In [50]:
```
%matplotlib inline
%load_ext autoreload
%autoreload 2 # Make it easier to test by autoreloading modules on executio
n
```

The autoreload extension is already loaded. To reload it, use:
  %reload_ext autoreload

In [51]:
```
import calphad.libcalphadcpp as lcp
from calphad.minimize.globmin import GlobalMinimizer
import numpy as np
import matplotlib.pyplot as plt
# Load thermodynamic database
maindb = lcp.Database("Ni-H-Austin.tdb")
if maindb == None:
        sys.exit("Failed to load database")

conds = lcp.evalconditions()
conds.statevars['T'] = 1073
conds.statevars['P'] = 101325
conds.statevars['N'] = 1
conds.elements.append('H')
conds.elements.append('NI')
conds.elements.append('VA')
conds.phases["FCC_A1"] = lcp.PhaseStatus.ENTERED

# Configure variable names
indices = lcp.IndexBiMap()
varmap = lcp.build_variable_map ( maindb.get_phases(), conds, indices )
cmps = {}
# Create phases
for ph in maindb.get_phases():
    status = conds.phases[ph.key()]
    if (status == lcp.PhaseStatus.ENTERED):
        cmps[ph.key()] = lcp.CompositionSet(ph.data(), maindb.get_parameter
_set(), varmap, indices)
```

In [52]:
```
# Initialize minimizer and sample points
engine = lcp.GlobalMinimizer()
engine.initial_subdivisions_per_axis = 20
engine.discard_unstable = False
points_1073 = engine.point_sample(cmps['FCC_A1'], varmap, conds)
conds.statevars['T'] = 1473
points_1473 = engine.point_sample(cmps['FCC_A1'], varmap, conds)
points_1073 = np.array(points_1073)
points_1473 = np.array(points_1473)
```
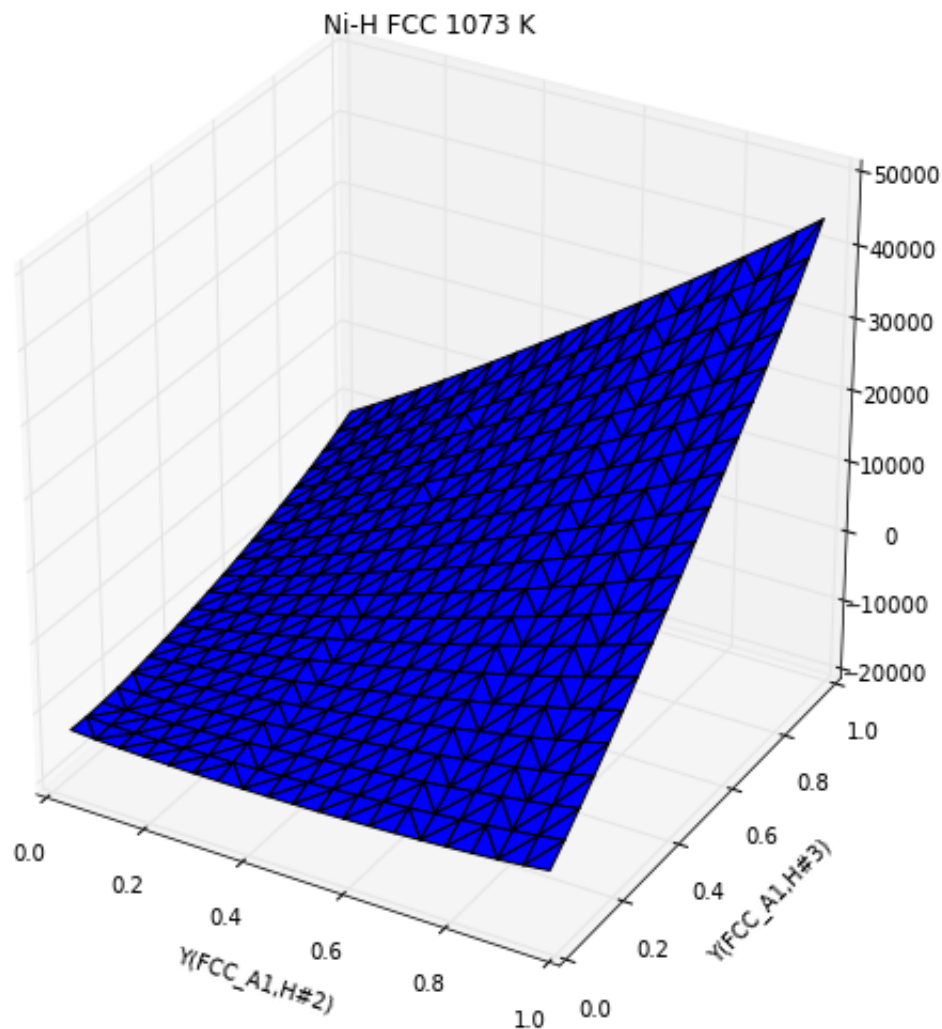
```
In [53]:  from mpl_toolkits.mplot3d import Axes3D
          import matplotlib.tri as tri
          fig = plt.figure(figsize=(9,9))
          ax = fig.add_subplot(111, projection='3d')


          triang = tri.Triangulation(points_1073[:,1],points_1073[:,3])

          # mask off the triangles on the side
          mask = np.any(np.any(np.where(points[triang.triangles,0:4] < 1e-6, True, Fa
          lse),axis=1), axis=1)
          triang.set_mask(mask)

          ax.plot_trisurf(triang,points[:,5], shade=False)
          plt.xlabel('Y(FCC_A1,H#2)')
          plt.ylabel('Y(FCC_A1,H#3)')
          plt.title('Ni-H FCC 1073 K')
          plt.show()
```



Ni-H FCC 1073 K
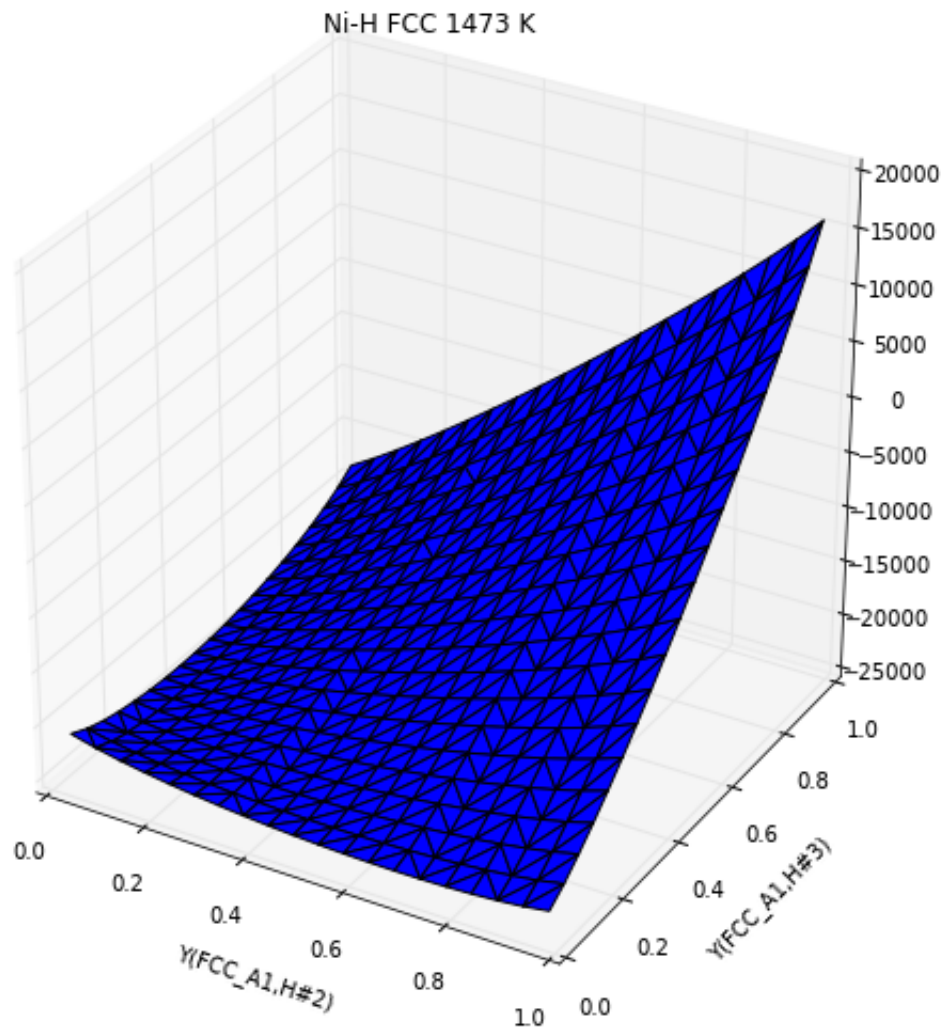
```
In [54]:  from mpl_toolkits.mplot3d import Axes3D
          import matplotlib.tri as tri
          fig = plt.figure(figsize=(9,9))
          ax = fig.add_subplot(111, projection='3d')


          triang = tri.Triangulation(points_1473[:,1],points_1473[:,3])

          # mask off the triangles on the side
          mask = np.any(np.any(np.where(points_1473[triang.triangles,0:4] < 1e-6, Tru
          e, False),axis=1), axis=1)
          triang.set_mask(mask)

          ax.plot_trisurf(triang,points_1473[:,5], shade=False)
          plt.xlabel('Y(FCC_A1,H#2)')
          plt.ylabel('Y(FCC_A1,H#3)')
          plt.title('Ni-H FCC 1473 K')
          plt.show()
```



Ni-H FCC 1473 K

# Documentation

A couple of things that might help to know for reproducing the figures. A small but finite Curie temperature was added to all the paramagnetic end-members to work around a bug in our implementation of the magnetic model.

```
In [55]: np.set_printoptions(threshold='nan')
         print(points_1073)
```

```
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```

```
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```

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```

```
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   4.25000000e-01  -1.19802204e+03]
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   3.25000000e-01   1.56211754e+02]
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   8.25000000e-01  -1.13425719e+04]
```

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   2.75000000e-01  -8.61845673e+01]
[  1.00000000e+00   2.25000000e-01   7.75000000e-01   6.75000000e-01
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```

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```

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   1.75000000e-01  -2.78554408e+03]
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   2.25000000e-01  -3.83838769e+03]
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   4.25000000e-01  -7.47407637e+03]
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   4.75000000e-01  -8.26198424e+03]
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   7.75000000e-01  -1.20129170e+04]
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   8.75000000e-01  -1.28019130e+04]
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   9.25000000e-01  -1.30529325e+04]
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             1.25000000e-01  -3.46061868e+03]
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             1.75000000e-01  -4.47131120e+03]
          [  1.00000000e+00   2.50000000e-02   9.75000000e-01   7.75000000e-01
             2.25000000e-01  -5.40385697e+03]
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          [  1.00000000e+00   2.50000000e-02   9.75000000e-01   3.25000000e-01
             6.75000000e-01  -1.14438918e+04]
          [  1.00000000e+00   2.50000000e-02   9.75000000e-01   2.75000000e-01
             7.25000000e-01  -1.18776349e+04]
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             9.25000000e-01  -1.29346437e+04]
          [  1.00000000e+00   2.50000000e-02   9.75000000e-01   2.50000000e-02
             9.75000000e-01  -1.28912291e+04]]
```

In [56]: 
```python
np.set_printoptions(threshold='nan')
print(points_1473)
```

```
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          [  1.00000000e+00   1.00000000e-12   1.00000000e+00   1.00000000e+00
             1.00000000e-12  -1.78512898e+04]
          [  1.00000000e+00   1.00000000e+00   1.00000000e-12   1.00000000e-12
             1.00000000e+00  -2.31248881e+04]
          [  1.00000000e+00   1.00000000e+00   1.00000000e-12   1.00000000e+00
             1.00000000e-12   1.90314389e+04]
          [  1.00000000e+00   9.75000000e-01   2.50000000e-02   9.75000000e-01
             2.50000000e-02   1.60067012e+04]
          [  1.00000000e+00   9.75000000e-01   2.50000000e-02   9.25000000e-01
             7.50000000e-02   1.30336994e+04]
          [  1.00000000e+00   9.75000000e-01   2.50000000e-02   8.75000000e-01
```

```
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 [  1.00000000e+00   9.75000000e-01   2.50000000e-02   8.25000000e-01
    1.75000000e-01   7.70993764e+03]
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    2.25000000e-01   5.22707241e+03]
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    4.25000000e-01  -3.91408004e+03]
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 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    8.75000000e-01
     1.25000000e-01   -1.48744647e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    8.25000000e-01
     1.75000000e-01   -1.59598085e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    7.75000000e-01
     2.25000000e-01   -1.69378731e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    7.25000000e-01
     2.75000000e-01   -1.78275587e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    6.75000000e-01
     3.25000000e-01   -1.86401315e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    6.25000000e-01
     3.75000000e-01   -1.93827111e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    5.75000000e-01
     4.25000000e-01   -2.00598243e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    5.25000000e-01
     4.75000000e-01   -2.06741749e+04]
 [  1.00000000e+00    2.25000000e-01    7.75000000e-01    4.75000000e-01
```

```
     5.25000000e-01  -2.12270324e+04]
 [  1.00000000e+00   2.25000000e-01   7.75000000e-01   4.25000000e-01
     5.75000000e-01  -2.17183973e+04]
 [  1.00000000e+00   2.25000000e-01   7.75000000e-01   3.75000000e-01
     6.25000000e-01  -2.21470006e+04]
 [  1.00000000e+00   2.25000000e-01   7.75000000e-01   3.25000000e-01
     6.75000000e-01  -2.25101393e+04]
 [  1.00000000e+00   2.25000000e-01   7.75000000e-01   2.75000000e-01
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 [  1.00000000e+00   2.25000000e-01   7.75000000e-01   1.25000000e-01
     8.75000000e-01  -2.31673835e+04]
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     9.25000000e-01  -2.30443100e+04]
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 [  1.00000000e+00   1.75000000e-01   8.25000000e-01   2.25000000e-01
     7.75000000e-01  -2.30959161e+04]
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 [  1.00000000e+00   1.75000000e-01   8.25000000e-01   1.25000000e-01
     8.75000000e-01  -2.30433514e+04]
 [  1.00000000e+00   1.75000000e-01   8.25000000e-01   7.50000000e-02
```

```
                9.25000000e-01  -2.28199720e+04]
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```

```
                               3.25000000e-01  -2.13994714e+04]
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    6.75000000e-01  -2.31949527e+04]
 [  1.00000000e+00   2.50000000e-02   9.75000000e-01   2.75000000e-01
```

```
                   7.25000000e-01  -2.30868475e+04]
 [  1.00000000e+00   2.50000000e-02   9.75000000e-01   2.25000000e-01
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 [  1.00000000e+00   2.50000000e-02   9.75000000e-01   1.75000000e-01
                   8.25000000e-01  -2.26280795e+04]
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                   8.75000000e-01  -2.22472595e+04]
 [  1.00000000e+00   2.50000000e-02   9.75000000e-01   7.50000000e-02
                   9.25000000e-01  -2.17229956e+04]
 [  1.00000000e+00   2.50000000e-02   9.75000000e-01   2.50000000e-02
                   9.75000000e-01  -2.09593835e+04]]
```

In [57]: 
```python
with open('Ni-H-Austin.tdb', 'r') as fin:
    print fin.read()
```

```
$ Database file written 2014- 6-12
$ From database: User data 2014. 6.12
 ELEMENT /-   ELECTRON_GAS               0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                     0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT H    1/2_MOLE_H2(GAS)           1.0079E+00  4.2340E+03  6.5285E+01!
 ELEMENT NI   FCC_A1                     5.8690E+01  4.7870E+03  2.9796E+01!

 FUNCTION F10598T    2.98150E+02  +211801.621+24.4989816*T-20.78611*T*LN(T)
;
       6.00000E+03   N !
 FUNCTION F10790T    2.98150E+02  +374456.652-34.0578028*T-24.054*T*LN(T)
      -.01185105*T**2+1.23611E-06*T**3-15550*T**(-1);  1.20000E+03   Y
       +362141.292+89.7695408*T-41.846*T*LN(T)-7.219E-04*T**2-4.367E-08*T**3
      +1525260*T**(-1);  3.10000E+03   Y
       +335048.906+118.55457*T-44.078*T*LN(T)-.0025659*T**2
      +1.23796667E-07*T**3+20792295*T**(-1);  5.70000E+03   Y
       -56310.2884+1055.69873*T-153.197*T*LN(T)+.01100975*T**2
      -1.93861667E-07*T**3+2.8526535E+08*T**(-1);  6.00000E+03   N !
 FUNCTION GHSERH2    2.98150E+02   -9522.97393+78.5273873*T-31.35707*T*LN(T)
      +.0027589925*T**2-7.46390667E-07*T**3+56582.3*T**(-1);  1.00000E+03   Y
       +180.10884-15.6128262*T-17.84857*T*LN(T)-.00584168*T**2
      +3.14618667E-07*T**3-1280036*T**(-1);  2.10000E+03   Y
       -18840.1661+92.3120249*T-32.05082*T*LN(T)-.0010728235*T**2
      +1.14281783E-08*T**3+3561002.5*T**(-1);  6.00000E+03   N !
 FUNCTION F13480T    2.98150E+02   +414972.341-18.8056393*T-24.34*T*LN(T)
      +.0046806645*T**2-3.40084167E-06*T**3;  4.00000E+02   Y
       +415486.817-40.9586295*T-20.26685*T*LN(T)-.006038615*T**2
      +1.2890125E-06*T**3;  8.00000E+02   Y
       +411065.296+18.3133675*T-29.24746*T*LN(T)+.0021365025*T**2
      -1.14496517E-07*T**3+412765.95*T**(-1);  2.60000E+03   Y
       +411224.713+11.7609247*T-28.29857*T*LN(T)+.001646801*T**2
      -7.78248167E-08*T**3+785084*T**(-1);  5.00000E+03   Y
       +406354.126+39.4541897*T-31.80175*T*LN(T)+.0024133565*T**2
      -1.0515525E-07*T**3;  1.00000E+04   N !
 FUNCTION F13543T    2.98150E+02   +638073.28-68.1901937*T-24.897*T*LN(T)
      -.0313584*T**2+5.93355333E-06*T**3-14215*T**(-1);  8.00000E+02   Y
       +611401.773+268.08482*T-75.25401*T*LN(T)+.01088525*T**2
      -7.08741667E-07*T**3+2633835*T**(-1);  2.10000E+03   Y
       +637459.339+72.071267*T-48.587*T*LN(T)-9.09E-05*T**2
```

```
                +9.12933333E-08*T**3-1191755*T**(-1);  4.50000E+03  Y
                 +564540.781+329.59901*T-80.11301*T*LN(T)+.00578085*T**2
                -1.08841667E-07*T**3+29137900*T**(-1);  6.00000E+03  N !
 FUNCTION GLIQH       2.98150E+02  +8035+25*T+2*T*LN(T)+.5*GHSERH2#;
     6.00000E+03   N !
 FUNCTION GHSERNI     2.98150E+02  -5179.159+117.854*T-22.096*T*LN(T)
     -.0048407*T**2;  1.72800E+03  Y
      -27840.655+279.135*T-43.1*T*LN(T)+1.12754E+31*T**(-9);  3.00000E+03
N
     !
 FUNCTION GLIQNI      2.98150E+02  +16414.686-9.397*T-3.82318E-21*T**7
     +GHSERNI#;  1.72800E+03  Y
      +18290.88-10.537*T-1.12754E+31*T**(-9)+GHSERNI#;  6.00000E+03  N !
 FUNCTION GBCCNI      2.98150E+02  +8715.084-3.556*T+GHSERNI#;   6.00000E+03

      N !
 FUNCTION GB2NIVA     2.98150E+02  +162397.3-27.40575*T;   6.00000E+03   N !
 FUNCTION LB2NIVA     2.98150E+02  -64024.38+26.49419*T;   6.00000E+03   N !
 FUNCTION GNIHENDO    2.98150E+02  -6943.19902+232.335861*T-.04484*T**2
     +7.69228E-06*T**3+414576.079*T**(-1)-33.0704558*T*LN(T);  3.00000E+03

      N !
 FUNCTION GNIHENDT   2.98150E+02  +8750.9+1192.79246*T+.08885*T**2
     -1.75912E-05*T**3+2999916.61*T**(-1)-183.864222*T*LN(T);  3.00000E+03

      N !
 FUNCTION GNIHENDF   2.98150E+02  +95728.2+3987.57995*T+.397102914*T**2
     -6.06166E-05*T**3+12316009.5*T**(-1)-611.369511*T*LN(T);  3.00000E+03

      N !
 FUNCTION UN_ASS     2.98150E+02  0.0 ;  3.00000E+02  N !

 TYPE_DEFINITION % SEQ *!
 DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
 DEFAULT_COMMAND DEF_SYS_ELEMENT VA /- !


 TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
 PHASE FCC_A1  %&  3 1   1   2 !
    CONSTITUENT FCC_A1  :NI : H,VA : H,VA :  !

   PARAMETER G(FCC_A1,NI:H:H;0)  2.98150E+02  +GNIHENDF#;   6.00000E+03    N

  REF0 !
   PARAMETER G(FCC_A1,NI:VA:H;0) 2.98150E+02  +GNIHENDT#;   6.00000E+03
N
  REF0 !
   PARAMETER G(FCC_A1,NI:H:VA;0) 2.98150E+02  +GNIHENDO#;   6.00000E+03
N
  REF0 !
   PARAMETER G(FCC_A1,NI:VA:VA;0)  2.98150E+02  +GHSERNI#;   6.00000E+03
N
  REF0 !
   PARAMETER TC(FCC_A1,NI:VA:VA;0) 2.98150E+02  633; 1.72830E+03  N REF0
!
   PARAMETER TC(FCC_A1,NI:VA:H;0)  2.98150E+02  1e-5;  6000  N REF0 !
```

```
        PARAMETER TC(FCC_A1,NI:H:VA;0)  2.98150E+02  1e-5;  6000  N REF0 !
        PARAMETER TC(FCC_A1,NI:H:H;0)  2.98150E+02  1e-5;  6000  N REF0 !
        PARAMETER BMAGN(FCC_A1,NI:VA:VA;0)  2.98150E+02  .52;  1.72830E+03  Y
        3;  6.00000E+03  N REF0 !

        LIST_OF_REFERENCES
        NUMBER  SOURCE
         !
```

In [57]: