1. **NaAlH4**

**For calculation = ‘Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

Al 0.8750000000 0.1250000000 0.2500000000

Al 0.1250000000 0.8750000000 0.7500000000

Na 0.3750000000 0.6250000000 0.2500000000

Na 0.6250000000 0.3750000000 0.7500000000

H 0.0634757715 0.7189029040 0.5869441028

H 0.7189029040 0.3495801257 0.0869441028

H 0.8058470067 0.9365242285 0.9130558972

H 0.6504198743 0.8058470067 0.4130558972

H 0.3495801257 0.1941529933 0.5869441028

H 0.9365242285 0.2810970960 0.4130558972

H 0.2810970960 0.6504198743 0.9130558972

H 0.1941529933 0.0634757715 0.0869441028

**End final coordinates**

**total energy = -279.14888607 Ry**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= 9.24**

0.00006559 0.00000000 0.00000000 9.65 0.00 0.00

0.00000000 0.00006559 0.00000000 0.00 9.65 0.00

0.00000000 0.00000000 0.00005720 0.00 0.00 8.41

**Calculation = ‘vc-relax’**

**total energy = -279.15002251 Ry**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= -0.11**

-0.00000120 -0.00000000 -0.00000000 -0.18 -0.00 -0.00

0.00000000 -0.00000120 -0.00000000 0.00 -0.18 -0.00

-0.00000000 -0.00000000 0.00000021 -0.00 -0.00 0.03

**CELL\_PARAMETERS (alat= 9.33732575)**

1.014253902 0.000000000 -0.000000000

-0.000000000 1.014253902 -0.000000000

0.507126951 0.507126951 1.126450927

1. **AlH3**

**Calculation = ‘Relax’**

ATOMIC\_POSITIONS (crystal)

Al -0.0000000000 0.0000000000 0.0000000000

Al 0.0000000000 0.5000000000 0.0000000000

Al 0.0000000000 0.0000000000 0.5000000000

Al 0.5000000000 -0.0000000000 -0.0000000000

H 0.3219677932 0.3219677932 0.9280322068

H 0.6780322068 0.0719677932 0.6780322068

H 0.9280322068 0.9280322068 0.3219677932

H 0.3219677932 0.9280322068 0.9280322068

H 0.0719677932 0.0719677932 0.6780322068

H 0.3219677932 0.9280322068 0.3219677932

H 0.6780322068 0.0719677932 0.0719677932

H 0.6780322068 0.6780322068 0.0719677932

H 0.0719677932 0.6780322068 0.6780322068

H 0.9280322068 0.3219677932 0.3219677932

H 0.9280322068 0.3219677932 0.9280322068

H 0.0719677932 0.6780322068 0.0719677932

End final coordinates

**total energy = -172.02282752 Ry**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= 11.75**

0.00007987 -0.00000000 -0.00000000 11.75 -0.00 -0.00

-0.00000000 0.00007987 -0.00000000 -0.00 11.75 -0.00

-0.00000000 -0.00000000 0.00007987 -0.00 -0.00 11.75

**Calculation = ‘vc-relax’**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= -0.35**

-0.00000239 -0.00000000 -0.00000000 -0.35 -0.00 -0.00

-0.00000000 -0.00000239 -0.00000000 -0.00 -0.35 -0.00

-0.00000000 -0.00000000 -0.00000239 -0.00 -0.00 -0.35

**total energy = -172.02444777 Ry**

**CELL\_PARAMETERS (alat= 16.96728396)**

0.505726285 0.505726285 -0.000000000

0.505726285 -0.000000000 0.505726285

-0.000000000 0.505726285 0.505726285

1. **Na3AlH6**

**Calculation =’Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

Al 0.5000000000 0.0000000000 0.0000000000

Al 0.5000000000 0.5000000000 0.5000000000

Na -0.0000000000 0.0000000000 0.5000000000

Na 0.0000000000 0.5000000000 0.0000000000

Na 0.2575387641 0.9529061849 0.2465724682

Na 0.7424612359 0.0470938151 0.7534275318

Na 0.7424612359 0.4529061849 0.2534275318

Na 0.2575387641 0.5470938151 0.7465724682

H 0.4015475728 0.7679252051 0.5631617623

H 0.5984524272 0.2320747949 0.4368382377

H 0.5984524272 0.2679252051 0.9368382377

H 0.4015475728 0.7320747949 0.0631617623

H 0.7291333023 0.8298476525 0.9564502687

H 0.2708666977 0.1701523475 0.0435497313

H 0.2708666977 0.3298476525 0.5435497313

H 0.7291333023 0.6701523475 0.4564502687

H 0.1828129401 0.9522814922 0.7826684429

H 0.8171870599 0.0477185078 0.2173315571

H 0.8171870599 0.4522814922 0.7173315571

H 0.1828129401 0.5477185078 0.2826684429

End final coordinates

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= 13.89**

0.00009473 0.00000000 0.00000010 13.93 0.00 0.02

0.00000000 0.00009335 0.00000000 0.00 13.73 0.00

0.00000010 0.00000000 0.00009520 0.02 0.00 14.00

Total energy = -665.33763309 Ry

**Calculation = ‘VC-RELAX’**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= -0.02**

0.00000025 0.00000000 0.00000043 0.04 0.00 0.06

0.00000000 -0.00000144 0.00000000 0.00 -0.21 0.00

0.00000043 0.00000000 0.00000072 0.06 0.00 0.11

**total energy = -665.34048474 Ry**

**CELL\_PARAMETERS (alat= 10.00307627)**

1.013534097 0.000000000 0.000296189

0.000000000 1.050516094 0.000000000

-1.012664219 0.000000000 1.459671107

1. **Na5AlH14**

**ATOMIC\_POSITIONS (crystal)**

Al 0.0000000000 0.0000000000 0.5000000000

Al 0.5000000000 0.5000000000 -0.0000000000

Al 0.0000000000 0.5000000000 0.0000000000

Al 0.5000000000 0.0000000000 0.5000000000

Al 0.0000000000 0.5000000000 0.5000000000

Al 0.5000000000 0.0000000000 -0.0000000000

Na 0.0000000000 0.0000000000 -0.0000000000

Na 0.5000000000 0.5000000000 0.5000000000

Na 0.7867926915 0.2867926915 0.2500000000

Na 0.7132073085 0.7867926915 0.2500000000

Na 0.2132073085 0.7132073085 0.2500000000

Na 0.7132073085 0.7867926915 0.7500000000

Na 0.2132073085 0.7132073085 0.7500000000

Na 0.2867926915 0.2132073085 0.2500000000

Na 0.2867926915 0.2132073085 0.7500000000

Na 0.7867926915 0.2867926915 0.7500000000

H 0.0448119173 0.3192088292 0.1184175414

H 0.4551880827 0.8192088292 0.3815824586

H 0.1807911708 0.4551880827 0.3815824586

H 0.4551880827 0.8192088292 0.6184175414

H 0.1807911708 0.4551880827 0.6184175414

H 0.9551880827 0.6807911708 0.1184175414

H 0.3192088292 0.9551880827 0.1184175414

H 0.9551880827 0.6807911708 0.8815824586

H 0.3192088292 0.9551880827 0.8815824586

H 0.6807911708 0.0448119173 0.1184175414

H 0.0448119173 0.3192088292 0.8815824586

H 0.6807911708 0.0448119173 0.8815824586

H 0.5448119173 0.1807911708 0.3815824586

H 0.8192088292 0.5448119173 0.3815824586

H 0.5448119173 0.1807911708 0.6184175414

H 0.8192088292 0.5448119173 0.6184175414

H 0.0000000000 0.0000000000 0.3285153115

H 0.5000000000 0.5000000000 0.1714846885

H 0.5000000000 0.5000000000 0.8285153115

H 0.0000000000 0.0000000000 0.6714846885

H 0.2520913161 0.5781773156 -0.0000000000

H 0.2479086839 0.0781773156 0.5000000000

H 0.9218226844 0.2479086839 0.5000000000

H 0.7479086839 0.4218226844 -0.0000000000

H 0.5781773156 0.7479086839 -0.0000000000

H 0.4218226844 0.2520913161 -0.0000000000

H 0.7520913161 0.9218226844 0.5000000000

H 0.0781773156 0.7520913161 0.5000000000

End final coordinates

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= 13.32**

0.00009117 0.00000000 0.00000000 13.41 0.00 0.00

0.00000000 0.00009117 0.00000000 0.00 13.41 0.00

0.00000000 0.00000000 0.00008937 0.00 0.00 13.15

**total energy = -1223.64057149 Ry**

**calculation = ‘VC-RELAX’**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= -0.27**

-0.00000197 0.00000000 0.00000000 -0.29 0.00 0.00

0.00000000 -0.00000197 0.00000000 0.00 -0.29 0.00

0.00000000 0.00000000 -0.00000158 0.00 0.00 -0.23

**total energy = -1223.64645231 Ry**

**CELL\_PARAMETERS (alat= 12.61135185)**

1.012667298 0.000000000 0.000000000

0.000000000 1.012667298 0.000000000

0.000000000 0.000000000 1.553073922

1. **NaH**

**Calculation = ‘Relax’**

**Computing stress (Cartesian axis) and pressure**

total stress (Ry/bohr\*\*3) (kbar) P= 9.65

0.00006563 0.00000000 -0.00000000 9.65 0.00 -0.00

0.00000000 0.00006563 -0.00000000 0.00 9.65 -0.00

0.00000000 -0.00000000 0.00006563 0.00 -0.00 9.65

**total energy = -96.54064924 Ry**

**Begin final coordinates**

**ATOMIC\_POSITIONS (crystal)**

Na 0.0000000000 0.0000000000 0.0000000000

H 0.5000000000 0.5000000000 0.5000000000

End final coordinates

**Calculation = ‘VC-RELAX’**

**Computing stress (Cartesian axis) and pressure**

**total stress (Ry/bohr\*\*3) (kbar) P= 0.16**

0.00000111 0.00000000 0.00000000 0.16 0.00 0.00

0.00000000 0.00000111 0.00000000 0.00 0.16 0.00

-0.00000000 0.00000000 0.00000111 -0.00 0.00 0.16

**total energy = -96.54091100 Ry**

**CELL\_PARAMETERS (alat= 9.01936044)**

0.506548187 0.506548187 -0.000000000

0.506548187 -0.000000000 0.506548187

-0.000000000 0.506548187 0.506548187