
Subject: Re: Molecule style & color
Posted by [nbehrnd](#) on Thu, 09 Jul 2020 07:57:52 GMT
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Hello Paul,

a quick work-around could employ the platform independent Jmol.(1) It is possible to save all of the conformers generated in one .sdf file in common -- just take care that the export retains the 3D coordinates (which is not the default).

In Jmol running, the entry File -> Console opens the programs' own little terminal. Then indicate Jmol the .sdf to read; it will recognize that the .sdf contains multiple models, but by default will display only the first one. This is the chance to disable the display of double / aromatic / triple bonds with more than one line (by the second command), to adjust the diameter of the sticks and balls (third command) and eventually display all models (here: all superimposed conformers) at once by the instruction of model 0.

The scene may be exported like below.

The interaction with Jmol may be scripted (e.g., 2,3,4) thus you may reuse instructions more than once. If the color of an atom type does not fit your needs, for example, you could alter the representation by

```
select hydrogen  
color gray
```

for all models load at once. You may return to the default color scheme by

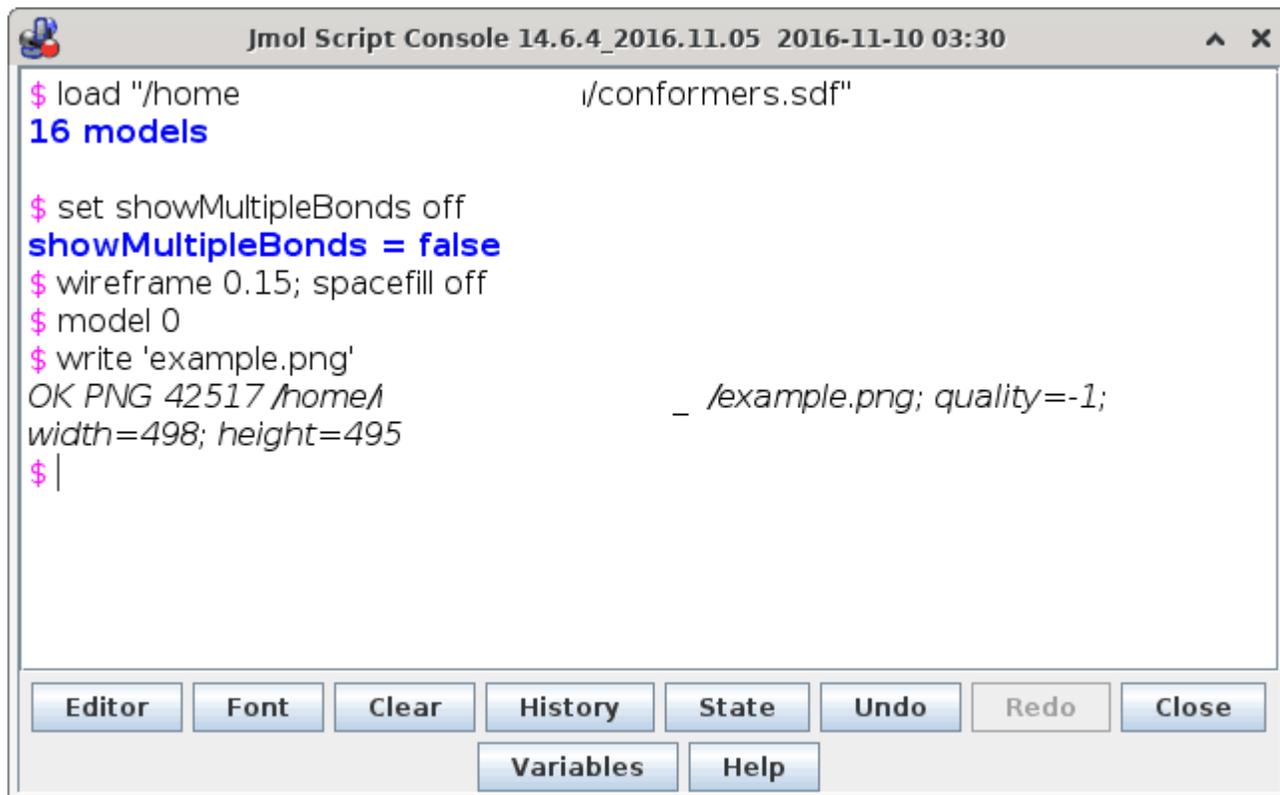
```
select all  
color cpk
```

Norwid

- 1) http://wiki.jmol.org/index.php/Main_Page
- 2) <https://chemapps.stolaf.edu/jmol/docs/>
- 3) https://earth.callutheran.edu/Academic_Programs/Departments/BioDev/omm/jsmol/scripting/molmast.htm#V
- 4) Hanson, J.Appl.Cryst.(2010).43, 12501260, doi: 10.1107/S0021889810030256

File Attachments

- 1) [console.png](#), downloaded 1307 times



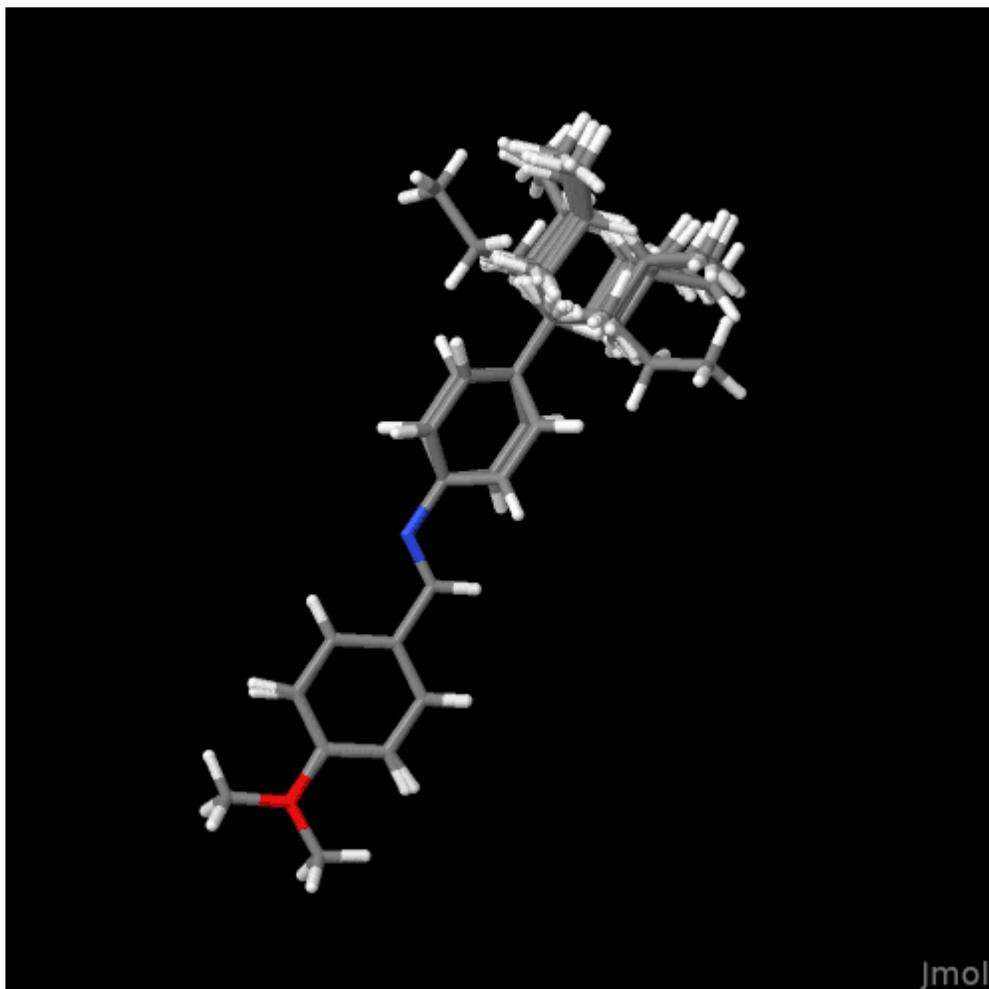
The screenshot shows a window titled "Jmol Script Console 14.6.4_2016.11.05 2016-11-10 03:30". The console contains the following text:

```
$ load "/home /conformers.sdf"
16 models

$ set showMultipleBonds off
showMultipleBonds = false
$ wireframe 0.15; spacefill off
$ model 0
$ write 'example.png'
OK PNG 42517 /home/ _ /example.png; quality=-1;
width=498; height=495
$ |
```

At the bottom of the window, there is a toolbar with buttons for "Editor", "Font", "Clear", "History", "State", "Undo", "Redo", "Close", "Variables", and "Help".

2) [example.png](#), downloaded 1300 times



- 3) [liquid_crystal.dwar](#), downloaded 699 times
- 4) [DW_conformer_generation.png](#), downloaded 745 times

Generate Conformers

Structure column: Structure

Algorithm: Random, low energy bias

Initial torsions: From crystallographic database

Minimize energy: Don't minimize

Max. conformer count: 16 per stereo isomer

Write into file: .../conformers.sdf Edit

File type: SD-File Version 3

Pool conformers of same compound

Remove small fragments

Neutralize remaining fragment

Skip compounds with more than 16 stereo isomers

Create proper protonation state(s) for pH= 7.4 +- 0

Help Cancel OK

5) [conformers.sdf](#), downloaded 741 times
