chem-bla-ics

CDK is now available from your nearest Debian mirror

Egon Willighagen

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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
```

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):

