TUCKEL

Author

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Homepage

The project is published in Github repository.
https://github.com/charlyqchm/TUCKEL

Source

The official sources are available for free download from the Github repository.
https://github.com/charlyqchm/TUCKEL

Reference

Bustamante Carlos Mauricio: TUCKEL (computer program), available from
https://github.com/charlyqchm/TUCKEL (2.7.2019).

Description & Use

TUCKEL is a simple extended Hückel calculation program. The current limitations are: (1) only closed shell molecules and ions are supported (when trying to input a radical/radical ion, incorrect charge is attributed as it were a related diamagnetic species), (2) elements H, B, C, N, O and F are parametrized.

Quick start

A typical input file contains:

```
[number of atoms / lines in xyz block]
[overall charge]
[atom] [x] [y] [z]
...
(blank line)
```

The inputfile must be saved as FOR005 to the same location where the TUCKEL executable resides.

Use in command line / shell:

```
tuckel
```
(in Windows command line)

or

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

The results FOR006 (output file) and FOR007 (output for Avogadro) will appear in the same location.

Program status

The current package contains TUCKEL binaries of primary version compiled for the particular Android hardware platforms.

License

TUCKEL

The original source is distributed under GNU Lesser GPL. This distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Bustamante Carlos Mauricio.

MinGW

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

BLAS

TUCKEL binaries for Android offered by us were statically linked to BLAS library (freely-available software package, available in the homepage). The Windows package contains the corresponding dynamic library.
http://www.netlib.org/blas/

LAPACK

TUCKEL binaries for Android offered by us were statically linked to LAPACK library (released under modified BSD license, check the homepage for details). The Windows package contains the corresponding dynamic library.
http://www.netlib.org/lapack/

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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