

Software & Tools

Size reduction of chemical structural formulas in $\hat{\text{X}}\text{M}\text{T}\text{E}\text{X}$ (Version 3.00)

Shinsaku Fujita* and Nobuya Tanaka

1 Introduction

The $\hat{\text{X}}\text{M}\text{T}\text{E}\text{X}$ system (Version 2.00) [1], which we released as an implementation of the $\hat{\text{X}}\text{M}$ Notation [2] and the $\hat{\text{X}}\text{M}$ Markup Language [3], has provided a convenient method for drawing complicated structural formulas. The $\hat{\text{X}}\text{M}\text{T}\text{E}\text{X}$ system has been designed to assure maximal portability within the scope of $\text{L}\text{A}\text{T}\text{E}\text{X}/\text{L}\text{A}\text{T}\text{E}\text{X} 2_{\epsilon}$ [4, 5]. The version 2.00

* To whom correspondence should be addressed.

has, however, suffered from a drawback that the size reduction of structural formulas has not been permitted. This has come from the fact that the $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ system has depended on the $\text{\L}\text{\A}\text{\T}\text{\E}\text{\X}$ picture environment that has been incapable of drawing short bonds (lines). Although the *epic* system [6] has been used to draw short lines so as to maintain such portability, it has occasionally given a split line. For example, the commands of the *epic* system,

```
\drawline(0,0)(171,103) and
\drawline(0,0)(171,-103),
```

are necessary to draw a benzene ring but give the following split lines:



when we encounter the worst-case situation (e.g., under $\text{\unitlength}=0.08\text{pt}$). If we lay stress on the portability of a drawing system [7], one of the most promising ways is to rely on the *epic* system after we analyze and revise the mechanism of giving split lines. Hence, the aim of this paper is to show how the $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ system (Version 3.00) [8] provides a method for permitting the size reduction of structural formulas within the scope of the $\text{\L}\text{\A}\text{\T}\text{\E}\text{\X}$ picture environment and the *epic* system.

2 Basic functions for size reduction

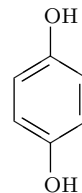
2.1 *sizedrc* package

The command \lineslope of *epic* has been used to convert the command \drawline of *epic* into the command \line of the $\text{\L}\text{\A}\text{\T}\text{\E}\text{\X}$ picture environment. In the process of obtaining the slope of a line, the command \lineslope has occasionally provided a rounding error, which has been found to cause such split lines as described above. A simple remedy for this phenomenon has been given in the *sizedrc* package (file name: *sizedrc.sty*) distributed as a part of the present version of $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$. According to this remedy, the drawing mechanism of the $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ system can be safely switched into the mechanism of *epic*, if \unitlength is set to be smaller than 0.1pt. Note that the unit length of the $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ system is stored by the command \unitlength , the standard value of which is 0.1pt.

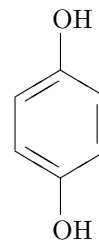
2.2 Changing unit lengths

The unit length of $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ can be changed by the command \changeunitlength , which is defined in the *sizedrc* 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{sizedrc}
\changeunitlength{0.08pt}
\begin{document}
\footnotesize
\bzdrv{1==OH;4==OH}
\end{document}
```



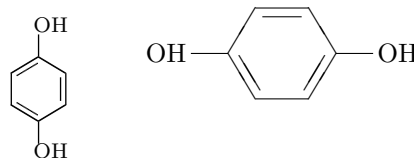
The font size of substituents can be changed by such a command as \footnotesize , as shown in the above formula. This should be compared with the counterpart drawn with the standard unit length (0.1pt) and the font size of \normalsize .



The command \changeunitlength can be declared at anywhere in a document; the setting of the command is effective after the declaration, until an alternative declaration is carried out. The grouping technique can be used to limit the effect of the setting within a pair of braces. For example, the codes represented by

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

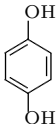
produce the following size-reduced formula and the corresponding formula of the standard dimension:



The command \changeunitlength sets a unit length given as an argument and declares a flag represented by $\text{\sizedreductiontrue}$ if the argument is less than 0.1pt. The flag is used to substitute the \drawline command of *epic* for the \line command

of L^AT_EX 2_ε. Hence, the following setting is equivalent to the setting derived from the declaration command `\changeunitlength{0.05pt}`.

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



3 Examples of size reduction

3.1 Size reduction of carbocycles

When `\sizereductiontrue` is not specified (i.e., `\sizereductionfalse`), the original picture environment of L^AT_EX 2_ε works. Table 1 shows the comparison between cases with and without the use of `sizedrc.sty`, which simulates the difference between X_YL^AT_EX Version 3.00 and Version 2.00.

Without using the `sizedrc` package, X_YL^AT_EX commands such as

```
{\unitlength=0.07pt \bzdrv{}} and
{\unitlength=0.06pt \bzdrv{}}
```

give incomplete formulas of benzene that have no inner double bonds (slanted lines), as found in the left column of Table 1. The disappearance of the inner bonds are in agreement with the original specification of the L^AT_EX picture environment. In fact, the `\line` command with slopes (5, 3) and (5, -3) cannot draw extremely short lines, although it is promised to draw longer lines under usual conditions (e.g., `\unitlength=0.1pt` or `0.08pt` without using the `sizedrc` package). By using the commands of `sizedrc` such as

```
{\changeunitlength{0.07pt}\bzdrv{}},
```

the slanted lines are revived to give complete formulas of benzene, as shown in the right column of Table 1.

3.2 Size Reduction of heterocycles







Table 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`.

3.3 Nested substitution

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

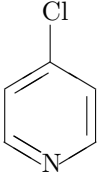
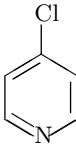
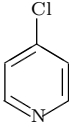
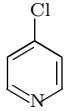


```
\changeunitlength{0.07pt}\scriptsize
\decaheterov[] {4a==N}{4D==O;7B==HO;%
{10}A}==H;%
```

Table 1: With and without `sizedrc.sty`

without <code>sizedrc.sty</code> (Version 2.00)	with <code>sizedrc.sty</code> (Version 3.00)
0.08pt 	0.08pt 
0.07pt ^a 	0.07pt 
0.06pt ^a 	0.06pt 

^aSlanted inner bonds disappear.

Table 2: Size reduction of 4-Chloropyridine

0.1pt ^a	0.08pt ^b	0.07pt ^c
		
0.06pt ^c 	0.05pt ^d 	0.04pt ^d 

^aA standard size.

^bThe font size is set by `\small`

^cThe font size is set by `\scriptsize`

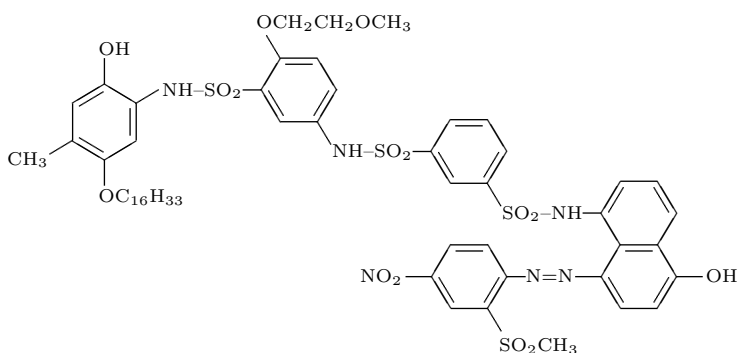
^dThe font size is set by `\tiny`

```

\changeunitlength{0.07pt}
\scriptsize
\bzdrv{1==OH;5==CH$_{3}$;4==OC$_{16}$H$_{33}$;2==\ryl(4==NH--SO$_{2}$)%
{4==\bzdrh{1==(y1);2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
5==\ryl(2==NH--SO$_{2}$){4==\bzdrh{1==(y1);5==\ryl(2==SO$_{2}$--NH)%
{4==\naphdrh{1==(y1);5==OH;8==\lyl(4==N=N){4==\bzdrh{4==(y1);%
1==NO$_{2}$;5==SO$_{2}$CH$_{3}$}}}}}}}}

```

(\changeunitlength{0.07pt})



(\changeunitlength{0.1pt})

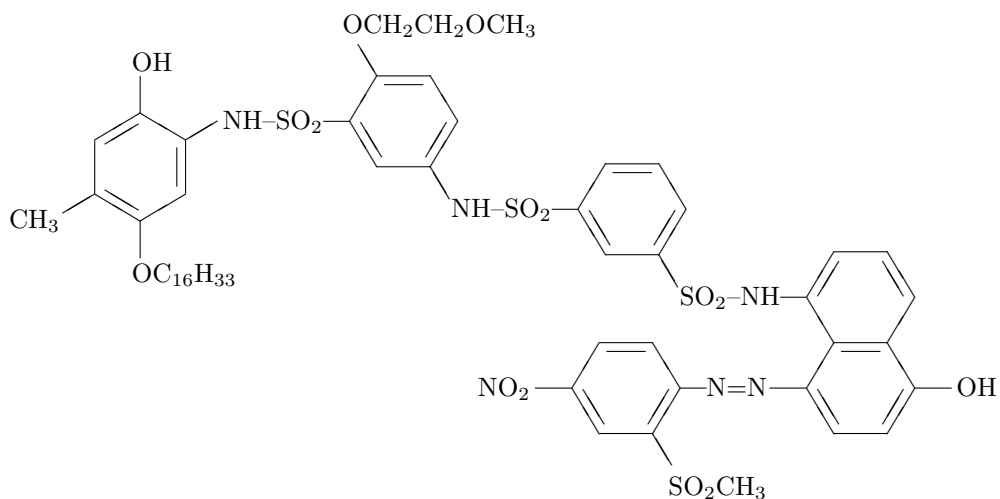
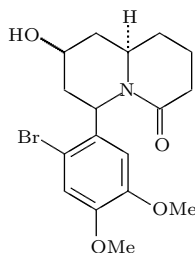


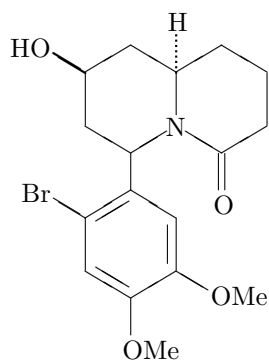
Figure 1: A cyan dye releaser drawn at unit lengths 0.07pt and 0.1pt

```
5==\bzdrv{3==OMe;4==OMe;6==Br;1==(y1)}
```

This code produces the formula shown below:



The formula of the standard dimension is drawn by the same code after returning to the default condition or by declaring `\changeunitlength{0.1pt}` explicitly.



A cyan dye releaser [9] has been drawn by using two or more `\ryl` and `\lyl` commands, as shown in the on-line manual of \XyMTeX Version 2.00 and has also been depicted in different ways (see Chapters 14 and 15 of the \XyMTeX book [10]). By virtue of the present version of \XyMTeX , the size of the formula can be reduced with the code shown in Fig. 1. It should be emphasized that the portability of the \XyMTeX system is still maintained in Version 3.00, where it is assured by the reliance on the \LaTeX picture environment and the `sizedc` package (a revision of `epic`).

References

- [1] Fujita S. & Tanaka N., “ \XyMTeX (Version 2.00) as Implementation of the \XyM Notation and the \XyM Markup Language”, *TUGboat*, **21** (1), 7–14 (2000).
- [2] Fujita S. & Tanaka N., “ \XyM Notation for electronic communication of organic chemical structures”, *J. Chem. Inf. Comput. Sci.*, **39**, 903–914 (1999).
- [3] Fujita S., “ \XyM Markup Language (\XyMML) for electronic communication of chemical documents containing structural formulas and reaction schemes”, *J. Chem. Inf. Comput. Sci.*, **39**, 915–927 (1999).
- [4] Lamport L., *LaTeX. A document Preparation System*, 2nd ed. for \LaTeX 2 ϵ , Addison-Wesley, Reading (1994).
- [5] Goossens M., Mittelbach F., & Samarin A., *The LaTeX Companion*, Addison-Wesley, Reading (1994).
- [6] For epic macros, see Podar S., “Enhancements to the picture environment of \LaTeX ”, Manual for Version 1.2 dated July 14, 1986.
- [7] For the portability of graphic applications of \TeX , \LaTeX and relevant systems, see Goossens, M., Rahtz, S., & Mittelbach, F., *LaTeX Graphics Companion*, Addison Wesley Longman, Reading (1997).
- [8] The system is now available from Fujita’s homepage via the Internet:
<http://imt.chem.kit.ac.jp/fujita/fujitas/fujita.html>
 A detailed manual is also available from this homepage.
- [9] Fujita S., Koyama K., & Ono S., “Dye Releasers for Instant Color Photography”, *Rev. Heteroatom Chem.*, **7**, 229–267 (1992).
- [10] Fujita S., *XyMTeX—Typesetting Chemical Structural Formulas*, Addison-Wesley, Tokyo (1997). The book title is abbreviated as “ \XyMTeX book” in the present article.

◇ Shinsaku Fujita
 Department of Chemistry and
 Materials Technology,
 Kyoto Institute of Technology,
 Matsugasaki, Sakyo-Ku, Kyoto,
 606-8585 Japan
fujitas@chem.kit.ac.jp

◇ Nobuya Tanaka
 Department of Chemistry and
 Materials Technology,
 Kyoto Institute of Technology,
 Matsugasaki, Sakyo-Ku, Kyoto,
 606-8585 Japan
nobuya@chem.kit.ac.jp