

CNINDO

Authors

John A. Pople and David L. Beveridge (original code)
Tytus Pikies and Aleksander Herman (reconstruction of the original code)

Homepage

Currently does not exist.

Source

Source code is available in the website of Gdańsk University of Technology.
<http://www.kchn.pg.gda.pl/download/CNINDO.rar>

Reference

John A. Pople, David L. Beveridge: Aproximate Molecular Orbital Theory, McGRAW-HILL BOOK COMPANY, 1970.

Description & Use

CNINDO performs CNDO and INDO calculations.

Quick start

Structure of a typical input file includes (cartesian system, lengths in Angstroms):

```
COMMENT
[endo\indo]
[open\closed]
[number of atoms]
[charge]
[multiplicity]
[atomic number] [X] [Y] [Z] }
[atomic number] [X] [Y] [Z] } number of atoms
... }
```

Use in command line / shell:

cnindo (input file must be saved as FOR005 in the same location before)
(in Windows command line)

or

`./cnindo` (input file must be saved as FOR005 in the same location before)
(in Android shell).

The result FOR006 will appear in the same location.

Program status

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

License

CNINDO

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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>