How to Install JSindo

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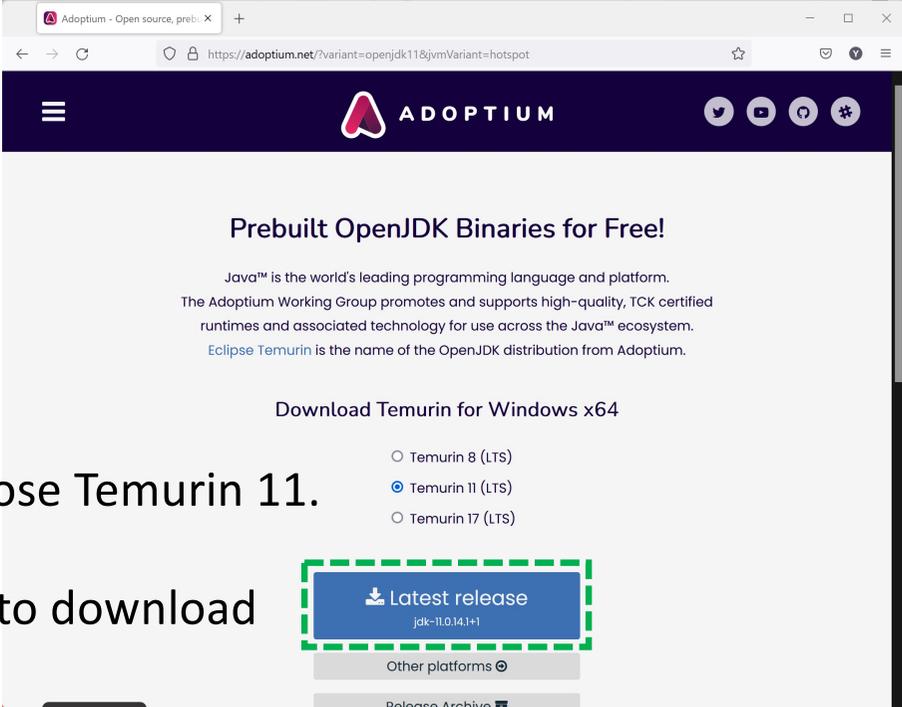
Theoretical Molecular Science Laboratory
RIKEN Cluster for Pioneering Research

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Windows

Download OpenJDK

https://adoptium.net/index.html

Choose Temurin 11.

Click to download

Execute (double click) the downloaded file, and follow the instruction.

Download sindo-4.0_xxxx.zip from our website:
    https://tms.riken.jp/en/research/software/sindo

Unzip (double click) the file, and then double click a jar file,
    sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar

You will see a control panel of JSindo.

You can copy this file to any place (e.g., Desktop), so that you can easily start up the program.

MacOS

Download OpenJDK

https://adoptium.net/index.html

Any version is OK.
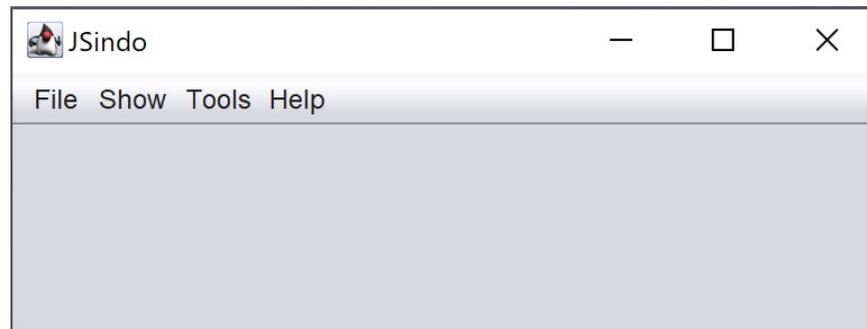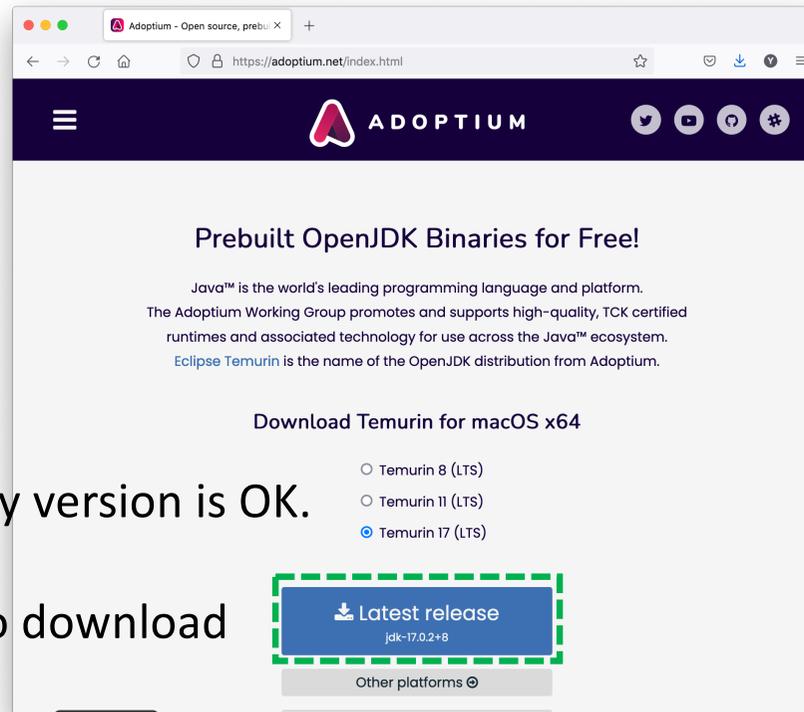
Click to download

Execute (double click) the downloaded file, and follow the instruction.

Download sindo-4.0_xxxx.zip from our website:
https://tms.riken.jp/en/research/software/sindo

Unzip (double click) the file, open a terminal, then type the following command:

```
java –jar /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar
```

or

```
java –cp /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar JSindo
```

You will see a control panel of JSindo.

You may add the following line in your ~/.bashrc,

```
alias jsindo='java –jar /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar'
```

After source, you can invoke the program by typing "jsindo" in the command.

```
> . ~/.bashrc
> jsindo
```

Linux

Download OpenJDK

Install Java 8 or Java 11 using the following command:

```
yum install java-1.8.0-openjdk
```
(CentOS)

```
apt install openjdk-8-jdk
```
(Debian, Ubuntu)

The newer version, Java 17, is also available through package tools, but currently JSindo doesn't work with Java 17.

Alternatively, you may obtain OpenJDK from here,

https://adoptium.net/index.html

This site provides a tarball. Extract the tarball and set the environment variables:

```
export JAVA_HOME=/path/to/jdk-11.0.14.1+1
export PATH=${JAVA_HOME}/bin:${PATH}
```

Download sindo-4.0_xxxx.zip from our website:
https://tms.riken.jp/en/research/software/sindo

Unzip (double click) the file, open a terminal, then type the following command:

```
java –jar /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar
```

or

```
java –cp /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar JSindo
```

You will see a control panel of JSindo.

You may add the following line in your ~/.bashrc,

```
alias jsindo='java –jar /path/to/sindo-4.0_xxxx/JSindo/jar/JSindo-4.0_fat.jar'
```
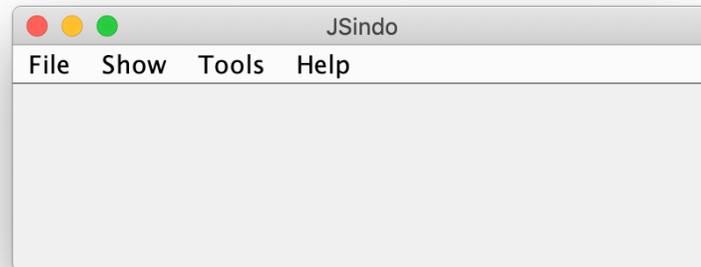
After source, you can invoke the program by typing "jsindo" in the command.

```
> . ~/.bashrc
> jsindo
```

Verify installation

Download doc-4.0_xxxx.zip from our website:
https://tms.riken.jp/en/research/software/sindo

Let's test the program. Sample files are included in
doc-4.0_xxxxxx/JSindo/sample_JSindo.

In JSindo control panel, click File -> Open, choose
"h2co.minfo", and click Open.
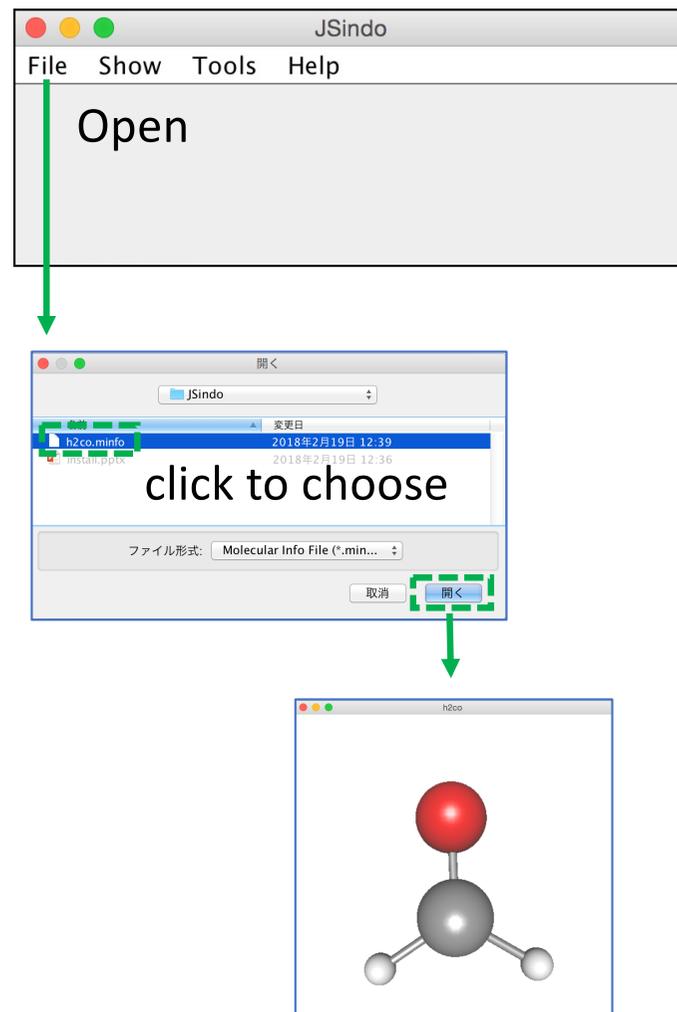
Then, goto Tools -> Harmonic Analysis. This should create a panel of "Normal modes".

If the panel appears, you're all set! Congratulations!

Check on "show vibrational coordinates", and choose a mode you want to see. Vibrational motion will be indicated by arrows. You can "Invert the arrows" by a check box, and change the magnitude using a slider.

Thanks for using JSindo!
Enjoy!
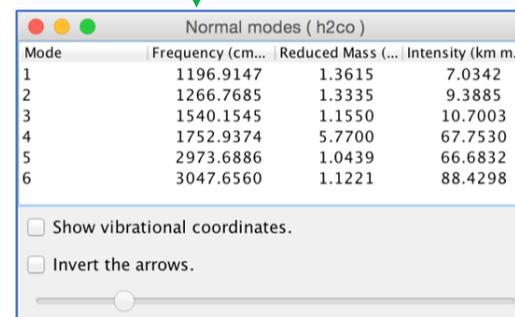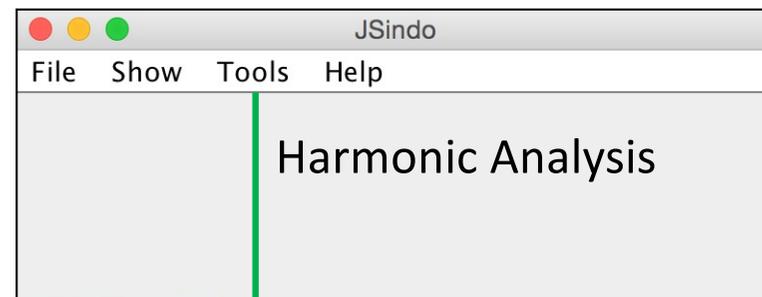
JSindo

File   Show   Tools   Help

Harmonic Analysis

Normal modes (h2co)

Mode	Frequency (cm...	Reduced Mass (...	Intensity (km m...
1	1196.9147	1.3615	7.0342
2	1266.7685	1.3335	9.3885
3	1540.1545	1.1550	10.7003
4	1752.9374	5.7700	67.7530
5	2973.6886	1.0439	66.6832
6	3047.6560	1.1221	88.4298

☐ Show vibrational coordinates.
☐ Invert the arrows.

h2co

FAQ
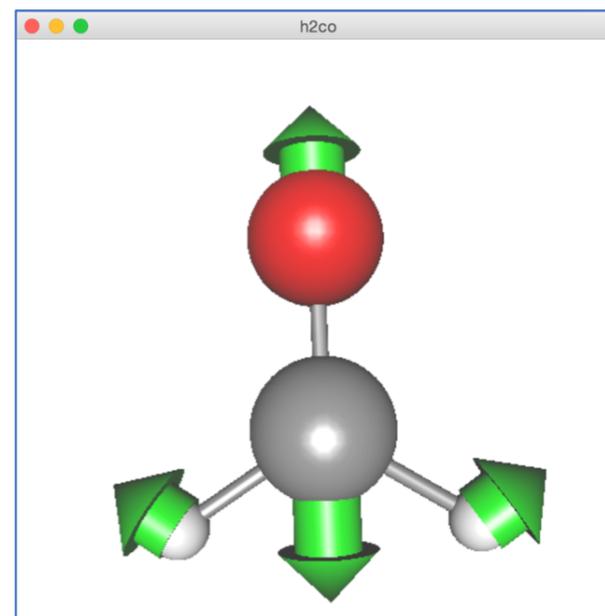
Which version of Java should I use?

Here is a table of available combination as far as I could check.

	Win	MacOS	Linux
Java8	NO	YES	YES
Java11	YES	YES	YES
Java17	NO	YES	NO

Note that this is far from complete.
The result may also depend on the version of OS.

JSindo stops with the following error:

```
Exception in thread "main" java.awt.HeadlessException
    at java.awt.GraphicsEnvironment.checkHeadless(GraphicsEnvironment.java:204)
    …
```

Some distrubutions have a headless version of Java by default. Try the following command to install OpenJDK

```
yum install java-1.8.0-openjdk
```
(CentOS)

```
apt install openjdk-8-jdk
```
(Debian, Ubuntu)

Win

I get JSindo start up, but fonts and icons are too tiny.

This is a general issue of Java/Swing applications when using Java 8 or older with a high DPI diplay. It is fixed after Java 9, so try with a newer version.

I get JSindo start up, but cannot open minfo file with the following error:

```
Exception in thread "AWT-EventQueue-0" java.lang.InternalError: XXX0
profile[1]: GL3bc -> profileImpl GL4bc !!! not mapped
…
```

This error happened to me when I didn't have the right driver installed for my GPU card (Quadro K600). It was solved after installing a NVIDIA driver.

MacOS, Linux

How can I switch the version of Java?

The version can be specified by setting a variable $JAVA_HOME and a path to it.

In MacOS, OpenJDK is installed to /Library/Java/JavaVirtualMachines, so,

```
export JAVA_HOME=/Library/Java/JavaVirtualMachines/temurin-11.jdk/Contents/Home/
export PATH=${JAVA_HOME}/bin:${PATH}
```

In Linux, OpenJDK is installed to /usr/lib/jvm, so

```
export JAVA_HOME=/usr/lib/jvm/java-11-openjdk-xxx
export PATH=${JAVA_HOME}/bin:${PATH}
```