



South Bohemian
Research Center
of Aquaculture
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of Hydrocenoses

Name of software (Czech): Ortho-elastic

Name of software (English): Ortho-elastic

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Description (Czech):

Softwarový balíček

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

Description (English):

A Package for calculating elastic tensors of orthorhombic structure by using second-order derivative with Wien2k code, this Package gives you the accurate values of the elastic constants of the orthorhombic 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 “**Ortho-elastic.tar.gz**” file in your computer. Then do the following:

```
tar -zxvf cubic-elastic.tar.gz
```

```
cd cubic-elastic
```

2_ Run **buildCIRelast_lapw**

This program helps you to provide "Makefile" and then compile cubic-elastic. Then define Environment Variable ELASTC_PATH and add it at the end of **.bashrc** file.

Requirements: Operation system Linux, Unix and WIEN2K code

Testing: the installation of software include some testing data

The source of financing: CENAKVA CZ.1.05/2.1.00/01.0024, GAJU 152/2010/Z