

# CDK is now available from your nearest Debian mirror

Egon Willighagen 

Published February 27, 2008

## Citation

Willighagen, E. (2008). CDK is now available from your nearest Debian mirror. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/g5s78-zqk90>

## Keywords

Cdk, Debian

## Copyright

Copyright © Egon Willighagen 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](http://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/
```

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`):

