## chem-bla-ics

# CDK is now available from your nearest Debian mirror



Published February 27, 2008

#### Citation

Willighagen, E. (2008, February 27). CDK is now available from your nearest Debian mirror. *Chembla-ics*. https://doi.org/10.59350/g5s78-zqk90

### Keywords

Cdk, Debian

#### **Abstract**

Some days have passed, and the Debian mirrors have now picked up the CDK package (unstable only so far), allowing you to sudo aptitude install libcdk-java from your favorite local mirror. The details are available from this packages.debian.org/libcdk-java page. The fact that it is listed as contrib is a small mistake; the package is really main material.

# Copyright

Copyright © None 2008. Distributed under the terms of the Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

#### chem-bla-ics

Some days have passed, and the Debian mirrors have now picked up the CDK package (unstable only so far), allowing you to **sudo aptitude install libcdk-java** from your favorite local mirror. The details are available from this packages.debian.org/libcdk-java page. The fact that it is listed as contrib is a small mistake; the package is really *main* material.

Now, also make sure to install BeanShell (sudo aptitude install bsh), which allows you to start scripting the CDK. For example, consider this simple script:

```
import org.openscience.cdk.Atom;
Atom atom = new Atom("C");
print(atom);
```

Save this as content of a file **simpleExample.bsh**, and run the bsh program to run the script. You will have to set the **CLASSPATH**, so the full command looks like this on my Linux desktop:

CLASSPATH=/usr/share/java/cdk-interfaces.jar:/usr/share/java/cdk-core.jar:/usr/share/java/cdk-data.jar:/usr/share/java/vecmath1.2-1.14.jar bsh simpleExample.bsh

A wrapper script **cdkbsh** that adds the CLASSPATH seems desirable here :) But you get the point.

Interestingly, BeanShell also comes with a graphical user interface, as well as a command line based scripting environment. Both make perfect set ups for quickly testing some code. The GUI version **xbsh** looks like (don't forget to set the CLASSPATH):

