

Software & Tools

$\X\TeX$ (Version 2.00) as Implementation of the \X Notation and the \X Markup Language

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Introduction

The $\X\TeX$ system [1, 2] has been accepted by \TeX / \LaTeX users as a tool for typesetting chemical structural formulas, since it incorporates several advantages over previous systems [3, 4]. The first version of the system (version 1.00, 1993) with a detailed on-line manual has been deposited to the @Nifty archives (FTEX library No. 11) by one of the authors [5] and to the CTAN by volunteers [6]. Articles on the construction and usage of $\X\TeX$ have appeared in Ref. [1, 2]. Although the packages (style files) of the $\X\TeX$ system were originally intended for use under the \LaTeX 2.09 system, they also work effectively under \LaTeX 2 ϵ [7, 8, 9] without any changes.

Version 1.01 of the $\X\TeX$ system was released in 1996. This version is available from the @Nifty archives [10] or from a CD-ROM that is attached to the reference manual published in 1997 [11, 12]. The main purpose of version 1.01 is the updating of $\X\TeX$ to meet the \LaTeX 2 ϵ way of preparing packages (option style files). The following items were revised or added to encourage $\X\TeX$ users to write articles in chemical fields.

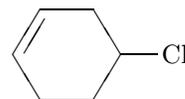
1. Each of the old sty files of $\X\TeX$ has been rewritten into a dtx file, from which we have prepared a new sty file by using the `docstrip` utility [8] of \LaTeX 2 ϵ . If you want to obtain the documentation for each source file, you may apply \LaTeX 2 ϵ to the corresponding drv file, which has also been prepared from the dtx file by using the `docstrip` utility.
2. Macros for drawing chair-form conformers of cyclohexane and for drawing adamantanes of an alternative type have been added.
3. Macros for drawing polymers have been added.
4. The package `chemist.sty`, which was originally prepared for [13], has been rewritten into a dtx file and added to $\X\TeX$ as a new component. This package enables us to use various functions such as
 - (a) the numbering and the cross-reference of chemical compounds and derivatives,

- (b) various arrows of fixed and flexible length for chemical equations,
- (c) ‘chem’ version and chemical environments for describing chemical equations, and
- (d) various box-preparing macros for chemical or general use.

The $\X\TeX$ command system can be regarded as a linear-notation system, which corresponds to the IUPAC nomenclature [14, 15] or to the CAS nomenclature [16]. For example, the command

```
\cyclohexaneh[a]{4==C1}/
```

for drawing **1** corresponds to the IUPAC name, 4-chlorocyclohex-1-ene, where the substituent “4-chloro” is generated by the code “4==C1” in the braces (a substitution list: SUBSLIST) and the endocyclic double bond “1-ene” comes from the code “a” in the brackets (a bond list: BONDLIST).

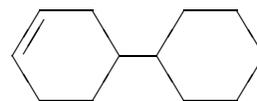


1

The chlorine atom in **1** is replaced by a cyclohexyl group so as to give 4-cyclohexylcyclohex-1-ene (**2**). According to this derivation, such a command as

```
\cyclohexaneh[a]{4==\cyclohexaneh{}}
```

should be capable of drawing the formula **2** in order that the $\X\TeX$ command system remains a linear-notation system. However, the latter command is incapable of drawing **2** within $\X\TeX$ version 1.01, since this version has postulated rather small substituents for the SUBSLIST.



2

Within the scope of $\X\TeX$ version 1.01, such a substituent with a complicated structure requires a direct description of layout data, as shown in Chapters 14 and 15 of the $\X\TeX$ book [11]. Thus, we can use the `picture` environment of \LaTeX :

```
\begin{picture}(1400,700)(0,0)
\put(0,0){\cyclohexaneh[a]{4==}}
\put(546,0){\cyclohexaneh{}}
\end{picture}
```

or the `\kern` command for horizontal adjustment and the `\lower` command for vertical adjustment in plain \TeX :

```
\cyclohexaneh[a]{4==\kern-25pt%
\lower37pt\hbox{\cyclohexaneh{}}}
```

Although these methods are useful for drawing complicated structures, such layout data should be hidden to realize a coherent system of drawing structural formulas. Moreover, the methods have another essential disadvantage: their codes give no, or at most partial, connectivity data between parts to be combined, though such parts appear to be combined as a picture. For example, the code

```
\cyclohexaneh[a]{4==\kern-25pt%
\lower37pt\hbox{\cyclohexaneh{3==Cl}}}
```

producing 4-(3-cyclohex-1-yl)cyclohex-1-ene (**3**) has no connectivity data at the 1-position to the 3-chlorine atom of the second cyclohexane ring:

**3**

For the purpose of overcoming the disadvantages, a new system to be developed should allow us to write such a code as `\cyclohexaneh{1==(y1)}` for representing the cyclohexyl substituent. Thus, we find the code for **2**:

```
\cyclohexaneh[a]{%
4==\cyclohexaneh{1==(y1)}}
```

where the code “1==(y1)” represents the substitution position. This specification of a substitution position is called a *yl*-function in the present paper. In order to represent the 3-cyclohex-1-yl substituent for 4-(3-cyclohex-1-yl)cyclohex-1-ene, the new system should enable us to use a code such as

```
\cyclohexaneh{1==(y1);3==Cl}
```

as found in the code for **3**:

```
\cyclohexaneh[a]{%
4==\cyclohexaneh{1==(y1);3==Cl}}
```

According to this approach, the $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ command system has been refined and extended to give a new linear-notation system, which is now called the *X_M Notation* [17, 18]. The abstract nature of the $\text{\X}\text{\M}$ Notation means that $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ is now regarded as a software application for $\text{\T}\text{\E}\text{\X}/\text{\L}\text{\A}\text{\T}\text{\E}\text{\X}$ printing, where the $\text{\X}\text{\M}$ Notation is parsed by virtue of $\text{\T}\text{\E}\text{\X}/\text{\L}\text{\A}\text{\T}\text{\E}\text{\X}$. It follows that a further system can be developed on the basis of the $\text{\X}\text{\M}$ Notation if another parsing system is available. Moreover, the $\text{\X}\text{\M}$ Notation can be used as an intermediate language, into which another language for representing structural formulas is translated so as to print out

Table 1: Package Files of $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$

| package name | included functions |
|--------------|---|
| aliphac.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 |
| 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 |

the formulas. This is the approach reported for the $\text{\X}\text{\M}$ Markup Language ($\text{\X}\text{\M}\text{\M}\text{\L}$) [19].

As clarified by the discussions described in the preceding paragraphs, the first goal of this article is to show a mechanism for the adjustment of substitution positions (or for concealing layout data), which has been developed in $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ version 2.00 to support the $\text{\X}\text{\M}$ Notation and $\text{\X}\text{\M}\text{\M}\text{\L}$. The second goal is to exhibit its scope and limitations by using illustrative examples.

$\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ Version 2.00

Overview Version 2.00 of $\text{\X}\text{\M}\text{\T}\text{\E}\text{\X}$ (1998 and 1999) supports the *yl*-function introduced by the $\text{\X}\text{\M}$ Notation [20], where a complicated substituent is treated as a modification of a substitution list (SUBSLIST). As an extension of this methodology, a bond list (BONDLIST) can be modified to treat ring

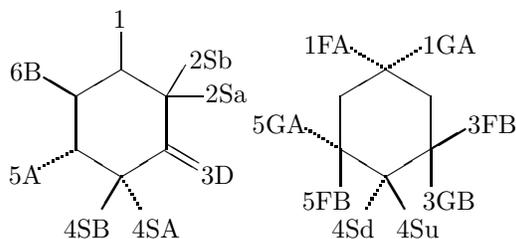


Figure 1: Examples of Locant Numbers and Bond Modifiers

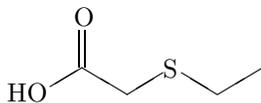
fusion, since each ring fusion is considered to be a kind of substitution on a bond. In addition, an atom list (ATOMLIST) can also be used to treat spiro rings, since each spiro ring is a kind of atom replacement at an appropriate vertex.

The $\text{\X}^{\text{M}}\text{T}_{\text{E}}\text{X}$ system (version 2.00) consists of the package files listed in Table 1. The package file `chemstr.sty` is the basic file that is automatically read within any other package file of $\text{\X}^{\text{M}}\text{T}_{\text{E}}\text{X}$. It contains macros for internal use, e.g., common commands for bond-setting and atom-setting. The other package files contain macros for users. The use of `xymtex.sty` calling all package files may sometimes cause the “ $\text{T}_{\text{E}}\text{X}$ capacity exceeded” error. In this case, you should call the necessary packages explicitly by using the `\usepackage` command.

Commands and Functions Added To expand the scope of the $\text{\X}^{\text{M}}\text{T}_{\text{E}}\text{X}$ system, several new functions have been introduced as follows.

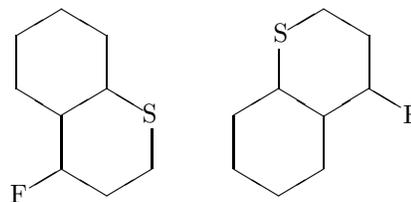
1. Several bond modifiers are added to draw alternative up- and down-bonds as well as to treat ring fusion, as shown in the right formula of Figure 1.
2. Commands for typesetting zigzag polymethylenes are developed (`methylen.sty`). For example, we obtain

```
\pentamethylenei{3==S}{1D==O;1W==HO}
```



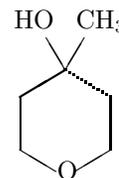
3. Commands for drawing six-six fused carbocycles and heterocycles are added. Thus, the suffixes “vb” and “vt” are used along with “v”, “vi”, “h” and “hi”:

```
\decaheterovb{1==S}{4==F}
\decaheterovt{1==S}{4==F}
```



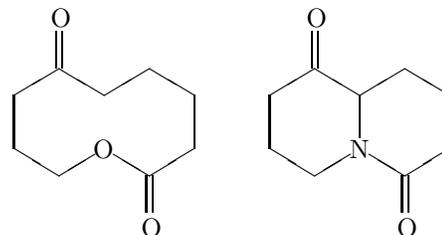
4. An optional argument (SKBONDLIST) for representing stereochemistry, e.g., (`{aA}{fB}`), is added to each command of general use for drawing boldfaced and dotted skeletal bonds.

```
\sixheterov({aA}{fB})%
{4==0}{1Sa==CH$_{3}$;1Sb==HO}
```



5. An optional argument (OMIT) is added to each command for drawing related skeletons by bond deletion. Compare the following structural formulas drawn by the codes with and without an OMIT argument (`[k]`).

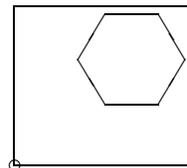
```
\decaheterov{9==O}{4D==O;8D==O}[k]
\decaheterov{9==N}{4D==O;8D==O}
```



Substitution Derivation

This section deals with the `yl`-function for complex substitution, where this type of derivation is called *substitution derivation* because of the usage of a substitution list (SUBSLIST).

Adjusting Mechanism For a usual drawing mode, each $\text{\X}^{\text{M}}\text{T}_{\text{E}}\text{X}$ command has its reference point of x and y -coordinates (0, 0), since $\text{\X}^{\text{M}}\text{T}_{\text{E}}\text{X}$ is based on the $\text{\L}^{\text{A}}\text{T}_{\text{E}}\text{X}$ picture environment. For example, the `\cyclohexaneh{}` command has the reference point shown by a circle in the following diagram:



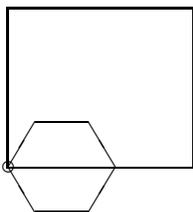
which is drawn by the code:

```
\begin{picture}(700,600)(0,0)
\put(0,0){\circle{40}}
\put(0,0){\cyclohexaneh{}}
\end{picture}
```

The frame is added to show the domain (700,600) of the picture environment, where the bottom-left vertex of the frame corresponds to the origin of (0,0), as shown by a small circle [22]. The reference point can be shifted to a vertex of the cyclohexane ring by means of the code:

```
\begin{picture}(700,600)(240,400)
\put(240,400){\circle{40}}
\put(0,0){\cyclohexaneh{}}
\end{picture}
```

where the second argument (240,400) specifies x - and y -shift values. Thereby, we obtain the following diagram:



Then the resulting structure with the reference point shifted is placed in the SUBSLIST of the outer skeleton.

The `\cyclohexaneh` command is defined on the basis of the `\sixheteroh` command, which involves the mechanism of shifting the reference point. The fundamentals of the mechanism are in turn implemented in its inner command `\@sixheteroh`. The definition of this command is cited from `heta-romh.sty` as follows:

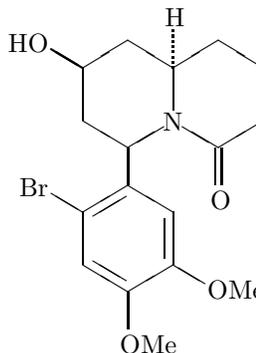
```
\def\@sixheteroh(#1)[#2]#3#4[#5]{%
\iniatom\iniflag%initialize
\test\vrtx@sixh{#3}%
\@reset@ylsw%
\ylpositionh{#4}{0}{0}{7}{0}%
\if@ylsw
\yl@shiftii=\@ylii
\yl@shifti=\@yli
\advance\yl@shiftii\yl@xdiff
\advance\yl@shifti\yl@ydiff
\begin{picture}(0,0)%
(-\yl@shiftii,-\yl@shifti)
\reset@yl@xydiff%
\else
\begin{picture}(880,800)(-240,-400)%
%(abbreviated)
\fi
%(abbreviated)
\end{picture}
}
```

The inner testing command `\ylpositionh` tests the SUBSLIST (the argument #4) to return a switch `\@ylswtrue` and shift values for adjustment, if a code (yl) is found in the list. Then, the reference point of the inner picture environment is shifted to the point $(-\yl@shiftii,-\yl@shifti)$.

Nested Substitution The `yl`-function is quite versatile, as indicated by the code

```
\decaheterov[] {4a==N}{4D==0;7B==HO;%
{{10}A}==H;5==\bzdrv{3==OMe;4==OMe;%
6==Br;1==(y1)}}}
```

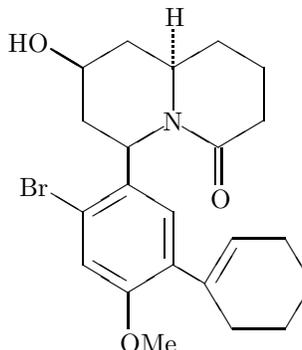
which produces the following structure:



where the substituted phenyl group is regarded as a substituent. In order that the phenyl substituent has a cyclohexenyl substituent in place of the methyl substituent, the code

```
\decaheterov[] {4a==N}{4D==0;7B==HO;%
{{10}A}==H;5==\bzdrv{4==OMe;%
3==\cyclohexaneh[a]{1==(y1)}};%
6==Br;1==(y1)}}}
```

is written to generate a formula with a nested substituent as follows:

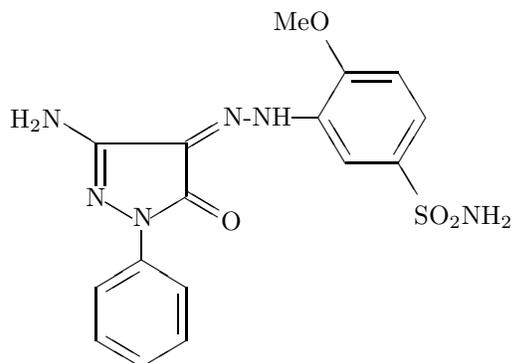


Linking Moieties The commands `\ryl` and `\lyl`, which are contained in the `chemstr` package (file name: `chemstr.sty`), are used to typeset linking moieties. For example, the command `\ryl` takes a linking unit (N–NH) as the first argument and

a substituent with the yl-function as the second argument, as found in the following code:

```
\fiveheterov[d]{1==N;5==N}{4==H$_{2}$N;%
1==\bzdrv{1==(y1)};2D==0;%
3D==\ryl(5==N-NH){4==\bzdrh{1==(y1)};%
2==\lmoiety{MeO};5==SO$_{2}$NH$_{2}$}}
```

This code typesets the following formula:

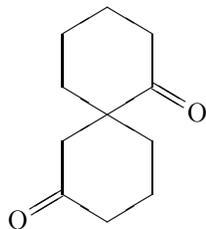


Atom Derivation

A new function for typesetting a spiro ring is introduced in each command for general use, in which a substituent generated by the yl-function is placed in its atom list (ATOMLIST). For example, the code

```
\sixheterov{1s==\sixheterov{}}%
{4==(y1)};3D==0}{5D==0}
```

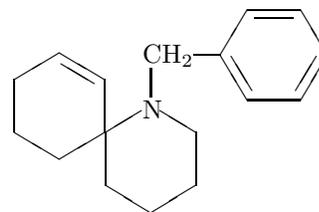
contains a code for a spiro-cyclohexanone ring, i.e., `\sixheterov{4==(y1)};3D==0` produced by the yl-function. Note that the atom modifier '1s' in the code represents the absence of a hetero-atom at the spiro 1-position. Thus, we can draw a spiro[5.5]undecane represented by the following formula:



The following code:

```
\sixheterov{1==N;%
6s==\cyclohexanev[a]{3==(y1)}}%
{1==\ryl(8==CH$_{2}$)}{4==\bzdrh{1==(y1)}}}
```

contains yl-functions in an atom list as well as in a substitution list. Using this, we can draw a 1-azaspiro[5.5]undecane,

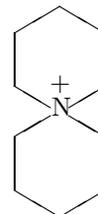


which is the skeleton present in histrionicotoxin.

When a hetero-atom is present at the spiro position, an atom modifier 'h' is used in place of 's'. For example, the code

```
\sixheterov{1h==\sixheterov{4+}}%
{4==N}{4==(y1)}}{}
```

typesets the following formula:



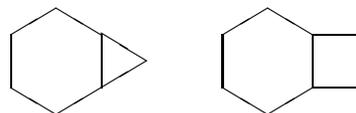
It should be noted that the BONDLIST of the inner `\sixheterov` contains the code `{4+}`, which is used for drawing a plus charge at an inner position of the cyclohexane ring.

Bond Derivation

Fusing Units Several fusing units (three- to six-membered units) have been developed (`fusering.sty`). For example, the codes

```
\cyclohexanev[{\B\threefuse{}}]{b}}{}
\cyclohexanev[{\B\fourfuse{}}]{D}}{}
```

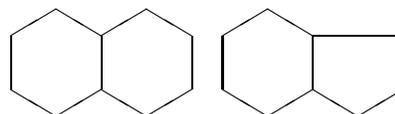
contain such three- and four-membered fusing units, `\threefuse` and `\fourfuse`. They generate fused cyclic compounds as follows.



In addition, five- and six-membered fusing units (`\fivefusev` and `\sixfusev`) contained in the code,

```
\cyclohexanev[{\B\fivefusev{}}]{D}}{}
\cyclohexanev[{\B\sixfusev{}}]{e}}{}
```

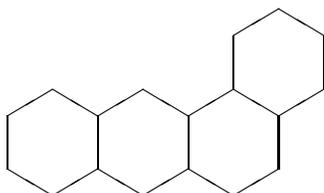
are used to typeset the following bicyclo compounds:



Ring Fusions Ring fusion is treated by adding a fusing unit to the BONDLIST of each command. A unit to be fused is written in the BONDLIST of a command with a bond specifier (a lowercase or uppercase alphabet) in one way. For example, the code

```
\hanthracenev[{\A\sixfusev{}}{d}]{}
```

generates a perhydroanthracene with a fused six-membered ring at the bond 'a' of the perhydroanthracene nucleus:



The letter 'A' of the code `{\A\sixfusev{}}{d}` is a bond specifier that represents the older terminal of the bond 'a' of the perhydroanthracene nucleus [21]. On the other hand, the code `\sixfusev{}}{d}` of `{\A\sixfusev{}}{d}` in the BONDLIST represents the fused six-membered ring with the bond 'd' omitted. The letter 'd' indicates that the fusing point of the unit is the younger terminal of the omitted bond 'd'. If the the fusing point of the unit is the other (older) terminal, the corresponding uppercase letter 'D' should be used.

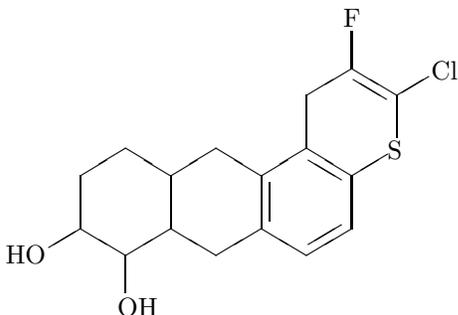
Accordingly, the same formula can be drawn by the code exchanging uppercase and lowercase letters, as found in the following code:

```
\hanthracenev[{\a\sixfusev{}}{D}]{}
```

We can use SUBSLISTs to specify substituents, BONDLISTs to specify endocyclic double bonds, and ATOMLISTs to specify heterocyclic atoms in such fused derivatives. For example, the code

```
\hanthracenev[aco{\A\sixfusev[a]{3==S}%  
{1==F;2==Cl}{d}]{5==OH;6==HO}
```

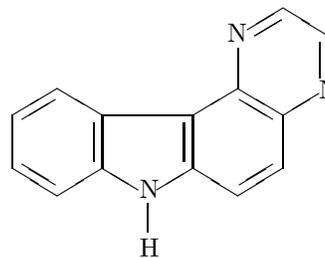
gives a tetracycle having additional substituents:



Nested Ring Fusions The `\sixfusev` command is capable of accomodating another `\sixfusev` command in a nested fashion. By this technique, the carbazole structure can take a further fused ring so as to produce the structural formula of 7*H*-pyrazino[2,3-*c*]carbazole. Thus, the code,

```
\nonaheterov[begj{b\sixfusev[%  
ac{\a\sixfusev[bf]{6==N;3==N}{D}}%  
{}}{e}]{1==N}{1==H}
```

gives the structural formula of the fused heterocycle:



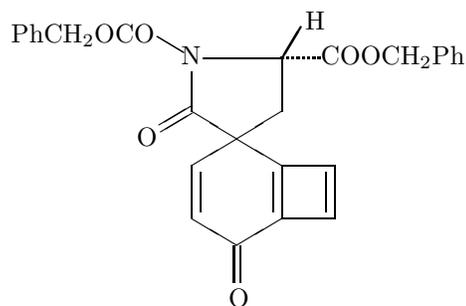
which is depicted by attaching a six-membered ring (`\sixfusev[ac]{}{e}`) to the bond 'b' of an indole nucleus.

Combined Derivations

Three types of derivations can be combined to draw complicated structural formulas. For example, the code

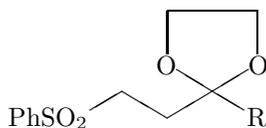
```
\sixheterov[be{B\fourfuse[b]{}{D}}]{%  
1s==\fiveheterov{4==N}{1==(y1)};3SB==H;%  
3SA==COOCH$_{2}$Ph;%  
4==PhCH$_{2}$OCO;5D==O}{4D==O}
```

involves a bond derivation (a 4–6 fused ring) and an atom derivation (a 5–6 spiro ring) to give the following formula:



Synonyms

The $\tilde{X}\tilde{M}$ notation system is so flexible in selecting mother skeletons that there can be several ways to draw structural formulas of the same meaning. For exmaple, a 1,3-dioxolane derivative

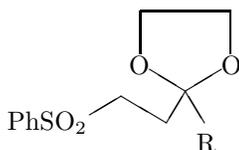


can be drawn by the code,

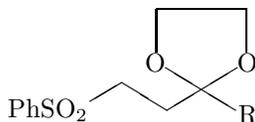
```
\fiveheterov{2==0;5==0;%
1s==\trimethylenei}{3==(y1);%
1W==PhSO$_{2}$;3W==R}{}
```

The same compound is also drawn by usual techniques as follows:

```
\fiveheterov{2==0;5==0}{%
1Sb==\dimethylenei%
}{2==(y1);1W==PhSO$_{2}$};1Sa==R}
```



```
\fiveheterov{2==0;5==0}{1G==\dimethylenei%
}{2==(y1);1W==PhSO$_{2}$};1F==R}
```



Conclusion

$\mathcal{X}\mathcal{M}\mathcal{T}\mathcal{E}\mathcal{X}$ (version 2.00) is regarded as an implementation of the $\mathcal{X}\mathcal{M}$ Notation, which is a linear notation for representing organic structures. The $\mathcal{X}\mathcal{M}$ Notation is an extension of the previous $\mathcal{X}\mathcal{M}\mathcal{T}\mathcal{E}\mathcal{X}$ command system (versions 1.00 and 1.01) and they are apparently akin to each other. However, they are conceptually different in that the former removes layout data by virtue of the newly introduced concepts of yl-function, substitution derivation, atom derivation, and bond derivation. Moreover, the $\mathcal{X}\mathcal{M}$ Markup Language ($\mathcal{X}\mathcal{M}\mathcal{M}\mathcal{L}$) has been developed as a markup language for representing organic structures. $\mathcal{X}\mathcal{M}\mathcal{M}\mathcal{L}$ is translated into the $\mathcal{X}\mathcal{M}$ Notation, which, in turn, can be used to print out structural formulas by means of the new version of $\mathcal{X}\mathcal{M}\mathcal{T}\mathcal{E}\mathcal{X}$.

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- [20] The system is now available from Fujita’s homepage via the Internet:
<http://www.chem.kit.ac.jp/fujita/fujitas/fujita.html>
 A detailed manual is also available from this homepage.
- [21] For the designation of the bonds of perhydroanthracene, see Chapter 5 of the X^MTEXbook. Note that the younger terminal of the bond ‘a’ is designated by the letter ‘a’. The word ‘older’ or ‘younger’ is concerned with the order of numbering of vertices. For a six-membered ring, the numbering 1—2—3—4—5—6—1 shows that the terminal 1 of the bond ‘a’ (1—2) is younger, while the terminal 2 of the bond ‘a’ is older. It should be noted that the terminal 6 of the bond ‘f’ (6—1) is younger, while the terminal 1 of the bond ‘f’ is older.
- [22] The `\cyclohexaneh` command of the present distribution of X^MTEX (version 2.00) contains a bug. Until the bug is fixed, please include the following code in the preamble of your article:
- ```
\makeatletter%bug for version 2.00
\def\cyclohexaneh{\@ifnextchar[%
{\@cyclohexaneh[@]{\@cyclohexaneh[@]}}
\makeatother
```
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