OpenBabel

Authors

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Homepage

The official website of Openbabel is located at
http://openbabel.org/wiki/Main_Page

Source

The official sources are available in the official website as well as in the Github and Sourceforge repositories.
http://openbabel.org/wiki/Main_Page
https://github.com/openbabel/openbabel
https://sourceforge.net/projects/openbabel/

Reference

N M O'Boyle, M Banck, C A James, C Morley, T Vandermeersch, and G R Hutchison. "Open Babel: An open chemical toolbox." J. Cheminf. (2011), 3, 33. DOI:10.1186/1758-2946-3-33
The Open Babel Package, version 2.3.1 http://openbabel.org (accessed Oct 2011)

Description & Use

OpenBabel is a favourite program which utilizes the interconversions of various input/output file formats.

Use in command line / shell:

e.g.
```
obabel -ixyz [name of .xyz file] -og [name of the converted file]
```
(in Windows command line)

or

```
./obabel -ixyz [name of .xyz file] -og [name of the converted file]
```
(in Android shell).

The result will appear in the same location.

Quick start

Available input/output file switches:

```
acr -- Carine ASCI Crystal
alc -- Alchemy format
arc -- Accelrys/MSI Biosym/Insight II CAR format [Read-only]
bgf -- MSI BGF format
box -- Dock 3.5 Box format
bs -- Ball and Stick format
c3d1 -- Chem3D Cartesian 1 format
c3d2 -- Chem3D Cartesian 2 format
caccrt -- Cacao Cartesian format
cache -- CAChe MolStruct format [Write-only]
cacint -- Cacao Internal format [Write-only]
can -- Canonical SMILES format
car -- Accelrys/MSI Biosym/Insight II CAR format [Read-only]
ccc -- CCC format [Read-only]
cdx -- ChemDraw binary format [Read-only]
cdxml -- ChemDraw CDXML format
cht -- Chemtool format [Write-only]
cif -- Crystallographic Information File
cml -- Chemical Markup Language
cmlr -- CML Reaction format
com -- Gaussian Cartesian Input [Write-only]
copy -- Copies raw text [Write-only]
crk2d -- Chemical Resource Kit 2D diagram format
crk3d -- Chemical Resource Kit 3D format
csr -- Accelrys/MSI Quanta CSR format [Write-only]
cssr -- CSD CSSR format [Write-only]
ct -- ChemDraw Connection Table format
dmol -- DMol3 coordinates format
ent -- Protein Data Bank format
fa -- FASTA format [Write-only]
fasta -- FASTA format [Write-only]
fch -- Gaussian formatted checkpoint file format [Read-only]
fchk -- Gaussian formatted checkpoint file format [Read-only]
fck -- Gaussian formatted checkpoint file format [Read-only]
feat -- Feature format
fh -- Fenske-Hall Z-Matrix format [Write-only]
fix -- SMILES FIX format [Write-only]
fpt -- Fingerprint format [Write-only]
fract -- Free Form Fractional format
fs -- Open Babel FastSearching database
fsa -- FASTA format [Write-only]
g03 -- Gaussian 98/03 Output [Read-only]
g98 -- Gaussian 98/03 Output [Read-only]
gam -- GAMESS Output [Read-only]
gamin -- GAMESS Input [Write-only]
gamout -- GAMESS Output [Read-only]
gau -- Gaussian Cartesian Input [Write-only]
gjc -- Gaussian Cartesian Input [Write-only]
gjf -- Gaussian Cartesian Input [Write-only]
gpr -- Ghemical format
gr96 -- GROMOS96 format [Write-only]
```

```
gzmat -- Gaussian Z-Matrix Input
hin -- HyperChem HIN format
inchi -- IUPAC InChI [Write-only]
inp -- GAMESS Input [Write-only]
ins -- ShelX format [Read-only]
jin -- Jaguar input format [Write-only]
jout -- Jaguar output format [Read-only]
mdl -- MDL MOL format
mmd -- MacroModel format
mmod -- MacroModel format
mol -- MDL MOL format
mol2 -- Sybyl Mol2 format
molreport -- Open Babel molecule report [Write-only]
moo -- MOPAC Output format [Read-only]
mop -- MOPAC Cartesian format
mopcrt -- MOPAC Cartesian format
mopin -- MOPAC Internal
mopout -- MOPAC Output format [Read-only]
mpc -- MOPAC Cartesian format
mpd -- Sybyl descriptor format [Write-only]
mpqc -- MPQC output format [Read-only]
mpqcin -- MPQC simplified input format [Write-only]
nw -- NWChem input format [Write-only]
nwo -- NWChem output format [Read-only]
pc -- PubChem format [Read-only]
pcm -- PCModel format
pdb -- Protein Data Bank format
pov -- POV-Ray input format [Write-only]
pqs -- Parallel Quantum Solutions format
prep -- Amber Prep format [Read-only]
qcin -- Q-Chem input format [Write-only]
qcout -- Q-Chem output format [Read-only]
report -- Open Babel report format [Write-only]
res -- ShelX format [Read-only]
rxn -- MDL RXN format
sd -- MDL MOL format
sdf -- MDL MOL format
smi -- SMILES format
sy2 -- Sybyl Mol2 format
tdd -- Thermo format
test -- Test format [Write-only]
therm -- Thermo format
tmol -- TurboMole Coordinate format
txyz -- Tinker MM2 format [Write-only]
unixyz -- UniChem XYZ format
vmol -- ViewMol format
xed -- XED format [Write-only]
xml -- General XML format [Read-only]
xyz -- XYZ cartesian coordinates format
yob -- YASARA.org YOB format
zin -- ZINDO input format [Write-only]
```

Program status

The current package contains OpenBabel binaries of version 2.4.9 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

OpenBabel

The distribution of OpenBabel binaries is published for free (under GPL v.2) at Mobile Chemistry Portal and Google Play Store with kind permission of Geoffrey Hutchison. Both the slightly modified source codes for generic Android binaries as well as for the binaries adapted to running in a standard Android filesystem (with defined hardlinks to each used file) are available for download below.

The included parameter files were taken from the OpenBabel official source distribution.

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.
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