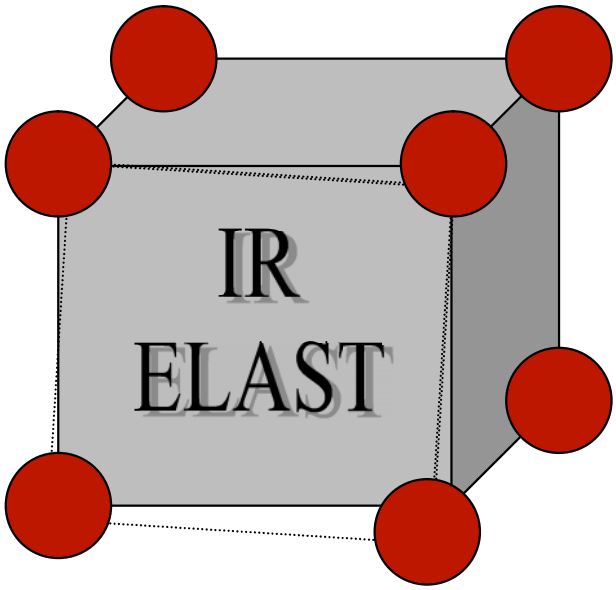

IR ELAST

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WIEN2k

A Package for calculating elastic tensors of hexagonal Phases *by using second-order derivative* with Wien2k Package

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User's guide, Elastic Hexagonal_12.1 (Release 06.02.2012)
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Installation guide

1_ Copy **“hex-elastic.tar.gz”** file in your computer in each Directory then do:
tar –zxvf hex-elastic.tar.gz
cd hex-elastic

2_ Run **buildHIRelast_lapw**

This program helps you to provide "Makefile" and then compile hex-elastic. Then define Environment Variable ELASTH_PATH and add it at the end of **.bashrc** file. Therefore you will able to call hex-elastic’s programs from each Directory.

Call Package

1_ Make struct file and we recommend then run "sgroupcheck_lapw".

2_ Do initialization (run "instgen_lapw" and "init_lapw" in Terminal).
It is not necessary to do step 2. This program can do that.

3_ If you want to do Spin-Orbit calculations run "command_initso_lapw" in Terminal.

4_ If you want to do LDA+U calculations run "command_initu_lapw" and then "auto_initu_lapw" in Terminal.

NOTE ABOUT STEPS 3 AND 4

After using distortion for calculation C11-C12 and C55, the symmetry of hexagonal compounds changes and maybe Number of atoms change. So when you run "command_initso_lapw" or "command_initu_lapw" ,in section name of atom, type "all name of atom" (e.g. all Mn). With this command, you use SO or LDA+U calculations for example for all Mn atoms.

5_ Run "H_set_elast_lapw" in Terminal.

6_Now you must modify job files according to your needs (you can run "H_modifyjob_lapw" in Terminal).

7_ Now you must run job files (you can run "H_calljob_lapw" in Terminal). It will take time.

Note 1: When you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials) **call “command_init_lapw”** and after that choose "answscf=no" in **“HEX.job”** files and a new "savename" (eg. "_use_pbe_rk8").

8_ Run "H_ana_elast_lapw" in Terminal.

Optionally you can specify more cases by rerunning "**H_setupcXX" (XX=11, 12,22,.. see Suppose section)**. Specify also your **''old'' cases**. The old results will then be taken automatically into account without recalculation (unless you modify **job** files i.e: set answscf=no).

NOTE ABOUT PROGRAMS

H_set_elast_lapw : makes elast-constant directory in present work directory (PWD) and c11+c11, c11-c12, c33, c55, and czz directories in elast-constant directory. Moreover H_set_elast_lapw program copies information of "PWD" in c11+c12, c11-c12, c33, c55, and czz directories and calls "command_init_lapw", H_setupc1112, H_setupc11m12, H_setupc33, H_setupc55, and H_setupczz programs.

H_modifyjob_lapw : Edits job files for modifying them according to your needs.

H_calljob_lapw : calls job files for running.

H_ana_elast_lapw : calls H_ana_elastc_lapw programs for calculation elastic constants **and makes an output file in elast-constant directory with name case.output_elastic.**

Moreover H_ana_elastc_lapw. makes an output with name ELC.output with in present work directory.

H_ana_elastorder_lapw : THIS PROGRAM CHECK THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT (This program saves these data in the **output-order** file in the elast-constant directory.). You can run it in the elats-constant directory. Moreover H_ana_elast_lapw calls H_ana_elastorder_lapw at the end of calculations.

TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

Moreover this program predicts **Bulk modulus** of your compound by using elastic constant values.

command_init_lapw : gets informations for making "auto_init_lapw".

sgroupcheck_lapw : finds best value of tol in sgroup program and copies case.struct_sgroup as case.struct.

Suppose

Suppose we only want to calculate c33.

We do these stages as following:

1) Make a directory for example c33.
2) Make "case" directory in c33 directory.
3) Make "case.struct" file in "case" directory and copy it as "init.struct".
Moreover make "pwdname" file and write in it "**case.**" and save it.
4) Run instgen_lapw **(It is not necessary. This program can do that.)**
5) Run command_init_lapw
6) For SO calculations, run command_initso_lapw.
7) For LDA+U calculations, run command_initu_lapw and auto_initu_lapw.
8) Run H_setupc33 program.
9) chmod +x HEX.job file.
10) Modify HEX.job file.
11) Call HEX.job
12) Call H_ana_elastc_lapw

Suppose we want to rerun czz with more data points.

We do these stages as following:

1) cd "elast-constant" directory.
2) cd "czz" directory.
3) cd "case" directory.
4) Run H_setupczz program.
5) If you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials) **call "command_init_lapw"** and after that choose "answscf=no" in **"HEX.job"** files and a new "savename" (eg. "_use_pbe_rk8").
6) Modify HEX.job file.
7) Call HEX.job
8) Call H_ana_elastc_lapw

_____
IMPORTANT NOTE

For calculation best values of elastic constants, please find EOS and then copy case.outputeos in "case" directory within c11+c11, c11-c12, c33, c55, and czz directories. **Otherwise this program set an arbitrary number for optimized volume (Vopt=999).**

Converged check

Since this package computes elastic constants by using second-order derivative (E”(ϵ)) of Polynomial fit (E=E(ϵ)) of Energy vs. Strains (ϵ) at zero strain (ϵ=0). So, you must use values of strain around zero and **from the viewpoint of fit convergence,** we usually expect to see a minimum when we plot Energy vs. strain (this Package plots it). Moreover I recommend to check the sensitivity of the results to the order of fit. This program shows them. You can see in the example.

We recommend to use more data-points, more k-points and larger RKmax for all calculations to reduce numerical noise.
TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

EXAMPLE

Calculation elastic-constants for Ti
You can find ti.struct and ti.outputeos in example-elastic directory of this package.

```
Ti
H   LATTICE,NONEQUIV.ATOMS:  1 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  5.574694  5.574694  8.843922 90.000000 90.000000120.000000
ATOM  -1: X=0.33333333 Y=0.66666665 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -1: X=0.66666667 Y=0.33333335 Z=0.25000000
Ti1        NPT=  781  R0=0.00005000 RMT=    2.4000   Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
```

Select Xc = PBE-GGA, R_Kmax = 7, L_max = 8, and nkpoint = 5000

Two dimensional of Equation Of State for ti by using 2Doptimize package.

```
Equation of state: EOS2 (PRB52,8064)        info           2
 a,b,c,d     -3413.342702        15.961321      -415.631334
1506.627412
 V0,B(GPa),BP,E0       234.6370       116.1081         3.7701

 Equation of state: Murnaghan                info           2
```

```
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0       234.6314       115.7348         3.7979      -
3415.259330
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
     214.2200    -3415.251234     0.000003     0.000003         12.583
     226.1212    -3415.258025    -0.000014    -0.000015          4.590
     238.0223    -3415.259167     0.000023     0.000026         -1.616
     249.9234    -3415.255761    -0.000017    -0.000020         -6.497
     261.8245    -3415.248898     0.000005     0.000006        -10.380
                  Sigma:          0.000014     0.000016

 Equation of state: Birch-Murnaghan                 info           2
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       234.6386       116.1166         3.7650      -
3415.259333
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
     214.2200    -3415.251234     0.000003               12.545
     226.1212    -3415.258025    -0.000013                4.603
     238.0223    -3415.259167     0.000023               -1.618
     249.9234    -3415.255761    -0.000017               -6.506
     261.8245    -3415.248898     0.000005              -10.353
                  Sigma:          0.000014
```

After running job files, you will find the below values for ELAST-CONSTANTS of Ti (**do not forget to copy ti.outputeos in "ti" directory within c11+c12, c11-c12, c33, c55, and czz directories**).

In the following examples you can find which percents I used for Strains.

```
########################################
#  H_ana_elast_lapw analyses Elastic  #
#            constant                #
#     C(2012) by Morteza Jamal       #
#           Ali H. Reshak            #
########################################

##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#             Ali H. Reshak              #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                  HEX.job               #
##########################################
-0.020000    -3415.258474
-0.010000    -3415.259248
 0.000000    -3415.259145
```

```
 0.010000    -3415.258204
 0.020000    -3415.256548
 ================================================================
Order of fit:  2 C11+C12 is:    255.0521 GPa, RMS: 0.231016E-04
Order of fit:  3 C11+C12 is:    255.0521 GPa, RMS: 0.440928E-05
Order of fit:  4 C11+C12 is:    264.5953 GPa, RMS: 0.352246E-12
 ****************************************
 Polynomial fit for C11+C12 done
A RMS of 0.231016E-04 was achieved using a polynome of degree :  2

At volume=  234.6314 bohr^3
 C11+C12 is:   0.017338 a.u or    255.0521 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#             Ali H. Reshak              #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                  HEX.job               #
##########################################
-0.020000    -3415.259032
-0.010000    -3415.259254
 0.000000    -3415.259145
 0.010000    -3415.258751
 0.020000    -3415.258066
 ================================================================
Order of fit:  2 C33 is:    187.8748 GPa, RMS: 0.622939E-05
Order of fit:  3 C33 is:    187.8748 GPa, RMS: 0.279662E-05
Order of fit:  4 C33 is:    175.7690 GPa, RMS: 0.203369E-12
 ****************************************
 Polynomial fit for C33 done
A RMS of 0.622939E-05 was achieved using a polynome of degree :  2

At volume=  234.6314 bohr^3
 C33 is:   0.012771 a.u or    187.8748 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
```

```
#             Ali H. Reshak              #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                  HEX.job               #
########################################
-0.020000    -3415.258881
-0.010000    -3415.259081
 0.000000    -3415.259145
 0.010000    -3415.259122
 0.020000    -3415.258927
 ============================================================
Order of fit:  2 Czz is:    353.0051 GPa, RMS: 0.899789E-05
Order of fit:  3 Czz is:    353.0051 GPa, RMS: 0.735610E-05
Order of fit:  4 Czz is:    209.7144 GPa, RMS: 0.287607E-12
 ****************************************
 Polynomial fit for Czz done
A RMS of 0.899789E-05 was achieved using a polynome of degree :  2

At volume=  234.6314 bohr^3
 Czz is:   0.023997 a.u or    353.0051 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

########################################
# H_ana_elastc_lapw analyses Elastic   #
#              constant                #
#       C(2012) by Morteza Jamal       #
#             Ali H. Reshak            #
#     using case.outputeos             #
#                          VstVene     #
#    which have been created by        #
#                  HEX.job             #
########################################
-0.020000    -3415.258482
-0.010000    -3415.259013
 0.000000    -3415.259145
 0.010000    -3415.258962
 0.020000    -3415.258437
 ============================================================
Order of fit:  2 C11-C12 is:    108.6240 GPa, RMS: 0.990173E-05
Order of fit:  3 C11-C12 is:    108.6240 GPa, RMS: 0.600696E-05
Order of fit:  4 C11-C12 is:     95.6228 GPa, RMS: 0.909495E-12
 ****************************************
 Polynomial fit for C11-C12 done
A RMS of 0.990173E-05 was achieved using a polynome of degree :  2

At volume=  234.6314 bohr^3
 C11-C12 is:   0.007384 a.u or    108.6240 GPa
 ****************************************

 Analyze done.....
```

```
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#             Ali H. Reshak              #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                  HEX.job               #
##########################################
-0.020000    -3415.273202
-0.010000    -3415.273652
 0.000000    -3415.273743
 0.010000    -3415.273652
 0.020000    -3415.273202
 ============================================================
Order of fit:  2 C55 is:     44.3437 GPa, RMS: 0.187853E-04
Order of fit:  3 C55 is:     44.3437 GPa, RMS: 0.187853E-04
Order of fit:  4 C55 is:     24.0148 GPa, RMS: 0.406738E-12
 ****************************************
 Polynomial fit for C55 done
A RMS of 0.187853E-04 was achieved using a polynome of degree :  2

At volume=  234.6314 bohr^3
 C55 is:   0.003014 a.u or     44.3437 GPa
 ****************************************


 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************
Printing final Elastic constant At voulme= 234.6314 bohr^3 .
==========================================================================
C11+C12 = 255.0521 GPa      C11-C12 = 108.6240 GPa
C33 = 187.8748 GPa            C55 = 44.3437 GPa
Czz = C11+C12+2C33-4C13 = 353.0051 GPa
==========================================================================
C11 = 181.8380 GPa                              C12 = 73.2140 GPa
                    C13 = 69.4491 GPa
C33 = 187.8748 GPa                              C55 = 44.3437 GPa
==========================================================================

Press enter key to continue....

################################################
# H_ana_elastorder_lapw analyses Elastic     #
#               constant                     #
#         C(2012) by Morteza Jamal           #
#               Ali H. Reshak                #
#             ELCorder.fit files             #
################################################
```

```
CHECK THE SENSITIVITY
      OF YOUR RESULT TO THE ORDER OF FIT

 Press enter key to continue....
 Order of fit for calculations were 4,4,4,4 and 4
 We select minimum value for ORDER OF FIT i.e. 4

 Press enter key to continue....
######## ORDER OF FIT IS :  2 , At volume = 234.6314 (bohr^3) ########
(c11-c12) = 108.624 (GPa)
(c11+c12) = 255.052 (GPa)
(c33) = 187.875 (GPa)
(c55) = 44.344 (GPa)
(czz=c11+c12+2c33-4c13) = 353.005 (GPa)
_____________________________________________
c11 = 181.838 (GPa)
c12 = 73.214 (GPa)
c13 = 69.449 (GPa)
c33 = 187.875 (GPa)
C55 = 44.344 (GPa)
==========================================================================
Prediction Bulk modulus by using elastic constant values = 108.419
(GPa)
==========================================================================
######## ORDER OF FIT IS :  3 , At volume = 234.6314 (bohr^3) ########
(c11-c12) = 108.624 (GPa)
(c11+c12) = 255.052 (GPa)
(c33) = 187.875 (GPa)
(c55) = 44.344 (GPa)
(czz=c11+c12+2c33-4c13) = 353.005 (GPa)
_____________________________________________
c11 = 181.838 (GPa)
c12 = 73.214 (GPa)
c13 = 69.449 (GPa)
c33 = 187.875 (GPa)
C55 = 44.344 (GPa)
==========================================================================
Prediction Bulk modulus by using elastic constant values = 108.419
(GPa)
==========================================================================
######## ORDER OF FIT IS :  4 , At volume = 234.6314 (bohr^3) ########
(c11-c12) = 95.623 (GPa)
(c11+c12) = 264.595 (GPa)
(c33) = 175.769 (GPa)
(c55) = 24.015 (GPa)
(czz=c11+c12+2c33-4c13) = 209.714 (GPa)
_____________________________________________
c11 = 180.109 (GPa)
c12 = 84.486 (GPa)
c13 = 101.604 (GPa)
c33 = 175.769 (GPa)
C55 = 24.015 (GPa)
==========================================================================
Prediction Bulk modulus by using elastic constant values = 123.486
(GPa)
==========================================================================
```

```
 You can find these data in the output-order file.
```

C11 = 182 GPa
C12 = 73 GPa
C13 = 69 GPa
C33 = 188 GPa
C55 = 44 GPa

	Our calculation	Other(TB)[1]	Exp[1]
C11	182	171	**160**
C12	73	58	**90**
C13	69	46	**60**
C33	188	203	**181**
C55	44	64	**47**

1) Michael J. Mehl and Dimitrios A. Papaconstantopoulos, PRB, 54, 1996.

Calculation c55 for Zr

```
Zr
H   LATTICE,NONEQUIV.ATOMS:  1194_P63/mmc
MODE OF CALC=RELA unit=bohr
  6.103818  6.103818  9.732094 90.000000 90.000000120.000000
ATOM  -1: X=0.33333334 Y=0.66666666 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -1: X=0.66666666 Y=0.33333334 Z=0.25000000
Zr         NPT=  781  R0=0.00001000 RMT=    2.6100   Z: 40.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24      NUMBER OF SYMMETRY OPERATIONS
```

Select Xc = PBE-GGA, R_Kmax = 7, L_max = 8, and nkpoint = 5000

```
Equation of state: EOS2 (PRB52,8064)        info           2
 a,b,c,d    -14388.300165      -113.741152       358.136832
132.514877
 V0,B(GPa),BP,E0       315.9043        92.8772         3.0467

 Equation of state: Murnaghan                info           7
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0       315.9113        92.6950         3.0216     -
14396.860209
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
     282.6068   -14396.847343     0.000002     0.000002         12.277
     298.3072   -14396.856860    -0.000007    -0.000008          5.803
```

```
     314.0075   -14396.860187     0.000012     0.000014          0.565
     329.7079   -14396.858405    -0.000009    -0.000010         -3.717
     345.4083   -14396.852503     0.000002     0.000003         -7.252
                  Sigma:          0.000007     0.000009

 Equation of state: Birch-Murnaghan               info           2
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       315.9004        93.0062         3.0637     -
14396.860213
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
     282.6068   -14396.847343     0.000001               12.245
     298.3072   -14396.856860    -0.000006                5.814
     314.0075   -14396.860187     0.000010                0.564
     329.7079   -14396.858405    -0.000007               -3.725
     345.4083   -14396.852503     0.000002               -7.230
                  Sigma:          0.000006

##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#             Ali. H. Reshak             #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                 HEX.job                #
##########################################
-0.020000   -14396.847677
-0.010000   -14396.848054
 0.000000   -14396.848175
 0.010000   -14396.848054
 0.020000   -14396.847677
 ================================================================
Order of fit:  2 C55 is:     29.1095 GPa, RMS: 0.129515E-05
Order of fit:  3 C55 is:     29.1095 GPa, RMS: 0.129515E-05
Order of fit:  4 C55 is:     28.0685 GPa, RMS: 0.000000E+00
 ****************************************
 Polynomial fit for C55 done
A RMS of 0.129515E-05 was achieved using a polynome of degree :  2

At volume=  315.9113 bohr^3
 C55 is:   0.001979 a.u or     29.1095 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************
```

	Our calculation	Other(TB)[1]	Exp[1]
C55	29	4	**33**

Calculation c55 for Ru

```
Ru
H   LATTICE,NONEQUIV.ATOMS:  1194_P63/mmc
MODE OF CALC=RELA unit=bohr
  5.121160  5.121160  8.088032 90.000000 90.000000120.000000
ATOM  -1: X=0.33333334 Y=0.66666666 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -1: X=0.66666666 Y=0.33333334 Z=0.25000000
Ru         NPT=  781  R0=0.00001000 RMT=    2.1500   Z: 44.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24      NUMBER OF SYMMETRY OPERATIONS
```

Select Xc = PBE-GGA, R_Kmax = 7, L_max = 8, and nkpoint = 5000

```
Equation of state: EOS2 (PRB52,8064)        info           2
 a,b,c,d    -18152.897773       533.739265     -3605.591959
7927.895698
 V0,B(GPa),BP,E0       187.0436       295.4639         5.5060

 Equation of state: Murnaghan                info           2
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0       187.0684       292.8903         5.3274     -
18127.426080
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
     165.3304   -18127.393108    -0.000034    -0.000026         51.190
     174.5154   -18127.416464     0.000150     0.000125         24.619
     183.7004   -18127.425227    -0.000249    -0.000226          5.587
     192.8854   -18127.424569     0.000183     0.000178         -8.276
     202.0705   -18127.415810    -0.000050    -0.000052        -18.527
                  Sigma:          0.000156     0.000143

 Equation of state: Birch-Murnaghan                info           2
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       187.0508       294.6235         5.4552     -
18127.426094
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
     165.3304   -18127.393108    -0.000031              50.922
     174.5154   -18127.416464     0.000142              24.694
     183.7004   -18127.425227    -0.000242               5.594
     192.8854   -18127.424569     0.000182              -8.322
     202.0705   -18127.415810    -0.000051             -18.433
                  Sigma:          0.000152
```

```
##########################################
# H_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#             Ali. H. Reshak             #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                  HEX.job               #
##########################################
-0.020000   -18127.371302
-0.010000   -18127.372798
 0.000000   -18127.373148
 0.010000   -18127.372798
 0.020000   -18127.371302
 ================================================================
Order of fit:  2 C55 is:    187.7497 GPa, RMS: 0.480220E-04
Order of fit:  3 C55 is:    187.7497 GPa, RMS: 0.480220E-04
Order of fit:  4 C55 is:    122.5682 GPa, RMS: 0.230086E-11
 ****************************************
 Polynomial fit for C55 done
A RMS of 0.480220E-04 was achieved using a polynome of degree :  2

At volume=  187.0684 bohr^3
 C55 is:   0.012763 a.u or    187.7497 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************
```

	Our calculation	Other(TB)[1]	Exp[1]
C55	188	214	181

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