



South Bohemian
Research Center
of Aquaculture
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of Hydrocenoses

Name of software (Czech): Tetra-elastický

Name of software (English): Tetra-elastic

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Description (Czech): Tento software se používá pro výpočet elastické konstanty v tetragonální strukture krystalu

Description (English): This software use to calculate the elastic constants of the Tetragonal structured crystals

Installation: - every thing described in the user guide,

1_ Copy “tetra-elastic.tar.gz” file in each Directory then do:

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

2_ Run **buildTIRElast_lapw**

This program helps you to provide "Makefile" and then compile tetra-elastic. Then define Environment Variable ELASTT_PATH and add it at the end of **.bashrc** file. Therefore you will be able to call tetra-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.

Requirements: - it need Linux, and Wien2k, moreover every thing described in the user guide,

Testing: - The testing is available in the user guide

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