[XΥMTEX-Tips 130208b-ps]
Caffeine with Coloring Substituents and Bonds

Shinsaku Fujita

Shonan Institute of Chemoinformatics and Mathematical Chemistry

February 8, 2013

Question:

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

Answer:

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

```
%testCaffeine.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 testCaffeine
```

Then, the resulting .dvi file (named testCaffeine.dvi) is converted into a .ps file by using dvips.

```
c:> dvips -Pdl -D2400 testCaffeine
```

Thereby, we obtain a .ps file (testCaffeine.ps), which contains the following structural formulas of caffeine:
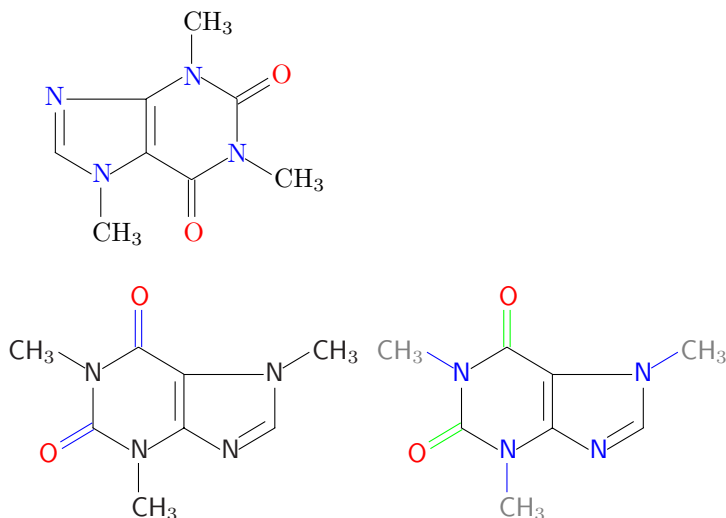
The .ps file can be converted into a .pdf file by using an appropriate converter such as the Adobe Distiller.
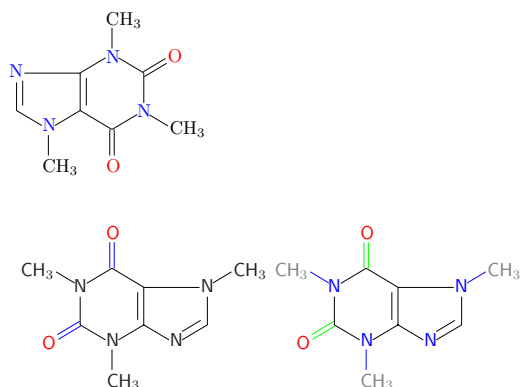
1   Getting .eps Files

For the purpose of obtaining an .eps 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 an .eps file as follows:

```
c:> dvips -E -D2400 -Pdl  -p1 -n1 testCaffeine.dvi -o testCaffeine.eps
```

The resulting .eps file (testCaffeine.eps) can be inserted into a .tex file by using the command of the graphicx package, i.e., `\includegraphics`.

```
\begin{center}
\includegraphics[scale=0.7]{testCaffeine.eps}
\end{center}
```

Thereby, we obtain the following diagram with size reduction:

References

[1] Manual for XƔMTEX version 5.00 (xymtex500PS.pdf)
    http://xymtex.com/fujita3/xymtex/index.html (Japanese)
    http://xymtex.com/fujita3/xymtex/indexe.html (English)