XyMTEX (Version 4.01) for Typesetting Chemical Structural Formulas. A Tool for DVI- and PostScript-Typsetting.

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Contents

Chapter 1

Introduction

1.1 History

The previous versions of the XyMTEX system are summarized in Table 1.1 [1, 2, 3]. The XyMTEX Version 2.00 supported the XyM Notation which we proposed as a linear notation of structural formulas [4, 5]. The XyMTEX Version 3.00 supported the size reduction of structural formulas, which expanded the scope of the XyMTEX system [6]. Up to Version 3.00, we laid stress on the portability within the scope of TEX/LATEX. Thus, to be as portable as possible, the XyMTEX system (up to Version 3.00) was designed to depend on the LATEX picture environment [7, 8] and the epic package [9].

A brief history has been described in the on-line manual attached to Version 2.00. The manual for Version 1.01 (distributed as a separate matter and published as a reference book [3]) and the manuals for Version 2.00 (attached to this distribution) and Version 3.00 (attached to this distribution) have described the specification and the usage of commands supported by the XyMTEX system. They are still effective for Version 4.01 [10].

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)	Size reduction (sizeredc.sty, version 1.01), and reconstruction of the command system
4.00 (2002)	(not released) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00)
4.01 (2004)	(this version) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00) and length-variable central atoms

During the last dacade (1990s), desktop publishing based on the PostScript language has developed remarkably so that conventional publishing systems have been linked with World Wide Web (WWW)

techniques. In particlular, PDF (Portable Document Format) based on PostScript has attracted anxious attention since it is capable of bringing a sound method to integrate publishing and WWW communication. The trend has influenced the TEX/LATEX typesetting system, paticularly in treating graphic data [11]. This implies that TEX/LATEX is recognized as a programing language to produce PostScript codes in place of TEX-original dvi (device-independent) codes. This recognition stems from the facts that TEX was originally equipped with the `¥special` funtion to accept such graphic data [12], that such versatile tools as PSTrick [13] has been developed to output PostScript codes via `¥special`, and that softwares to translate dvi codes (including the codes due to `¥special`) to PostScript codes have become easily available.

To catch up the expansion of new techniques, XyMTEX has been updated as Version 4.00 so that the portability within TEX/LATEX and the capability of PostScript printing can coexist with each other by developing a mechanism to switch the two modes of usage.

1.2 Package Files of XyMTEX Version 4.01

The XyMTEX system (version 4.00) consists of package files listed in Table 1.2, where two packages, xymtx-px and chmst-px, have been developed for PostScript printing. Macros for PostScript printing are contained in xymtx-px added in Version 4.01. They are substituted for several drawing macros contained in the chemstr package. The chmst-ps package for PostScript printing corresponds to the chemist package for the LATEX picture environment.

Table 1.2: Package Files of XyMTEX and Related Files

package name	included functions
XyMTEX Files	
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 carbocyles.
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 numeres
polymers.sty	commands for drawing polymers
fusering.sty	commands for drawing units for ring fusion
methylen.sty	commands for drawing zigzag polymethylene chains
sizeredc.sty	commands for size reduction (Version 1.01)
xymtx-ps.sty	macros for PostScript printing (Version 1.00). These macros are substituted for several macros contained in the chemstr package.
XyMTEX Utilities	
xymtex.sty	a package for calling all package files except xymtx-ps.sty (no PostScript)
xymps.sty	a package for calling all package files (PostScript, i.e. with xymtx-ps.sty)
Related Files	
chemist.sty	commands for using 'chem' version and chemical environments
chmst-ps.sty	macros for PostScript printing. These macros are substituted for several macros contained in chemist package.

Chapter 2

PostScript Printing of Structural Formulas

2.1 Using the xymtx-ps Package

To draw the structural formula of 4-fluorophenol, we write the following codes in a tex file (named 400test1.tex, for example), where the included packages carom and xymtx-ps are part of the XyMTeX symtem. The standard unit length of drawing is initially set to be 0.1pt. The size of the formula can be reduced by using ¥changeunitlength.

```
%400test1.tex
¥documentclass[draft]{article}
¥usepackage{carom}
¥usepackage{xymtx-ps}
¥begin{document}
¥bzdrv{1==OH;4==F}
{¥changeunitlength{0.08pt}
¥bzdrv{1==OH;4==F}}
{¥changeunitlength{0.06pt}
¥bzdrv{1==OH;4==F}}
¥end{document}
```

Then the file is compiled by means of the TEX/LATEXsystem by inputting the following command in the command line of a personal computer.[1]

```
C:¥fujita¥doc400>platex␣400test1
```

Thereby, the TEX/LATEX processing starts to include carom.sty and xymtx-ps.sty, where the latter is a key package of the XyMTeX Version 4.01 for PostScript printing. The carom.sty package further includes chemstr.sty, hetarom.sty, and hetaromh.sty, all of which are part of XyMTEX system. The xymtx-ps.sty package internally includes pstricks.sty, pstricks.tex, and pstricks.con, which are distributed as part of the PSTricks system.

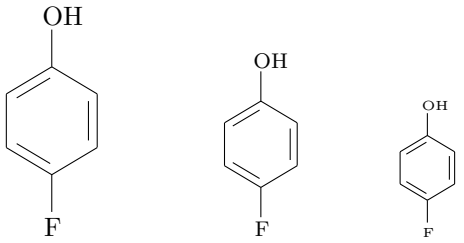
The resulting dvi file (named 400test1.dvi) should be converted into the correspoding ps file (named 400test1.ps) by inputting the following command:[2]

```
C:¥fujita¥doc400>dvipsk␣400test1
```

[1] The command 'platex' starts pLATEX 2_ε, which is distributed by ASCII Co., Ltd. as a well-known Japanese version of LATEX 2_ε.

[2] The converter 'dvipsk' is a Japanese version of 'dvips', which permits Japanese characters. Any other converters from DVI to PostScript can be used.

The ps file is displayed or printed by an appropriate PostScript viewer or printer. By using GhostScript and GSview, for example, we obtain the following formulas of various sizes.

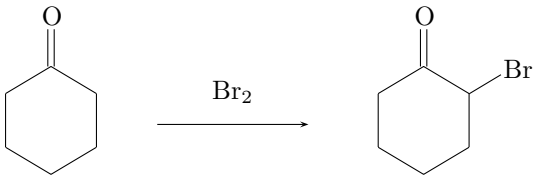


2.2 Using the chmst-ps Package

To draw reaction schemes which contain various reaction arrows, we additionally use the chmst-ps package. The chmst-ps package automatically includes the chemist package.

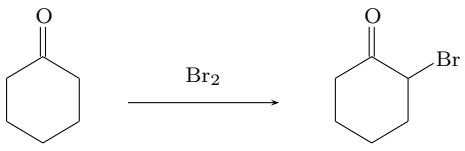
```
%400test2.tex
¥documentclass[draft]{article}
¥usepackage{carom}
¥usepackage{xymtx-ps,chmst-ps}
¥begin{document}
¥cyclohexanev{1D==O}
¥reactrarrow{40pt}{2cm}{Br$_{2}$}{¥strut}
¥cyclohexanev{1D==O;2==Br}
¥end{document}
```

This code produces the following reaction scheme, which represents a bromination of cyclohexanone. The command ¥reactrarrow is defined in the chmst-ps package for PostScript printing and in the chemist package for using the LaTeX picture environment.



Since the font size in the reagent section on or below a reaction arrow is not obeyed the size reduction due to ¥changeunitlength, such a command as ¥footnotesize should be declared explicitly.

```
{¥changeunitlength{0.08pt}¥footnotesize
¥cyclohexanev{1D==O}
¥reactrarrow{32pt}{2cm}{Br$_{2}$}{¥strut}
¥cyclohexanev{1D==O;2==Br}}
```



2.3 Using the Original Picture Environment

2.3.1 Without Including the xymtx-ps Package

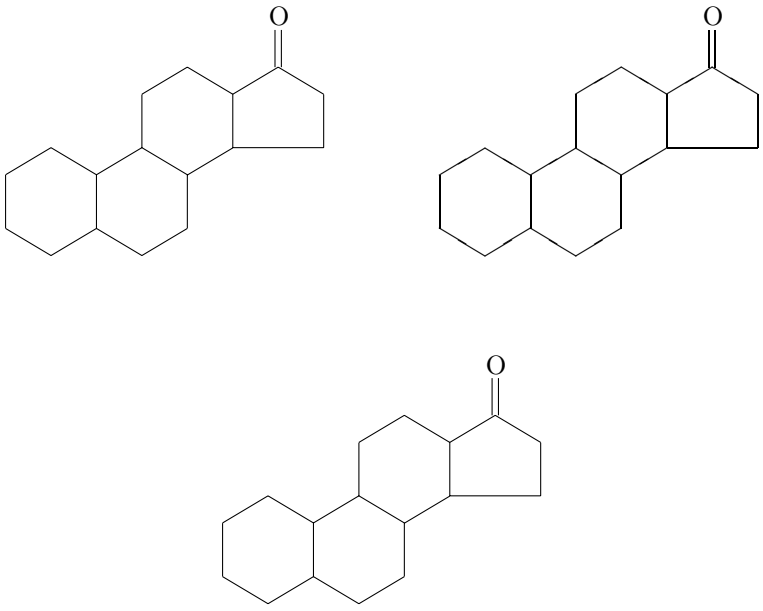
The functions of the PSTrick system (for PostScript) are used only in the packages xymtx-ps and chmst-ps that have been added in Version 4.01 of the XyMTEX system. Hence, you can use the XyMTEX system in the original LATEX picture environment, so long as you do not include these packages. Since the resulting dvi files depend on the native functions of TEX/LATEX, they can be previewed and printed out by virtue of a dvi-ware without converting them into ps files.

2.3.2 Switching to the Original Picture Environment

Even if the xymtx-ps package is included, the original LATEX picture environment can be used by a switching declaration `¥orignalpicture`. For example, in the present article that has included the xymtx-ps package, we write down following code:

```
¥steroid{{17}D==O}
{¥originalpicture
¥steroid{{17}D==O}}
¥steroid{{17}D==O}
```

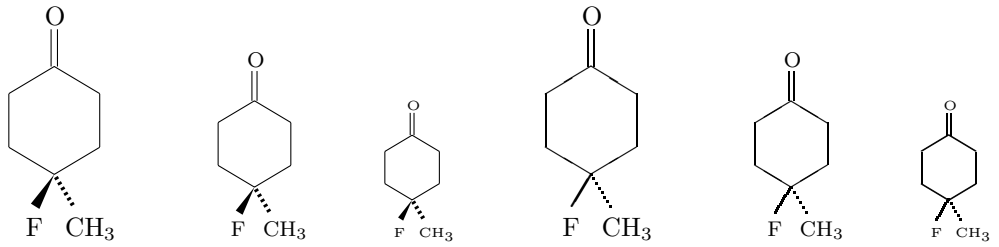
The declaration of `¥orignalpicture` is effective until another switching declaration will be inputted. This example shows that a grouping restricts the effect of `¥orignalpicture` within a pair of braces, where the second formula of a steroid is typeset by virtue of the original LATEX picture environment and the remaining two formulas are drawn by PostScript (by using the PSTricks sysetm).



Since the original LATEX picture environment gives an insufficient result of reducing formula sizes, the sizeredc package (distibuted form Version 3.00) should be included additionally by using `¥usepackage`. Once the sizeredc package is additionally included, the original LATEX picture environment can be used by a switching declaration `¥reducedsizepicture` in order to reduce the sizes of formulas. For example, a minimal set of packages are used in the following code:

```
%400test3.tex
¥documentclass[draft]{article}
¥usepackage{carom}
¥usepackage{sizeredc}
¥usepackage{xymtx-ps}
¥begin{document}
{¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}}
{¥reducedsizepicture
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}}
¥end{document}
```

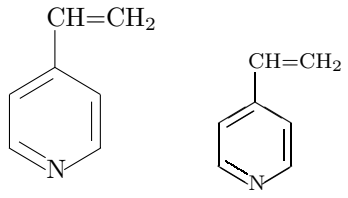
Thereby, we obtain structural formulas with various sizes. The top three formulas are drawn in PostScript and the remaining three are typeset within the picture environment and the epic package.



The declaration command `¥reducedsizepicture` can take an optional argument, by which the unit length of the picture enviroment is specified.

```
%400test4.tex
¥documentclass{article}
¥usepackage{hetarom}
¥usepackage{sizeredc}
¥usepackage{xymtx-ps}
¥begin{document}
¥pyridinevi{4==CH=CH$_{2}$}
¥reducedsizepicture[0.08pt]
¥pyridinevi{4==CH=CH$_{2}$}
¥end{document}
```

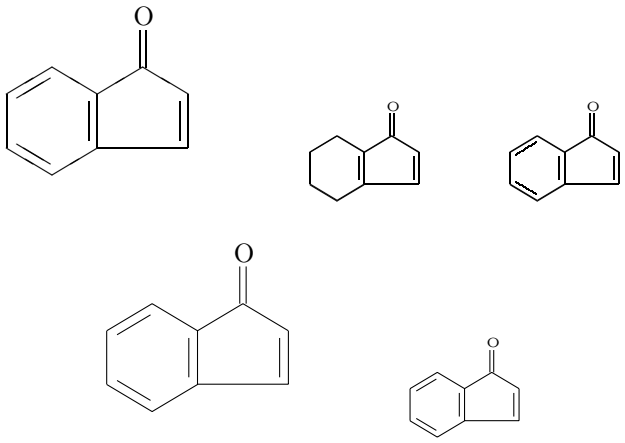
This code produces the following two formulas. The first formula is drawn in PostScript at the standard unit length of 0.1pt, while the second one is typeset in the LaTeX picture environment (plus the epic package) at the unit length of 0.08pt.



If the text mode is run under ¥originalpicture, the declaration ¥setxymtxps is used to return to the PostScript drawing mode.

```
%400test5.tex
¥documentclass{article}
¥usepackage{lowcycle}
¥usepackage{sizeredc}
¥usepackage{xymtx-ps}
¥begin{document}
¥originalpicture%original picture environment
¥indanevi{1D==0}
¥changeunitlength{0.06pt}
¥indanevi{1D==0}
{¥reducedsizepicture[0.06pt]
¥indanevi{1D==0}} ¥¥
¥setxymtxps%PostScript drawing
¥indanevi{1D==0}
¥changeunitlength{0.06pt}
¥indanevi{1D==0}
¥end{document}
```

This code produces the following formulas. The first two formulas in the top row are typeset within the original LaTeX picture environment,[3] while the last one in the top row is typeset by the picture enviroment plus the epic package. In contrast, the two formulas in the bottom row are drawn in PostScript.



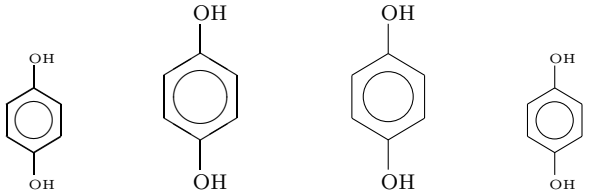
The declaration ¥setxymtxps can take an optional argument, which specifies the unit length when returned to the PostScript drawing mode.

```
%400test6.tex
¥documentclass{article}
¥usepackage{carom}
¥usepackage{sizeredc}
¥usepackage{xymtx-ps}
¥begin{document}
¥reducedsizepicture[0.06pt]
¥bzdrv[A]{1==OH;4==OH}
¥changeunitlength{0.08pt}
```

[3]Note that the LaTeX picture environment is incapable of drawing short lines. Hence, two inner slanted lines disappear in the benzene ring of the second formula.

```
¥bzdrv[A]{1==OH;4==OH}
¥setxymtxps[0.08pt]
¥bzdrv[A]{1==OH;4==OH}
¥changeunitlength{0.06pt}
¥bzdrv[A]{1==OH;4==OH}
¥end{document}
```

The top two of the resulting formulas are typeset within the LaTeX picture environment and the epic package, while the remaining two after the declaration `¥setxymtxps[0.08pt]` are drawn in PostScript.



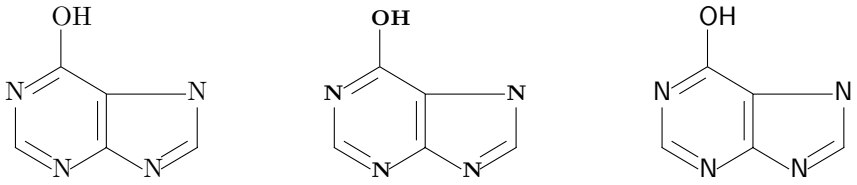
2.4 Fonts

The font for drawing substituents and atoms in a default mode is selected by the following setting:

```
¥let¥substfont=¥normalfont
¥let¥substfontsize=¥normalsize
```

According to this specification,[4] the font and its size can be changed by substituting `¥substfont` and `¥substfontsize` as follows:

```
¥purinev{4==OH}
{¥let¥substfont=¥bfseries
¥let¥substfontsize=¥footnotesize
¥purinev{4==OH}}
{¥let¥substfont=¥sffamily
¥purinev{4==OH}}
```



[4] This specification is different from that of the previous versions (version 3.00 and the older versions).

Chapter 3

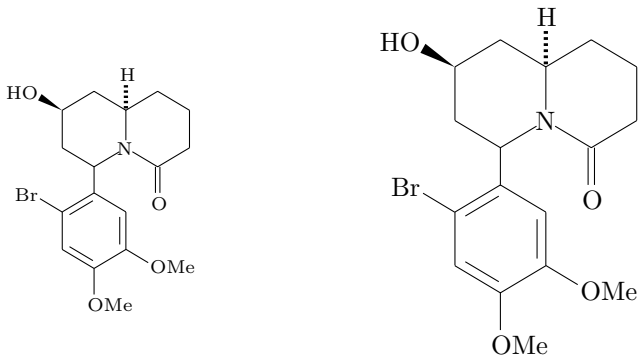
Complicated Compounds

3.1 Nested Substitution

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

```
{¥changeunitlength{0.07pt}
¥decaheterov{4a==N}{4D==O;7B==HO;{{10}A}==H;%
5==¥bzdrv{3==OMe;4==OMe;6==Br;1==(yl)}}¥hskip2cm
¥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:

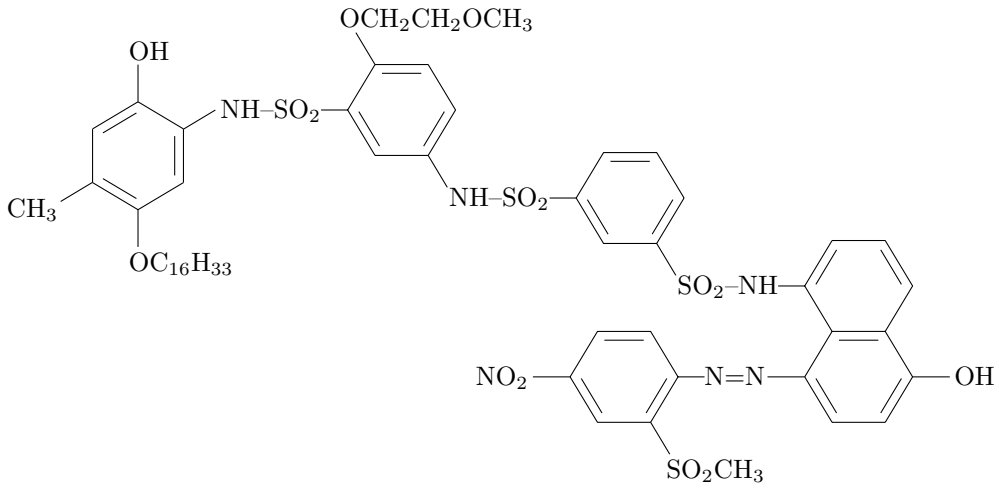


The right formula is drawn by the same code with the standard unit length (0.1pt).

A cyan dye releaser has been drawn by using two or more `¥ryl` and `¥lyl` commands, as shown in the on-line manual of XƎMTEX Version 2.00 and has also been depicted in different ways (see Chapters 14 and 15 of the XƎMTEXbook [3]). First, we define `¥cyandyereleaser` as being

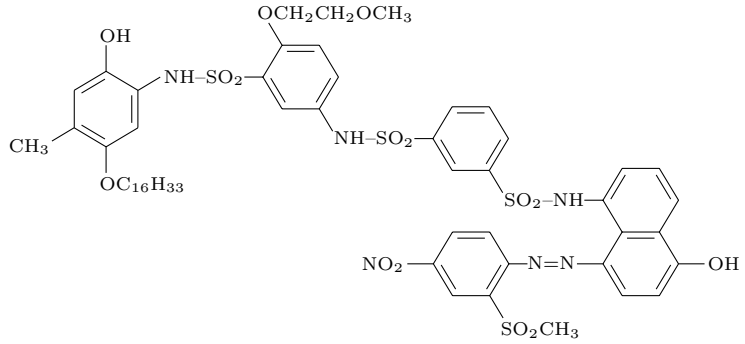
```
¥def¥cyandyereleaser{%
¥bzdrv{1==OH;5==CH$_{3}$;4==OC$_{16}$H$_{33}$;%
2==¥ryl(4==NH--SO$_{2}$){4==¥bzdrh{1==(yl);2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
5==¥ryl(2==NH--SO$_{2}$){4==¥bzdrh{1==(yl);%
5==¥ryl(2==SO$_{2}$--NH){4==¥naphdrh{1==(yl);5==OH;%
8==¥lyl(4==N=N){4==¥bzdrh{4==(yl);1==NO$_{2}$;5==SO$_{2}$CH$_{3}$}}}}}}}}}}
```

Then, we write down the command `¥cyandyereleaser`. Thereby, we obtain a target formula:

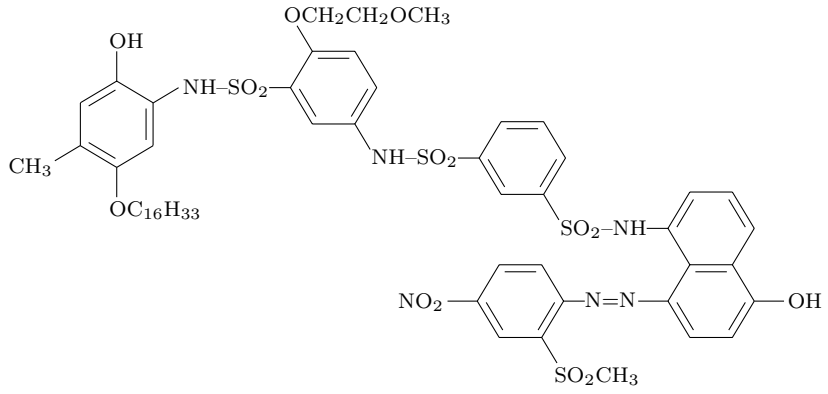


The size of the formula can be reduced by declaring the command `¥changeunitlength`.

—0.07pt: (`¥changeunitlength{0.07pt}`)

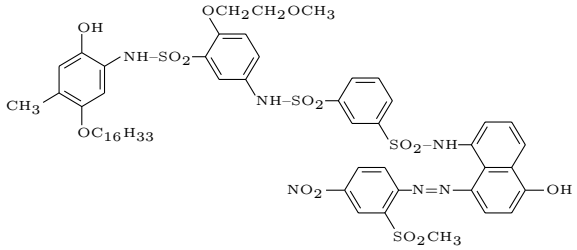


—0.08pt: (`¥changeunitlength{0.08pt}`)



A further reduction is possible. The following example shows the case of `¥unitlength=0.05pt`.

—0.05pt: (`¥changeunitlength{0.05pt}`)

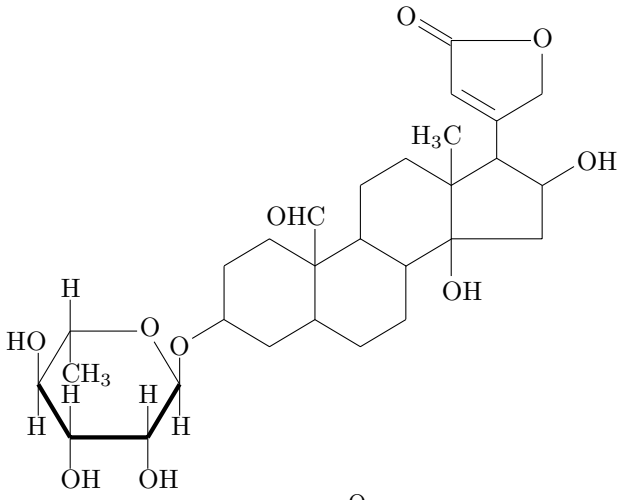


The structural formula of adonitoxin, which has once been depicted in a different way in Chapter 15 of the XyMTEXbook [3], can be drawn by the code defined as follows:

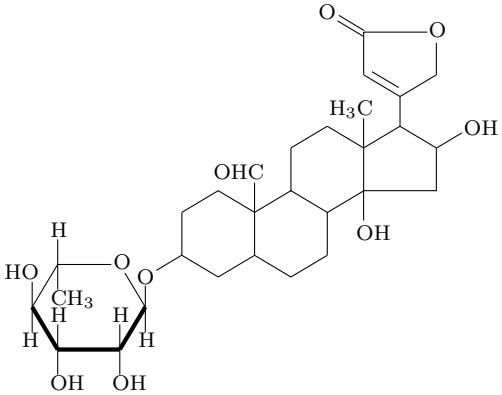
```
¥def¥adonitoxin{%
¥steroid{{{10}}=¥lmoiety{OHC};{{14}}=OH;%
{{13}}=¥lmoiety{H$_{3}$C};{{16}}=OH;%
{{17}}=¥fiveheterov[e]{3=O}{4D=O;1=(yl)};%
3=¥lyl(3=O){8=%
¥pyranose{1Sb=(yl);1Sa=H;2Sb=H;2Sa=OH;3Sb=H;3Sa=OH;4Sb=HO;%
4Sa=H;5Sb=H;5Sa=CH$_{3}$}}}}
```

Then, we write down the defined command `¥adonitoxin`. If it is necessary to reduce the size of a formula, the command `¥changeunitlength` is declared.

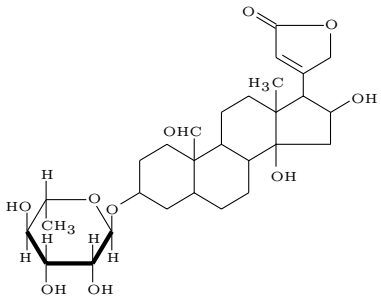
—0.1pt



—0.08pt



—0.06pt

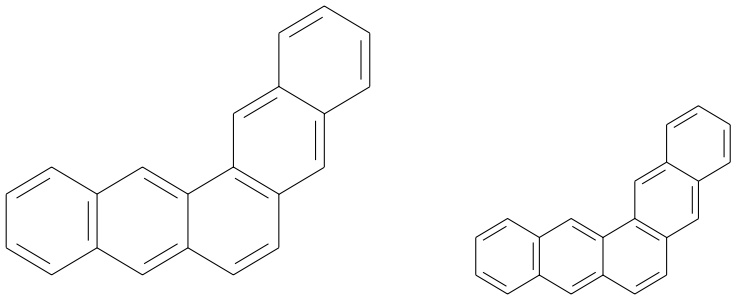


3.2 Nested Ring Fusion

A pentacyclic aromatic compound named pentaphene can be drawn by the code:

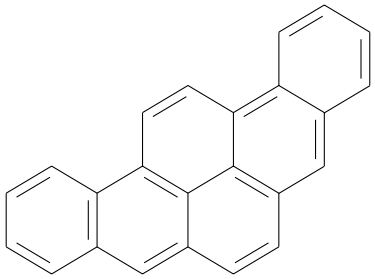
```
¥hanthracenev[acehjmp%
{a¥sixfusev[bf%
{a¥sixfusev[bf]{}{}{D}}
]{}{}{D}}%
]{}
```

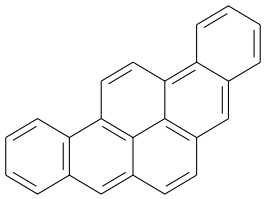
The mode of nesting is designated by 666(↓6(↓6)), where 666 represents an anthracene ring and ↓6 represents the fusion of a six-membered unit. The formula appearing in the right-hand side is drawn under declaring `¥changeunitlength{0.07pt}`



The fusion of a six-membered unit on the formula of pentaphene generates benzo[*rst*]pentaphene, which is drawn by the code:

```
¥hanthracenev[acehjmp%
{a¥sixfusev[bf%
{a¥sixfusev[bf]{}{}{D}}%
]{}{}{D}}%
{m¥sixfusev[f]{}{}{D}[bc]}%
]{}
```

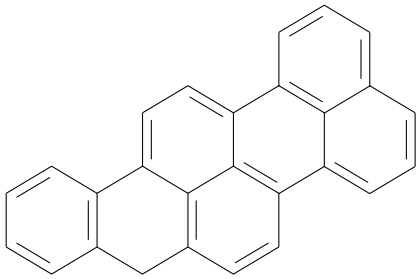


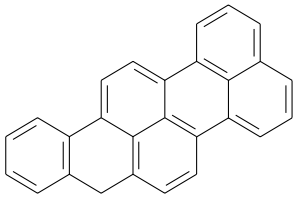


Note that the bay area represented by *rst* in pentacene corresponds to the bond 'm' of the mother skeleton ¥hanthracenev.[1] The last optical argument [bc] in the code m¥sixfusev[f]{}{}{D}[bc] designates bonds to be deleted.

A further fusion generates 9*H*-dibeno[*de,rst*]pentaphene as follows:

```
¥hanthracenev[chojp%
{a¥sixfusev[d%
{a¥sixfusev[bdf]{}{}{D}}
{b¥sixfusev[bd]{}{}{E}[f]}
]{}{}{D}}%
{m¥sixfusev[ae]{}{}{D}[bc]}%
]{}
```

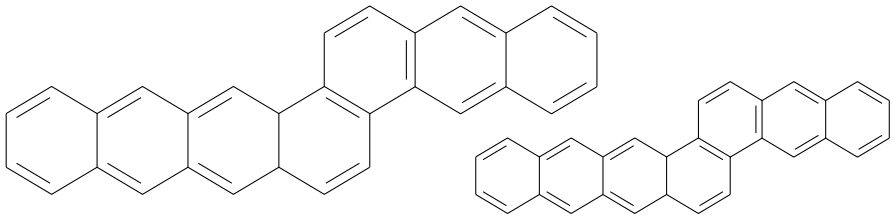




The formula of anthra[2,1-a]nathphacene can be generated by the nesting that is represented to be 66(←6(←6(↓6(←6(←6))))).

```
¥decaheterov[dfhj%
{b¥sixfusev[df{b¥sixfusev[ac%
{a¥sixfusev[bf%
{b¥sixfusev[ac{b¥sixfusev[ac]{}{}{E}}]{}{}{E}}%
]{}{}{D}}%
]{}{}{E}}]{}{}{E}}%
]{}{}{}
```

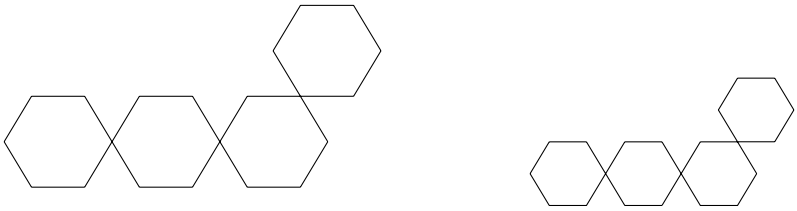
[1] Since the bond 'm' is not considered as a proper fused position under usual derivation, a XyMTEX warning appears in the present drawing. However, ther is no problem to draw such improper fusing.



3.3 Nested Spiro Compounds

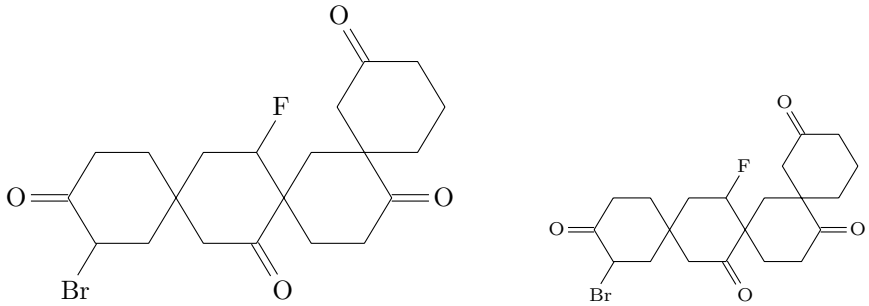
Spiro compounds can be drawn by using so-called "atom derivation", where a spiro ring is designated the atom list (atomlist) argument of a mother skeleton. The following example shows a multi-nested drawing of a spiro-compound. The formula appearing in the right-hand side is drawn under declaring ¥changeunitlength{0.07pt}

```
¥sixheteroh{4s==¥sixheteroh{4s==¥sixheteroh{%
3s==¥sixheteroh{}{6==(yl)}}{1==(yl)}}{1==(yl)}}{}
```



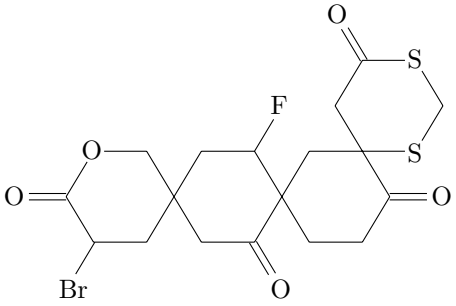
Each component of the formula can take substituents, which are designated by using the coressponding substitution list (substlist).

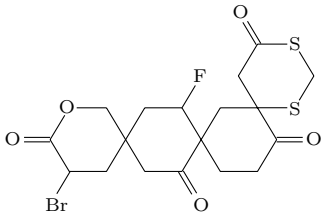
```
¥sixheteroh{4s==¥sixheteroh{%
4s==¥sixheteroh{3s==¥sixheteroh{}{6==(yl);2D==O}}{1==(yl);4D==O}}%
{1==(yl);5D==O;3==F}}{1D==O;6==Br}
```



Hetero atoms can be placed on the vertices of each component, where they are designated by using the atom list (atomlist).

```
¥sixheteroh{2==O;4s==¥sixheteroh{%
4s==¥sixheteroh{3s==¥sixheteroh{3==S;5==S}{6==(yl);2D==O}}{1==(yl);4D==O}}%
{1==(yl);5D==O;3==F}}{1D==O;6==Br}
```


O
S
F
O
S
O
O
O
Br
O


O
S
F
O
S
O
O
Br
O

Chapter 4

Dirty Tricks

4.1 Meisenheimer Complexes

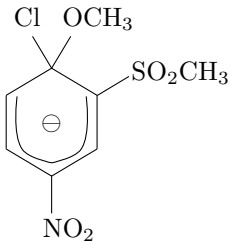
A nucleophilic substitution on a benzene ring includes a so-called Meisenheimer-type complex. To draw such an ionic intermediate, we first define ¥benzeniumionelement to draw a pentadienyl anionic species.

```
¥def¥benzeniumionelement{%
¥begin{pspicture}(200,200)
¥pscurve[linewidth=0.4pt](0,50)(110,100)(130,300)
¥pscurve[linewidth=0.4pt](0,50)(-110,100)(-130,300)
¥rput(0,200){$¥ominus$}
¥end{pspicture}}
```

The command ¥benzeniumionelement depicts the following element:

Then, this element is designated in the atom list of ¥sixheterov.

```
¥sixheterov{4s==¥benzeniumionelement}{%
1Sb==Cl;1Sa==OCH$_{3}$;2==SO$_{2}$CH$_{3}$;4==NO$_{2}$}
```

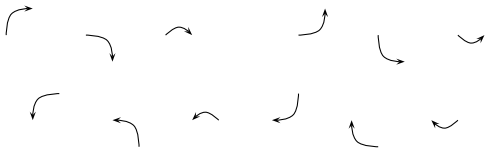


4.2 Electron Shifts

To illustrate the mechanisms of organic reactions, curved arrows are used to show an electron shift. The macros for drawing such curved arrows are defined in the chmst-ps package: ¥electronrshiftarrow and ¥electronlshiftarrow.

Several curved arrows generated by these commands are shown as examples:

```
¥electronrshiftarrow(0,0)(100,100)¥qquad
¥electronrshiftarrow(0,0)(100,-100)¥qquad
¥electronrshiftarrow(0,0)(100,0)¥qquad¥qquad
¥electronrshiftarrow[1](0,0)(100,100)¥qquad
¥electronrshiftarrow[1](0,0)(100,-100)¥qquad
¥electronrshiftarrow[1](0,0)(100,0) ¥¥[20pt]
¥electronlshiftarrow(0,0)(100,100)¥qquad
¥electronlshiftarrow(0,0)(100,-100)¥qquad
¥electronlshiftarrow(0,0)(100,0)¥qquad
¥electronlshiftarrow[1](0,0)(100,100)¥qquad
¥electronlshiftarrow[1](0,0)(100,-100)¥qquad
¥electronlshiftarrow[1](0,0)(100,0)
```

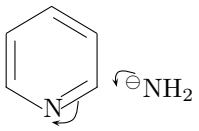


An attack of an amide anion $^{\ominus}NH_2$ on the 2-position of pyridine is illustrated as follows. According to the specification of the XyMTEXsystem, the code `1==N` should be placed at the last part of the atom list of `¥sixheterovi`.[1]

```
¥sixheterovi[ace]{2==¥futuresubst{$^{¥ominus}$NH$_{2}$};
2s==¥electronlshiftarrow(70,0)(140,50);%
1s==¥electronlshiftarrow[1](0,-30)(100,50);1==N}{}
```

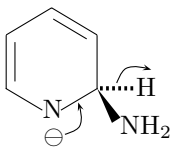
The command `¥futuresubst` is defined to show the amide anion $^{\ominus}NH_2$ that will be involved as a future substituent.

The command `¥electronlshiftarrow` for drawing a left curly arrow is designated in the atom list of the command `¥sixheterovi`.



Similarly, the command `¥electronrshiftarrow` is used to draw a right curly arrow.

```
¥sixheterovi[ce]{%
1s==¥electronrshiftarrow[1](50,-70)(100,50);%
2s==¥electronrshiftarrow(70,20)(200,70);1==¥downnobond{N}{$¥ominus$}%
}{2SB==NH$_{2}$;2SA==H}
```



[1] Otherwise, the flag for truncating a vertex is deleted.

Chapter 5

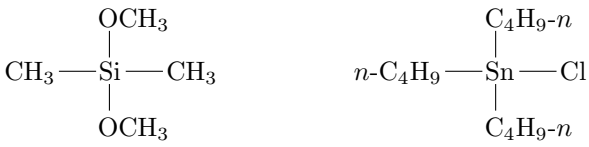
Variable Lengths of Horizontal and Vertical Bonds

5.1 Automatic Adjustment for Two- or More-Character Central Atoms

5.1.1 Tetrahedral Molecules

The specification of the command `¥tetrahedral` in XƎMTEX Versions 3.00 (published) and 4.00 (private) allows us to draw a one-character central atom only, which is output in the centralized position of the domain of the central atom. This means that an atom represented by two characters (Si, Zn, etc.) or a group such as CH and CH_2 cannot be placed properly as a central atom, where the central atom and an incident bond may overlap each other. The command `¥tetrahedral` in XƎMTEX Vesion 4.01 is improved to allow a length-variable central atoms.

1. Examples of Metal Complexes:



which are drawn by the following codes:

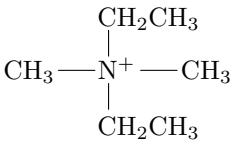
```
¥tetrahedral{0==Si;4==CH$_{3}$;2==CH$_{3}$;1==OCH$_{3}$;3==OCH$_{3}$}
¥hskip3cm
¥tetrahedral{0==Sn;1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;2==$n$-C$_{4}$H$_{9}$;4==Cl}
```

2. As for quaternary ammonium salts, e.g.,

the specification of XyMTEX Versions 3.00 and 4.00 has forced us to write the following codes:

```
¥tetrahedral{0==N¥rlap{$^{^{+}}$};4==CH$_{3}$;2==CH$_{3}$;%
1==CH$_{2}$CH$_{3}$;3==CH$_{2}$CH$_{3}$}
¥hskip 3cm
¥tetrahedral[{0+}]{0==N;4==CH$_{3}$;2==CH$_{3}$;%
1==CH$_{2}$CH$_{3}$;3==CH$_{2}$CH$_{3}$}
```

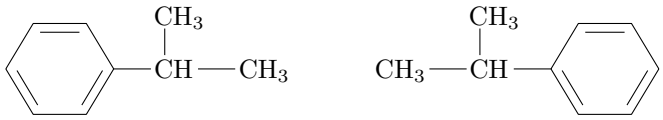
On the other hand, the version 4.01 can draw a quaternary salt in the following way:



by inputting as follows:

```
¥tetrahedral{0==N$^{+}$;4==CH$_{3}$;2==CH$_{3}$;%
1==CH$_{2}$CH$_{3}$;3==CH$_{2}$CH$_{3}$}
```

3. Cumene (isopropylbenzene or 2-propylbenzene) can be drawn as follows:



They are drawn by the following codes containing a “yl function”:

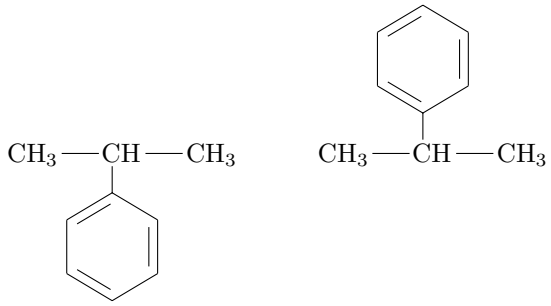
```
¥bzdrh{4==¥tetrahedral{2==(yl);0==CH;1==CH$_{3}$;4==CH$_{3}$}}
¥hskip4cm
¥bzdrh{1==¥tetrahedral{4==(yl);0==CH;1==CH$_{3}$;2==CH$_{3}$}}
```

Cumene can be drawn as a derivative of propane, i.e., 2-phenylpropane. Thus, we have:

These formulas are drawn by inputting following codes:

```
¥tetrahedral{2==¥bzdrh{4==(yl)};0==CH;1==CH$_{3}$;4==CH$_{3}$}
¥hskip3cm
¥tetrahedral{4==¥bzdrh{1==(yl)};0==CH;1==CH$_{3}$;2==CH$_{3}$}
```

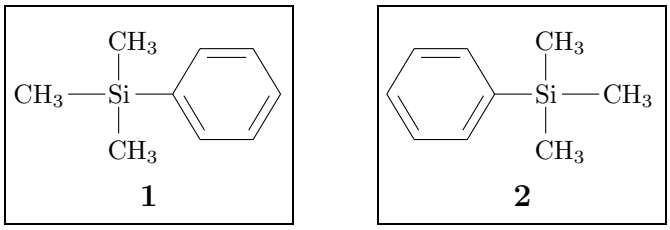
The direction of a phenyl group can be changed:



These formulas are drawn by inputting following codes:

```
¥tetrahedral{3==¥bzdrv{1==(yl)};0==CH;2==CH$_{3}$;4==CH$_{3}$}
¥hskip2cm
¥tetrahedral{1==¥bzdrv{4==(yl)};0==CH;2==CH$_{3}$;4==CH$_{3}$}
```

4. The formulas of trimethylsilylbenzene (**1** and **2**) represented by:



are drawn by the following codes

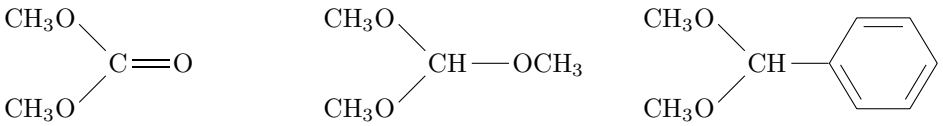
```
¥fbox{%
¥begin{XyMcompd}(900,600)(-300,100){cpd:2}{}
¥bzdrh{1==¥tetrahedral{4==(yl);0==Si;1==CH$_{3}$;2==CH$_{3}$;3==CH$_{3}$}}
¥end{XyMcompd}}
¥hskip1cm
¥fbox{%
¥begin{XyMcompd}(900,600)(300,100){cpd:3}{}
¥bzdrh{4==¥tetrahedral{2==(yl);0==Si;1==CH$_{3}$;4==CH$_{3}$;3==CH$_{3}$}}
¥end{XyMcompd}}
```

in which the XyMcompd environment is used to specify the drawing domain of each structural formula (surrounded by the `¥fbox` command). Moreover, the cross references of the fomulas can be accomplished by using `¥cref` or `¥ref`.

5.1.2 Trigonal Units

The same situation described above occurs in the use of the commands `¥ltrigonal` and `Ltrigonal` of the previous versions of XyMTEX. These commands are also improved to allow a length-variable central atoms in XyMTEX Vesion 4.01.

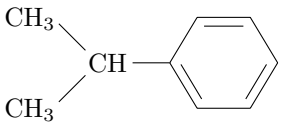
1. For example, the command `¥ltrigonal` is used to draw structural formulas having a two-character group (CH) as follows:



where the first formula is drawn as a reference formula with a centeral atom of a single character (C). These formulas are drawn by the following codes:

```
¥ltrigonal{0==C;2==CH$_{3}$O;1D==O;3==CH$_{3}$O}
¥hskip 2cm
¥ltrigonal{0==CH;2==CH$_{3}$O;1==OCH$_{3}$;3==CH$_{3}$O}
¥hskip2cm
¥ltrigonal{0==CH;2==CH$_{3}$O;1==¥bzdrh{1==(yl)};3==CH$_{3}$O}
```

The following formula (**3**) is drawn by regarding cumene as 2-propenylbenzene:

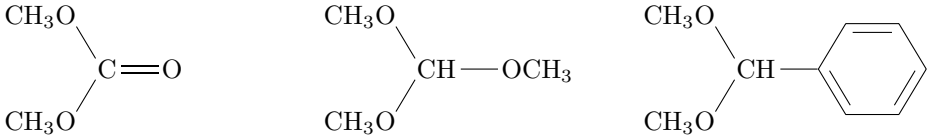


3

which is drawn by the code:

```
¥begin{XyMcompd}(1000,500)(-400,200){cpd:4}{}
¥bzdrh{1==¥ltrigonal{1==(yl);0==CH;2==CH$_{3}$;3==CH$_{3}$}}
¥end{XyMcompd}
```

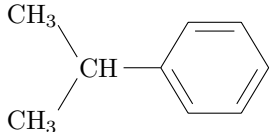
2. The command `¥Ltrigonal` is defined in the same guideline as `¥ltrigonal` described above. The command is used to draw the same formulas having a two-character group (CH) as follows:



These formulas are drawn by the following codes:

```
¥Ltrigonal{0==C;2==CH$_{3}$O;1D==O;3==CH$_{3}$O}
¥hskip 2cm
¥Ltrigonal{0==CH;2==CH$_{3}$O;1==OCH$_{3}$;3==CH$_{3}$O}
¥hskip2cm
¥Ltrigonal{0==CH;2==CH$_{3}$O;1==¥bzdrh{1==(yl)};3==CH$_{3}$O}
```

The following formula (**4**) is drawn by regarding cumene as 2-propenylbenzene:



4

which is drawn by the code:

```
¥begin{XyMcompd}(1000,500)(-400,200){cpd:5}{}
¥bzdrh{1==¥Ltrigonal{1==(yl);0==CH;2==CH$_{3}$;3==CH$_{3}$}}
¥end{XyMcompd}
```

3. On the other hand, the previous definitions of the commands `¥rtrigonal` and `¥Rtrigonal` remain unchanged in XƎMTEX vertion 4.01, because even a group of two or more characters can be accommodated as a central atom.


```
¥bzdrh{4==¥rtrigonal{0==CH;3==CH$_3$;2==CH$_3$;1==(yl)}}
¥hskip3cm
¥bzdrh{4==¥Rtrigonal{0==CH;3==CH$_3$;2==CH$_3$;1==(yl)}}
```

4. On the same line, the previous definitions of the commands `¥utrigonal` and `¥Utrigonal` remain unchanged in XƎMTEX vertion 4.01.


```
¥utrigonal{1==¥bzdrv{1==(yl)};0==CH;2==CH$_{3}$;3==CH$_{3}$}
¥hskip3cm
¥Utrigonal{1==¥bzdrv{1==(yl)};0==CH;2==CH$_{3}$;3==CH$_{3}$}
```

5. The previous definitions of the commands `¥dtrigonal` and `¥Dtrigonal` remain also unchanged in XƎMTEX vertion 4.01.

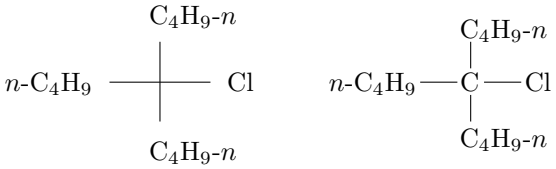

```
¥dtrigonal{1==¥bzdrv{4==(yl)};0==CH;2==CH$_{3}$;3==CH$_{3}$}
¥hskip3cm
¥Dtrigonal{1==¥bzdrv{4==(yl)};0==CH;2==CH$_{3}$;3==CH$_{3}$}
```

5.1.3 Omission of Central Atoms

A central atom could not be omitted in the old version of the ¥tetrahedral command so that a vacancy was resulted if the central atom is not specified. In XyMTEXxVersion 4.01, the ¥tetrahedral command allows the omission of such a central atom, where a vacancy is deleted. For example, the codes

```
¥tetrahedral{1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;2==$n$-C$_{4}$H$_{9}$;4==Cl}
¥hskip2cm
¥tetrahedral{0==C;1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;2==$n$-C$_{4}$H$_{9}$;4==Cl}
```

produce the following structures:



The ¥tetrahedral command can be used in another command in a nested fashion. The following examples show the use of the ¥tetrahedral command in the argument of the ¥bzdrh command. Thus, the codes:

```
¥bzdrh{4==%
¥tetrahedral{2==(yl);1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;4==Cl}}
¥hskip3cm
¥bzdrh{4==%
¥tetrahedral{2==(yl);0==C;1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;4==Cl}}
```

produce the following structures:

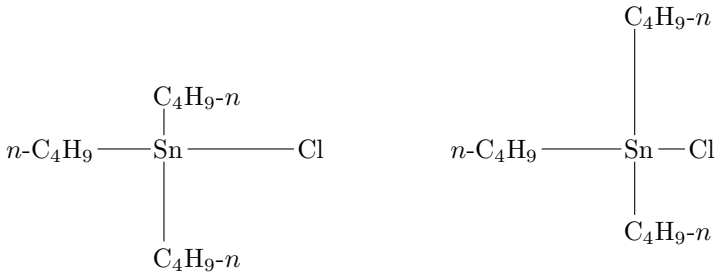
Note: In XyMTEXxVersion 4.01, the ¥trigonal command etc. do not support this function so that a vacancy was resulted if the central atom is not specified.

5.2 Variable Bond Lengths

In XyMTEXxVersion 4.01, the ¥tetrahedral command takes an additional optional argument, which specifies the bond length of each horizontal or vertical bond by the unit ¥unitlength (= 0.1pt for the standard situation). For example, the codes

```
¥tetrahedral{0==Sn;1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;2==$n$-C$_{4}$H$_{9}$;4==Cl}<100,200,300,400>
¥hskip2cm
¥tetrahedral{0==Sn;1==C$_{4}$H$_{9}$-$n$;%
3==C$_{4}$H$_{9}$-$n$;2==$n$-C$_{4}$H$_{9}$;4==Cl}<400,300,200,100>
```

produce the following structures:

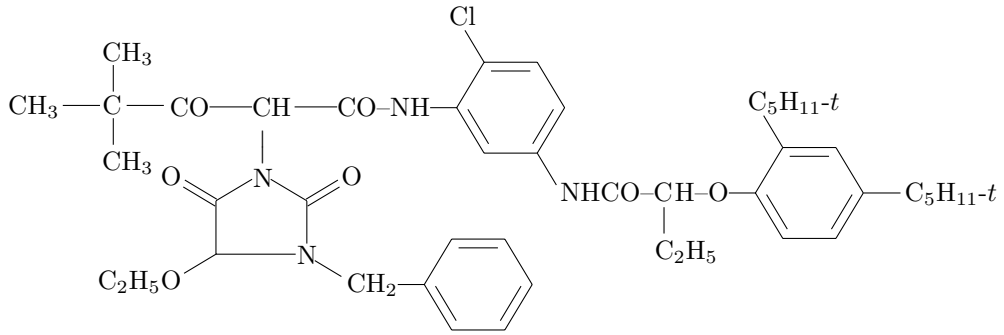


In 2004, I have published a monograph entitled "Organic Chemistry of Photography" [14]. In this book, I have extensitively used XƎMTEX (Version 4.00) for typesetting chemical structural formulas. However, a direct method has been applied as follows, because the version 4.00 did not support the function of variable bond lengths. Thus, the codes:

```
¥makeatletter
¥begingroup
¥def¥methineunitCA#1{¥vtop{%
¥hbox to0.8em{CH¥hss}¥nointerlineskip
¥hbox to0.8em{¥hss
$¥big|$¥rule[-1.7ex]{0pt}{5ex}%
¥hss}¥nointerlineskip
¥hbox to0.8em{¥hss¥kern#1%
%¥fiveheterovi{1==N;3==N}{1==(yl);2D==O;5D==O;4==C$_{2}$H$_{5}$;%
¥fiveheterovi{1==N;3==N}{1==(yl);2D==O;5D==O;4==C$_{2}$H$_{5}$O;%
3==¥ryl(3==CH$_{2}$){4==¥bzdrh{1==(yl)}}}¥hss}¥nointerlineskip
¥hbox to1.6em{}%
}}


%EX-Y yellow coupler
%¥fbox{%
¥begin{tabular}{c}
¥begin{XyMcompd}(3600,1500)(-100,-700){}{}
¥tetrahedral{O==C;1==CH$_{3}$;2==CH$_{3}$;3==CH$_{3}$;%
4==¥raisebox{.5ex}{¥ryl(4=={CO¥sbond¥methineunitCA{1pt}¥sbond CO--NH}){%%
4==¥bzdrh{1==(yl);2==Cl;5==%
¥ryl(3==NHCO--%
¥vtop{¥hbox{C}¥nointerlineskip
¥hbox to0.8em{¥hss¥rule[-1.2ex]{0pt}{3.5ex}$|$¥hss}¥nointerlineskip
¥hbox to0.8em{¥hss C¥rlap{$_{2}$H$_{5}$}¥hss}%
}%
H--O){4==¥bzdrh{1==(yl);2==C$_{5}$H$_{11}$-$t$;%
4==C$_{5}$H$_{11}$-$t$}}};%
}}%%
}%
¥end{XyMcompd} ¥¥
¥compd¥label{cpd:ch1-00LL1a} ¥¥
¥end{tabular}
%}
¥endgroup
¥makeatother
```

produce the following structure of a two-equivalent yellow coupler:



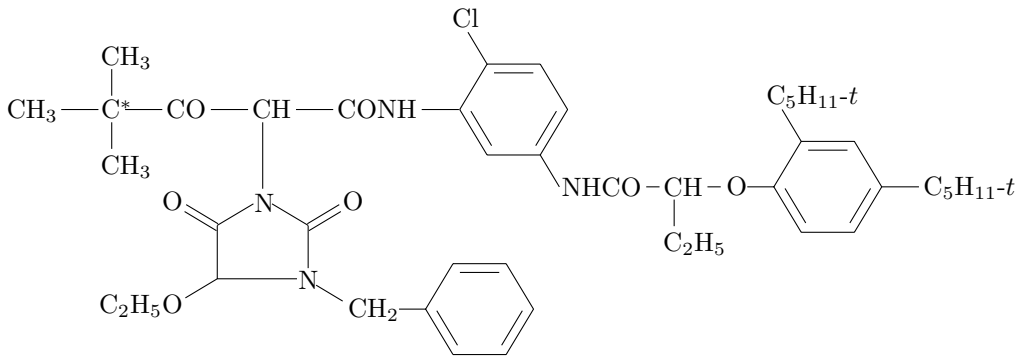
5

This direct method contains layout data in the form of the command `¥methineunitCA` etc. Such layout data should be concealed from the souce list of the book for the consistency of the XyMTEX methodology.

The function of variable bond lengths supported by XyMTEX (Version 4.01) provides us with a more elegant solution to draw this type of compounds. The same structure as **5** can be drawn by using the redefined command `¥tetrahedral`. Thus, the codes:

```
%¥fbox{%
¥begin{XyMcompd}(3800,1500)(-100,-700){cpd:06}{}
¥tetrahedral{0==C¥rlap{$^{*}$};1==CH$_{3}$;2==CH$_{3}$;3==CH$_{3}$;%
4==¥tetrahedral{0==CO;2==(yl);%
4==¥tetrahedral{0==CH;2==(yl);%
3==¥fiveheterovi{1==N;3==N}{1==(yl);2D==O;5D==O;4==C$_{2}$H$_{5}$O;%
3==¥ryl(3==CH$_{2}$){4==¥bzdrh{1==(yl)}}};%
4==¥tetrahedral{0==CONH;2==(yl);%
4==¥bzdrh{1==(yl);2==Cl;%
5==¥tetrahedral{0==NHCO;2==(yl);%
4==¥tetrahedral{0==CH;2==(yl);3==C$_{2}$H$_{5}$;%
4==¥ryl(4==O){4==¥bzdrh{1==(yl);2==C$_{5}$H$_{11}$-$t$;%
4==C$_{5}$H$_{11}$-$t$}%
}}<,,,50>}<,,,50>}}}<,,250,>}}%
¥end{XyMcompd}%
%}
```

typeset the following structure:



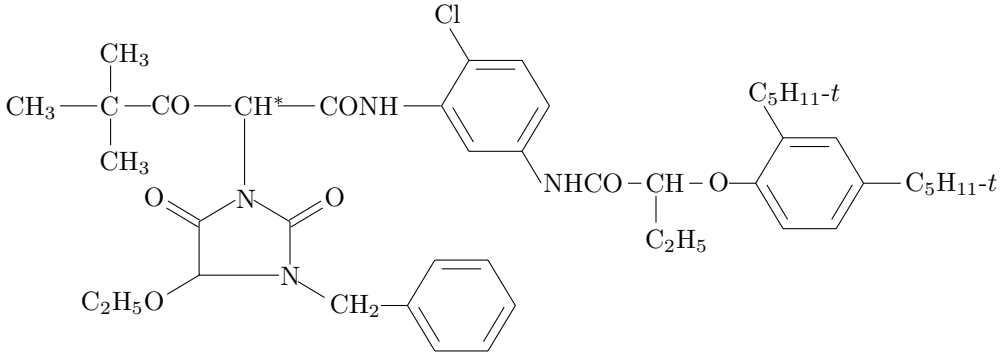
6

It should be noted that this drawing is started at the asterisked carbon by using the redefined command `¥tetrahedral`.

The start of drawing at another carbon is possible. For example, the following codes:

```
%¥fbox{%
¥begin{XyMcompd}(3800,1500)(-600,-700){cpd:07}{}
¥tetrahedral{0==CH¥rlap{$^{*}$};%
2==¥lyl(4==CO){%
4==¥tetrahedral{4==(yl);0==C;1==CH$_{3}$;2==CH$_{3}$;3==CH$_{3}$}};%
3==¥fiveheterovi{1==N;3==N}{1==(yl);2D==O;5D==O;4==C$_{2}$H$_{5}$O;%
3==¥ryl(3==CH$_{2}$){4==¥bzdrh{1==(yl)}}};%
4==¥tetrahedral{0==CONH;2==(yl);%
4==¥bzdrh{1==(yl);2==Cl;%
5==¥tetrahedral{0==NHCO;2==(yl);%
4==¥tetrahedral{0==CH;2==(yl);3==C$_{2}$H$_{5}$;%
4==¥ryl(4==O){4==¥bzdrh{1==(yl);2==C$_{5}$H$_{11}$-$t$;%
4==C$_{5}$H$_{11}$-$t$}%
}}<,,,50>}<,,,50>}}}<,,250,>
¥end{XyMcompd}%
%}
```

produce almost the same structure:



7

where the startin carbon atom is designaed by an asterisk.

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] Fujita, S.; Tanaka, N. "XYMTEX (Version 2.00) as Implementation of the XYM Notation and the XYM Markup Language", *TUGboat*, **21** (1), 7 (1995).

[6] Fujita, S.; Tanaka, N., *TUGboat*, **22** (4), 285 (2001).

[7] Lamport L., *LATEX. A document Preparation System*, 2nd ed. for LATEX 2$_\varepsilon$, 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] For epic macros, see Podar S., "Enhancements to the picture environment of LATEX", Manual for Version 1.2 dated July 14, 1986.

[10] XYMTEX Version 4.01 is available from
http://imt.chem.kit.ac.jp/fujita/fujitas/fujita.html

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

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

[13] van Zandt, T., Girou, D., "Inside PSTricks", *TUGboat*, **15** (3), 239 (1995).

[14] Fujita, S. *Organic Chemistry of Photography*, Springer-Verlag, Berlin-Hidelberg (2004).