
Elastic constants calculation for α -Pt₂Si step by step

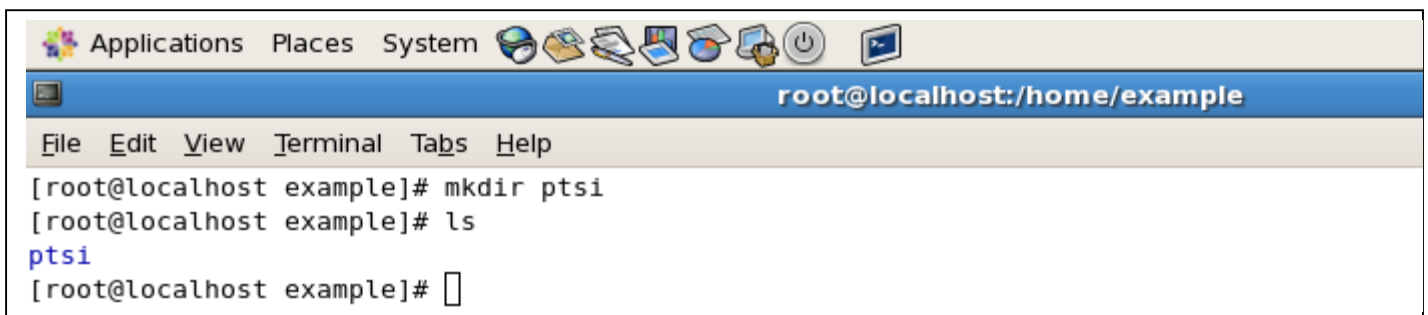
Morteza Jamal
(09.02.2013)

α -Pt₂Si compound is a test case for elastic constants calculation. It has tetragonal symmetry with space group I4/mmm with number 139. The α -Pt₂Si structure (**PtSi.struct**) is described in detail in the following:

```
alpha Pt2Si
B LATTICE,NONEQUIV.ATOMS: 2139_I4/mmm
MODE OF CALC=RELA unit=bohr
 7.461000 7.461000 11.268000 90.000000 90.000000 90.000000
ATOM -1: X=0.00000000 Y=0.50000000 Z=0.25000000
      MULT= 2 ISPLIT=-2
      -1: X=0.00000000 Y=0.50000000 Z=0.75000000
Pt      NPT= 781 R0=0.00000500 RMT= 2.4100 Z: 78.0
LOCAL ROT MATRIX: 0.7071068-0.7071068 0.0000000
                  0.7071068 0.7071068 0.0000000
                  0.0000000 0.0000000 1.0000000
ATOM -2: X=0.00000000 Y=0.00000000 Z=0.00000000
      MULT= 1 ISPLIT=-2
Si      NPT= 781 R0=0.00010000 RMT= 2.1300 Z: 14.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                  0.0000000 1.0000000 0.0000000
                  0.0000000 0.0000000 1.0000000
16      NUMBER OF SYMMETRY OPERATIONS
```

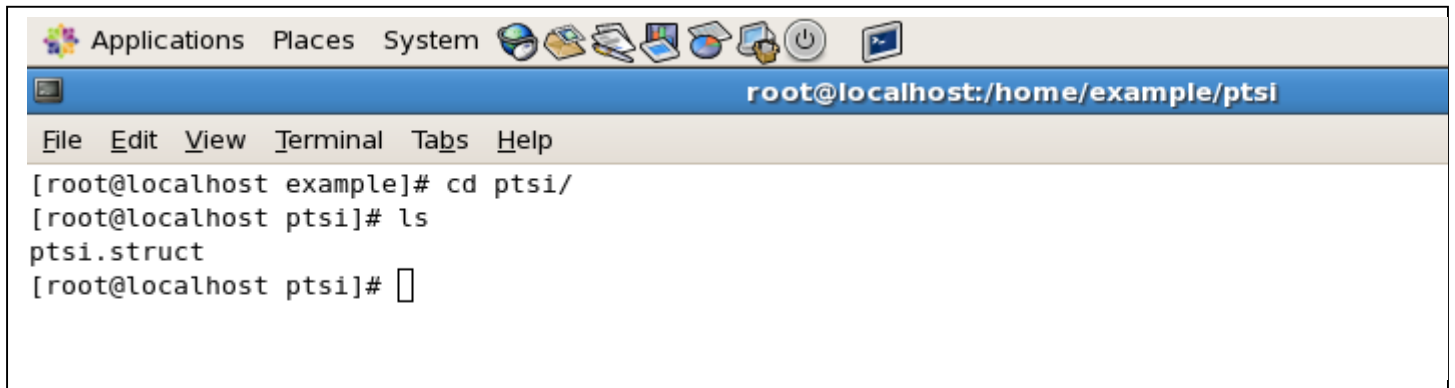
You can find it from example directory.

- Make a directory with name **ptsi** .



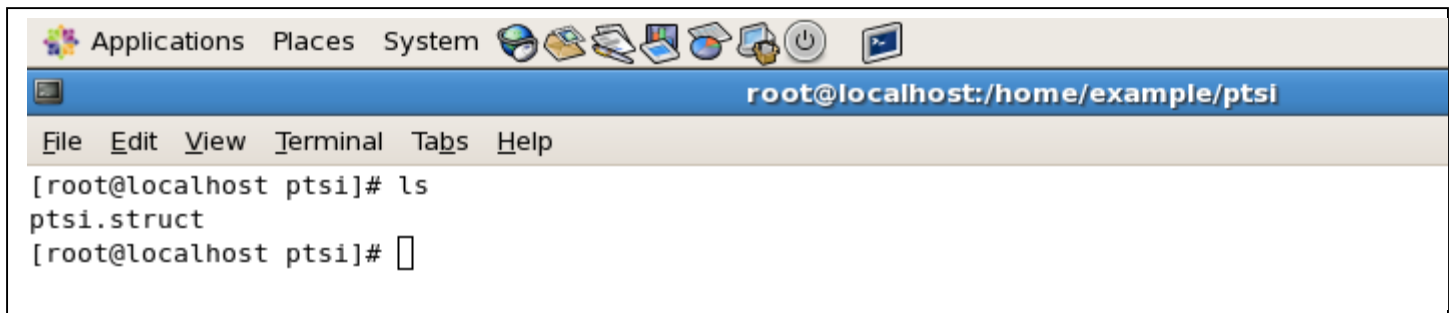
```
Applications Places System [network icons] [power icon] [terminal icon]
root@localhost:/home/example
File Edit View Terminal Tabs Help
[root@localhost example]# mkdir ptsi
[root@localhost example]# ls
ptsi
[root@localhost example]#
```

- Change to **ptsi** directory and copy **ptsi.struct** within it from example directory.



A terminal window with a blue title bar containing the text "root@localhost:/home/example/ptsi". The menu bar includes "File", "Edit", "View", "Terminal", "Tabs", and "Help". The terminal content shows the following commands and output:

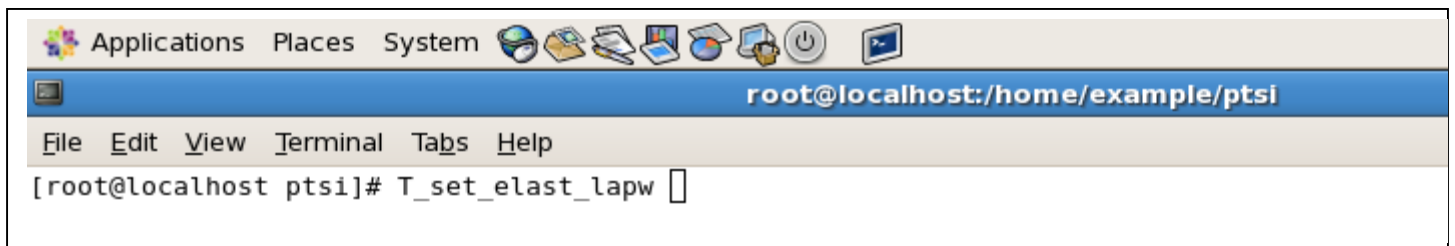
```
[root@localhost example]# cd ptsi/  
[root@localhost ptsi]# ls  
ptsi.struct  
[root@localhost ptsi]#
```



A terminal window with a blue title bar containing the text "root@localhost:/home/example/ptsi". The menu bar includes "File", "Edit", "View", "Terminal", "Tabs", and "Help". The terminal content shows the following commands and output:

```
[root@localhost ptsi]# ls  
ptsi.struct  
[root@localhost ptsi]#
```

➤ Run `T_set_elast_lapw`



A terminal window with a blue title bar containing the text "root@localhost:/home/example/ptsi". The menu bar includes "File", "Edit", "View", "Terminal", "Tabs", and "Help". The terminal content shows the following command and output:

```
[root@localhost ptsi]# T_set_elast_lapw
```

➤ I selected the following parameters for calculation :

RMT reduction = default (RMT not changed), Xc = default (PBE), Energy separation = -9.0, R_Kmax = 7, L_max = 8, Type of Fermi calculation = default (TETRA), mixing factor = default (0.2), nkpoint = 5000, and Spin-polarized calculation = default (no).

```
Applications Places System [icons]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help

#####
#      C(2009) by Morteza Jamal      #
#      Making auto_init_lapw      #
#####

#####
Start for making COMMAND for Initialization
#####

---->RMT reduction by X % (default: RMT not changed):

  recommended: 13: GGA (Perdew-Burke-Ernzerhof 96)
                 5: LSDA
                 11: GGA (Wu-Cohen 2006)
                 19: PBEsol-GGA (Perdew etal. 2008)
---->VXC option (default: 13 = PBE ):

---->Energy separation between core/valence (default: -6.0 Ry): -9.0

---->RKMAX (default: 7.0, not changed):

To avoid Gibbs Like Oscilation select LMAX~RKMAX
---->LMAX (default: 8.0):


(GAUSS,ROOT,TEMP,TETRA)
---->Type of Fermi calculation (default: TETRA):

---->Select mixing factor (default: 0.2, not changed):

---->Number of k-points in full BZ (default: 3000): 5000

---->Spin-polarized calculation (default: no)(y/n): n
```

➤ Define **command run**

```
Applications Places System 
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help

#####
#      C(2009) by Morteza Jamal      #
#      Making auto_init_lapw      #
#####

#####
Start for making COMMAND for Initialization
#####

---->RMT reduction by X % (default: RMT not changed):

recommended: 13: GGA (Perdew-Burke-Ernzerhof 96)
              5: LSDA
              11: GGA (Wu-Cohen 2006)
              19: PBEsol-GGA (Perdew etal. 2008)
---->VXC option (default: 13 = PBE ):

---->Energy separation between core/valence (default: -6.0 Ry): -9.0

---->RKMAX (default: 7.0, not changed):


To avoid Gibbs Like Oscilation select LMAX~RKMAX
---->LMAX (default: 8.0):


(GAUSS,ROOT,TEMP,TETRA)
---->Type of Fermi calculation (default: TETRA):

---->Select mixing factor (default: 0.2, not changed):

---->Number of k-points in full BZ (default: 3000): 5000

---->Spin-polarized calculation (default: no)(y/n): n

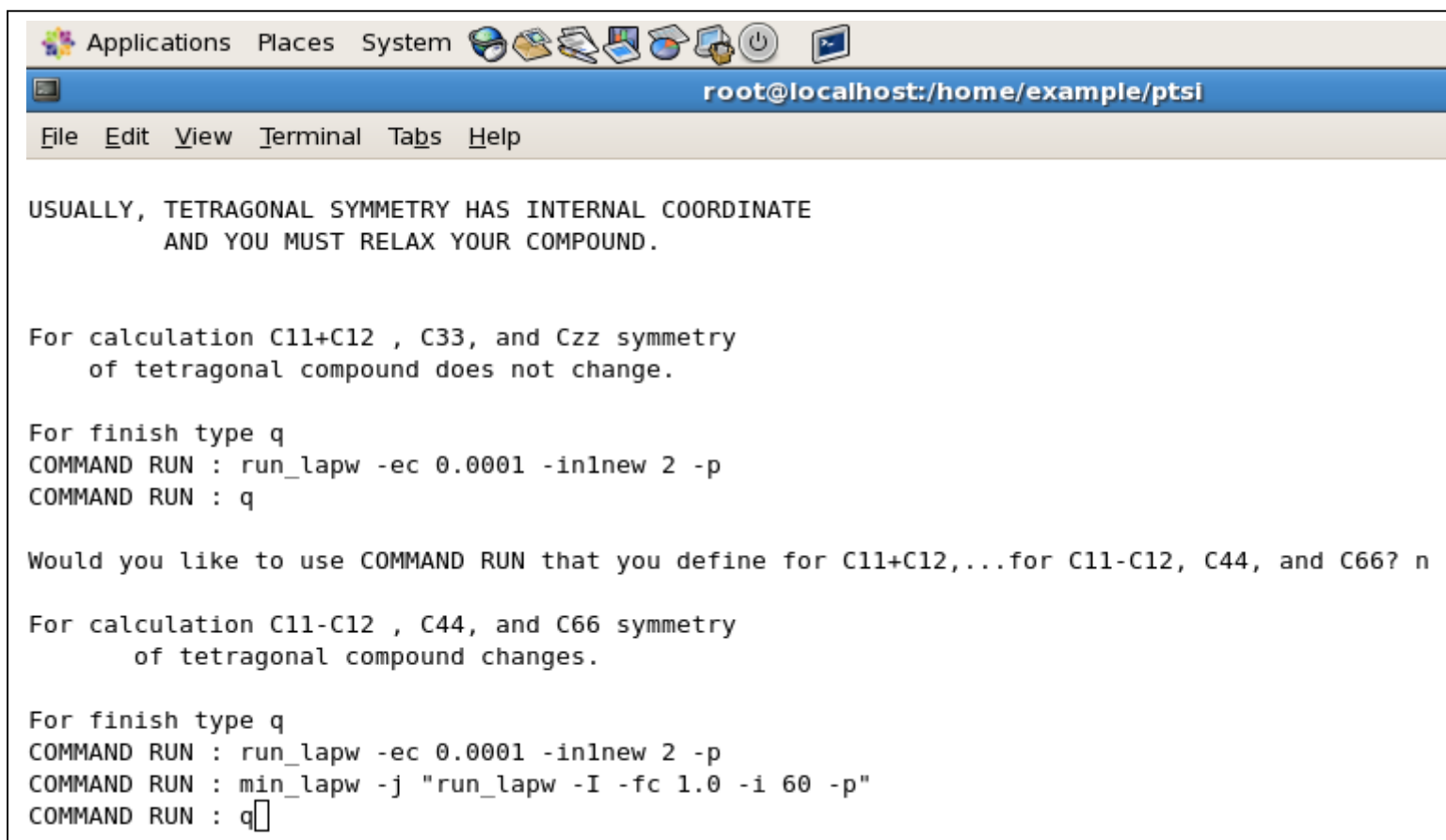
Would you like to define COMMAND RUN here?(Y/n) y 
```

```
Applications Places System 
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help

USUALLY, TETRAGONAL SYMMETRY HAS INTERNAL COORDINATE
AND YOU MUST RELAX YOUR COMPOUND.

For calculation C11+C12 , C33, and Czz symmetry
of tetragonal compound does not change.

For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -inlnew 2 -p
COMMAND RUN : q
```



The image shows a terminal window with a standard Linux desktop environment. The title bar indicates the user is root at localhost in the directory /home/example/ptsi. The terminal content consists of several paragraphs of text and command-line interactions. The first paragraph states that tetragonal symmetry has internal coordinates and that the compound must be relaxed. The second paragraph explains that for calculations with C11+C12, C33, and Czz symmetry, the tetragonal symmetry of the compound does not change. The user is then prompted to finish by typing 'q', and the terminal shows the execution of 'run_lapw -ec 0.0001 -inlnew 2 -p' followed by 'q'. The third paragraph asks if the user wants to use a specific command for C11-C12, C44, and C66, with a trailing 'n' on the line. The fourth paragraph explains that for calculations with C11-C12, C44, and C66 symmetry, the tetragonal symmetry of the compound changes. The user is again prompted to finish by typing 'q', and the terminal shows the execution of 'run_lapw -ec 0.0001 -inlnew 2 -p', 'min_lapw -j "run_lapw -I -fc 1.0 -i 60 -p"', and finally 'q' with a cursor.

```
Applications Places System [icons] [power] [terminal]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help

USUALLY, TETRAGONAL SYMMETRY HAS INTERNAL COORDINATE
AND YOU MUST RELAX YOUR COMPOUND.

For calculation C11+C12 , C33, and Czz symmetry
of tetragonal compound does not change.

For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -inlnew 2 -p
COMMAND RUN : q

Would you like to use COMMAND RUN that you define for C11-C12,...for C11-C12, C44, and C66? n

For calculation C11-C12 , C44, and C66 symmetry
of tetragonal compound changes.

For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -inlnew 2 -p
COMMAND RUN : min_lapw -j "run_lapw -I -fc 1.0 -i 60 -p"
COMMAND RUN : q
```

Now, we see

```
Applications Places System [icons] [power] [terminal]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help

For calculation C11-C12 , C44, and C66 symmetry
of tetragonal compound changes.

For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -inlnew 2 -p
COMMAND RUN : min_lapw -j "run_lapw -I -fc 1.0 -i 60 -p"
COMMAND RUN : q

#####
Please wait. I am making c11+c12 Directory and copying information in c11+c12 for running
#####

#####
Please wait. I am making c33 Directory and copying information in c33 for running
#####

#####
Please wait. I am making czz Directory and copying information in czz for running
#####

#####
Please wait. I am making c11-c12 Directory and copying information in c11-c12 for running
#####

#####
Please wait. I am making c44 Directory and copying information in c44 for running
#####

#####
Please wait. I am making c66 Directory and copying information in c66 for running
#####
```

- I didn't use default parameters for (C11+C12) calculations. I selected number of changes 6 and value of changes -2, -1, 0, 1, 2, 3.

File Edit View Terminal Tabs Help

```
*****
** Setup for ELASTIC constant calculations**
**      TETRAGONAL SYMMETRY      **
**                               **
**      Start to calculation C11+C12  **
**      by distortion matrices D1    **
**-----**
**      D1 does not change          **
**      the symmetry of the lattice  **
*****
```

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Ali. H. Reshak

```
*****
** Setup for ELASTIC constant calculations**
**      TETRAGONAL SYMMETRY      **
*****
```

Do you want to use default parameters ?(y/n)
(-2%, -1%, 0, 1%, 2%)

n

Number of changes?

6

***** 0.0 value MUST be calculated for analysis *****

Enter value 1 in %

-2

Enter value 2 in %

-1

Enter value 3 in %

0

Enter value 4 in %

1

Enter value 5 in %

2

Enter value 6 in %

3

```
Applications Places System [icons]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
*****
Do you want to use default parameters ?(y/n)
(-2%, -1%, 0, 1%, 2%)
n
Number of changes?
6
***** 0.0 value MUST be calculated for analysis *****

Enter value          1 in %
-2
Enter value          2 in %
-1
Enter value          3 in %
0
Enter value          4 in %
1
Enter value          5 in %
2
Enter value          6 in %
3

Styp1_-2.0.struct
Styp1_-1.0.struct
Styp1_0.0.struct
Styp1_1.0.struct
Styp1_2.0.struct
Styp1_3.0.struct

        6 struct files generated.

Now TETRA.job file is ready.

Please modify running command in job file
according to your needs and then run it.
```

- I didn't use default parameters for (C33) calculations. I selected number of changes 7 and value of changes -2, -1, 0, 1, 2, 3, 4.

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```
*****  
** Setup for ELASTIC constant calculations**  
**      TETRAGONAL SYMMETRY      **  
**                               **  
**      Start to calculation C33   **  
**      by distortion matrices D3  **  
**-----**  
**      D3 does not change        **  
**      the symmetry of the lattice **  
*****
```

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Ali. H. Reshak







```
*****  
** Setup for ELASTIC constant calculations**  
**      TETRAGONAL SYMMETRY      **  
*****
```

Do you want to use default parameters ?(y/n)
(-2%, -1%, 0, 1%, 2%)

n
Number of changes?
7

***** 0.0 value MUST be calculated for analysis *****

Enter value 1 in %
-2
Enter value 2 in %
-1
Enter value 3 in %
0
Enter value 4 in %
1
Enter value 5 in %
2
Enter value 6 in %

```
Applications Places System      
root@localhost:/home/example/ptsi/elastic-constant/c33/pts
File Edit View Terminal Tabs Help
Do you want to use default parameters?(y/n)
(-2%, -1%, 0, 1%, 2%)
n
Number of changes?
7
***** 0.0 value MUST be calculated for analysis *****

Enter value          1 in %
-2
Enter value          2 in %
-1
Enter value          3 in %
0
Enter value          4 in %
1
Enter value          5 in %
2
Enter value          6 in %
3
Enter value          7 in %
4

Styp3_-2.0.struct
Styp3_-1.0.struct
Styp3__0.0.struct
Styp3__1.0.struct
Styp3__2.0.struct
Styp3__3.0.struct
Styp3__4.0.struct

          7 struct files generated.

Now TETRA.job file is ready.

Please modify running command in job file
according to your needs and then run it.
```

➤ I used default parameters for (Czz) calculations.

```
#####  
Setup information for (Czz) elastic constant calculations  
#####
```

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```
*****  
** Setup for ELASTIC constant calculations**  
**      TETRAGONAL SYMMETRY          **  
**                                     **  
**      Start to calculation Czz      **  
**      by distortion matrices D5     **  
**-----**  
**      D5 is volume conserved and keeps **  
**      the symmetry of the lattice    **  
*****
```

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```
*****  
** Setup for ELASTIC constant calculations**  
**      TETRAGONAL SYMMETRY          **  
*****
```

Do you want to use default parameters ?(y/n)
(-2%, -1%, 0, 1%, 2%)

y

```
Applications Places System [Icons] [Power] [Terminal Icon]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
(C) 2012 by Morteza Jamal
*****
** Setup for ELASTIC constant calculations**
**      TETRAGONAL SYMMETRY          **
**                                  **
**      Start to calculation Czz      **
**      by distortion matrices D5     **
**-----**
**      D5 is volume conserved and keeps **
**      the symmetry of the lattice     **
*****

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      Ali. H. Reshak
*****
** Setup for ELASTIC constant calculations**
**      TETRAGONAL SYMMETRY          **
*****

Do you want to use default parameters ?(y/n)
(-2%, -1%, 0, 1%, 2%)
y

Styp5_-2.0.struct
Styp5_-1.0.struct
Styp5_0.0.struct
Styp5_1.0.struct
Styp5_2.0.struct

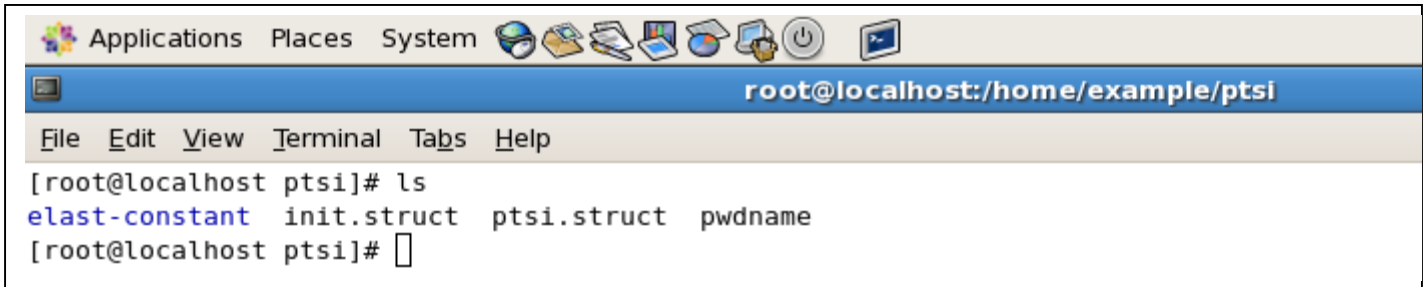
      5 struct files generated.

Now TETRA.job file is ready.

Please modify running command in job file
according to your needs and then run it.
```

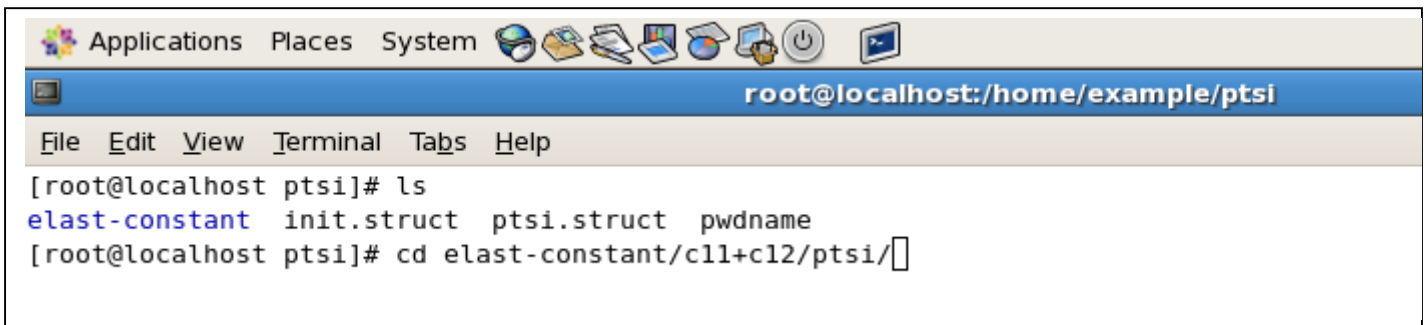
- I used default parameters for (C44), (C11-C12), and (C66) calculations. I did the same producer such as above pictures .

Now, if we get a list we will see a directory with name **elast-constant**

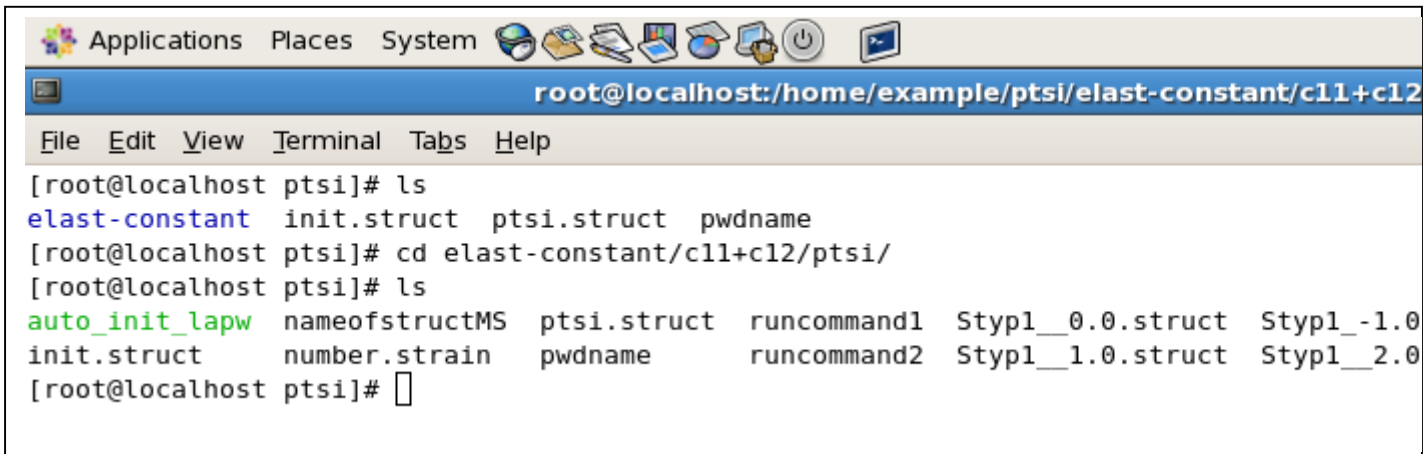


```
Applications Places System [Icons] [Power] [Terminal]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ls
elast-constant  init.struct  ptsi.struct  pwdname
[root@localhost ptsi]#
```

- Now, we have to run created **TETRA.job** file. You can use **T_calljob_lapw** but, I prefer to run them by hand because I want to check steps of running by WIEN2k. For this goal, I change to **elast-constant** directory and then to **c11+c12** and **ptsi**.



```
Applications Places System [Icons] [Power] [Terminal]
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ls
elast-constant  init.struct  ptsi.struct  pwdname
[root@localhost ptsi]# cd elast-constant/c11+c12/ptsi/
```



```
Applications Places System [Icons] [Power] [Terminal]
root@localhost:/home/example/ptsi/elast-constant/c11+c12
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ls
elast-constant  init.struct  ptsi.struct  pwdname
[root@localhost ptsi]# cd elast-constant/c11+c12/ptsi/
[root@localhost ptsi]# ls
auto_init_lapw  nameofstructMS  ptsi.struct  runcommand1  Styp1__0.0.struct  Styp1__-1.0
init.struct     number.strain   pwdname      runcommand2  Styp1__1.0.struct  Styp1__2.0
[root@localhost ptsi]#
```

- Now, I call **TETRA.job** and calculations start. It will take time.

```
Applications Places System [system icons]
root@localhost:/home/example/ptsi/elastic-constant/c11+c1
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ./TETRA.job
```

Now, we see

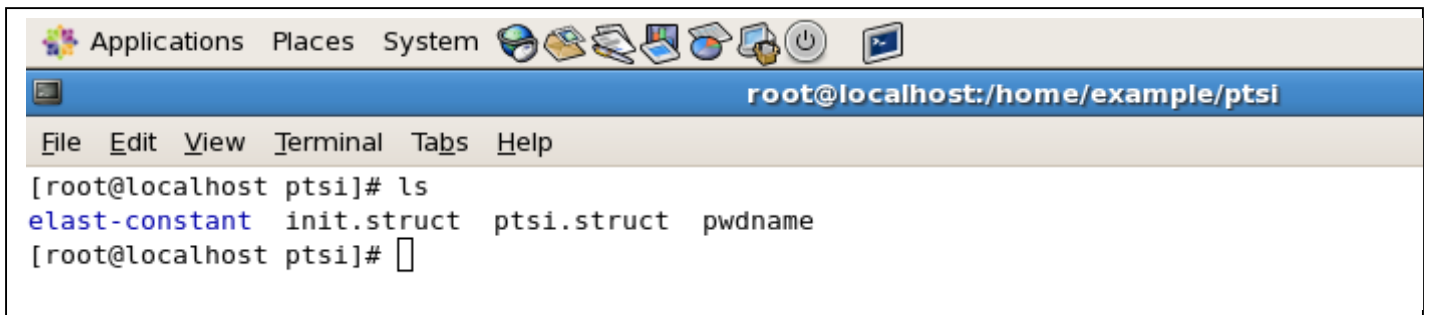
```
Applications Places System [system icons]
root@localhost:/home/example/ptsi/elastic-constant/c11+c1
File Edit View Terminal Tabs Help
NN ENDS
0.001u 0.004s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
> sgroup (21:17:16) 0.000u 0.000s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
Names of point group: -4m2 -4m2 D2d
Names of point group: 4/mmm 4/m 2/m 2/m D4h
Number and name of space group: 139 (I 4/m m m)
> symmetry (21:17:16) 0.001u 0.001s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
SELECT XCPOT:
recommended: 13: PBE-GGA (Perdew-Burke-Ernzerhof 96)
5: LSDA
11: WC-GGA (Wu-Cohen 2006)
19: PBEsol-GGA (Perdew et al. 2008)
SELECT ENERGY to separate core and valence states:
recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
ALTERNATIVELY: specify charge localization
(between 0.97 and 1.0) to select core state
LSTART ENDS
> inputfiles prepared (21:17:16)
NUMBER OF K-POINTS IN WHOLE CELL: (0 allows to specify 3 divisions of G)
length of reciprocal lattice vectors: 1.017 1.017 1.203 16.169 16.169 19.124
Shift of k-mesh allowed. Do you want to shift: (0=no, 1=shift)
405 k-points generated, ndiv= 17 17 17
KGEN ENDS
> dstart (21:17:17) DSTART ENDS
2.348u 0.010s 0:02.36 99.5% 0+0k 0+0io 0pf+0w
-----> new ptsi.in0 generated
init_lapw finished ok

DSTART ENDS
2.352u 0.009s 0:02.36 99.5% 0+0k 0+0io 0pf+0w
0.017u 0.011s 0:00.02 100.0% 0+0k 0+0io 0pf+0w
clmextrapol_lapw has generated a new ptsi.clmsum
LAPW0 END
LAPW1 END
LAPW1 END
LAPW1 END
LAPW1 END
```

- We repeat the same steps for running **TETRA.job** within c11-c12 , c33, czz, c44, and c66 directories.

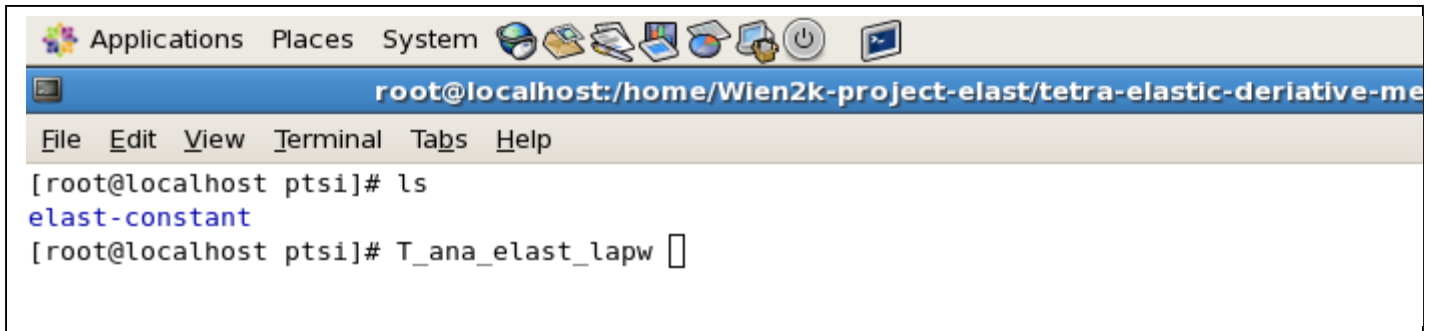
After calculations, we analyze our calculation for finding C11 , C12 , C44 and
For this goal, we change to main directory i.e. **ptsi** directory and run

- **T_ana_elast_lapw**



A terminal window with a menu bar (Applications, Places, System) and a toolbar. The title bar shows the current directory: root@localhost:/home/example/ptsi. The terminal content shows the command 'ls' being executed, resulting in the output: 'elast-constant', 'init.struct', 'ptsi.struct', and 'pwdname'.

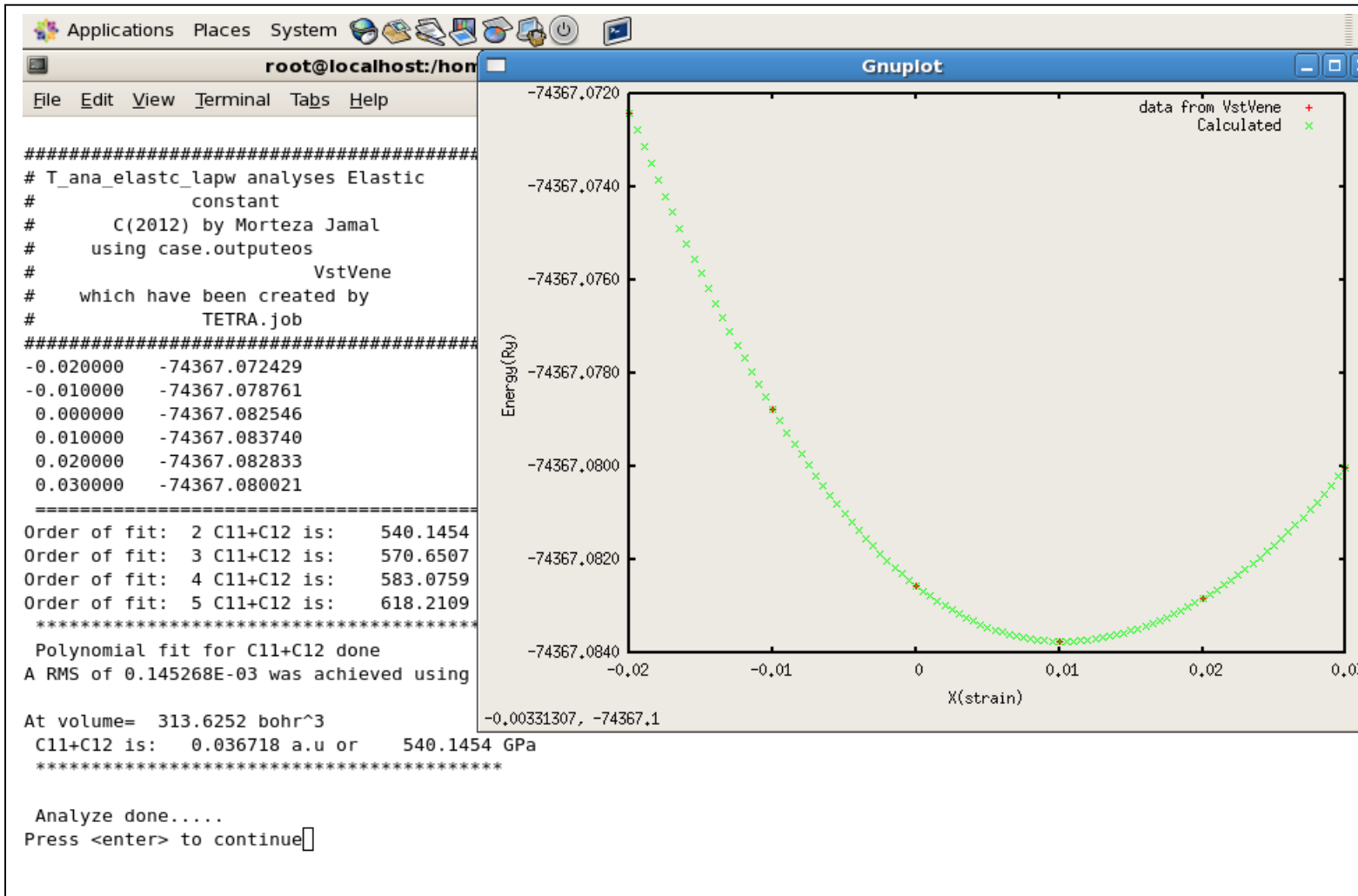
```
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ls
elast-constant  init.struct  ptsi.struct  pwdname
[root@localhost ptsi]#
```



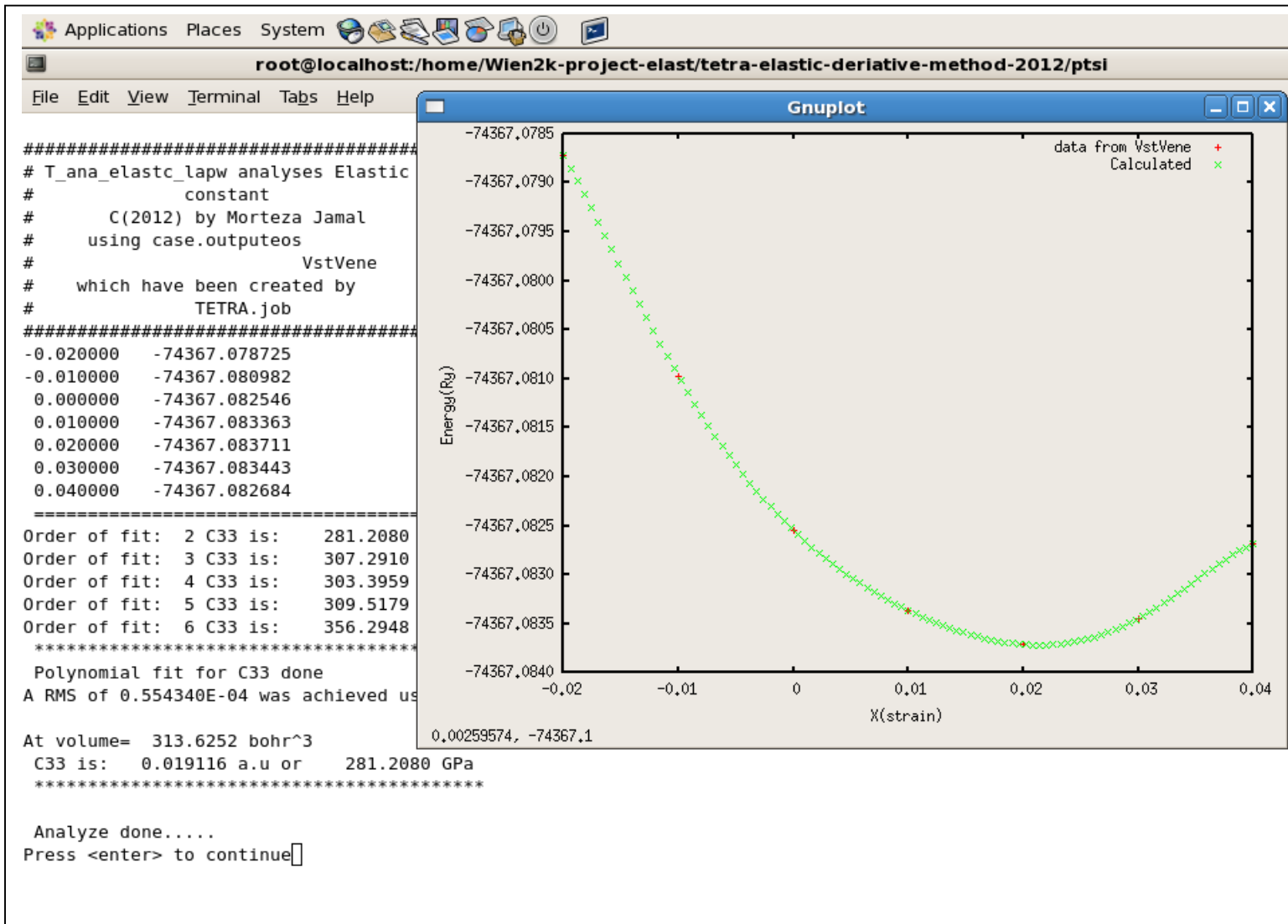
A terminal window with a menu bar (Applications, Places, System) and a toolbar. The title bar shows the current directory: root@localhost:/home/Wien2k-project-elast/tetra-elastic-derivative-me. The terminal content shows the command 'ls' being executed, resulting in the output: 'elast-constant'. Below that, the command 'T_ana_elast_lapw' is entered and followed by a cursor.

```
root@localhost:/home/Wien2k-project-elast/tetra-elastic-derivative-me
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ls
elast-constant
[root@localhost ptsi]# T_ana_elast_lapw
```

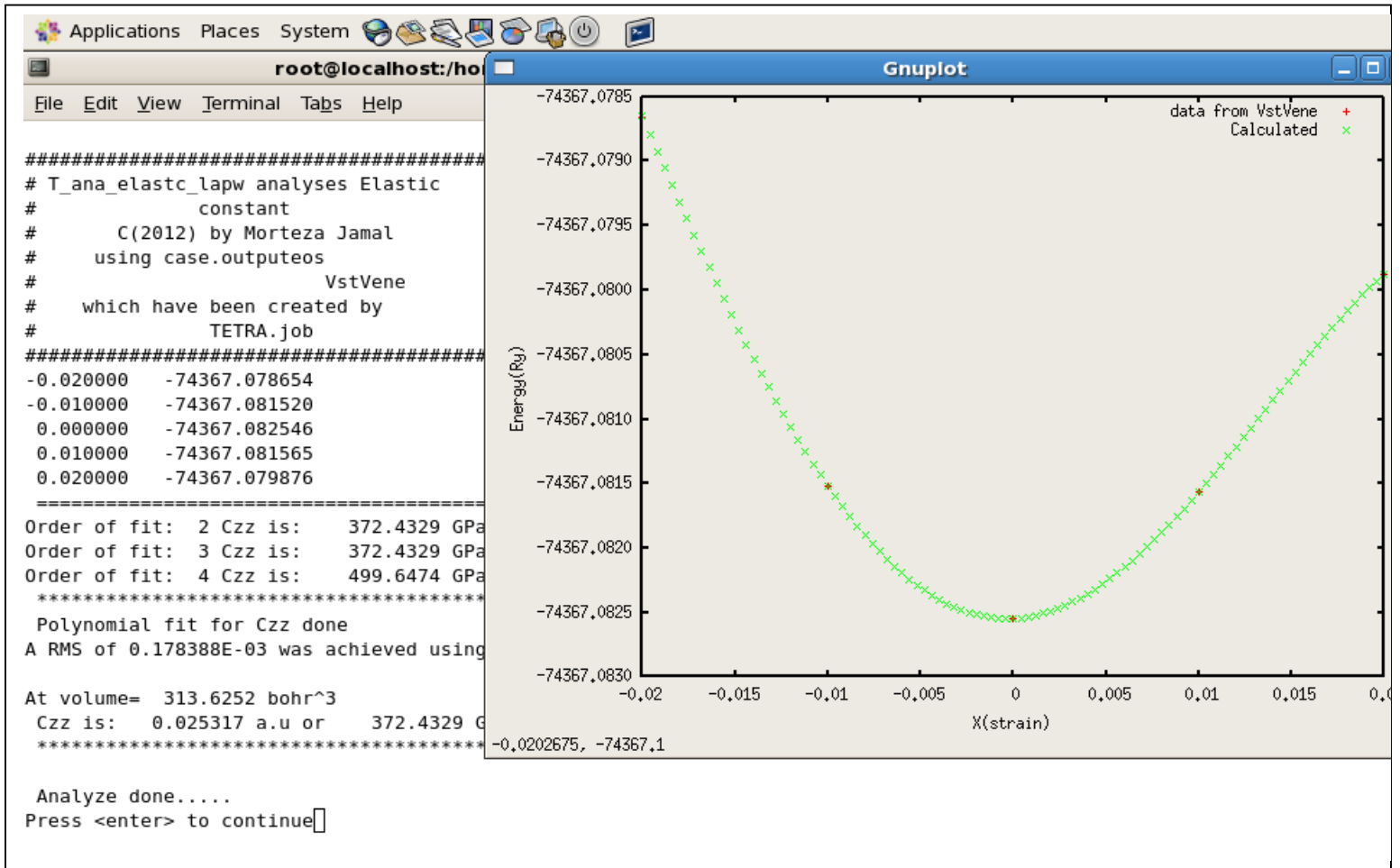
Now, we see



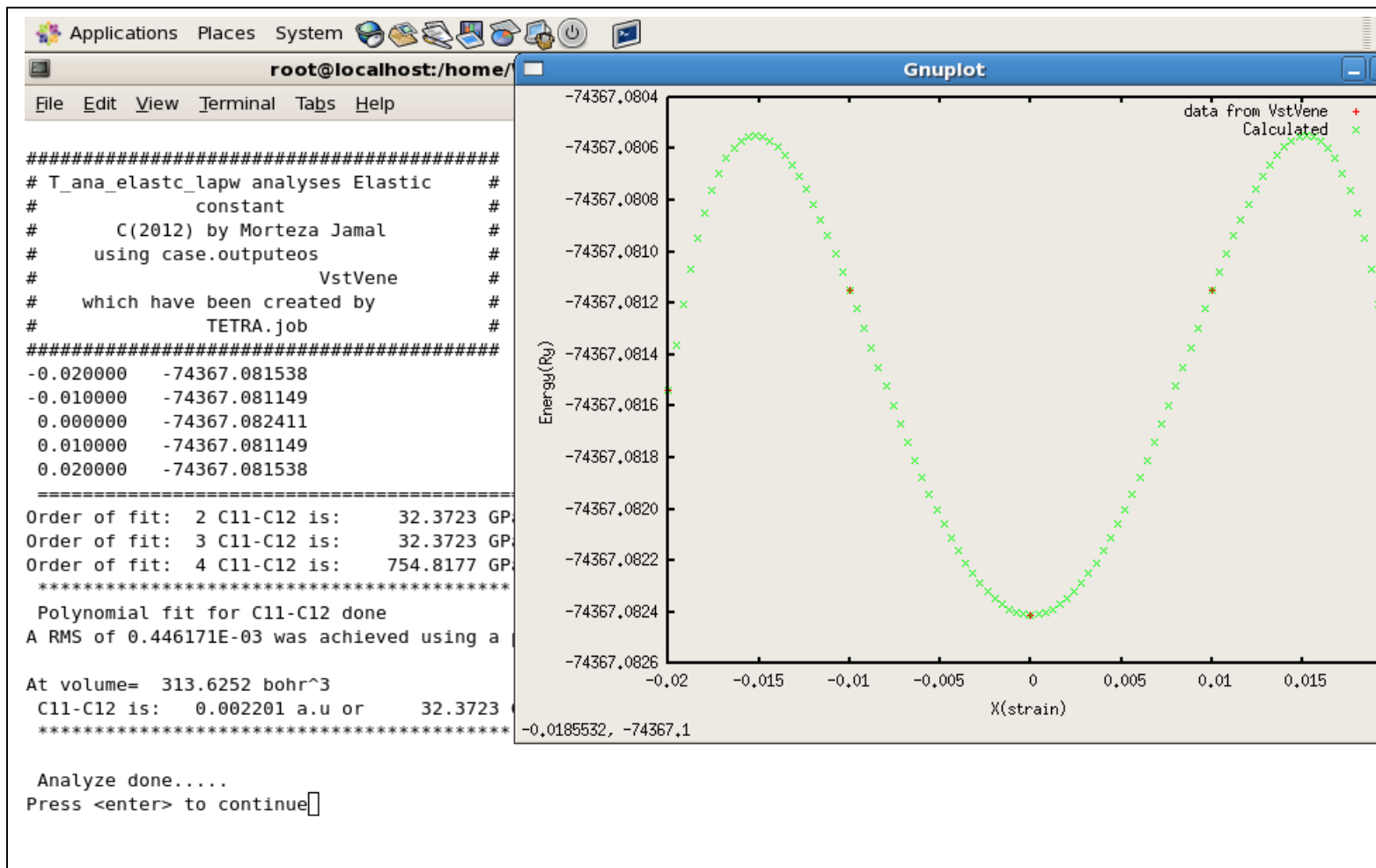
And then



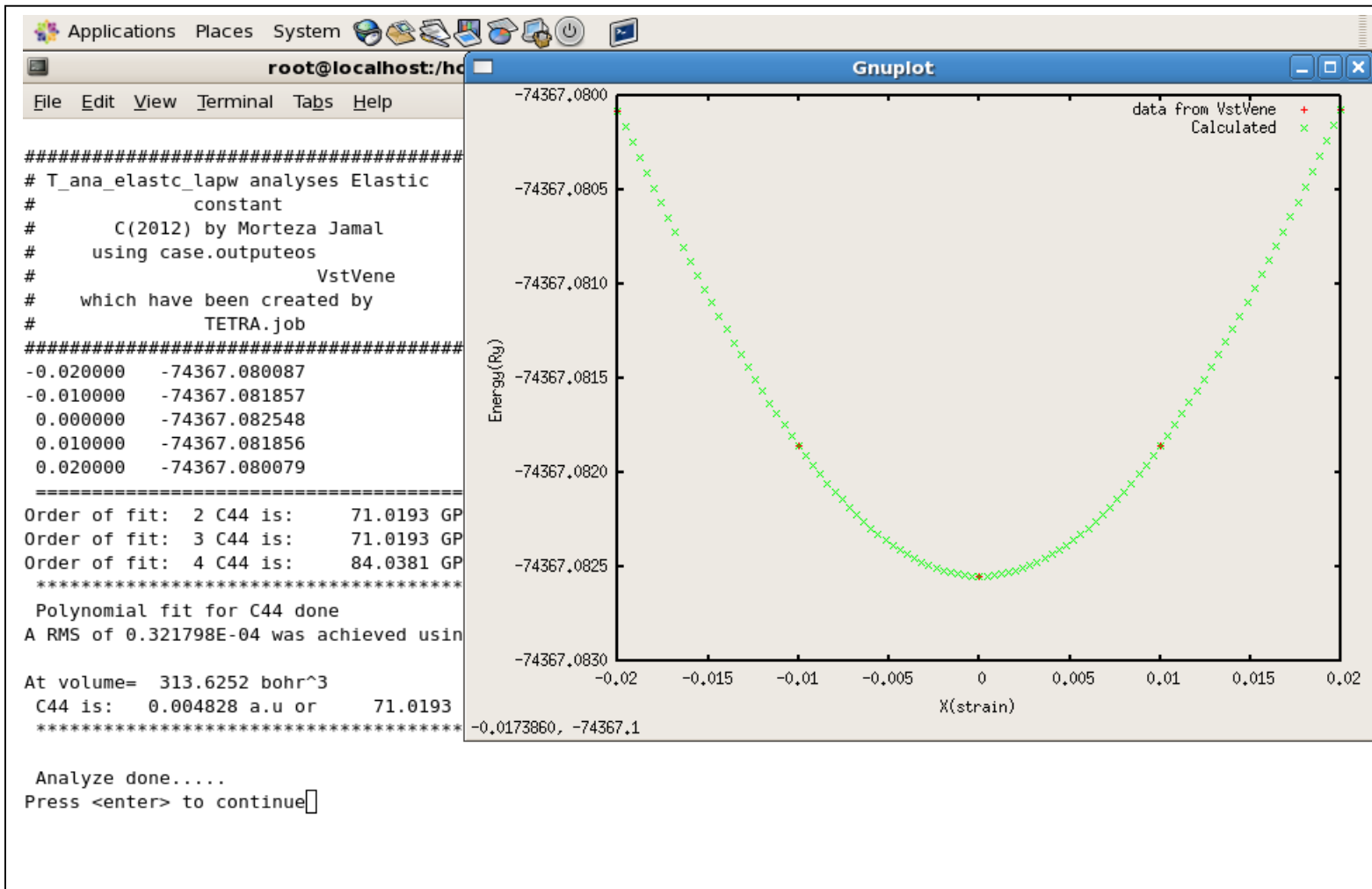
And after that



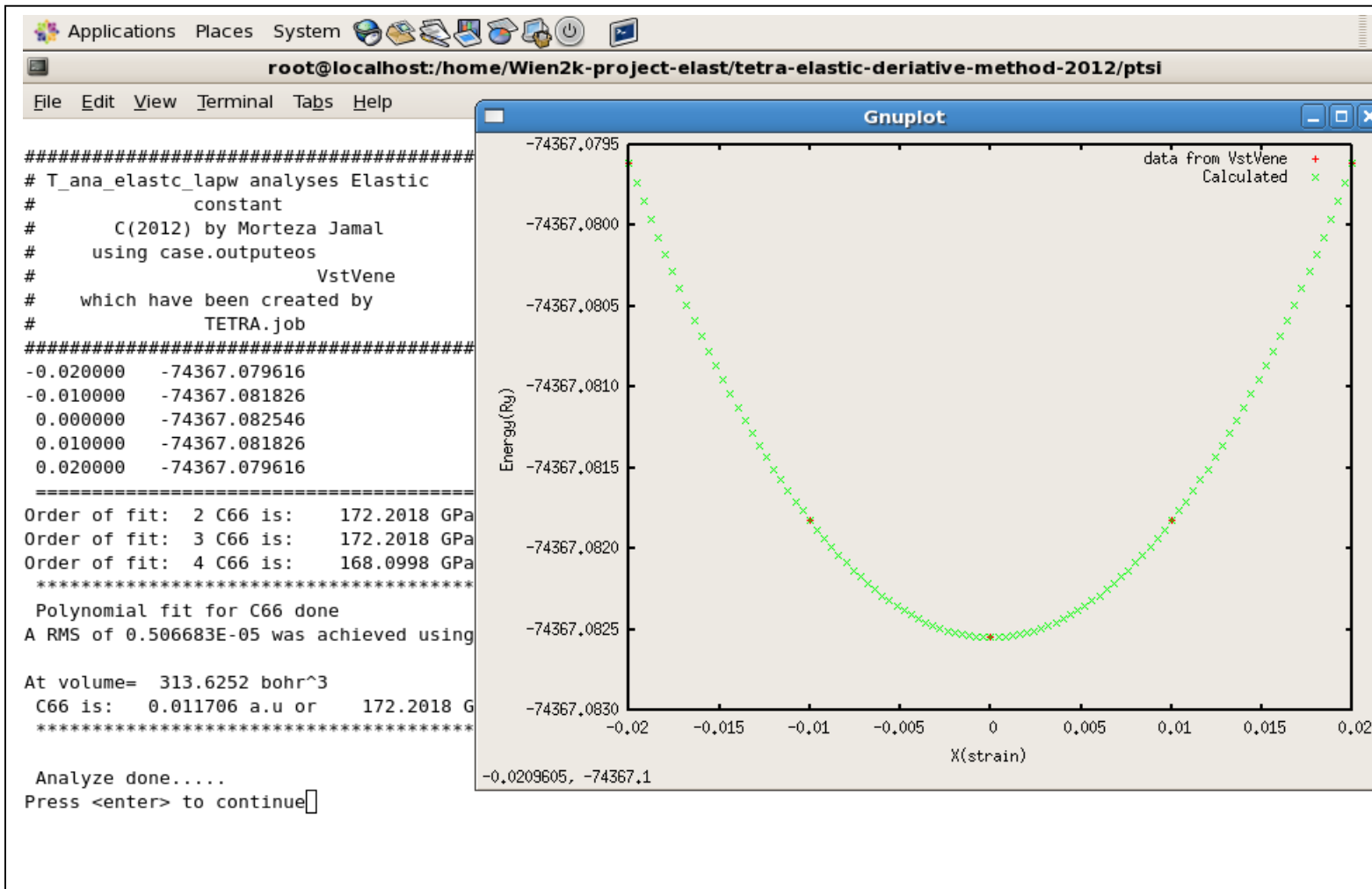
And then




And after that



And at the end



Now, we see results

```
Applications Places System 
root@localhost:/home/Wien2k-project-elast/tetra-elastic-derivative-met
File Edit View Terminal Tabs Help
Printing final Elastic constant At voulme= 313.6252 bohr^3 .
=====
C11+C12 = 540.1454 GPa      C11-C12 = 32.3723 GPa
C33 = 281.2080 GPa        C44 = 71.0193 GPa
Czz = C11+C12+2C33-4C13 = 372.4329 GPa
C66 = 172.2018 GPa
=====
C11 = 286.2588 GPa          C12 = 253.8865 GPa
      C13 = 182.5321 GPa
C33 = 281.2080 GPa          C44 = 71.0193 GPa
      C66 = 172.2018 GPa


Prediction VOIGT Bulk modulus by using elastic constant values = 232.403 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values = 228.919 (GPa)
Prediction HILL Bulk modulus by using elastic constant values = 230.661 (GPa)

Prediction VOIGT Shear modulus by using elastic constant values = 78.499 (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.776 (GPa)
Prediction HILL Shear modulus by using elastic constant values = 61.637 (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 211.665 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 126.105 (GPa)
Prediction HILL Young modulus by using elastic constant values = 169.787 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .348
Prediction REUSS Poisson's coefficient by using elastic constant values = .408
Prediction HILL Poisson's coefficient by using elastic constant values = .377
=====
Press enter key to continue....
```

And then checks the sensitivity of your results to the order of fit.

```
Applications Places System 
root@localhost:/home/Wien2k-project-elast/tetra-elastic-deriativ
File Edit View Terminal Tabs Help

=====
##### ORDER OF FIT IS : 3 , At volume = 313.62518 (bohr^3) #####
(c11-c12) = 32.372 (GPa)
(c11+c12) = 570.651 (GPa)
(c33) = 307.291 (GPa)
(c44) = 71.019 (GPa)
(czz=c11+c12+2c33-4c13) = 372.433 (GPa)
(c66= 172.202 (GPa)

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c11 = 301.511 (GPa)
c12 = 269.139 (GPa)
c13 = 203.200 (GPa)
c33 = 307.291 (GPa)
c44 = 71.019 (GPa)
c66 = 172.202 (GPa)

=====
Prediction VOIGT Bulk modulus by using elastic constant values = 251.265 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values = 249.106 (GPa)
Prediction HILL Bulk modulus by using elastic constant values = 250.185 (GPa)

Prediction VOIGT Shear modulus by using elastic constant values = 78.499 (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.910 (GPa)
Prediction HILL Shear modulus by using elastic constant values = 61.704 (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 213.285 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 127.092 (GPa)
Prediction HILL Young modulus by using elastic constant values = 171.049 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .358
Prediction REUSS Poisson's coefficient by using elastic constant values = .414
Prediction HILL Poisson's coefficient by using elastic constant values = .386

=====
##### ORDER OF FIT IS : 4 , At volume = 313.62518 (bohr^3) #####
(c11-c12) = 754.818 (GPa)
(c11+c12) = 583.076 (GPa)
(c33) = 303.396 (GPa)
(c44) = 84.038 (GPa)
(czz=c11+c12+2c33-4c13) = 499.647 (GPa)
(c66= 168.100 (GPa)
```

Now, change to **elast-constant** directory. You can see the results in **ptsi.output_elastic**

```
Applications Places System [system tray icons]
root@localhost:/home/Wien2k-project-elastic/tetra-elastic-derivative-method-2012/ptsi/elastic-c
File Edit View Terminal Tabs Help
[root@localhost ptsi]# cd elast-constant/
[root@localhost elast-constant]# gedit ptsi.output_elastic
pts_i.output_elastic (/home/Wien2k-project-elastic/tetra-elastic...erivative-method-2012/ptsi/elastic-constan
File Edit View Search Tools Documents Help
New Open Save Print... Undo Redo Cut Copy Paste Find Replace
pts_i.output_elastic x
Final Elastic constants for ptsi At voulme= 313.6252 bohr^3 are.
C11 = 286.2588 GPa          C12 = 253.8865 GPa
      C13 = 182.5321 GPa
C33 = 281.2080 GPa          C44 = 71.0193 GPa
      C66 = 172.2018 GPa

Prediction VOIGT Bulk modulus by using elastic constant values = 232.403 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values = 228.919 (GPa)
Prediction HILL Bulk modulus by using elastic constant values = 230.661 (GPa)

Prediction VOIGT Shear modulus by using elastic constant values = 78.499 (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.776 (GPa)
Prediction HILL Shear modulus by using elastic constant values = 61.637 (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 211.665 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 126.105 (GPa)
Prediction HILL Young modulus by using elastic constant values = 169.787 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .348
Prediction REUSS Poisson's coefficient by using elastic constant values = .408
Prediction HILL Poisson's coefficient by using elastic constant values = .377
```

Good luck
Morteza Jamal