

# Submitting articles to CDK News

A tutorial for writing  $\LaTeX$  articles for the CDK News newsletter.

by Egon Willighagen

## Latex

Articles for this newsletter are written in  $\LaTeX$  for its superior layout mechanism [1]. We understand that some users prefer to use Word or OpenOffice, but for this newsletter we will stick to  $\LaTeX$ .

For those who are not familiar with  $\LaTeX$ , it is a documentation tool that separates to a large extent content from layout. This means for the editors that they do not need to bother about designing each issue;  $\LaTeX$  will do that for them. The article source for a submission, however, does not just contain the content, but also mark up about the function of some content. This allows  $\LaTeX$  to properly layout the content to create the nice design of this newsletter.

For example, the title is marked up like `\title{Some Title}`.

A complete example of a CDK News article is as follows:

```
\title{Submitting articles to CDK News}
\subtitle{A tutorial for writing \LaTeX
articles for the \CDKnews newsletter.}
\author{by Egon Willighagen}
```

```
\maketitle
```

```
\section*{Latex}
```

```
Articles for this newsletter are written
in \LaTeX for its superior layout mechanism
\cite{art2:LaTeX}. We understand that some
users prefer to use Word or OpenOffice, but
for this newsletter we will stick to \LaTeX.
```

```
For those who are not familiar with \LaTeX,
it is a documentation tool that separates to
a large extent content from layout. Etc.
```

```
\address{Egon Willighagen\
University of Nijmegen, The Netherlands\
\email{egonw@sci.kun.nl}}
```

Not that complex, is it? Note that new paragraphs are started by having an empty line in the source code. Many other things are marked up using commands, e.g. `\LaTeX`. There are many of them, and a number are special to this newsletter.

There are a number of  $\LaTeX$  commands which are very useful for writing articles. Here are a few supported by the newsletter stylesheet:

`\code` Indicate text that is a literal example of a piece of a program.

`\kbd` Indicate keyboard input.

`\file` Indicate the name of a file.

`\command` Indicate a command name, such as `ls`.

`\dfn` Indicate the introductory or defining use of a term.

`\acronym` Use for abbreviations written in all capital letters, such as 'CDK'.

`\class` Indicate a CDK class, such as **Atom**.

`\pkg` Indicate a java package, such as `java.util`.

`\module` Indicate a CDK module, such as **core**.

`\url` Indicate a URL, such as `http://cdk.sf.net/`.

For example, a command line example should be marked up as `\code{\command{cdk-view} -h}`, resulting in this output: `cdk-view -h`.

Also, the full capabilities of  $\LaTeX$  are at hand. Defining equations is, thus, done as in normal LaTeX. Many  $\LaTeX$  tutorial explain how to include them. Here are a few useful examples.

The verbatim environment is used to wrap multi line source code:

```
\begin{verbatim}
AtomContainer container = new AtomContainer();
container.addAtom(new Atom("C"));
\end{verbatim }
```

of which the output will look like:

```
AtomContainer container = new AtomContainer();
container.addAtom(new Atom("C"));
```

A enumerated list can be made with the `enumerate` environment:

```
\begin{enumerate}
\item First item.
\end{enumerate}
```

The output looks like:

1. First item.

And a simple dotted list with:

```
\begin{itemize}
\item First item.
\end{itemize}
```

The output looks like:

- First item.

The capabilities of  $\LaTeX$  go far beyond this very short introduction. Googling the web for "latex tutorial" will give a list with many sources for further information. Furthermore, the editors may be contacted for assistance.

## 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  $\text{\LaTeX}$  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 formatted using the 'CDKnews.sty' stylesheet the  $\text{\LaTeX}$  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}
```

## CDK ChangeLog

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

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 explicitly 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"
  );
```

```
\end{document}
```

The stylesheet should be placed in the same directory as the two  $\text{\TeX}$  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  $\text{\LaTeX}$  for writing articles for this newsletter. Good luck and send in those articles!

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## Bibliography

- [1] L. Lamport.  *$\text{\LaTeX}$ : 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.

- 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 do-let. This makes compiling of a specific module much easier, and makes it easier to under-