HFCXX

Author

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Homepage

The author´s homepage contains a brief annotation.
http://www.ivofilot.nl/software/hfcxx
The project is located at GitHub as well.
https://github.com/ifilot/hfcxx

Source

Source code is available at GitHub.
https://github.com/ifilot/hfcxx

Description & Use

HFCXX performs HF calculations with STO-3G and STO-6G bases.

Quick start

Structure of a typical input file includes e.g.:

```
basis = [sto-3g/sto-6g]
charge = [charge]
atoms = [number of atoms]
units = angstrom
[atom] [x] [y] [z]
...
```

Use in command line / shell:

```
hfcxx [input file] > [output file]
```
(in Windows command line)

or

```
./hfcxx [input file] > [output file]
```
(in Android shell).

The result will appear in the same location.

Program status

The current package contains HFCXX binaries of primary version compiled for x86 based Windows operating system.

License

HFCXX

The original source code is published under GPL v.3 in the homepage. This distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Ivo Filot.

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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 Růžičková (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.
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