1. **NaGaH4**

**For calculation = ‘Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

Ga 0.8418726390 0.1581273610 0.7500000000

Ga 0.1581273610 0.8418726390 0.2500000000

Na 0.6579193184 0.3420806816 0.2500000000

Na 0.3420806816 0.6579193184 0.7500000000

H 0.6891700272 0.3108299728 0.5696546507

H 0.6891700272 0.3108299728 0.9303453493

H 0.3108299728 0.6891700272 0.0696546507

H 0.3108299728 0.6891700272 0.4303453493

H 0.1766627347 0.1930537308 0.7500000000

H 0.1930537308 0.1766627347 0.2500000000

H 0.8233372653 0.8069462692 0.2500000000

H 0.8069462692 0.8233372653 0.7500000000

**End final coordinates**

**total energy = -755.96425163 Ry**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 9.02**

**0.00005375 0.00000000 0.00000000 7.91 0.00 0.00**

**-0.00000000 0.00007015 0.00000000 -0.00 10.32 0.00**

**0.00000000 0.00000000 0.00006003 0.00 0.00 8.83**

**Calculation = ‘vc-relax’**

**total energy = -755.96622438 Ry**

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

total stress (Ry/bohr\*\*3) (kbar) P= -0.20

-0.00000170 0.00000000 0.00000000 -0.25 0.00 0.00

0.00000000 -0.00000112 0.00000000 0.00 -0.17 0.00

0.00000000 0.00000000 -0.00000127 0.00 0.00 -0.19

**CELL\_PARAMETERS (alat= 13.16555183)**

0.509473081 -0.461686891 0.000000000

0.509473081 0.461686891 0.000000000

0.000000000 0.000000000 1.028229683

1. **GaH3**

**Calculation = ‘Relax’**

ATOMIC\_POSITIONS (crystal)

B 0.1421475330 0.5436581385 0.6443004729

B 0.8578524670 0.4563418615 0.3556995271

B 0.8578524670 0.0436581385 0.8556995271

B 0.1421475330 0.9563418615 0.1443004729

H 0.0878937199 0.0049810536 0.3109590124

H 0.9121062801 0.9950189464 0.6890409876

H 0.9121062801 0.5049810536 0.1890409876

H 0.0878937199 0.4950189464 0.8109590124

H 0.1417569354 0.1321189147 0.0241757751

H 0.8582430646 0.8678810853 0.9758242249

H 0.8582430646 0.6321189147 0.4758242249

H 0.1417569354 0.3678810853 0.5241757751

H 0.3874343926 0.6515319688 0.6714651309

H 0.6125656074 0.3484680312 0.3285348691

H 0.6125656074 0.1515319688 0.8285348691

H 0.3874343926 0.8484680312 0.1714651309

End final coordinates

**total energy = -39.61400683 Ry**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 9.29**

**0.00006124 0.00000000 -0.00000056 9.01 0.00 -0.08**

**0.00000000 0.00006669 0.00000000 0.00 9.81 0.00**

**-0.00000056 0.00000000 0.00006159 -0.08 0.00 9.06**

**Calculation = ‘vc-relax’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 0.37**

**0.00000272 0.00000000 -0.00000081 0.40 0.00 -0.12**

**0.00000000 0.00000090 0.00000000 0.00 0.13 0.00**

**-0.00000081 0.00000000 0.00000386 -0.12 0.00 0.57**

**total energy = -39.62207456 Ry**

CELL\_PARAMETERS (alat= 8.10805891)

1.113857385 0.000000000 -0.011867227

0.000000000 1.624450407 0.000000000

-0.733754376 0.000000000 1.388013903

1. **Na3GaH6**

**Calculation =’Relax’**

**Begin final coordinates**

ATOMIC\_POSITIONS (crystal)

Ga 0.5000000000 0.0000000000 0.0000000000

Ga 0.5000000000 0.5000000000 0.5000000000

Na -0.0000000000 0.0000000000 0.5000000000

Na 0.0000000000 0.5000000000 0.0000000000

Na 0.2698437578 0.8589447414 0.3576009595

Na 0.7301562422 0.1410552586 0.6423990405

Na 0.7301562422 0.3589447414 0.1423990405

Na 0.2698437578 0.6410552586 0.8576009595

H 0.3375176526 0.8530816440 0.5396757471

H 0.6624823474 0.1469183560 0.4603242529

H 0.6624823474 0.3530816440 0.9603242529

H 0.3375176526 0.6469183560 0.0396757471

H 0.6666520995 0.8954879063 0.9947078768

H 0.3333479005 0.1045120937 0.0052921232

H 0.3333479005 0.3954879063 0.5052921232

H 0.6666520995 0.6045120937 0.4947078768

H 0.2219905859 0.9145000132 0.8323668933

H 0.7780094141 0.0854999868 0.1676331067

H 0.7780094141 0.4145000132 0.6676331067

H 0.2219905859 0.5854999868 0.3323668933

End final coordinates

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

**total stress (Ry/bohr\*\*3) (kbar) P= -13.94**

**-0.00010011 0.00000000 -0.00009340 -14.73 0.00 -13.74**

**0.00000000 -0.00009063 0.00000000 0.00 -13.33 0.00**

**-0.00009340 0.00000000 -0.00009364 -13.74 0.00 -13.78**

Total energy = -1141.47358166 Ry

**Calculation = ‘VC-RELAX’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 0.31**

**0.00004092 0.00000000 0.00000185 6.02 0.00 0.27**

**0.00000000 -0.00002118 0.00000000 0.00 -3.12 0.00**

**0.00000185 0.00000000 -0.00001342 0.27 0.00 -1.97**

**total energy = -1142.00018105 Ry**

CELL\_PARAMETERS (alat= 14.09520260)

0.722297196 0.000000000 -0.004681104

0.000000000 0.745801375 0.000000000

-0.714135671 0.000000000 1.066146605

1. **Na5Ga3H14**

**ATOMIC\_POSITIONS (crystal)**

Ga 0.0000000000 0.0000000000 0.5000000000

Ga 0.5000000000 0.5000000000 0.0000000000

Ga 0.0000000000 0.5000000000 0.0000000000

Ga 0.5000000000 0.0000000000 0.5000000000

Ga 0.0000000000 0.5000000000 0.5000000000

Ga 0.5000000000 0.0000000000 0.0000000000

Na 0.0000000000 0.0000000000 -0.0000000000

Na 0.5000000000 0.5000000000 0.5000000000

Na 0.7873693316 0.2873693316 0.2500000000

Na 0.7126306684 0.7873693316 0.2500000000

Na 0.2126306684 0.7126306684 0.2500000000

Na 0.7126306684 0.7873693316 0.7500000000

Na 0.2126306684 0.7126306684 0.7500000000

Na 0.2873693316 0.2126306684 0.2500000000

Na 0.2873693316 0.2126306684 0.7500000000

Na 0.7873693316 0.2873693316 0.7500000000

H 0.0420161654 0.3246583315 0.1149741256

H 0.4579838346 0.8246583315 0.3850258744

H 0.1753416685 0.4579838346 0.3850258744

H 0.4579838346 0.8246583315 0.6149741256

H 0.1753416685 0.4579838346 0.6149741256

H 0.9579838346 0.6753416685 0.1149741256

H 0.3246583315 0.9579838346 0.1149741256

H 0.9579838346 0.6753416685 0.8850258744

H 0.3246583315 0.9579838346 0.8850258744

H 0.6753416685 0.0420161654 0.1149741256

H 0.0420161654 0.3246583315 0.8850258744

H 0.6753416685 0.0420161654 0.8850258744

H 0.5420161654 0.1753416685 0.3850258744

H 0.8246583315 0.5420161654 0.3850258744

H 0.5420161654 0.1753416685 0.6149741256

H 0.8246583315 0.5420161654 0.6149741256

H 0.0000000000 0.0000000000 0.3342268228

H 0.5000000000 0.5000000000 0.1657731772

H 0.5000000000 0.5000000000 0.8342268228

H 0.0000000000 0.0000000000 0.6657731772

H 0.2530104651 0.5703088820 0.0000000000

H 0.2469895349 0.0703088820 0.5000000000

H 0.9296911180 0.2469895349 0.5000000000

H 0.7469895349 0.4296911180 0.0000000000

H 0.5703088820 0.7469895349 0.0000000000

H 0.4296911180 0.2530104651 0.0000000000

H 0.7530104651 0.9296911180 0.5000000000

H 0.0703088820 0.7530104651 0.5000000000

End final coordinates

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

**total stress (Ry/bohr\*\*3) (kbar) P= -63.31**

**-0.00042243 0.00000000 0.00000000 -62.14 0.00 0.00**

**0.00000000 -0.00042243 0.00000000 0.00 -62.14 0.00**

**0.00000000 0.00000000 -0.00044636 0.00 0.00 -65.66**

**total energy = -2651.20509353 Ry**

**calculation = ‘VC-RELAX’**

1. **GaH3**

**Calculation = ‘Relax’**

**total stress (Ry/bohr\*\*3) (kbar) P= -1.86**

**-0.00005043 0.00000000 -0.00000000 -7.42 0.00 -0.00**

**0.00000000 -0.00005043 0.00000000 0.00 -7.42 0.00**

**0.00000000 0.00000000 0.00006295 0.00 0.00 9.26**

**total energy = -281.21444027 Ry**

**Begin final coordinates**

**ATOMIC\_POSITIONS (crystal)**

**Ga 0.0000000000 0.0000000000 0.0000000000**

**H 0.7500000000 0.2500000000 0.5000000000**

**H 0.2500000000 0.7500000000 0.5000000000**

**H 0.5000000000 0.5000000000 0.0000000000**

End final coordinates

**Calculation = ‘VC-RELAX’**

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

**total stress (Ry/bohr\*\*3) (kbar) P= 0.30**

**0.00000100 -0.00000000 -0.00000000 0.15 -0.00 -0.00**

**-0.00000000 0.00000100 -0.00000000 -0.00 0.15 -0.00**

**-0.00000000 -0.00000000 0.00000415 -0.00 -0.00 0.61**

**total energy = -281.21545168 Ry**

CELL\_PARAMETERS (alat= 5.41880856)

0.990258509 0.000000000 -0.000000000

0.000000000 0.990258509 -0.000000000

0.495129255 0.495129255 1.155597721