



South Bohemian
Research Center
of Aquaculture
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of Hydrocenoses

Name of software (Czech): Hex-elastic

Name of software (English): Hex-elastic

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Description (Czech):

Softwarový balíček pro výpočet elastických tenzorů u šestihranných struktur pomocí derivací druhého řádu v kódu Wien2k, tento balíček počítá přesné hodnoty elastických konstant v hexagonálním systému. Výsledky získané pomocí tohoto balíčku jsou ve velmi dobré shodě s měřeními. Další podrobnosti jsou uvedeny v příložených souborech, které jsou k dispozici online.

Description (English):

A Package for calculating elastic tensors of Hexagonal structure by using second-order derivative with Wien2k code, this Package gives you the accurate values of the elastic constants of the hexagonal system. Results obtained by using this package are in very good agreement with the measured once. More details are described in the files attached to the package which are available online.

Installation:

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 be able to call hex-elastic's programs from each Directory.

Requirements: Operation system Linux, Unix and WIEN2K code

Testing: the installation of software include some testing data

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