YAeHMOP

Author

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Homepage

The project homepage contains the sources, binaries, manuals and lots of other usefull stuff. The project is located at sourceforge as well.
http://yaehmop.sourceforge.net/
https://sourceforge.net/projects/yaehmop/

Source

Source code is available in the project homepage and at sourceforge.
http://yaehmop.sourceforge.net/
https://sourceforge.net/projects/yaehmop/

Reference

Landrum, G. A., and W. V. Glassey. "YAeHMOP (Yet Another Extended Hückel Molecular Orbital Package)." Cornell University, Ithaca, NY (1995).

Description & Use

YAeHMOP is used for extended Hückel method for both molecular and condensed state. It consists of two main (and few other additional) codes: bind (the core executable) and viewkel (visualization program, not actualy compiled for Android).

Quick start

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

```
; the title
[title]

; it's a molecular calculation, tell the program that
molecular

; Cartesian coordinates in Angstroms
geometry
[number of atoms]
[atom symbol] [x] [y] [z]
... (this part actually corresponds to a standard .xyz file,
produced e.g. by Atomdroid)

charge
[overall charge]

orbital occupations
; the number of occupations to change
[number]
; the orbitals and new occupation
[number of orbital] [number of electrons inside]
...

print
distance matrix
charge mat transpose
wave func transpose
net charges
overlap pop
reduced overlap pop
end_print
```

The input file and parameter file must be saved in the same location where the YAeHMOP executable resides.

Use in command line / shell:

```
bind [input file] [parameter file]
```
(in Windows command line)

or

```
./ bind [input file] [parameter file]
```
(in Android shell).

The result will appear in the same location.

Program status

The current package contains YAeHMOP binaries of version 3.0 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

YAeHMOP

The distribution is published for free at Mobile Chemistry Portal and Google Play Store with kind permission of Greg Landrum.


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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

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