XyMTEX for Typesetting Chemical Structural Formulas. Size Reduction and Added Commands for Version 3.00

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Contents

Chapter 1

Introduction

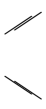
1.1 History

The previous versions of the XyMTEX system are summarized in Table 1.1. A brief history has been described in the on-line manual attached to Version 2.00. The manual for Version 1.01 (attached to this distribution and published as a reference book [3]) and the manual for Version 2.00 (attached to this distribution) have described the specification and the usage of commands supported by the XyMTEX system. They are still effective for Version 3.00.

Table 1.1: Versions of XyMTEX

version	package files and comments
1.00 (1993)	(for LaTeX2.09) See Ref. [1, 2]. aliphat.sty, carom.sty, lowcycle.sty, hetarom.sty, hetaromh.sty, hcycle.sty, chemstr.sty, locant.sty, xymtex.sty
1.01 (1996)	(for LaTeX 2_ε) See Ref. [3]. ccycle.sty, polymers.sty, chemist.sty
1.02 (1998)	(not released) Nested substitution by 'yl'-function.
2.00 (1998)	Enhanced version based on the XyM Notation. See Ref. [4]. fusering.sty, methylen.sty
2.01 (2001)	(not released) Size reduction, sizeredc.sty (version 1.00)
3.00 (2002)	(this version) Size reduction (sizeredc.sty, version 1.01), and reconstruction of the command system

To be as portable as possible, the XyMTEX system has been designed to depend on the LaTeX picture environment and only one command of epic.sty (`\dottedline`), since the mechanism of epic.sty for obtaining the slope of a line sometimes provides an erroneous result so that it occasionally gives a split line. For example, the commands `\drawline(0,0)(171,103)` and `\drawline(0,0)(171,-103)` of epic.sty under `\unitlength=0.08pt` give the following split lines if we encounter the wrongest situation:



This is because we have adopted the `\dottedline` of epic.sty only in the XyMTEX system. This means, however, that the previous versions of XyMTEX have no methods of reducing the size of a formula into

less than `\unitlength=0.1pt`, since the original picture environment of LaTeX 2_ε cannot draw a short line.

The XymTEX version 2.00 permits us to a nested usage of commands, where many flags (`\@acliptrue` etc.) have been declared for designating vertices to be clipped. It follows that these flags may interfere each other in a nested condition.

Accordingly, the purposes of the present version (3.00) are

1. to give functions for reducing sizes of structural formulas (sizeredc.sty),
2. to give a more reliable mechanism for clipping (truncating) vertices, and
3. to add further commands for drawing cyclic sugars (hcycle.sty).

1.2 Package Files of XymTEX Version 3.00

The XymTEX system (version 3.00) consists of package files listed in Table 1.2.

Table 1.2: Package Files of XymTEX

package name	included functions
aliphat.sty	macros for drawing aliphatic compounds
carom.sty	macros for drawing vertical and horizontal types of carbocyclic compounds
lowcycle.sty	macros for drawing five-or-less-membered carbocycles.
ccycle.sty	macros for drawing bicyclic compounds etc.
hetarom.sty	macros for drawing vertical types of heterocyclic compounds
hetaromh.sty	macros for drawing horizontal types of heterocyclic compounds
hcycle.sty	macros for drawing pyranose and furanose derivatives (added further commands for cyclic sugars in Version 3.00)
chemstr.sty	basic commands for atom- and bond-typesetting
locant.sty	commands for printing locant numbers
polymers.sty	commands for drawing polymers
fusering.sty	commands for drawing units for ring fusion
methylen.sty	commands for drawing zigzag polymethylene chains
xymtex.sty	a package for calling all package files
chemist.sty	commands for using 'chem' version and chemical environments
sizeredc.sty	commands for size reduction (Version 1.01)

The use of xymtex.sty calling all package files may sometimes cause the "TEX capacity exceeded" error. In this case, you should call necessary packages distinctly by using the `\usepackage` command in the following way:

```
\documentclass{article}
%\usepackage{xymtex}% to use for large capacity of computer
\usepackage{carom}
\usepackage{hetaromh}
\usepackage{aliphat,hcycle}
\usepackage{fusering}
\usepackage{locant}
\usepackage{epic}
\usepackage{sizeredc}
```

```
\usepackage{xymman}
\begin{document}
(texts and formulas)
\end{document}
```

Chapter 2

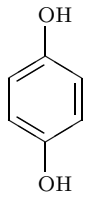
Size Reduction

2.1 Basic Functions

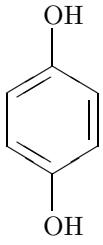
2.1.1 Changing Unit Lengths

The default unit length of the XeLaTeX system is equal to 0.1pt. This setting can be changed by the command `\changeunitlength`, which is defined in the sizeredc.sty package. As shown in the following code, the setting by `\changeunitlength` can be done in the preamble of a document if the value is used in the whole document.

```
\documentclass{article}
\usepackage{carom}
\usepackage{sizeredc}
\changeunitlength{0.08pt}
\begin{document}
\bzdrv{1==OH;4==OH}
\end{document}
```



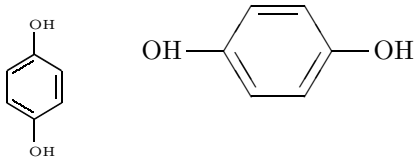
Compare this formula with the counterpart with the standard unit length (0.1pt).



The command `\changeunitlength` can be declared at any place of a document, where the setting of the command is effective after the declaration place until an alternative declaration is carried out afterward. The grouping technique can be used to limit the effect of the setting within a pair of braces. For example, the code represented by

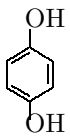
```
{%grouping by braces
\changeunitlength{0.06pt}
\bzdrv{1==OH;4==OH}}
\qquad \bzdrh{1==OH;4==OH}
```

produces a size-reduced formula as follows:



The \changeunitlength sets a unit length given as an argument and declares a flag represented by \sizereductiontrue if the argument is less than 0.1pt. The flag is used to substitute the \drawline command of epic.sty for the \line command of LaTeX 2_ε. Hence, the following setting is equivalent to the setting derived from the declaration command \changeunitlength{0.05pt} within the TeX/LaTeX compatible mode.

```
{%
\scriptsize
\unitlength=0.05pt
\sizereductiontrue
\bzdrv{1==OH;4==OH}
}
```



2.1.2 Size Reduction of Carbocycles

When the \sizereductiontrue is not declared (i.e. \sizereductionfalse), the original picture environment of LaTeX 2_ε works. The following example shows the comparison between cases with and without the use of sizeredc.sty. Note Version 4.00 requires the declaration of \originalpicture.

```
\begin{table}
\caption{With and Without \textsf{sizeredc.sty}}
\label{tt:300c}
\begin{center}
\begin{tabular}{ll}
\hline
without \textsf{sizeredc.sty} & with \textsf{sizeredc.sty} \\
\hline
0.08pt &  \\
{\originalpicture\unitlength=0.08pt \bzdrv{}} &
{\changeunitlength{0.08pt}\bzdrv{}} \\
0.07pt & \\
{\originalpicture\unitlength=0.07pt\bzdrv{}} &
{\changeunitlength{0.07pt}\bzdrv{}} \\
0.06pt & \\
{Version 4.00 \originalpicture\unitlength=0.06pt \bzdrv{}} &
{\changeunitlength{0.06pt}\bzdrv{}} \\
\hline
\end{tabular}
\end{center}
\end{table}
```

Table 2.1: With and Without sizeredc.sty

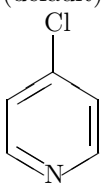
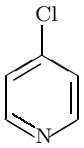
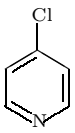
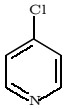
without sizeredc.sty	with sizeredc.sty
0.08pt	
	
0.07pt	
	
0.06pt	
	

This code gives the results shown in Table 2.1. Without sizeredc.sty, the resulting formulas (0.07pt and 0.06pt in the left column) have no slanting lines (inner double bonds) in agreement with the original specification of the LaTeX 2_ε picture environment.[1] By using sizeredc.sty, the slanted lines are revived, as shown in the right column of Table 2.1.

2.1.3 Size Reduction of Heterocycles

Table 2.2 shows the effect of size reduction to the drawing of 4-chloropyridine, where `\unitlength` is changed from 0.1pt (default value) to 0.04pt by using `\changeunitlength`.

Table 2.2: Size Reduction of 4-Chloropyridine

0.1pt (default)	0.08pt	0.07pt	0.06pt	0.05pt	0.04pt
					

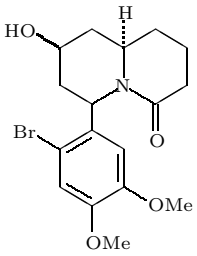
[1] Note that XeTeX is based on the LaTeX 2_ε picture environment without using sizeredc.sty. The slanted lines of the benzene ring are drawn by the \line command with slopes $(5, 3)$ and $(5, -3)$.

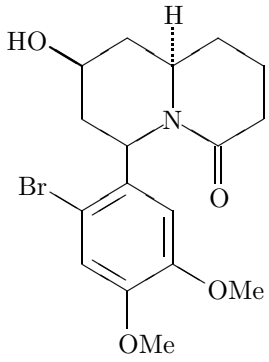
2.1.4 Nested Substitution

Formulas by nested substitution can be totally reduced in size by the following code:

```
\changeunitlength{0.07pt}
\scriptsize
\decaheterov[]{4a==N}{4D==O;7B==HO;{{10}A}==H;%
5==\bzdrv{3==OMe;4==OMe;6==Br;1==(yl)}}
```

This code produces the left formula shown below:

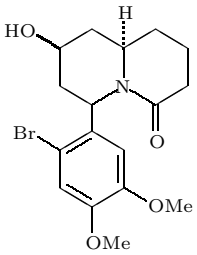




The right formula is drawn by the same code with the standard unit length (0.1pt).

Spaces between dots in a dotted line can be changed by redefining the command `\dottedline` as follows.

```
\makeatletter
\let\olddottedline=\dottedline
\def\dottedline#1(#2,#3)(#4,#5){\ifsizereduction
\olddottedline{30}(#2,#3)(#4,#5)\else
\olddottedline{#1}(#2,#3)(#4,#5)\fi}
\makeatother
\changeunitlength{0.07pt}
\scriptsize
\decaheterov[]{4a==N}{4D==O;7B==HO;{{10}A}==H;%
5==\bzdrv{3==OMe;4==OMe;6==Br;1==(yl)}}
```

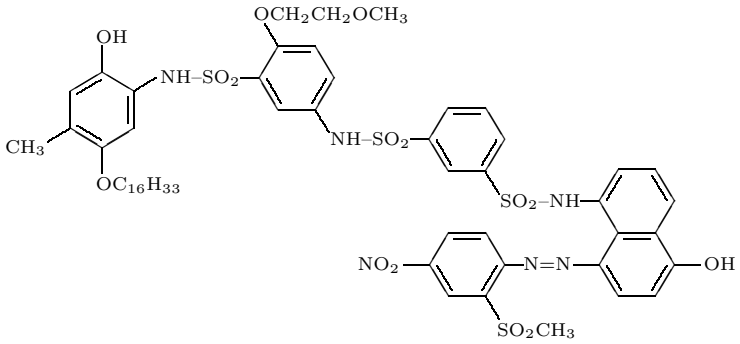


A cyan dye releaser has been drawn by using two or more `\ryl` and `\lyl` commands, as shown in the on-line manual of XΥMTEX Version 2.00 and has also been depicted in different ways (see Chapters 14 and 15 of the XΥMTEXbook [3]). The size of the formula can be reduced with a code represented by

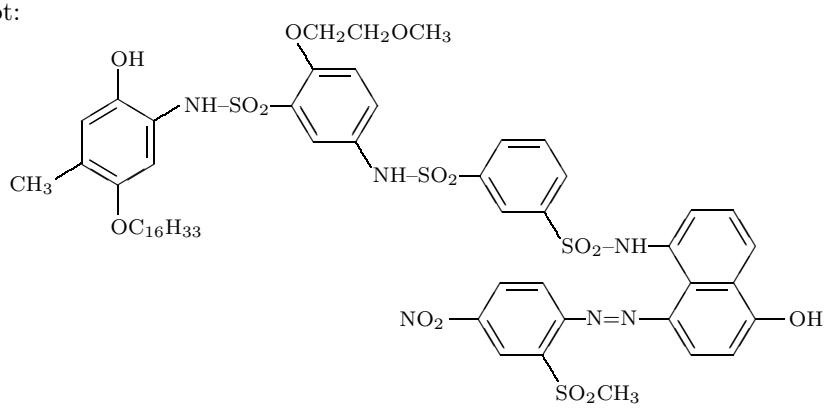
```
\changeunitlength{0.07pt}
%\changeunitlength{0.08pt}
\scriptsize
\bzdrv{1==OH;5==CH$_{3}$;4==OC$_{16}$H$_{33}$;%
2==\ryl(4==NH--SO$_{2}$){4==\bzdrh{1==(yl);2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
5==\ryl(2==NH--SO$_{2}$){4==\bzdrh{1==(yl);%
5==\ryl(2==SO$_{2}$--NH){4==\naphdrh{1==(yl);5==OH;%
8==\lyl(4==N=N){4==\bzdrh{4==(yl);1==NO$_{2}$;5==SO$_{2}$CH$_{3}$}}}}}}}}}
```

Thereby, we obtain a target formula:

—0.07pt:

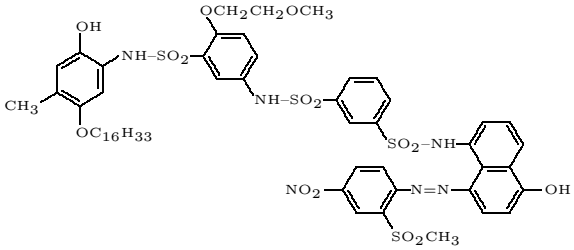


—0.08pt:



A further reduction is possible. The following example shows the case of `\unitlength=0.05pt` and font size of `\tiny`.

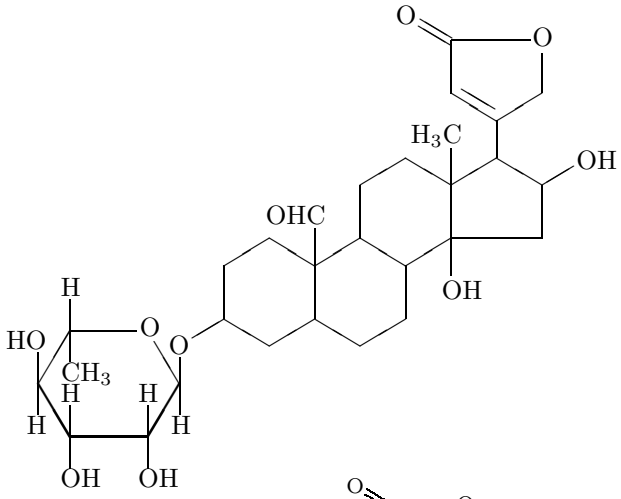
—0.05pt:



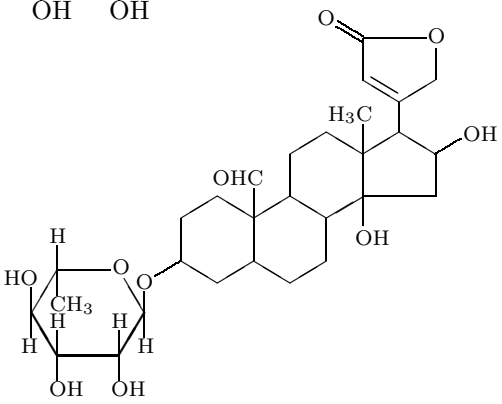
The structural formula of adonitoxin, which has once been depicted in a different way in Chapter 15 of the XyMTEXbook can be obtained by the code,

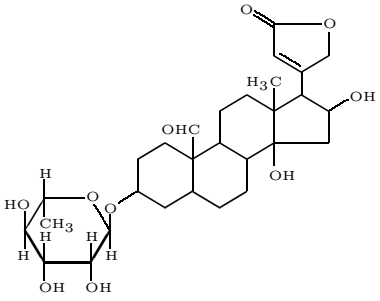
```
\steroid{{{10}}==\lmoiety{OHC};{{14}}==OH;%
{{13}}==\lmoiety{H$_{3}$C};{{16}}==OH;%
{{17}}==\fiveheterov[e]{3==O}{4D==O;1==(yl)};%
3==\lyl(3==O){8==%
\pyranose{1Sb==(yl);1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==CH$_{3}$}}}
```

—0.1pt



—0.08pt





Bibliography

[1] Fujita S., "Typesetting structural formulas with the text formatter TEX/LATEX", *Comput. Chem.*, **18**, 109 (1994).

[2] Fujita S., "XYMTEX for Drawing Chemical Structural Formulas", *TUGboat*, **16** (1), 80 (1995).

[3] Fujita, S., *XYMTEX—Typesetting Chemical Structural Formulas*, Addison-Wesley, Tokyo (1997). The book title is abbreviated as "XYMTEXbook" in the present manual.

[4] Fujita, S.; Tanaka, N. "XyM Notation for Electronic Communication of Organic Chemical Structures", *J. Chem. Inf. Comput. Sci.*, **39**, 903 (1999).

[5] NIFTY-Serve achieves, FPRINT library No. 7, Item Nos. 201, 202, 204.

[6] CTAN, tex-archive/macros/latex209/contrib/xymtex/.

[7] Lamport L., *LATEX. A document Preparation System*, 2nd ed. for LATEX 2ε, Addison-Wesley, Reading (1994). See also Lamport L., *LATEX. A document Preparation System*, Addison-Wesley, Reading (1986).

[8] Goossens, M., Mittelbach, F., & Samarin, A., *The LATEX Companion*, Addison-Wesley, Reading (1994).

[9] NIFTY-Serve achieves, FPRINT library No. 7, Item Nos. 385, 386.

[10] http://imt.chem.kit.ac.jp/fujita/fujitas/fujita.html

[11] For the TEX system, see Knuth D. E., *The TEXbook*, Addison-Wesley, Reading (1984).

[12] For the ChemTEX macros, see Haas R. T. & O'Kane K. C., *Comput. Chem.*, **11**, 251 (1987).

[13] For drawing chemical formulas by TEX, see Ramek, M., in Clark, M. (ed), TEX: Applications, Uses, Methods, Ellis Horwood, London (1990), p. 277.

[14] For chemical application of the LATEX system, see Fujita S., *Kagakusha-Seikagakusha no tame no LATEX (LATEX for Chemists and Biochemists)*, Tokyo Kagaku Dozin, Tokyo (1993).

[15] For epic macros, see Podar S., "Enhancements to the picture environment of LATEX", Manual for Version 1.2 dated July 14, 1986.

[16] For graphic applications of TEX, LATEX and relevant systems, see Goossens, M., Rahtz, S., & Mittelbach, F., *LATEX Graphics Companion*, Addison Wesley Longman, Reading (1997).