Subject: Re: Molecule style & color
Posted by nbehrnd on Thu, 09 Jul 2020 07:57:52 GMT
View Forum Message <> Reply to Message

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

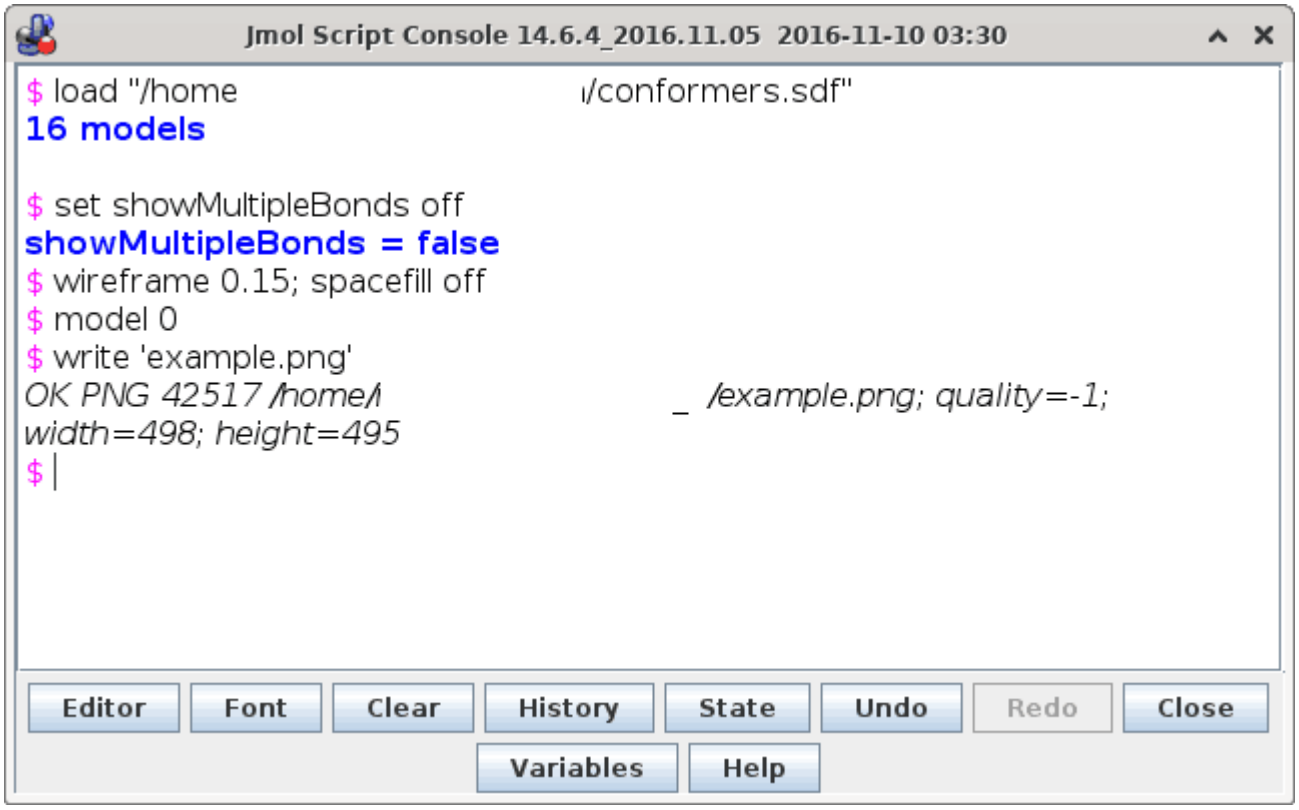
select all
color cpk

Norwid

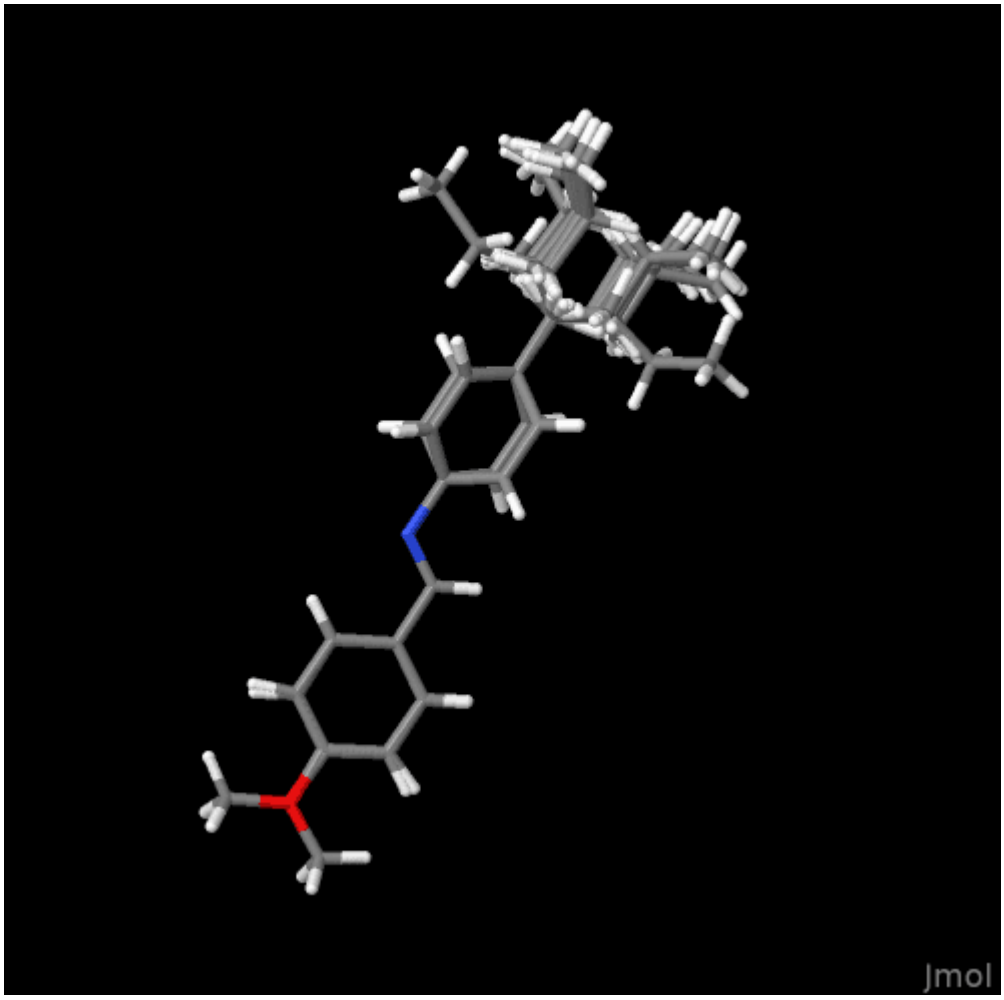
1) http://wiki.jmol.org/index.php/Main_Page
2) https://chemapps.stolaf.edu/jmol/docs/
3) https://earth.callutheran.edu/Academic_Programs/Departments/BioDev/omm/jsmol/scripting/molmast.htm#V
4) Hanson, J.Appl.Cryst.(2010).43, 12501260, doi: 10.1107/S0021889810030256

File Attachments

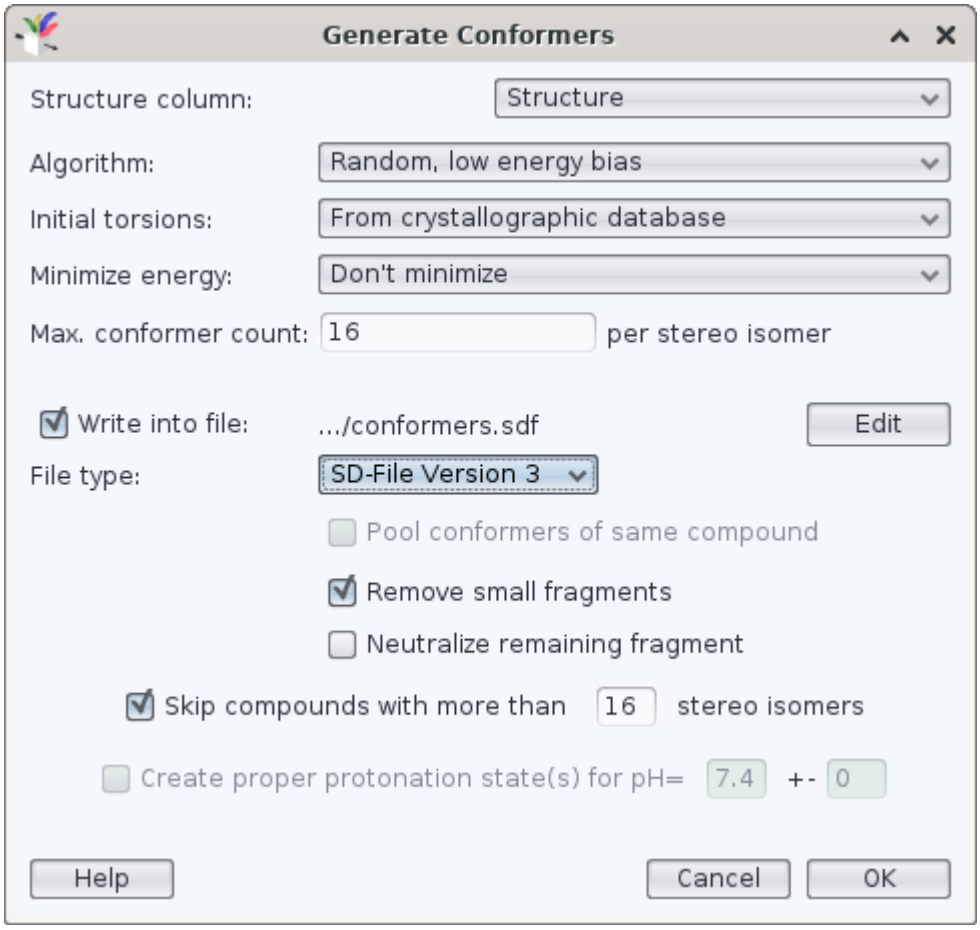
1) console.png, downloaded 1042 times



2) example.png, downloaded 1060 times



3) liquid_crystal.dwar, downloaded 652 times
4) DW_conformer_generation.png, downloaded 537 times



5) conformers.sdf, downloaded 645 times