CINDO

Authors

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Homepage

The project is hosted at Computer Physics Communications Program Library (search for keyword „cindo" or type the name „AECN_v1_0"). Modified parts are published by Aoyama Iwao in his Github repository.
http://www.cpc.cs.qub.ac.uk/
https://github.com/brhr-iwao/cindo_windows

Source

The official source code is available in Computer Physics Communications Program Library (keyword: CINDO or AECN_v1_0). Useful modifications which help when compiling for Windows platform posted by Aoyama Iwao are available in his Github repository.
http://www.cpc.cs.qub.ac.uk/
https://github.com/brhr-iwao/cindo_windows

Reference

Sridhar Sahu, Alok Shukla: Fortran 90 implementation of the Hartree–Fock approach within the CNDO/2 and INDO models, Computer Physics Communications 180(5) 2009, 724-734.

Description & Use

CINDO enables performing CNDO/2 and INDO calculations of species containing elements from the first to third period. Apart from the standard output it contains several other facilities such as generating custom orbital / spectrum datasheets.

Quick start

A typical input file contains answers to the original version prompts:

```
[total number of atoms]
[proton number of atom 1] [proton number of atom 2] ...
[x] [y] [z] (for the first atom)
[x] [y] [z] (for the second atom)
...
[CNDO / INDO]
[RHF / UHF]
```

```
[overall charge]
[convergence threshold, max.iterations] (e.g. 1.d-7,100)
[DAMP / NODAMP]
MULLIK
[ORBPLT / DENPLT / BOTHPLT / NOPLT]
[further keywords...]
[DIPOLE / NODIPOLE]
OPTICS
[frequency step, min., max. freq. range, line width of the excited states]
(e.g. 0.25,0.0,10.d0,0.01,1.d0)
(blank line)
(blank line)
(blank line)
(blank line)
```

For more details, please check the included manual and example file.

The input file is saved as FOR005 to the folder where the CINDO executable is present.

Use in command line / shell:

`cindo` (in Windows command line)

or

`./cindo` (in Android shell).

The resulting output file(s) will appear in the same location.

Program status

The current package contains CINDO binaries of primary version compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

CINDO

The distribution of CINDO binaries is published for free (under GPL v.3) at Mobile Chemistry Portal and Google Play Store with kind permission of Alok Shukla under the condition that you will cite the original reference paper (Sridhar Sahu, Alok Shukla: Fortran 90 implementation of the Hartree–Fock approach within the CNDO/2 and INDO models, Computer Physics Communications 180(5) 2009, 724-734.) in case of obtaining some results for publication purposes. By downloading, installing and using the program you automatically comply with this condition and are fully responsible for keeping the copyright rules. The included manual file was taken from the official source code distribution.

MinGW

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

```
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SOFTWARE.
```

BLAS

CINDO 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

CINDO 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/

<u>Advanced Installer</u>

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),
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Website: http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm