

YAeHMOP

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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 x86 based Windows operating system.

License

YAeHMOP

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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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Website: <http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm>