

OpenBabel et Jmol

OpenBabel

[OpenBabel](#) est un ensemble de programme permettant de manipuler et convertir les fichiers de description de molécules dans différents formats.

- Site officiel : http://openbabel.org/wiki/Main_Page
- Interfaçage en Python : <http://openbabel.org/wiki/Python>

Jmol

[Jmol](#) est un logiciel libre de visualisation de structures chimiques en 3D, écrit en Java et donc multi-plateformes (Windows, Mac OS X, Linux,...).

C'est un programme idéal pour visualiser des molécules dont les fichiers de description ont été obtenus par OpenBabel (ou d'autres logiciels de chimie).

- Site officiel : <http://jmol.sourceforge.net/index.fr.html>

Exemple de programme Python

```
<sxh python; title : generate_alcohols-01.py> #!/usr/bin/env python # -*- coding: utf-8 -*- #
génération à partir du code smile d'alcools ddes caractéristiques 3D # et de fichiers .pdb lisible par
Jmol # références : # http://openbabel.org/wiki/Python #
http://openbabel.org/docs/current/UseTheLibrary/PythonDoc.html#using-iterators #
http://pythonchem.blogspot.be/2012/08/fun-and-little-disappointment-with.html #
https://gist.github.com/cstein/3294891 # http://nullege.com/codes/search/openbabel
```

```
import openbabel
```

```
def OBMolMinimize(mol):
```

```
    """Minimize a molecule
    """
    ff = openbabel.OBForceField.FindForceField("MMFF94")
    ff.Setup(mol)
    ff.ConjugateGradients(100, 1.0e-5)
    ff.GetCoordinates(mol)
    return mol
```

```
def OBStructureFromSmiles(smilesstring, filename=None):
```

```
    mol = openbabel.OBMol()
    obConversion = openbabel.OBConversion()
```

```
obConversion.SetInAndOutFormats("smi", "pdb")
obConversion.ReadString(mol, smilesstring)
mol.AddHydrogens()
builder = openbabel.OBBuilder()
builder.Build(mol)
mol = OBMolMinimize(mol)
if filename is None: return mol
# save structures in subfolder molecules
obConversion.WriteFile(mol, "molecules/%s.pdb" % filename)
```

def getAlcohols():

```
molecules = dict()
molecules['methanol'] = 'CO'
molecules['ethanol'] = 'CCO'
molecules['1-propanol'] = 'CCCO'
molecules['isopropanol'] = 'CC(O)C'
molecules['n-butanol'] = 'CCCCO'
molecules['butan-2-ol'] = 'CC(O)CC'
molecules['isobutanol'] = 'CC(C)CO'
molecules['tert-butanol'] = 'CC(C)(C)O'
molecules['1-Pentanol'] = 'CCCCCO'
return molecules
```

if name == 'main':

```
etab = openbabel.OBElementTable()
dico = getAlcohols()
for elem in dico:
    OBStructureFromSmiles(dico[elem], elem)
```

```
# Determine the charge of a molecule
for file_in in dico:
    obConversion = openbabel.OBConversion()
    obConversion.SetInFormat("pdb")
    mol = openbabel.OBMol()
    obConversion.ReadFile(mol, "molecules/%s.pdb" % file_in)
    # get the charges of the atoms
    charge_model = openbabel.OBChargeModel.FindType("MMFF94")
    charge_model.ComputeCharges(mol)
    partial_charges = charge_model.GetPartialCharges()
    print file_in, '- Formula = ', mol.GetFormula()
    print 'mol wt = ', mol.GetMolWt(), '- Numb atoms = ', mol.NumAtoms(),
'- Numb bonds = ', mol.NumBonds()
    for atom in openbabel.OBMolAtomIter(mol):
        z=atom.GetAtomicNum()
        v3=atom.GetVector()
        print atom.GetAtomicMass(), z, etab.GetSymbol(z), 'x=',v3.GetX(),
'y=',v3.GetY(), 'z=',v3.GetZ()
```

```
print 'partial charges = ', partial_charges
print 'total charge = ', "%i" % int(sum(partial_charges))
print '*****'
```

</sxh> Pour le méthanol, ce programme sort ces informations :

```
methanol - Formula = CH4O
mol wt = 32.04186 - Numb atoms = 6 - Numb bonds = 5
12.0107 6 C x= 0.956 y= -0.086 z= -0.056
15.9994 8 O x= 0.488 y= -1.374 z= 0.299
1.00794 1 H x= 0.587 y= 0.64 z= 0.672
1.00794 1 H x= 0.584 y= 0.177 z= -1.05
1.00794 1 H x= 2.049 y= -0.08 z= -0.052
1.00794 1 H x= 0.831 y= -1.996 z= -0.365
partial charges = (0.28, -0.68, 0.0, 0.0, 0.0, 0.4)
total charge = 0
```

References

- [Open Babel: An open chemical toolbox](#), Noel M O'Boyle, Michael Banck, Craig A James, Chris Morley, Tim Vandermeersch and Geoffrey R Hutchison, Journal of Cheminformatics 2011, 3:33 doi:10.1186/1758-2946-3-33

From:

<https://dvillers.umons.ac.be/wiki/> - **Didier Villers, UMONS - wiki**

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Last update: **2014/02/27 22:42**

