 3 Fe 1 Ni 4 | -1.245| 425.0825293  | 3.2539555 |
| Pr 4 Ho 4 Ga 8      | -1.245| 92.15403512  | 3.2539555 |
| Pr 4 Dy 4 Ga 8      | -1.244| 90.00434745  | 3.2544716 |
| Ba 4 Y 4 Ga 8       | -1.243| 348.4244475  | 3.2549877 |
| Ba 4 Sr 4 Ni 8      | -1.241| 830.6034559  | 3.2560199 |
| Y 4 Ho 4 Ga 8       | -1.24 | 82.99657195  | 3.256536  |
| Sr 4 Ba 4 Sc 2 Ni 6 | -1.239| 588.2483985  | 3.2570521 |
| Ba 8 Y 4 Co 4       | -1.238| 245.8857092  | 3.2575682 |
| Sr 4 Ba 4 Al 2 Ni 6 | -1.238| 635.6333761  | 3.2575682 |
| Sr 4 Ba 4 Al 1 Ni 7 | -1.235| 670.126541    | 3.2591165 |
| Ba 6 Zr 2 Zn 2 Ni 6 | -1.233| 745.2791945  | 3.2601487 |
| Dy 4 Y 4 Ga 8       | -1.233| 81.726855    | 3.2601487 |
| Ba 6 Hf 2 Zn 2 Ni 6 | -1.232| 797.3632545  | 3.2606648 |
| Nd 4 Y 4 Ga 8       | -1.231| 79.07980342  | 3.2611809 |
| Pr 4 Nd 4 Ga 8      | -1.225| 74.56373534  | 3.2642775 |
| Ca 4 Y 4 Ga 8       | -1.224| 288.3272051  | 3.2647936 |
| Sr 2 Y 6 Ga 8       | -1.224| 192.4399565  | 3.2647936 |
| Sr 2 Ba 6 Sc 1 Ni 7 | -1.22 | 633.9212317  | 3.266858  |
| Ba 8 Fe 2 Ni 6      | -1.22 | 638.676464   | 3.266858  |
| Sr 2 Y 6 Sc 8       | -1.219| 120.4591182  | 3.2673741 |
| Sr 2 Ba 6 Y 2 Ni 6  | -1.218| 583.6983181  | 3.2678902 |
| Y 8 Mg 1 Sc 7       | -1.216| 79.20833369  | 3.2689224 |
| Ba 8 Zn 2 Fe 6      | -1.216| 345.3246223  | 3.2689224 |
| Pr 4 Sm 4 Ga 8      | -1.216| 82.92662983  | 3.2689224 |
| Sr 8 In 2 Ni 6      | -1.214| 638.3999239  | 3.2699546 |
| Ba 4 Sr 4 Al 6 Fe 2 | -1.212| 366.1720247  | 3.2709868 |
| Sr 4 Ba 4 In 4 Co 4 | -1.212| 336.2168512  | 3.2709868 |
| Ba 4 Y 4 Sc 8       | -1.209| 207.1861857  | 3.2725351 |
| Ba 8 Mn 2 Ni 6      | -1.209| 616.283022   | 3.2725351 |
| Ba 2 Pr 6 Ga 8      | -1.206| 198.3563235  | 3.2740834 |
| Ca 2 Y 6 Ga 8       | -1.206| 179.3471695  | 3.2740834 |
| Ba 8 Y 2 Ni 6       | -1.204| 564.7827476  | 3.2751156 |
| Ca 4 Pr 4 Ga 8      | -1.203| 285.9401669  | 3.2756317 |
| Sr 4 Ba 4 Ga 1 Ni 7 | -1.201| 672.9121922  | 3.2766639 |
| Sr 2 Ba 6 Y 1 Ni 7  | -1.198| 642.0419768  | 3.2782122 |
| Structure | ΔG (eV) | E (eV) | E (eV) |
|-----------|---------|-------|-------|
| Sr 6 Zn 2 Ni 8 | -1.198 | 903.7533597 | 3.2782122 |
| Ba 2 Pr 6 Sc 8 | -1.195 | 115.0208732 | 3.2797605 |
| Sm 4 Y 4 Ga 8 | -1.195 | 82.90154417 | 3.2797605 |
| Sr 4 Ba 4 In 1 Ni 7 | -1.192 | 666.9713797 | 3.2813088 |
| Sr 2 Ba 6 Sc 2 Ni 6 | -1.187 | 574.077078 | 3.2838893 |
| Ba 4 Pr 4 Sc 8 | -1.186 | 192.3737259 | 3.2844054 |
| Sr 4 Ba 4 Y 2 Ni 6 | -1.184 | 604.7471386 | 3.2854376 |
| Sr 2 Ba 6 Ga 4 Fe 4 | -1.183 | 288.9661179 | 3.2859537 |
| Ca 2 Y 6 Sc 8 | -1.182 | 125.1627653 | 3.286498 |
| Ba 8 Ga 8 | -1.181 | 439.4478259 | 3.2869859 |
| Ba 4 Sr 4 Fe 4 Cu 4 | -1.18 | 528.7626909 | 3.287502 |
| Sr 8 Mg 4 V 4 | -1.176 | 221.0588574 | 3.2895664 |
| Sr 2 Ba 6 Al 1 Ni 7 | -1.174 | 659.0317205 | 3.2905986 |
| Sr 4 Y 4 Ga 8 | -1.174 | 302.338029 | 3.2905986 |
| Ca 2 Pr 6 Ga 8 | -1.174 | 177.5044044 | 3.2905986 |
| Sr 8 Sc 4 Ni 4 | -1.173 | 461.083928 | 3.2911147 |
| Sr 4 Ba 4 Al 4 Ni 4 | -1.17 | 572.055534 | 3.292663 |
| Ba 8 Fe 1 Ni 7 | -1.168 | 702.4408557 | 3.2936952 |
| Ba 4 Pr 4 Ga 8 | -1.168 | 315.3707314 | 3.2936952 |
| Sr 4 Y 4 Sc 8 | -1.167 | 201.4358621 | 3.2942113 |
| Y 8 Mg 1 Ga 7 | -1.165 | 111.8132485 | 3.2952435 |
| Y 8 Mg 2 Sc 6 | -1.164 | 134.2935431 | 3.2957596 |
| Ba 8 Ni 7 Co 1 | -1.164 | 726.8315198 | 3.2957596 |
| Sr 2 Ba 6 In 4 Co 4 | -1.164 | 319.3083203 | 3.2957596 |
| Ba 8 Sc 1 Ni 7 | -1.163 | 623.2091612 | 3.2962757 |
| Pr 8 Mg 1 Sc 7 | -1.161 | 71.89846084 | 3.2973079 |
| Sr 2 Ba 6 Al 2 Ni 6 | -1.16 | 625.6065556 | 3.297824 |
| Ba 8 Mn 1 Ni 7 | -1.158 | 735.8887935 | 3.2988562 |
| Ba 8 Cu 8 | -1.158 | 706.6057089 | 3.2988562 |
| Y 8 Mg 2 Ga 6 | -1.155 | 157.0373629 | 3.3004045 |
| Ba 6 Zn 2 Ni 8 | -1.152 | 941.1204116 | 3.3019528 |
| Pr 8 Mg 1 Ga 7 | -1.152 | 109.8950685 | 3.3019528 |
| Sr 2 Pr 6 Ga 8 | -1.151 | 185.7875382 | 3.3024689 |
| Sr 4 Pr 4 Ga 8 | -1.15 | 285.2592284 | 3.302985 |
| Ba 8 Y 1 Ni 7 | -1.147 | 627.5879063 | 3.3045333 |
| Sr 4 Ba 4 Ga 2 Ni 6 | -1.147 | 641.1569286 | 3.3045333 |
| Ba 8 Sc 2 Ni 6 | -1.145 | 562.3185075 | 3.3055655 |
| Sr 4 Ba 4 In 4 Fe 4 | -1.145 | 253.4567339 | 3.3055655 |
| Sr 2 Pr 6 Sc 8 | -1.143 | 98.68802881 | 3.3065977 |
| Compound          | E (eV) | Heat Capacity (J/mol) | Entropy (J/mol/K) |
|-------------------|--------|-----------------------|-------------------|
| Y\textsubscript{8}Mg\textsubscript{4}Sc\textsubscript{4}   | -1.142 | 240.966962            | 3.3071138         |
| Pr\textsubscript{8}Mg\textsubscript{2}Sc\textsubscript{6} | -1.142 | 122.5804012           | 3.3071138         |
| Ca\textsubscript{4}Y\textsubscript{4}Sc\textsubscript{8}  | -1.141 | 222.8939064           | 3.3076299         |
| Pr\textsubscript{8}Mg\textsubscript{2}Ga\textsubscript{6} | -1.14  | 152.4017451           | 3.308146          |
| Ba\textsubscript{8}Mn\textsubscript{4}Ni\textsubscript{4} | -1.137 | 496.157979            | 3.3096943         |
| Sr\textsubscript{2}Ba\textsubscript{6}Ga\textsubscript{1}Ni\textsubscript{7} | -1.137 | 660.1236217           | 3.3096943         |
| Ba\textsubscript{4}Sr\textsubscript{4}Zn\textsubscript{8} | -1.136 | 699.7820966           | 3.3102104         |
| Y\textsubscript{8}Mg\textsubscript{4}Ga\textsubscript{4}   | -1.133 | 247.3678419           | 3.3117587         |
| Sr\textsubscript{2}Ba\textsubscript{6}In\textsubscript{1}Ni\textsubscript{7} | -1.133 | 650.6703092           | 3.3117587         |
| Sr\textsubscript{4}Pr\textsubscript{4}Sc\textsubscript{8}  | -1.131 | 173.1372871           | 3.3127909         |
| Ba\textsubscript{8}Zr\textsubscript{3}Fe\textsubscript{1}Cu\textsubscript{4} | -1.131 | 397.3003513           | 3.3127909         |
| Ca\textsubscript{2}Pr\textsubscript{6}Sc\textsubscript{8}  | -1.128 | 115.7311854           | 3.3143392         |
| Ba\textsubscript{8}In\textsubscript{4}Co\textsubscript{4}  | -1.127 | 298.5130388           | 3.3148553         |
| Pr\textsubscript{8}Mg\textsubscript{4}Sc\textsubscript{4}  | -1.119 | 221.0850319           | 3.3189841         |
| Sr\textsubscript{4}Ba\textsubscript{4}Sc\textsubscript{4}Ni\textsubscript{4} | -1.119 | 469.9275911           | 3.3189841         |
| Sr\textsubscript{4}Ba\textsubscript{4}In\textsubscript{2}Ni\textsubscript{6} | -1.119 | 625.3365534           | 3.3189841         |
| Ca\textsubscript{4}Pr\textsubscript{4}Sc\textsubscript{8}  | -1.117 | 210.7571004           | 3.3200163         |
| Ba\textsubscript{8}Ni\textsubscript{8}                  | -1.117 | 805.2925649           | 3.3200163         |
| Pr\textsubscript{8}Mg\textsubscript{4}Ga\textsubscript{4} | -1.114 | 237.7283484           | 3.3215646         |
| Sr\textsubscript{8}Ga\textsubscript{4}Ni\textsubscript{4} | -1.113 | 544.7329672           | 3.3220807         |
| Sr\textsubscript{2}Ba\textsubscript{6}Al\textsubscript{4}Ni\textsubscript{4} | -1.112 | 570.0417257           | 3.3225968         |
| Ba\textsubscript{8}Al\textsubscript{6}Fe\textsubscript{2} | -1.111 | 364.3330943           | 3.3231129         |
| Nd\textsubscript{2}Y\textsubscript{6}Ga\textsubscript{8}  | -1.109 | 76.84371871           | 3.3241451         |
| Ba\textsubscript{8}Al\textsubscript{1}Ni\textsubscript{7} | -1.107 | 650.30215             | 3.3251773         |
| Sr\textsubscript{2}Ba\textsubscript{6}In\textsubscript{4}Fe\textsubscript{4} | -1.107 | 235.715203            | 3.3251773         |
| Ba\textsubscript{8}Al\textsubscript{2}Ni\textsubscript{6} | -1.098 | 617.2347351           | 3.3298222         |
| Ba\textsubscript{8}Zr\textsubscript{5}Fe\textsubscript{1}Cu\textsubscript{2} | -1.091 | 217.1117991           | 3.3334349         |
| Ba\textsubscript{4}Sr\textsubscript{4}Zn\textsubscript{4}Fe\textsubscript{4} | -1.091 | 464.5173361           | 3.3334349         |
| Sm\textsubscript{2}Y\textsubscript{6}Ga\textsubscript{8}  | -1.081 | 77.23771408           | 3.3385959         |
| Ba\textsubscript{8}Ga\textsubscript{4}Fe\textsubscript{4} | -1.08  | 287.2828583           | 3.339112          |
| Sr\textsubscript{2}Ba\textsubscript{6}Ga\textsubscript{2}Ni\textsubscript{6} | -1.079 | 627.9721081           | 3.3396281         |
| Ba\textsubscript{2}Ca\textsubscript{6}Zr\textsubscript{8} | -1.077 | 0                     | 3.3406603         |
| Sr\textsubscript{2}Ba\textsubscript{6}Sc\textsubscript{4}Ni\textsubscript{4} | -1.074 | 458.9407706           | 3.3422086         |
| Ba\textsubscript{8}In\textsubscript{1}Ni\textsubscript{7}  | -1.074 | 636.8019887           | 3.3422086         |
| Dy\textsubscript{2}Y\textsubscript{6}Ga\textsubscript{8}  | -1.067 | 75.6574945            | 3.3458213         |
| Ba\textsubscript{4}Sr\textsubscript{4}Fe\textsubscript{2}Cu\textsubscript{6} | -1.064 | 626.3372704           | 3.3473696         |
| Ba\textsubscript{8}Ga\textsubscript{1}Ni\textsubscript{7} | -1.064 | 649.9593012           | 3.3473696         |
| Sr\textsubscript{2}Ba\textsubscript{6}In\textsubscript{2}Ni\textsubscript{6} | -1.064 | 604.3427329           | 3.3473696         |
| Sr\textsubscript{8}Y\textsubscript{4}Ni\textsubscript{4}  | -1.054 | 514.8814393           | 3.3525306         |
| Compound                  | Energy   | Energy_1  | Energy_2  |
|--------------------------|----------|-----------|-----------|
| Ba$_8$Fe$_4$Cu$_4$        | -1.053   | 501.5170499 | 3.3530467 |
| Ba$_4$Ca$_4$Zr$_8$        | -1.045   | 679.4408168 | 3.3571755 |
| Ba$_8$Zn$_8$              | -1.043   | 218.128635  | 3.3582077 |
| Ba$_8$In$_4$Fe$_4$        | -1.036   | 558.1114052  | 3.3618204 |
| Ba$_8$Al$_4$Ni$_4$        | -1.032   | 449.6689501  | 3.3638848 |
| Ba$_8$Sc$_4$Ni$_4$        | -1.03    | 628.3974124  | 3.36917   |
| Ba$_8$Ga$_2$Ni$_6$        | -1.02    | 617.1985376  | 3.370078  |
| Ba$_8$Zn$_4$Fe$_4$        | -1.011   | 449.3468538  | 3.3747229 |
| Ba$_4$Sr$_4$Zr$_8$        | -1.001   | 575.8687045  | 3.3798839 |
| Ba$_4$Sr$_4$Zn$_6$Fe$_2$  | -1.001   | 484.9633212  | 3.3819483 |
| Ba$_8$Zn$_4$Fe$_4$        | -0.992   | 557.416251   | 3.3845288 |
| Sr$_4$Ba$_4$Y$_4$Ni$_4$   | -0.997   | 302.8047955  | 3.3865932 |
| Ba$_8$Y$_8$               | -0.988   | 567.9653364  | 3.3881415 |
| Sr$_8$Ba$_4$Ga$_4$Ni$_4$  | -0.985   | 329.9975333  | 3.3938186 |
| Ba$_8$Zr$_5$Zn$_2$Fe$_1$  | -0.96    | 462.9645007  | 3.3948508 |
| Sr$_4$Ba$_4$Ga$_6$Fe$_2$  | -0.962   | 412.3486599  | 3.4000118 |
| Sr$_8$In$_4$Ni$_4$        | -0.952   | 182.606731   | 3.401044  |
| Sr$_8$Zr$_8$              | -0.952   | 442.7626802  | 3.4051728 |
| Ca$_8$Zr$_8$              | -0.95    | 584.4185483  | 3.4051728 |
| Ba$_8$Y$_4$Ni$_4$         | -0.936   | 361.4694343  | 3.4134304 |
| Sr$_2$Ba$_6$Ga$_4$Ni$_4$  | -0.936   | 601.9186294  | 3.4191075 |
| Ba$_8$Zr$_3$Zn$_4$Fe$_1$  | -0.92    | 537.4111131  | 3.421688  |
| Sr$_4$Ba$_4$In$_4$Ni$_4$  | -0.915   | 548.8275853  | 3.4242685 |
| Ba$_8$Zn$_6$Fe$_2$        | -0.92    | 512.2518303  | 3.4309778 |
| Sr$_2$Ba$_6$In$_4$Ni$_4$  | -0.871   | 402.3889671  | 3.4469769 |
| Ba$_8$Ga$_6$Fe$_2$        | -0.864   | 582.4945102  | 3.452654  |
| Ba$_8$Ga$_4$Ni$_4$        | -0.86    | 494.4612598  | 3.4758785 |