[XꟿMTEX-Tips 130208b-pdf]
Caffeine with Coloring Substituents and Bonds

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Question:

How can I draw caffeine with coloring substituents and bonds by XꟿMTEX?

Answer:

The PDF mode of XꟿMTEX (as well as the PostScript mode) supports coloring substituents and bonds [1]. For example, the following code for the PostScript mode (named "testCaffeineA.tex") is first executed by the LATEX system:

```
%testCaffeineA.tex
\documentclass{article}
%\usepackage{xymtexps}%PostScript mode: dvi--- (dvips) --- ps file
\usepackage{xymtexpdf}%PDF mode: dvi --- (dvipdfmx) ---pdf file
\usepackage{graphicx}
%\pagestyle{empty}% for conversion into eps file
\begin{document}

\sixheterov[e{e\fivefusev[d]{1=={\blue N};4=={\blue N}}{1==CH$_{3}$}{b}}]
{1=={\blue N};3=={\blue N}}
{1==CH$_{3}$;3==CH$_{3}$;2D=={\red O};4D=={\red O}}
\\ \vskip.5cm
{%
\let\substfont=\sffamily
\purinev[aj]{3==CH$_{3}$;%
4D=={\red\aftergroup\blue O};5==CH$_{3}$;%
6D=={\red\aftergroup\blue O};7==CH$_{3}$}
\quad
\def\gray{\color{gray}}%necessary in the PDF mode
\def\colorBgAr#1{\red\aftergroup\green #1}
\def\colorBgyAr#1{\gray\aftergroup\blue #1}
\nonaheterov[aj]{1=={\blue N};3=={\blue N};5=={\blue N};7=={\blue N}}%
{3==\colorBgyAr{CH$_{3}$};%
4D==\colorBgAr{O};5==\colorBgyAr{CH$_{3}$};%
6D==\colorBgAr{O};7==\colorBgyAr{CH$_{3}$}}}
}

\end{document}
```

The execution is conducted by writing the following command in the command line of a command-prompt window of Windows:

```
c:> latex testCaffeineA
```

Then, the resulting .dvi file (named testCaffeineA.dvi) is converted into a .pdf file by using dvips.
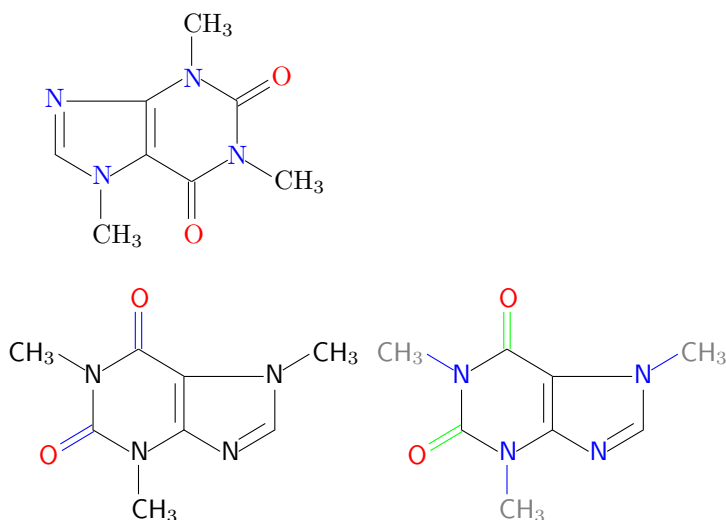
```
c:> dvipdfmx -d5 testCaffeineA
```

> **Note**
>
> The use of `dvipdfmx` in processing the resulting dvi files containing these coloring codes may result in the appearance of a warning:
>
> ```
> ** WARNING ** Color stack underflow. Just ignore.
> ```
>
> In spite of this warning, we can obtain the correct printing of structural formulas. So we just ignore this warning.

Thereby, we obtain a .pdf file (testCaffeineA.pdf), which contains the following structural formulas of caffeine:
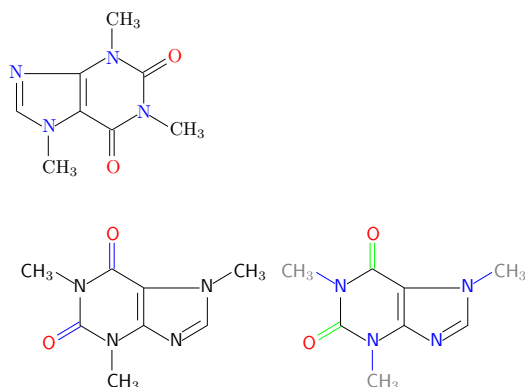

The .pdf file can be browsed by an appropriate browser such as the Adobe Reader.

Including .pdf Files into a .tex File

For the purpose of including .pdf Files into a .tex File, the commented line "`%\pagestyle{empty}`" is revived to be effective ("`\pagestyle{empty}`") and the modified .tex file is processed by LaTeX. The resulting .dvi file is converted into a .pdf file as described above: The resulting .pdf file (testCaffeineA.pdf) can be inserted into a .tex file by using the command of the graphicx package, i.e., `\includegraphics`.

```
\includegraphics[bb=133 515 408 720, scale=0.7]{testCaffeineA.pdf}
```

The setting of bb corresponds to the "BoundingBox: 133 515 408 720", where the set of values determined in big points indicates a clipped rectangle decided by the lowerleft point (133, 515) and the upperright point (408, 720). Thereby, the following diagram is inserted:
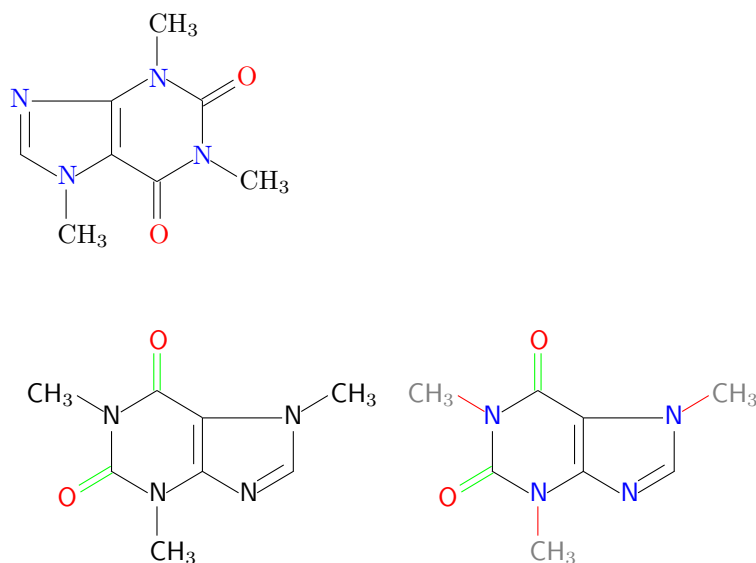
Avoiding "** WARNING ** Color stack underflow"

To avoid the warning "** WARNING ** Color stack underflow" during processing by the dvipdfmx converter, command-type commands such as `\redx` and `\bluex` can be used in the PDF mode (as well as the PostScript mode) in place of declare-type commands such as `\red` and `\blue`. Moreover, the `\addbscolor` command can be used to color bonds and substituents.

```
\documentclass{article}
%\usepackage{xymtexps}
\usepackage{xymtexpdf}
\usepackage{graphicx}
\pagestyle{empty}
\begin{document}

\sixheterov[e{e\fivefusev[d]{1==\bluex{N};4==\bluex{N}}{1==CH$_{3}$}{b}}]
{1==\bluex{N};3==\bluex{N}}
{1==CH$_{3}$;3==CH$_{3}$;2D==\redx{O};4D==\redx{O}}
\\ \vskip0.5cm
{%
\let\substfont=\sffamily
\purinev[aj]{3==CH$_{3}$;%
4D==\addbscolor{\green}{\redx{O}};5==CH$_{3}$;%
6D==\addbscolor{\green}{\redx{O}};7==CH$_{3}$}
\qquad
\def\grayx#1{\xymcolor{gray}{#1}}
\nonaheterov[aj]{1==\bluex{N};3==\bluex{N};5==\bluex{N};7==\bluex{N}}%
{3==\addbscolor{\red}{\grayx{CH$_{3}$}};%
4D==\addbscolor{\green}{\redx{O}};5==\addbscolor{\red}{\grayx{CH$_{3}$}};%
6D==\addbscolor{\green}{\redx{O}};7==\addbscolor{\red}{\grayx{CH$_{3}$}}}
}

\end{document}
```

This code contains the definition of a new command-type command `\grayx`. The successive treatment of the code by LaTeX and dvipdfmx produces the following diagram:

References

[1] Manual for XΥMTEX version 5.00 (xymtex500.pdf)
http://xymtex.com/fujita3/xymtex/index.html (Japanese)
http://xymtex.com/fujita3/xymtex/indexe.html (English)