

# **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

CONFLEX Installer Setup	CONFLEX Installer Setup X
etup - CONFLEX	License Agreement Please read the following license agreement. You must accept the term contained in this agreement before continuing with the installation.
elcome to the CONFLEX Setup Wizard.	
	End-User License Agreement
	CONFLEX Corporation
	End-User License Agreement for CONFLEX®
	PLEASE CAREFULLY REVIEW THE FOLLOWING TERMS AND CONDITIONS OF THIS SOFTWARE LICENSE CHTE "LICENSE AGREEMENT"). THIS LICENSE IS A LEGALLY BINDING CONTRACT BETWEEN YOU (THE "LICENSEE") AND CONFLEX COrporation. ("CONFLEX").
	• I accept the license.
	I do not accept the license.
Next > Quit	< <u>B</u> ack Next > Cancel
ii) Click "Next".	iii) Select "I accept the license" and click "Next"
ii) Click "Next".	iii) Select "I accept the license" and click "Next"
ii) Click "Next".	iii) Select "I accept the license" and click "Next"
ii) Click "Next". CONFLEX Installer Setup	iii) Select "I accept the license" and click "Next" CONFLEX Installer Setup
ii) Click "Next". CONFLEX Installer Setup to Install s now ready to begin installing CONFLEX on your computer. tion will use 216.78 MB of disk space.	iii) Select "I accept the license" and click "Next" CONFLEX Installer Setup Completing the CONFLEX Wizard Click Finish to exit the CONFLEX Wizard.
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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 xcbutil-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 :	Send MAC address X
Address :	
ZIP code :	Please register your informations.
Phone No. :	MAC address of this machine is :
FAX No. :	00:11:22:33:44:55
E-Mail address :	Request License Register License
MAC address : 11:22:33:44:55:66	

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

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

when the following screen is shown, click "OK".

		CONFLEX	×
?	This license is for :	Username	OK Cancel

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

CONFLEX		×
<b>()</b>	License file validat	ed
4	Username	
ОК	Hide Details	s
Conflex Corporation Shinagawa Center Bldg. 6F, 3-23-17 Takanawa Minato-ku, Tokyo 108-0074 Japan + 81-3-6380-8290		

## 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				
<pre>[root@centos-linux-7 ~]# ls /usr/local/conflex/Sample_Files/</pre>					
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) <u>Double-click</u> 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) <u>Double-click</u> the job in "Job Manager" window after finished calculation. C17H34-F.sdf is opened, and the conformation list is displayed in "Property Box" window.

