Typesetting Chemical Formulae

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April 11, 2006

Abstract

This is brief introduction to typesetting chemical formulae in LaTeX. Two packages `pst-rel-points.sty` and `pst-chem-formula` (both developed by yours truly!) make it easy to typeset chemical formulae.

1 Examples

First we show a few examples. Then we describe the main commands which are used. This is the first forumula $\underset{\substack{| \\ \mathrm{Br}}}{\mathrm{CH_3CH}}\,\overset{\substack{\mathrm{CL} \\ |}}{\mathrm{C}}\mathrm{HCH{=}CHCH_3}$ and the second formula is $\mathrm{CH_3CO_2}\overset{\substack{\mathrm{CH_2} \\ \|}}{\mathrm{C}}\mathrm{CH_3}$. Observe how the full stop appeared on the next line. This is because the horizontal space provided for the `pspicture` environment is a little less than required. A bit of experimentation should get it right. It is possible to get more spacing by splitting the text chunks. Thus the modified second formula with additional horizontal space is $\mathrm{CH_3\ CO_2}\ \overset{\substack{\mathrm{CH_2} \\ \|}}{\mathrm{C}}\ \mathrm{CH_3}$. One needs to fix the height and the width of the `pspicture` envirnonment While adjusting the height, one also needs to change the value of the parameter to `\raisebox` command. Actually we need negative raisebox only if we have a line below the main fragment of the formula which is horizontally aligned with the text line. The trick to get the height, width, and horizontal spacing right is to use `\psframe` command with the same parameters as `pspicture` environment. The last formula below exemplifies it.

The third example $\mathrm{CH_3}\underset{\substack{| \\ \mathrm{NHCH_3}}}{\overset{\substack{\mathrm{CL} \\ |}}{\mathrm{C}}}\mathrm{H\ CHCH{=}CHCH_3}$ is a slight modification of the first formula in which the top branch has been shifted a bit and a longer string has been included in the bottom branch. Our final formula is $\boxed{\mathrm{CH_3CH_2}{-\!\!-}\overset{\substack{\mathrm{CH_2} \\ \|}}{\mathrm{C}}{-\!\!-}\mathrm{CH\ (CH_3)_2}}$.

2 Commands

We need to use the `pspicture` environment from `pstricks` package. The LaTeX source of this document is also bundled with the tarball so it should be easy to figure out. Basically we need to specify

- The width and the height of the box to be created.
- The amount by which the box should be lowered (using `raisebox` command) for three line formulae so that the main fragment alings properly with the text line.

- The amount by which the main fragment should be raised in the lowered box (using `\sety` command).

- The amount by which the upper and the lower branches should be seprated from the main fragment (using `\setdy` command). The default value is 10.

For `pst-rel-points` to be of any help, we need to set the `unit` to be very small (may be `1mm` or `.9mm`).

Having specified the above, main commands to be used within the `pspicture` environment are:

- `\fpnode{nodeName}{stuffToTypeset}`. This is the *first* box which appears in the formula. If this is not contained, then the LaTeX file won't compile.

- `\apnode{nodeName}{predNode}{stuffToTypeset}{lineStyle}`. This command puts the `stuffToTypeset` *a*bove the `predNode` (by an amount `dy` set by `\setdy` command). The `lineStyle` can be
  - `sline` for a single line,
  - `dline` for a double line,
  - empty for no line (empty as in `{}` and not `empty`).

- `\bpnode{nodeName}{predNode}{stuffToTypeset}{lineStyle}`. Exactly same as `apnode` except that this puts the `stuffToTypeset` *b*elow the `predNode`.

- `\rpnode{nodeName}{predNode}{stuffToTypeset}{lineStyle}{deltax}`. Same as `apnode` and `bpnode` except that in this case the `stuffToTypeset` is put on the *r*ight of the `predNode`. It requires an additional parameter `deltax` because there is no way of knowing where the `predNode` box ended.

We reproduce the source of the first formula below to illustrate the commands.

```
\newcommand{\firstformula}{%
\sety{6}%
\setdy{8}%
\psset{unit=.95mm}%
\raisebox{-2.8em}{%
\begin{pspicture}(0,-5)(41,17)
%\psframe(0,-5)(41,17)
\fpnode{n1}{CH$_3$}
\rpnode{n2}{n1}{CH}{}{7}
\bpnode{n21}{n2}{Br}{sline}
\rpnode{n3}{n2}{CHCH}{}{6}
\apnode{n31}{n3}{CL}{sline}
\rpnode{n4}{n3}{CHCH$_3$}{dline}{14}
\end{pspicture}
}%
}
```

Observe the use of `%` at the end of some of the lines. This prevents spurious spaces in the output.

3 Epilogue

The tarball containing all of the above is available at

`http://www.cse.iitb.ac.in/~uday/latex/chemFormulae.tgz`

Some day I hope to write a similar document for `pst-rel-points` package also. I ended up writing this document because someone (he-who-need-not-be-named!) wanted to typeset chemical formulae. Thanks to he-who-need-not-be-named.