



IR ELAST

+

WIEN2k

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

User's guide, Elastic Hexagonal_11.1(Release 07.08.2011)

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TO thank P. Blaha and A. H. Reshak

Installation guide

1_ Copy “**hex-elastic.tar.gz**” file in your computer in each Directory that you would like.

```
tar -zxvf hex-elastic.tar.gz
cd hex-elastic
```

2_Edit "Makefile" and select your Fortran compiler (FC) and Fortran compiler options (FOPT) and the path of MKL library (LDFLAGS) and then save it (you can type options that used for compiling Wien2k Package). Now type in Terminal environment:

```
make
make clean
```

3_Run “H_addbash_lapw” program (type H_addbash_lapw in terminal). This program define Environment Variable ELASTH_PATH and add it at the end of **.bashrc** file. Therefore you will able to call hex-elastic’s programs in 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).
- 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

Since for calculation C55 and (C11-C12) we use from Strains and then run "sgroupcheck_lapw", may be Number of atoms in new struct file 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) choose "answscf=no" in **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_set_elast_lapw**” (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_elastic1112_lapw, H_ana_elastic11m12, H_ana_elastic33_lapw, H_ana_elastic55_lapw, and H_ana_elasticzz_lapw programs for calculation elastic constants **and makes an output file in elast-constant directory with name case.output_elastic.**

Moreover H_ana_elastic1112_lapw, H_ana_elastic11m12, H_ana_elastic33_lapw, H_ana_elastic55_lapw, and H_ana_elasticzz_lapw programs produce aLattice.output, ortho.output, cLattice.output, Tri.output, and coa.output, respectively.

H_ana_elastorder_lapw : In this calculations, I use the highest polynomial for the final results. Usually this is VERY BAD!!!. It follows all your numerical noise and although such a fit may go through all points (leading to the smallest RMS), it may strongly oscillate between the points and give wrong results. **SO, WE HIGHLY RECOMMEND TO CHECK THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT by using H_ana_elastorder_lapw program and then select suitable values for Elastic Constants** (This program saves these data in the **output-order** file in the elast-constant directory.).

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

You can run it in the elast-constant directory. Moreover H_ana_elast_lapw calls H_ana_elastorder_lapw at the end of calculations.

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
- 5) Run 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 c33.job file.
- 10) Modify c33.job file.
- 11) Call c33.job
- 12) Call H_ana_elastic33_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) Modify czz.job file.
- 6) Call czz.job
- 7) Call H_ana_elasticzz_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.

Converged check

Since this package computes elastic constants by using second-order derivative ($E''(\epsilon)$) of Polynomial fit ($E=E(\epsilon)$) of Energy vs. Strains (ϵ) at zero strain ($\epsilon=0$). 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 we expect the behavior of elastic constants (second-order derivative of Energy vs. strain) vs. strains around zero strain (for example [-0.005 , +0.005]) to be plateau and you can find these data in unit of GPa vs. strain in the “case” directory within in c11+c12, c11-c12, c33, c55, and czz directories with name **aLatticediv2.fit, orthodiv2.fit, cLatticediv2.fit, Tridiv2.fit, and coadiv2.fit** respectively. I recommend to plot them and check this behavior for different data. 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.

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 90.000000 120.000000
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 = 11, L_max = 12, and nkpoint = 9000

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
 $E = E_0 + 9/16*(B/14703.6)*V_0*[(\eta^{**2}-1)**3*BP + (\eta^{**2}-1)**2*(6-4*\eta^{**2})]$

--> $\eta = (V_0/V)**(1/3)$

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+c11, c11-c12, c33, c55, and czz directories).

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

```
#####
# H_ana_elasticl1m12_lapw analyses Elastic #
# constant #
# C(2011) by Morteza Jamal #
# using case.outputeos #
# ortho.strain #
# which have been generated by #
# c11m12.job #
#####
-0.039999 -3415.271482
-0.029999 -3415.272397
-0.019999 -3415.273055
-0.009999 -3415.273509
0.000000 -3415.273751
0.009999 -3415.273502
0.020000 -3415.273011
0.030000 -3415.272252
0.040000 -3415.271089
```

Is -0.040000

```
=====  
Order of fit: 2, C11-C12 is: 93.7715 GPa, RMS: 0.531053E-04  
Order of fit: 3, C11-C12 is: 93.7713 GPa, RMS: 0.339176E-04  
Order of fit: 4, C11-C12 is: 100.5270 GPa, RMS: 0.294820E-04  
Order of fit: 5, C11-C12 is: 100.5271 GPa, RMS: 0.292761E-04  
Order of fit: 6, C11-C12 is: 127.1294 GPa, RMS: 0.153318E-04  
Order of fit: 7, C11-C12 is: 127.1293 GPa, RMS: 0.153243E-04
```

Order of fit: 8, C11-C12 is: 176.6953 GPa, RMS: 0.338949E-12

Polynomial fit or orthorhombic strain done

A RMS of 0.338949E-12 was achieved using a polynome of degree : 8

At volume= 234.6314 bohr^3

C11-C12 is: 0.012011 a.u or 176.6953 GPa

Analyze done.....

Press <enter> to continue

Do you want a hardcopy? (y/N)

You can find data in ortho.output file.

#####

H_ana_elastc1112_lapw analyses Elastic

constant

C(2011) by Morteza Jamal

using case.outputeos

aLattice.strain

which have been created by

c1112.job

#####

-0.040001 -3415.268296

-0.030000 -3415.271063

-0.020000 -3415.272861

-0.010001 -3415.273742

0.000000 -3415.273732

0.010000 -3415.272941

0.019999 -3415.271361

0.029999 -3415.269075

0.040000 -3415.266136

=====

Order of fit: 2, C11+C12 is: 255.7724 GPa, RMS: 0.110042E-03

Order of fit: 3, C11+C12 is: 255.7717 GPa, RMS: 0.489854E-05

Order of fit: 4, C11+C12 is: 255.9623 GPa, RMS: 0.487563E-05

Order of fit: 5, C11+C12 is: 255.9623 GPa, RMS: 0.486445E-05

Order of fit: 6, C11+C12 is: 253.4698 GPa, RMS: 0.426643E-05

Order of fit: 7, C11+C12 is: 253.4698 GPa, RMS: 0.426390E-05

Order of fit: 8, C11+C12 is: 239.6812 GPa, RMS: 0.371300E-12

Polynomial fit or a-Lattice changes done

A RMS of 0.371300E-12 was achieved using a polynome of degree : 8

At volume= 234.6314 bohr^3

C11+C12 is: 0.016293 a.u or 239.6812 GPa

Analyze done.....

Press <enter> to continue
Do you want a hardcopy? (y/N)

You can find data in aLattice.output file.

H_ana_elastc33_lapw analyses Elastic #
constant #
C(2011) by Morteza Jamal #
using case.outputeos #
cLattice.strain #
which have been created by #
c33.job #
#####

-0.150000	-3415.235135
-0.100000	-3415.258322
-0.050000	-3415.270870
0.000000	-3415.273746
0.019999	-3415.272687
0.049999	-3415.269095
0.099999	-3415.258636
0.149999	-3415.244097

=====
Order of fit: 2, C33 is: 188.9120 GPa, RMS: 0.152636E-02
Order of fit: 3, C33 is: 190.2842 GPa, RMS: 0.656246E-04
Order of fit: 4, C33 is: 192.4389 GPa, RMS: 0.542324E-04
Order of fit: 5, C33 is: 192.7923 GPa, RMS: 0.242531E-04
Order of fit: 6, C33 is: 187.5345 GPa, RMS: 0.220928E-05
Order of fit: 7, C33 is: 187.3238 GPa, RMS: 0.533239E-12

Polynomial fit or c-Lattice changes done
A RMS of 0.533239E-12 was achieved using a polynome of degree : 7

At volume= 234.6314 bohr^3
C33 is: 0.012734 a.u or 187.3238 GPa

Analyze done.....
Press <enter> to continue
Do you want a hardcopy? (y/N)

You can find data in cLattice.output file.

```
#####
# H_ana_elastc55_lapw analyses Elastic #
#      constant                          #
#      C(2011) by Morteza Jamal          #
#      using case.outputeos             #
#      Tri.strain                        #
#      which have been created by       #
#      c55.job                           #
#####
```

```
-0.020000    -3415.273091
 0.000000    -3415.273751
 0.020000    -3415.273091
 0.030000    -3415.272327
```

```
=====  
Order of fit:  2, C55 is:      49.9222 GPa, RMS: 0.121492E-04  
Order of fit:  3, C55 is:      51.7358 GPa, RMS: 0.393823E-12
```

```
*****  
Polynomial fit or triclinic changes done  
A RMS of 0.393823E-12 was achieved using a polynome of degree :  3
```

```
At volume=  234.6314 bohr^3  
C55 is:  0.003517 a.u or      51.7358 GPa  
*****
```

```
Analyze done.....  
Press <enter> to continue  
Do you want a hardcopy? (y/N)
```

```
*****  
You can find data in Tri.output file.  
*****
```

```
#####
# H_ana_elastczz_lapw analyses Elastic #
#      constant                          #
#      C(2011) by Morteza Jamal          #
#      using case.outputeos             #
#      coa.strain                        #
#      which have been created by       #
#      czz.job                           #
#####
```

```
-0.060000    -3415.271608
-0.040000    -3415.272846
-0.030001    -3415.273267
-0.020001    -3415.273560
```

-0.010001 -3415.273716
0.000000 -3415.273757
0.010000 -3415.273676
0.020000 -3415.273478
0.040000 -3415.272736

=====
Order of fit: 2, Czz is: 349.0863 GPa, RMS: 0.130588E-04
Order of fit: 3, Czz is: 340.6188 GPa, RMS: 0.169003E-05
Order of fit: 4, Czz is: 340.1537 GPa, RMS: 0.167541E-05
Order of fit: 5, Czz is: 335.1572 GPa, RMS: 0.132060E-05
Order of fit: 6, Czz is: 334.0748 GPa, RMS: 0.114695E-05
Order of fit: 7, Czz is: 324.7455 GPa, RMS: 0.999698E-06
Order of fit: 8, Czz is: 344.7134 GPa, RMS: 0.428740E-12

Polynomial fit or c/a changes done
A RMS of 0.428740E-12 was achieved using a polynome of degree : 8

At volume= 234.6314 bohr^3
Czz is: 0.023433 a.u or 344.7134 GPa

Analyze done.....
Press <enter> to continue
Do you want a hardcopy? (y/N)

You can find data in coa.output file.

Since the values of TRICLINIC strain were not more(4), I removed it from TO CHECK THE SENSITIVITY OF OUR RESULT TO THE ORDER OF FIT.

IN THIS CALCULATIONS, WE USE the highest polynomial for the final results.
Usually this is VERY BAD. It follows all your numerical noise and although such a fit may go through all points (leading to the smallest RMS),
it may strongly oscillate between the points and give wrong results.

SO, WE HIGHLY RECOMMEND TO CHECK THE SENSITIVITY
OF YOUR RESULT TO THE ORDER OF FIT

Order of fit for calculations were 8,7,3,8 and 8
We select minimum value for ORDER OF FIT i.e. 7

ORDER OF FIT IS : 2 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 93.772 (GPa)
(c11+c12) = 255.772 (GPa)
(c33) = 188.912 (GPa)
(c55) = 49.922 (GPa)
(czz=c11+c12+2c33-4c13) = 349.086 (GPa)

c11 = 174.772 (GPa)
c12 = 81.000 (GPa)

c13 = 71.127 (GPa)
c33 = 188.912 (GPa)
C55 = 49.922 (GPa)
ORDER OF FIT IS : 3 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 93.771 (GPa)
(c11+c12) = 255.772 (GPa)
(c33) = 190.284 (GPa)
(c55) = 51.736 (GPa)
(czz=c11+c12+2c33-4c13) = 340.619 (GPa)

c11 = 174.771 (GPa)
c12 = 81.000 (GPa)
c13 = 73.930 (GPa)
c33 = 190.284 (GPa)
C55 = 51.736 (GPa)
ORDER OF FIT IS : 4 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 100.527 (GPa)
(c11+c12) = 255.962 (GPa)
(c33) = 192.439 (GPa)
(c55) = 51.736 (GPa)
(czz=c11+c12+2c33-4c13) = 340.154 (GPa)

c11 = 178.244 (GPa)
c12 = 77.717 (GPa)
c13 = 75.171 (GPa)
c33 = 192.439 (GPa)
C55 = 51.736 (GPa)
ORDER OF FIT IS : 5 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 100.527 (GPa)
(c11+c12) = 255.962 (GPa)
(c33) = 192.792 (GPa)
(c55) = 51.736 (GPa)
(czz=c11+c12+2c33-4c13) = 335.157 (GPa)

c11 = 178.244 (GPa)
c12 = 77.717 (GPa)
c13 = 76.597 (GPa)
c33 = 192.792 (GPa)
C55 = 51.736 (GPa)
ORDER OF FIT IS : 6 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 127.129 (GPa)
(c11+c12) = 253.470 (GPa)
(c33) = 187.535 (GPa)
(c55) = 51.736 (GPa)
(czz=c11+c12+2c33-4c13) = 334.075 (GPa)

c11 = 190.299 (GPa)
c12 = 63.170 (GPa)
c13 = 73.616 (GPa)
c33 = 187.535 (GPa)
C55 = 51.736 (GPa)
ORDER OF FIT IS : 7 , At volume = 234.6314 (bohr^3) #####
(c11-c12) = 127.129 (GPa)
(c11+c12) = 253.470 (GPa)
(c33) = 187.324 (GPa)
(c55) = 51.736 (GPa)
(czz=c11+c12+2c33-4c13) = 324.746 (GPa)

c11 = 190.299 (GPa)
 c12 = 63.170 (GPa)
 c13 = 75.843 (GPa)
 c33 = 187.324 (GPa)
 C55 = 51.736 (GPa)

After checking the sensitivity of our results to the order of fit, I prefer to select:

C11 = 178 GPa
C12 = 78 GPa
C13 = 74 GPa
C33 = 188 GPa
C55 = 52 GPa

	Our calculation	Other(TB) ¹	Exp ¹
C11	178	171	160
C12	78	58	90
C13	74	46	60
C33	188	203	181
C55	52	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
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
  
```

Pressure(GPa)	vol	energy	de(EOS2)	de(Murnaghan)	
282.6068	282.6068	-14396.847343	0.000002	0.000002	12.277
298.3072	298.3072	-14396.856860	-0.000007	-0.000008	5.803
314.0075	314.0075	-14396.860187	0.000012	0.000014	0.565
329.7079	329.7079	-14396.858405	-0.000009	-0.000010	-3.717
345.4083	345.4083	-14396.852503	0.000002	0.000003	-7.252
		Sigma:	0.000007	0.000009	

Equation of state: Birch-Murnaghan info 2
 $E = E_0 + 9/16*(B/14703.6)*V_0*[(\eta^{**2}-1)**3*BP + (\eta^{**2}-1)**2*(6-4*\eta^{**2})]$

--> $\eta = (V_0/V)**(1/3)$
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

Pressure(GPa)	vol	energy	de(Birch-Murnaghan)	Pressure(GPa)
282.6068	282.6068	-14396.847343	0.000001	12.245
298.3072	298.3072	-14396.856860	-0.000006	5.814
314.0075	314.0075	-14396.860187	0.000010	0.564
329.7079	329.7079	-14396.858405	-0.000007	-3.725
345.4083	345.4083	-14396.852503	0.000002	-7.230
		Sigma:	0.000006	

```
#####
# H_ana_elastic55_lapw analyses Elastic #
# constant #
# C(2011) by Morteza Jamal #
# using case.outputeos #
# Tri.strain #
# which have been created by #
# c55.job #
#####
```

```
-0.030000 -14396.846682
-0.020000 -14396.847373
0.000000 -14396.847979
0.020000 -14396.847373
```

```
=====  
Order of fit: 2, C55 is: 33.7993 GPa, RMS: 0.136539E-04  
Order of fit: 3, C55 is: 35.3131 GPa, RMS: 0.128622E-11
```

```
*****  
Polynomial fit or triclinic changes done  
A RMS of 0.128622E-11 was achieved using a polynome of degree : 3
```

```
At volume= 315.9113 bohr^3  
C55 is: 0.002401 a.u or 35.3131 GPa  
*****
```

```
Analyze done.....  
Press <enter> to continue  
Do you want a hardcopy? (y/N)
```

```
*****  
You can find data in Tri.output file.  
*****
```

	Our calculation	Other(TB)¹	Exp¹
C55	35	4	33

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