1. **KAlH4**

**For calculation = ‘Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

K 0.1764602255 0.2500000000 0.1652784563

K 0.3235397745 0.7500000000 0.6652784563

K 0.8235397745 0.7500000000 0.8347215437

K 0.6764602255 0.2500000000 0.3347215437

Al 0.0687993182 0.2500000000 0.6791431807

Al 0.4312006818 0.7500000000 0.1791431807

Al 0.9312006818 0.7500000000 0.3208568193

Al 0.5687993182 0.2500000000 0.8208568193

H 0.0780832498 0.0193196199 0.8118385343

H 0.4219167502 0.5193196199 0.3118385343

H 0.4219167502 0.9806803801 0.3118385343

H 0.9219167502 0.5193196199 0.1881614657

H 0.9219167502 0.9806803801 0.1881614657

H 0.5780832498 0.4806803801 0.6881614657

H 0.5780832498 0.0193196199 0.6881614657

H 0.0780832498 0.4806803801 0.8118385343

H 0.0911078360 0.7500000000 0.4345192055

H 0.4088921640 0.2500000000 0.9345192055

H 0.9088921640 0.2500000000 0.5654807945

H 0.5911078360 0.7500000000 0.0654807945

H 0.2169189313 0.2500000000 0.5433093303

H 0.2830810687 0.7500000000 0.0433093303

H 0.7830810687 0.7500000000 0.4566906697

H 0.7169189313 0.2500000000 0.9566906697

**End final coordinates**

**total energy = -629.07405623 Ry**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 5.06**

0.00003560 0.00000000 0.00000000 5.24 0.00 0.00

0.00000000 0.00003249 0.00000000 0.00 4.78 0.00

0.00000000 0.00000000 0.00003519 0.00 0.00 5.18

**Calculation = ‘vc-relax’**

**total energy = -629.07593479 Ry**

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

**total stress (Ry/bohr\*\*3) (kbar) P= -0.17**

-0.00000259 0.00000000 0.00000000 -0.38 0.00 0.00

0.00000000 0.00000095 0.00000000 0.00 0.14 0.00

0.00000000 0.00000000 -0.00000180 0.00 0.00 -0.26

**CELL\_PARAMETERS (alat= 16.56925094)**

1.013712397 0.000000000 0.000000000

0.000000000 0.661804274 0.000000000

0.000000000 0.000000000 0.841492913

1. **Na3AlH6**

**Calculation =’Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

K 0.7429433753 0.5281183457 0.2490437660

K 0.2570566247 0.4718816543 0.7509562340

K 0.2570566247 0.0281183457 0.2509562340

K 0.7429433753 0.9718816543 0.7490437660

K -0.0000000000 0.0000000000 0.5000000000

K 0.0000000000 0.5000000000 0.0000000000

Al 0.5000000000 0.0000000000 0.0000000000

Al 0.5000000000 0.5000000000 0.5000000000

H 0.6317091292 0.7390654155 0.4641293597

H 0.3682908708 0.2609345845 0.5358706403

H 0.3682908708 0.2390654155 0.0358706403

H 0.6317091292 0.7609345845 0.9641293597

H 0.7080581533 0.1718112348 0.9707961772

H 0.2919418467 0.8281887652 0.0292038228

H 0.2919418467 0.6718112348 0.5292038228

H 0.7080581533 0.3281887652 0.4707961772

H 0.7630006381 0.5194887107 0.7037187813

H 0.2369993619 0.4805112893 0.2962812187

H 0.2369993619 0.0194887107 0.7962812187

H 0.7630006381 0.9805112893 0.2037187813

End final coordinates

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

**total stress (Ry/bohr\*\*3) (kbar) P= 6.82**

0.00004592 0.00000000 -0.00000000 6.76 0.00 -0.00

0.00000000 0.00004554 0.00000000 0.00 6.70 0.00

-0.00000000 0.00000000 0.00004753 -0.00 0.00 6.99

Total energy = -771.38277563 Ry

**Calculation = ‘VC-RELAX’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= -0.15**

**-0.00000069 0.00000000 0.00000018 -0.10 0.00 0.03**

**0.00000000 -0.00000150 0.00000000 0.00 -0.22 0.00**

**0.00000018 0.00000000 -0.00000092 0.03 0.00 -0.14**

**total energy = -771.38406034 Ry**

**CELL\_PARAMETERS (alat= 11.29137816)**

1.008992867 0.000000000 0.000091320

0.000000000 1.014962038 0.000000000

-0.994769294 0.000000000 1.432589018

1. **NaH**

**Calculation = ‘Relax’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 1.58**

0.00001071 0.00000000 0.00000000 1.58 0.00 0.00

0.00000000 0.00001071 0.00000000 0.00 1.58 0.00

0.00000000 0.00000000 0.00001071 0.00 0.00 1.58

**total energy = -114.20719569Ry**

**Begin final coordinates**

**ATOMIC\_POSITIONS (crystal)**

K 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= 0.43**

0.00000294 0.00000000 -0.00000000 0.43 0.00 -0.00

0.00000000 0.00000294 0.00000000 0.00 0.43 0.00

-0.00000000 0.00000000 0.00000294 -0.00 0.00 0.43

**total energy = -114.20721727 Ry**

**CELL\_PARAMETERS (alat= 10.71947144)**

0.501330435 0.501330435 0.000000000

0.501330435 0.000000000 0.501330435

0.000000000 0.501330435 0.501330435