

ICON-EDiT

Author

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Homepage

All the information about the code is presented in the project homepage.

<https://calzaferri.dcb.unibe.ch/program/iconedit.html>

Source

Source code is available in the project homepage.

<https://calzaferri.dcb.unibe.ch/program/iconedit.html>

Reference

Reference for the code - please see the project homepage.

<https://calzaferri.dcb.unibe.ch/program/iconedit.html>

Included database files were extended using following reference:

Alvarez, S.: Tables of parameters for extended Hückel calculations, Universitat de Barcelona 1989.

Description & Use

ICON-EDiT performs extended Hückel calculations.

Quick start

Structure of a typical input is complicated. For input file creation it is recommended to use the inputc program which guides the user by dialogue. The inputc is executed as

```
inputc  
(in Windows command line)
```

or

```
./inputc  
(in Android shell).
```

The best choice is to create directly the cartesian coordinate file (.kar). It is ready to be submitted to the main program iconc:

```
iconc < [input file].kar > [output file].out
```

(in Windows command line)

or

```
./iconc < [input file].kar > [output file].out
```

(in Android shell).

The resulting file appears in the same location.

Program status

The current package contains ICON-EDiT binaries of version `97 compiled for x86 based Windows operating system.

License

ICON-EDiT

The original source code is published under GPL v.2 in the homepage. This distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Gion Calzaferri.

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MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime.
<http://www.mingw.org/>

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X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.

<http://x11-basic.sourceforge.net/>

<https://www.libsdl.org/>

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).

<https://www.advancedinstaller.com/>

<https://www.advancedinstaller.com/top-freeware-features.html>

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžicková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.

Website: <http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm>