

CONFLEX 8 Revision B Installation Manual and Quick Start For Linux

0. Download the installer

When you receive e-mail from us including download site, you can download CONFLEX 8.B installers for Linux from the links. In this document, the installer “CONFLEX8B_eng_gui_flex” is downloaded and used as example.

1. Install and copy sample files

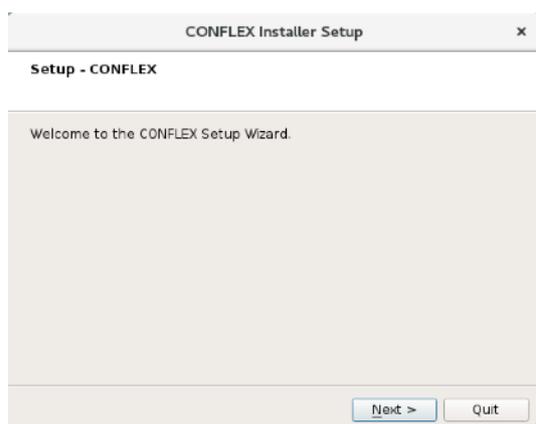
If the file “CONFLEX8B_eng_gui_flex” does not have execution authority, please execute

```
chmod +x CONFLEX8B_eng_gui_flex
```

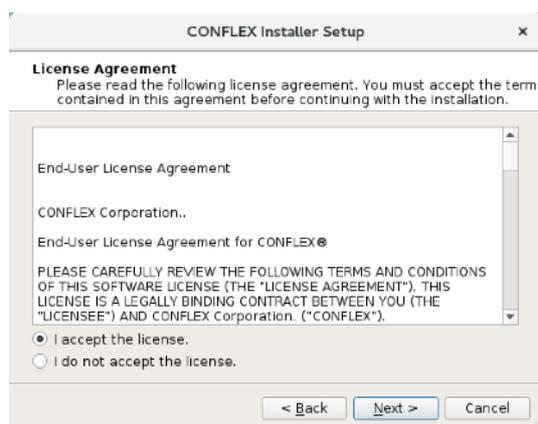
before installation.

i) Execute below command as root:

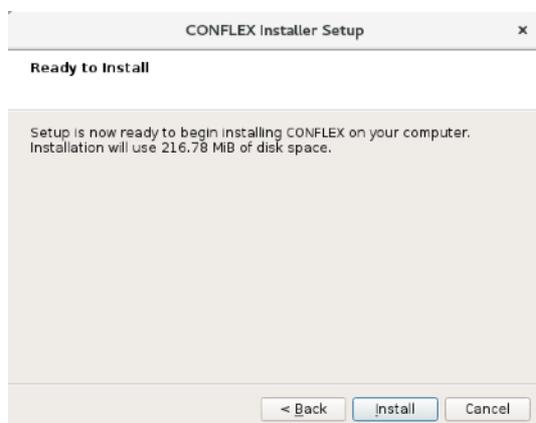
```
sudo ./CONFLEX8B_eng_gui_flex
```



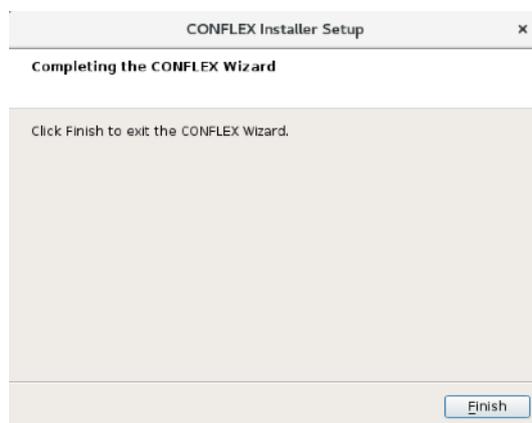
ii) Click “Next”.



iii) Select “I accept the license” and click “Next”.



iv) Click “Install”.



v) Click “Finish” after finished installation.

After installation is completed, CONFLEX8.B is installed in /usr/local/conflex. Please set the environment variable as below:

```
export LD_LIBRARY_PATH=/usr/local/conflex/lib:$LD_LIBRARY_PATH
```

*When CONFLEX Interface cannot run with below messages,

```
This application failed to start because it could not find or load the Qt
platform plugin "xcb"
```

or

```
qt.qpa.plugin: Could not load the Qt platform plugin "xcb" in "" even
though it was found.
```

```
This application failed to start because no Qt platform plugin could be
initialized. Reinstalling the application may fix this problem.
```

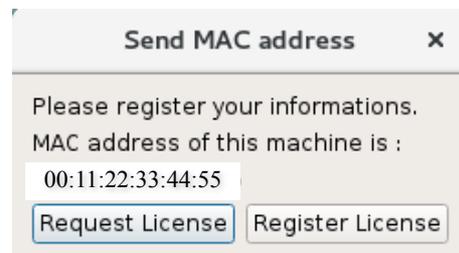
please run command below to install the necessary libraries:

```
yum install libxcb xcb-util-renderutil xcb-util-keysyms xcb-util-wm xcb-
util-image compat-libxcb xcb-util
```

2. Send Information and Activation

To activate your authorized license for CONFLEX, you need to send information of your machine to us. When you run CONFLEX and click [Request License] in "Send MAC address" window, the E-mail software starts automatically and below message is appeared:

Your Name :
Affiliation :
Address :
ZIP code :
Phone No. :
FAX No. :
E-Mail address :
MAC address : 11:22:33:44:55:66



Please fill in the form and send it to info@conflex.co.jp. We will send license file (license.dat) to you in a day or two. The activation procedure is below:

- Save attached license.dat file
- Run CONFLEX as root
- Click "Register License" on "Send MAC address" window (see above)
- Browse to the location where you saved the license.dat and Select it

when the following screen is shown, click “OK”.



click “OK” to complete activation. The license.dat is copied in /usr/local/conflex/par/.



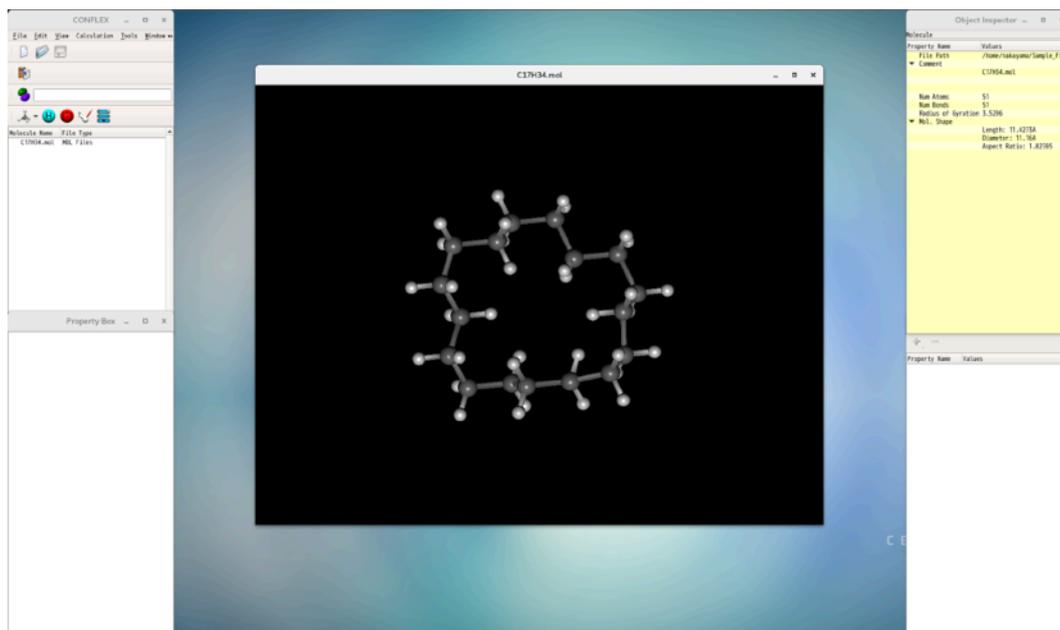
3. Geometry Optimization and Conformation Search using Sample File

Please copy “Sample_Files” folder in /usr/local/conflex/ for the test calculation.

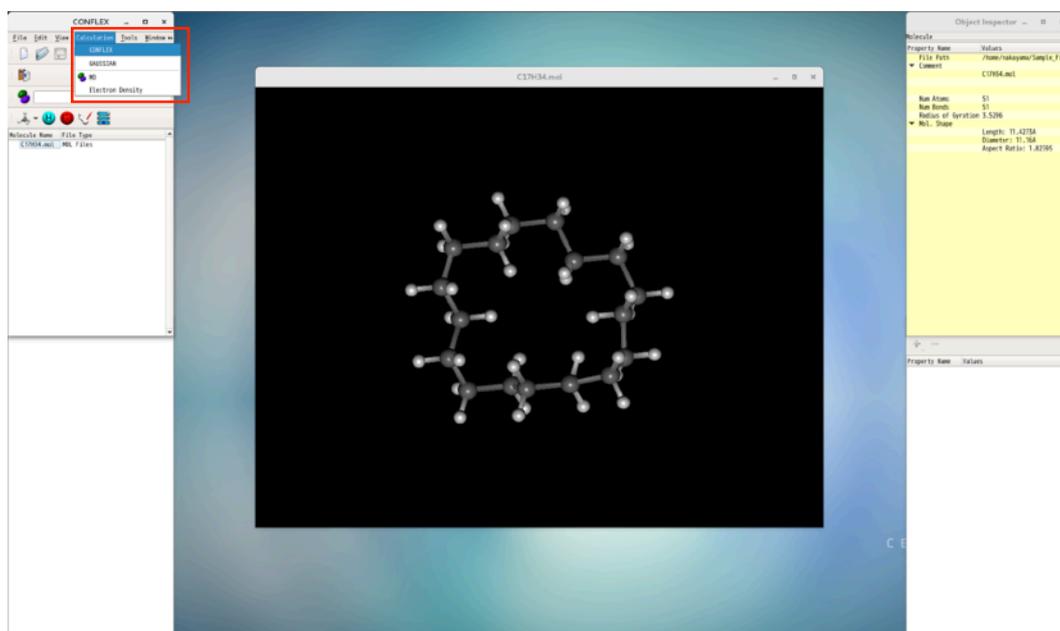
```
[root@centos-linux-7 ~]# ls /usr/local/conflex/
CONFLEX                               components.xml      maintenancetool.ini
CONFLEX_Scheme_Editor.exe             dat                network.xml
CONFLEX_Spectra_Analyzer.exe          doc                par
InstallationLog.txt                   icon.png           platforms
Licenses                               lib                schemes
Sample_Files                           maintenancetool   xcbglintegrations
bin                                     maintenancetool.dat

[root@centos-linux-7 ~]# ls /usr/local/conflex/Sample_Files/
CONFLEX GAMESS Gaussian
[root@centos-linux-7 ~]#
```

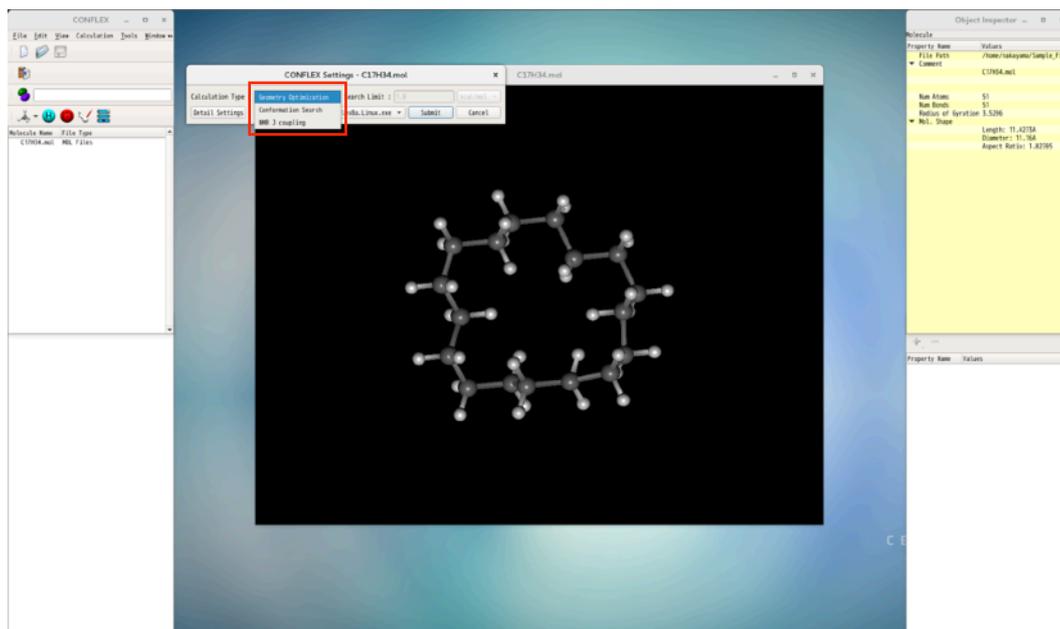
a) Run CONFLEX and open C17H34.mol in “Sample_Files/CONFLEX/conformation_search” folder.



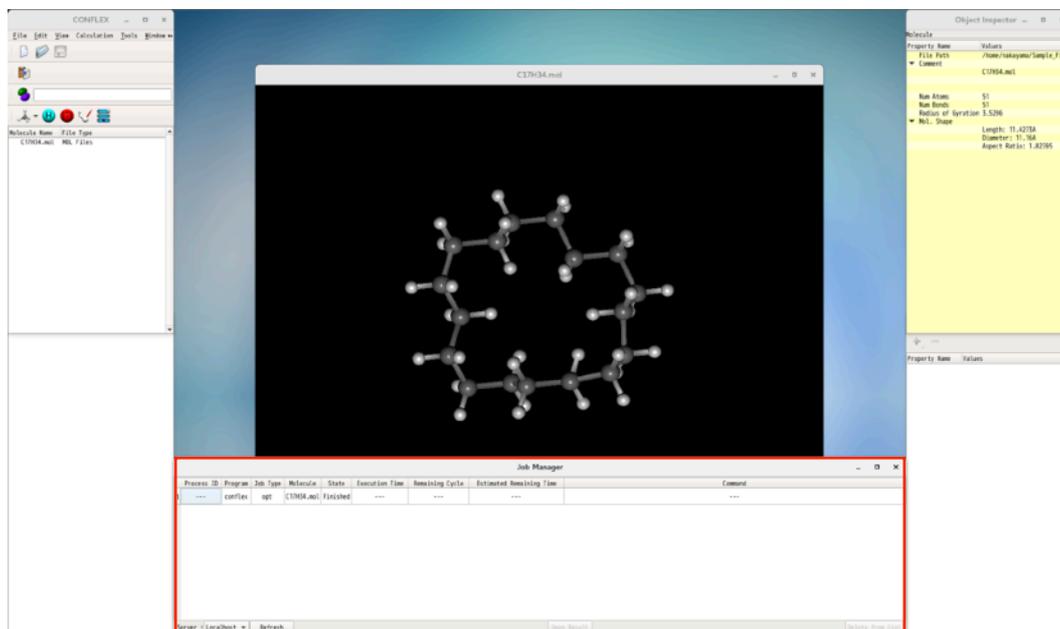
b) Select “CONFLEX” from [Calculation] menu.



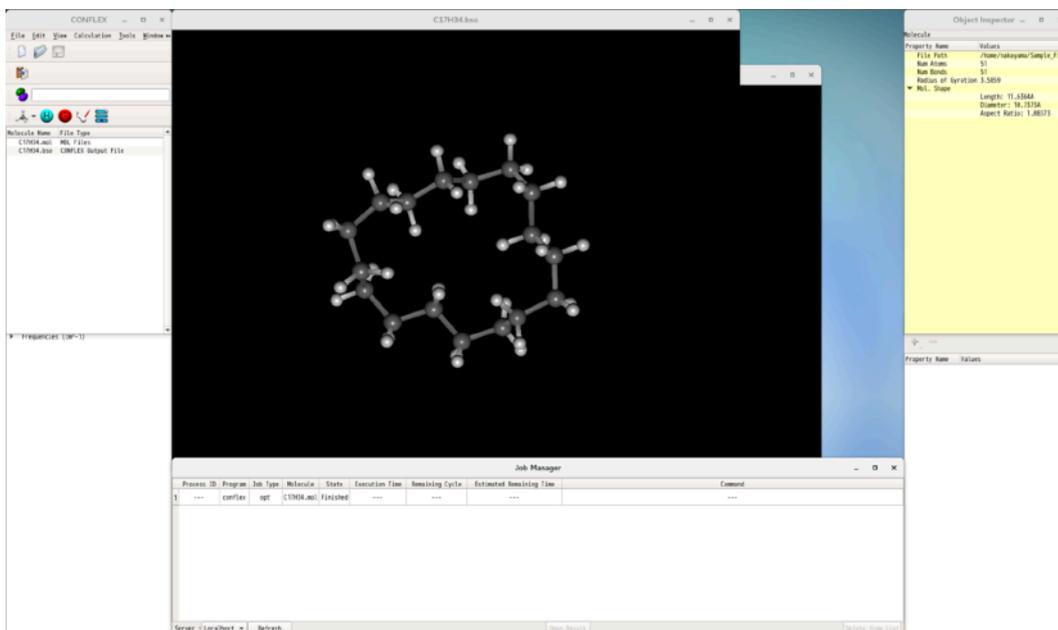
c) Select “Geometry Optimization” and Click “Submit”.



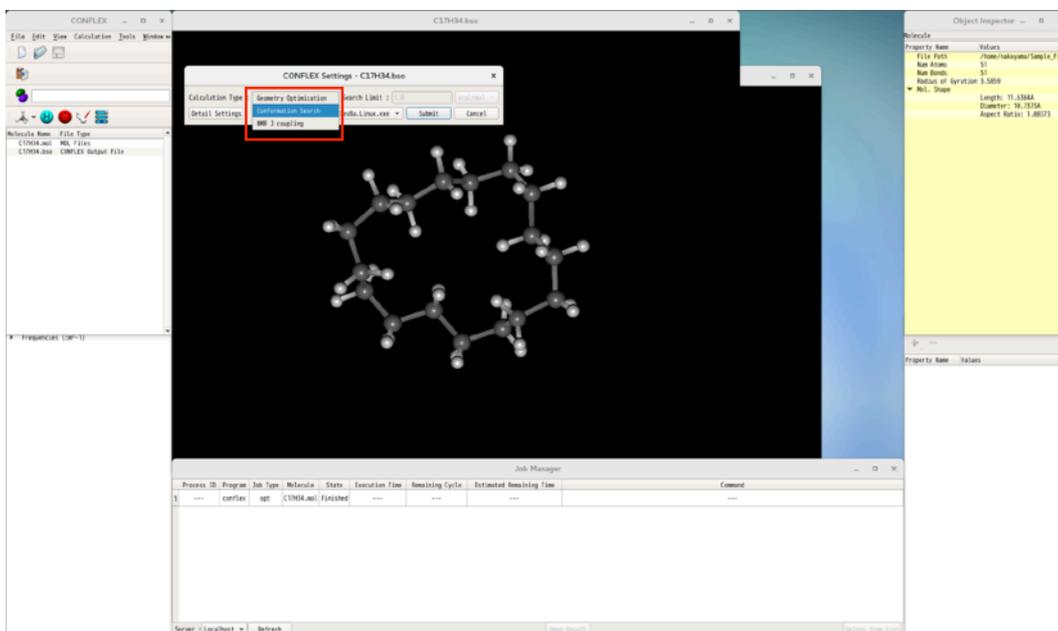
d) Start calculation and appear “Job Manager” window.



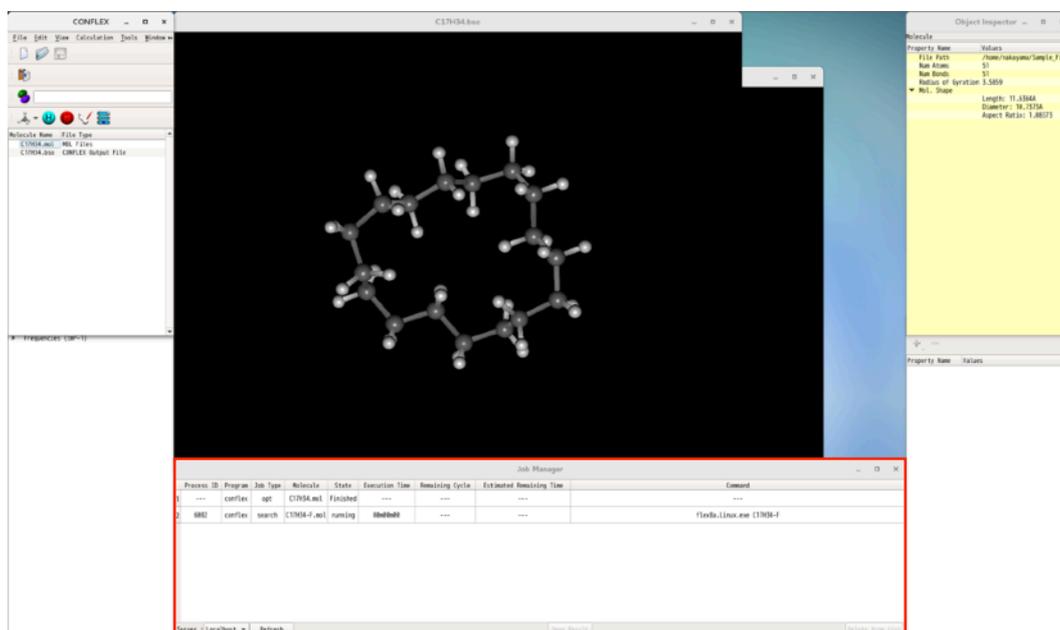
e) Double-click the job in “Job Manager” window after “Running” in the [State] column is changed to “Finished”. C17H34.bso file is opened, and vibrational frequencies can be seen in “Property Box” window.



f) Select “Conformation Search” and Click “Submit”.



g) During the conformation search, the number of remaining cycle and estimated remaining time are displayed in “Job Manager” window.



h) Double-click the job in “Job Manager” window after finished calculation. C17H34-F.sdf is opened, and the conformation list is displayed in “Property Box” window.

