The stylesheet

If you would like to layout the document in the format as it will appear in this newsletter you will need to download a LaTeX distribution. The most common is TeTeX [2] which runs on Unix systems, but also on the Windows platform using CygWin [3]. On the CDK website an example article can be downloaded, as well as the 'CDKnews.sty' stylesheet.

To see what an article will look like when formated using the 'CDKnews.sty' stylesheet the LaTeX source for the article can be wrapped in another file, e.g. 'wrapper.tex', which looks like:

```
\documentclass[a4paper]{report}
\usepackage{CDKnews}

\bibliographystyle{unsrt}

\begin{document}

\begin{article}
  \input{art}
\end{article}

\end{document}
```

The stylesheet should be placed in the same directory as the two TeX files. A PDF file can then be created with the command `pdflatex wrapper.tex`.

I hope that this tutorial helps anyone getting started with using LaTeX for writing articles for this newsletter. Good luck and send in those articles!

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Bibliography

[1] L. Lamport. *LaTeX: A Document Preparation System*. Reading, Massachusetts, 1994.

[2] The teTeX HomePage. `http://www.tug.org/teTeX/`, 2004.

[3] Cygwin Information and Installation. `http://www.cygwin.com/`, 2004.

CDK ChangeLog

"CDK ChangeLog" is a series in the newsletter summarizing the changes in the CDKlibrary since the previous newletter.

by Egon Willighagen

This series gives an overview of recent changes in the CDK library, but in this special case - this is the first newsletter - it will focus on the last few releases. For each release the important changes are given.

The 20040120 Release

- An important change in the release made on 20 January 2004 is the addition of the **ValencyChecker** as an alternative for the older **SaturationChecker**. The difference lies in the list of atom types it uses. The new class uses a list of atom types which explicitely gives the formal charge of the atom type. The **HydrogenAdder** has been adapted to be able to use both checkers; when constructing the object the valency checker that needs to be used can be given:

  ```
  HydrogenAdder hAdder =
    new HydrogenAdder(
      "org.openscience.cdk." +
      "tools.ValencyChecker"
    );
  ```

- The lazyCreation patch was applied to the **ChemObject** improving the memory usage and time to create a new **ChemObject** considerably. This patch was already available in previous releases, but was only applied when specified. The patch delays the memory allocation and initialization of a few object fields until the variable is really used.

- The coordinate system of the **Renderer2D** has changed to match a more commonly used system with (0,0) in the lower-left corner, instead of the top-left corner common in Java. It is important to note that this modification changes wedge bond based stereochemistry!

Many other bug fixes, addition and other changes are documented in the complete CHANGELOG which can be found online [1].

The 20040202 Release

- This release was mostly a bug fix version of the 20040120 release, but also includes a reworked build process: module information is now extracted for the '.java' files using a JavaDoc doclet. This makes compiling of a specific module much easier, and makes it easier to under-

stand dependencies between classes and modules. The doclet creates '*.javafiles' in the src/ directory which explicitely lists all classes in a specific module. And only those get grouped into the jar file for that module.

- Release 20040202 also included updates to the **io** module: a **HINReader** and **HINWriter** for HyperChem (`http://www.hyper.com/`) files were added, the **CMLWriter** can now write namespaced CML, and a stereochemistry writing bug was fixed in the **MDLWriter**.

The 20040324 Release

- The most important change in this release is the generalization of the way in which the **UniversalIsomorphismTester** compares bonds and atoms. The comparison is now customizable with the default being the comparisons that were used sofar: bond order match, and element symbol match. This makes it possible to use more complex ways to compare atoms, and the SMARTS substructure search mentioned elsewhere in this issue is based on this extension.

- Support for reactions was improved in this release. Reaction SMILES can now be parsed and created. These one line representations extend normal SMILES by listing which molecules are reactants, products or agents, like catalysts. The following strings describes the reaction of acetic acid and ethanol under acidic conditions: CC(=O)O.OCC>[H+]>CC(=O)OCC.O.

- Finally, I would like to mention the fix of the **IterationMDLReader** which was introduced in the previous release. This reader allows parsing a SDF file molecule by molecule allowing to process files with thousands of molecules without running out of memory.

Wrap up

A lot of changes are not mentioned in this article. As mentioned earlier, check the full changelog for a complete list of changes [1]. Especially, the API change sections are important, indicating changes which could break your CDK based software.

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Bibliography

[1] CDK ChangeLog. `http://cdk.sf.net/changelog.html`.

 ISSN 1614-7553