1. **K5Al3h14**

**Calculation = ‘Relax’**

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

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

**0.00002051 0.00000000 0.00000000 3.02 0.00 0.00**

**0.00000000 0.00002051 0.00000000 0.00 3.02 0.00**

**0.00000000 0.00000000 -0.00004660 0.00 0.00 -6.86**

**total energy = -1400.35941843 Ry**

**Begin final coordinates**

**ATOMIC\_POSITIONS (crystal)**

K 0.0000000000 0.0000000000 0.5000000000

K 0.5000000000 0.5000000000 0.0000000000

K 0.2917230712 0.7917230712 0.2500000000

K 0.2082769288 0.2917230712 0.2500000000

K 0.7082769288 0.2082769288 0.2500000000

K 0.2082769288 0.2917230712 0.7500000000

K 0.7082769288 0.2082769288 0.7500000000

K 0.7917230712 0.7082769288 0.2500000000

K 0.7917230712 0.7082769288 0.7500000000

K 0.2917230712 0.7917230712 0.7500000000

Al 0.0000000000 0.0000000000 -0.0000000000

Al 0.5000000000 0.5000000000 0.5000000000

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

H 0.5433039353 0.8348610650 0.1051107069

H 0.9566960647 0.3348610650 0.3948892931

H 0.6651389350 0.9566960647 0.3948892931

H 0.9566960647 0.3348610650 0.6051107069

H 0.6651389350 0.9566960647 0.6051107069

H 0.4566960647 0.1651389350 0.1051107069

H 0.8348610650 0.4566960647 0.1051107069

H 0.4566960647 0.1651389350 0.8948892931

H 0.8348610650 0.4566960647 0.8948892931

H 0.1651389350 0.5433039353 0.1051107069

H 0.5433039353 0.8348610650 0.8948892931

H 0.1651389350 0.5433039353 0.8948892931

H 0.0433039353 0.6651389350 0.3948892931

H 0.3348610650 0.0433039353 0.3948892931

H 0.0433039353 0.6651389350 0.6051107069

H 0.3348610650 0.0433039353 0.6051107069

H 0.0000000000 0.0000000000 0.1521826764

H 0.5000000000 0.5000000000 0.3478173236

H 0.5000000000 0.5000000000 0.6521826764

H 0.0000000000 0.0000000000 0.8478173236

H 0.7542896291 0.0580343515 0.0000000000

H 0.7457103709 0.5580343515 0.5000000000

H 0.4419656485 0.7457103709 0.5000000000

H 0.2457103709 0.9419656485 0.0000000000

H 0.0580343515 0.2457103709 -0.0000000000

H 0.9419656485 0.7542896291 -0.0000000000

H 0.2542896291 0.4419656485 0.5000000000

H 0.5580343515 0.2542896291 0.5000000000

End final coordinates

**Calculation = ‘VC-RELAX’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 0.04**

**0.00000040 0.00000000 0.00000000 0.06 0.00 0.00**

**0.00000000 0.00000040 0.00000000 0.00 0.06 0.00**

**0.00000000 0.00000000 -0.00000008 0.00 0.00 -0.01**

**total energy = -1400.36282068 Ry**

CELL\_PARAMETERS (alat= 13.62507654)

1.015239953 0.000000000 0.000000000

0.000000000 1.015239953 0.000000000

0.000000000 0.000000000 1.575349781