CHEMSOL

Authors

Jan Florián and Arieh Warshel

Homepage

The project homepage contains the sources as well as the documentation.
https://laetro.usc.edu/software.html

Source

Source code is available in the project homepage.
https://laetro.usc.edu/software.html

Reference

Florián, J., and A. Warshel. "ChemSol, version 2.1." University of Southern California, Los Angeles (1999).

Description & Use

CHEMSOL enables the calculation of solvation energies by using the Langevin Dipole model of the solvent and ab-initio calculations.

Quick start

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

```
Title
number of atoms, number of different structures
XXXX-X
e.g.
  14 1
      (blank line)
Symbol, atom number, charge, x, y, z
e.g.
 H 1.0 0.4196 -0.0213 1.9586 0.0000
...
      (blank line)
      (blank line)
```

The structural data usually comes from another calculation (e.g. geometry optimization in vacuum). For obtaining reliable results, the previous calculation (to obtain well geometry and charges) is recommended to be carried out at at least B3LYP/6-31G(d) level (check the original manual for details). The calculation may last long, depending on size of the species.

Use in command line / shell:

```
chemsol [parameter file] [input file] > [output file]
```
(in Windows command line)

or

```
./ chemsol [parameter file] [input file] > [output file]
```

(in Android shell).

The result will appear in the same location.

Program status

The current package contains CHEMSOL binaries of version 2.1 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

CHEMSOL

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