XΥMTEX (Versions 5.00) for Typesetting Chemical Structural Formulas: I. Portable-Document-Format-(PDF-)Compatible Mode Supported by the **xymtx-pdf** Package and the **chmst-pdf** Package, as Well as II. Coloring Bonds Supported by the **bondcolor**.

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(Revised)

This document has been typeset by the PDF-compatible mode and the resulting dvi file has been converted into a PDF file by using the `dvipdfmx` converter.

Contents

Chapter 1

Introduction

1.1 History of the XΥMTeX System

The history of the XΥMTeX system is summarized in Table 1.1. The boldfaced versions have provided substantial improvements for drawing chemical structural formulas. The present version (version 5.00) contains two main improvements, i.e., the development of the PDF mode and the development of bond coloring.

Recent books on LaTeX 2$_{\varepsilon}$ have referred to the XΥMTeX system, e.g., pages 520–540 of [14] and pages 551–598 of Vol. II of [15].

1.2 Backgrounds and Motivations of XΥMTeX Version 5.00

1.2.1 PDF Printing

The previous version (version 4.06) of the XΥMTeX system has supported the TeX/LaTeX mode based on the LaTeX picture environment as well as the PostScript mode based on the PSTricks package linked with the LaTeX picture environment. The latter PostScript mode requires after-processing by the `dvips` converter (dvi files → ps files), where resulting PostScript files can be browsed by using the Ghostscript system (coupled with Ghostview). The PostScript files are further transformed into PDF files by using an appropriate converter (e.g., Adobe Distiller). It follows that the PDF printing of XΥMTeX structural formulas is available via such a route as

$$< \text{tex with XΥMTeX codes} > \xrightarrow{\text{TeX/LaTeX}} < \text{dvi} > \xrightarrow{\text{dvips}} < \text{ps} > \xrightarrow{\text{Distiller}} < \text{PDF} >.$$

On the other hand, structural formulas drawn by the XΥMTeX system can also be transformed into EPS (encapsulated PostScript) files by using the Ghostscript utilities so as to be incorporated into PDF files. This means that we are alternatively able to use the dvipdfm(x) converter in order to convert LaTeX document files with XΥMTeX structural formulas (EPS files) into PDF files, i.e.,

$$< \text{tex with XΥMTeX EPS files} > \xrightarrow{\text{TeX/LaTeX}} < \text{dvi} > \xrightarrow{\text{dvipdfm(x)}} < \text{PDF} >.$$

The PDF printing of XΥMTeX structural formulas has been discussed under the title "Articles, Books, and Internet Documents with Structural Formulas Drawn by XΥMTeX — Writing, Submission, Publication, and Internet Communication in Chemistry." [16], where such state-of-the-art routes as described above have been compared in preparing PDF documents with XΥMTeX structural formulas.

Although the above-mentioned methods are capable of providing PDF documents of high quality, they are incapable of converting dvi files into PDF files, when the dvi files have been prepared from LaTeX document files containing XΥMTeX codes (not EPS files). In other words, the dvi files cannot be treated directly by the dvipdfm(x) converter. Because PDF files become more and more popular in

Table 1.1: Versions of XΥMTEX

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 2ε) 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 XΥM Notation. See Ref. [4, 5, 6]. 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. See Ref. [7]
4.00 (2002)	(not released) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00)
4.01 (2004)	The xymtx-ps package for PostScript printing and length-variable central atoms [8]
4.02 (2004)	PostScript printing and wedges bonds for stereochemistry
4.03 (2005)	PostScript printing and wavy bonds for stereochemistry. See Ref. [9]
4.04 (2009)	Macros for drawing steroids (steroid.sty, ver 1.00). See Ref. [10]
4.05 (2009)	Macros for drawing Lewis structures of the lewissturc package (lewisstruc.sty, version 1.00), revised and improved macros added to the chemist package (ver 4.05) [and the chmst-ps package (ver 1.02)], and the first release of the chemtimes package (ver 1.00)
4.06 (2009)	The chmst-ps package (ver 1.03) for supporting bent (curved) harpoons. See Refs. [11, 12, 13]
5.00 (2010)	The present version: the xymtx-pdf package (ver 5.00) for supporting PDF printing, the bondcolor package (ver 5.00) for coloring double bonds and skeletal bonds as well as the assurelatexmode package for assuring compatibility of the three modes. This version also contains the chmst-pdf package (ver 5.00) for extending the chemist package to support PDF printing and the assurechemist package for assuring compatibility of the three modes.

writing, publication and internet documentation, and because the dvipdfm(x) converter becomes the de facto standard for preparing PDF files, it is highly desirable to develop a direct route for processing dvi files prepared from TeX/LaTeX documents with XΥMTEX codes, i.e.,

$$< \text{tex with XΥMTEX codes} > \xrightarrow{\text{TeX/LaTeX}} < \text{dvi} > \xrightarrow{\text{dvipdfm(x)}} < \text{PDF} >.$$

Such a direct route is now available by the present XΥMTEX system (version 5.00), where the xymtx-pdf package added as part of the XΥMTEX 5.00 supports the PDF-compatible mode for using the dvipdfm(x) converter or equivalent.

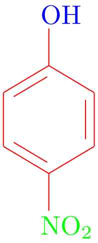
Because the drawing mechanism of structural formulas in the XΥMTEX 5.00 relies on graphic utilities of the pgf package developed by T. Tantau [18], you should download the the pgf package from his site: `http://sourceforge.net/projects/pgf`.

1.2.2 Bond Coloring

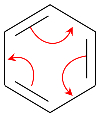
Even within the scope of the previous version (4.06), the code:

```
{\red \bzdrv{1=={\blue OH};4=={\green NO$_{2}$}}}
```

produces the following colored structure:



On a similer line, electron shifts in a resonance structure of benzene can be colored as follows:



by writing the following code:

```
\sixheterov[bdf]
{2s=={\red\electronrshiftarrow(-40,-90)(-90,-240)};%
4s=={\red\electronlshiftarrow(-160,200)(-70,100)};%
6s=={\red\electronrshiftarrow[1](100,20)(260,20)}}{}
```

However, there has been no systematic way of coloring a specific bond to be emphasized. For example, the substitution bond between the OH group and the aromatic ring in the first example cannot be colored differently from other portions of the molecule. The three double bonds of the benzene ring in the second example cannot be colored if we rely on the previous techniques of XΥMTEX version 4.06.

Hence, it is highly desirable to differentiate a specific bond by color if we pursue intuitively- and visually-understandable documentation. The bondcolor package newly added in the XΥMTEX version 5.00 supports commands for coloring double bonds, skeletal bonds and others.

1.3 About On-Line Manuals for XΥMTEX Version 5.00

Two on-line manuals (xymtx500.pdf and xymtx500PS.pdf) are available for XΥMTEX Version 5.00, where their contents are substantially the same. The manual xymtx500.pdf has been processed by the PDF-compatible mode, i.e.,

$$< \text{tex with XΥMTEX codes} > \xrightarrow{\text{TEX/LATEX}} < \text{dvi} > \xrightarrow{\text{dvipdfm(x)}} < \text{PDF} >$$

where the preamble of the corresponding tex file has been described as follows:

```
%xymtx500.tex
\documentclass{book}
%%\usepackage[dvips]{xymtexpdf}%draft making
\usepackage{xymtexpdf}
\usepackage{chmst-pdf}
\begin{document}
<text with XyMTeX codes>
\end{document}
```

The resulting dvi file has been converted into the PDF file (xymtx500.pdf) by means of the dvipdfmx converter (cf. Section 2.2). Note that `\usepackage[dvips]{xymtexpdf}` has been used during draft making, where the resulting PostScript file has been browsed by GSview coupled with Ghostscript (cf. Section 2.3).

On the other hand, the manual xymtx500PS.pdf has been processed by the PostScript-compatible mode, i.e.,

$$< \text{tex with X\!\Upsilon\!M\TeX\ codes} > \xrightarrow{\text{\TeX/\LaTeX}} < \text{dvi} > \xrightarrow{\text{dvips}} < \text{ps} > \xrightarrow{\text{Distiller}} < \text{PDF} >$$

where the preamble of the corresponding tex file has been described as follows:

```
%xymtx500PS.tex
\documentclass{book}
\usepackage{xymtexps}
\usepackage{chmst-ps}
\begin{document}
<text with XyMTeX codes>
\end{document}
```

The text `<text with XyMTeX codes>` of the PostScript-compatible mode is essentially the same as the counterpart of the PDF-compatible mode described above. The resulting dvi file has been converted into the PDF file (xymtx500PS.pdf) via a PostScript file (dvips and Adobe Distiller).

Although these two manuals have essentially the same context, they are different in their document sizes (xymtx500.pdf ca. 3.5 Mbyte vs. xymtx500PS.pdf ca. 1 Mbyte).

Chapter 2

XΥMTEX Version 5.00

2.1 Package Files of XΥMTEX Version 5.00

The XΥMTEX system (version 5.00) consists of the package files listed in Table 2.1, where the package xymtx-pdf.sty has been developed to realize the PDF-compatible mode.

The XΥMTEX system (version 5.00) supports three modes of structural drawing.

1. **TEX/LATEX Mode**: The declaration of `\usepackage{xymtex}` in the preamble of a tex file results in the reading of all the package files listed in the XΥMTEX Structural Files of Figure 2.1, which permits XΥMTEX drawing according to the LATEX picture environment and the epic package (modified slightly). Please consult the on-line manuals of XΥMTEX version 4.06 and before.

2. **PostScript-Compatible Mode**: The declaration of `\usepackage{xymtexps}` in the preamble of a tex file results in the reading of the xymtx-ps package as well as all the package files listed in the XΥMTEX Structural Files of Figure 2.1. The drawing of structural formulas is based on the LATEX picture environment and the pstricks package [17]. Please consult the on-line manuals of XΥMTEX version 4.06 and before. A dvi file produced by TEX/LATEX processing should be further converted into a ps file by dvips (or equivalents) in order to browse XΥMTEX structural formulas:

   $$<\text{tex with XΥMTEX codes}> \xrightarrow{\text{TEX/LATEX}} <\text{dvi}> \xrightarrow{\text{dvips}} <\text{ps}> \xrightarrow{\text{Distiller}} <\text{PDF}>.$$

   Of course, an alternative process using a tex file with XΥMTEX EPS files:

   $$<\text{tex with XΥMTEX EPS files}> \xrightarrow{\text{TEX/LATEX}} <\text{dvi}> \xrightarrow{\text{dvips}} <\text{ps}> \xrightarrow{\text{Distiller}} <\text{PDF}>$$

   is also effective in this mode. As a result, a tex file for drawing structural formulas is permitted to contain both XΥMTEX codes and XΥMTEX EPS files.

3. **PDF-Compatible Mode**: The declaration of `\usepackage{xymtexpdf}` in the preamble of a tex file results in the reading of the xymtx-pdf package as well as all the package files listed in the XΥMTEX Structural Files of Figure 2.1. The drawing of structural formulas is based on the LATEX picture environment and the pgf package [18]. A dvi file produced by TEX/LATEX processing should be further converted into a PDF file by dvipdfm(x) in order to browse XΥMTEX structural formulas by means of Adobe Reader. The direct process described on Page 8:

   $$<\text{tex with XΥMTEX codes}> \xrightarrow{\text{TEX/LATEX}} <\text{dvi}> \xrightarrow{\text{dvipdfm(x)}} <\text{PDF}>.$$

   is now realized by the PDF-compatible mode.

   Of course, the previous process using a tex file with XΥMTEX EPS files:

Table 2.1: Package Files of XΥMTEX and Related Files

package name	included functions
XΥMTEX Structural 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 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 macros for atom- and bond-typesetting
locant.sty	macros for printing locant numbers
polymers.sty	macros for drawing polymers
fusering.sty	macros for drawing units for ring fusion
methylen.sty	macros for drawing zigzag polymethylene chains
sizeredc.sty	macros for size reduction
steroid.sty	macros for drawing steroid derivatives contained in the steroid package
lewissturc	macros for drawing Lewis structures
bondcolor	macros for coloring double bonds and skeletal bonds (XΥMTEX Version 5.00)
assurelatexmode	dummy declaration for compatibility of the three modes (XΥMTEX Version 5.00)
Packages for PostScript- and PDF-Compatible Modes	
xymtx-ps.sty	macros for PostScript printing (XΥMTEX Version 4.02). These macros are substituted for several macros contained in the chemstr package.
xymtx-pdf.sty	macros for PDF printing (XΥMTEX Version 5.00). These macros are substituted for several macros contained in the chemstr package.
XΥMTEX Utilities	
xymtex.sty	a package for calling all package files (listed in XΥMTEX Structural Files) without loading xymtx-ps.sty and xymtx-pdf.sty (for the TEX/LATEX mode)
xymtexps.sty	a package for calling all package files (listed in XΥMTEX Structural Files) and xymtx-ps.sty (for the PostScript-compatible mode). Not with xymtx-pdf.sty
xymtexpdf.sty	a package for calling all package files (listed in XΥMTEX Structural Files) and xymtx-pdf.sty (for the PDF-compatible mode). Not with xymtx-ps.sty
Related Files	
chemist.sty	commands for using 'chem' version and chemical environments
assurechemist.sty	dummy commands for compatibility of the three modes (Version 5.00)
chmst-ps.sty	macros for PostScript printing. These macros are substituted for several macros contained in chemist package.
chmst-pdf.sty	macros for PDF printing. These macros are substituted for several macros contained in chemist package.

$$< \text{tex with XΥMTEX EPS files} > \xrightarrow{\text{TEX/LATEX}} < \text{dvi} > \xrightarrow{\text{dvipdfm(x)}} < \text{PDF} >$$

is also effective in this mode. It follows that a tex file is permitted to contain both XΥMTEX codes and XΥMTEX EPS files for drawing structural formulas.

The TEX/LATEX mode and the PostScript-compatible mode can be switched in a tex file. On a similar line, the TEX/LATEX mode and the PDF-compatible mode can be switched in a tex file.

It should be noted, however, that the PostScript-compatible mode and the PDF-compatible mode cannot coexist in a tex file. More precisely speaking, XΥMTEX Version 5.00 does not support simultaneous loading of the xymtexps package and the xymtexpdf package or, in more basic levels, simultaneous loading of the pstricks package and the pgf package. Hence, raw commands of the pstricks package (e.g., `\psline`) cannot be used in the PDF-compatible mode, while raw commands of the pgf package (e.g., `\draw`) cannot be used in the PostScript-compatible mode.

The exclusive loading between the PostScript-compatible mode and the PDF-compatible mode, however, is not an essential drawback in practical use of the XΥMTEX system. Because the commands defined in the package files of the XΥMTEX Structural Files (Figure 2.1) are common in the three modes, they are unnecessary to be rewritten even if one selected mode is changed into another. It follows that the PostScript-compatible mode and the PDF-compatible mode can be switched only by exchanging the declarations: `\usepackage{xymtexps}` ↔ `\usepackage{xymtexpdf}` (cf. Section 1.3).

2.2 PDF-Compatible Mode of XΥMTEX

The present on-line manual mainly describes the PDF-compatible mode of the XΥMTEX system.

2.2.1 Templates for the PDF-Compatible Mode

The macro codes for the PDF-compatible mode of XΥMTEX are defined in xymtx-pdf.sty, which is incompatible with xymtx-ps.sty for the PostScript-compatible mode. The following template (named test1.tex) indicates a typical format for loading xymtexpdf.sty for the PDF-compatible mode of the XΥMTEX system.

```
%test1.tex
\documentclass{article}
\usepackage{xymtexpdf}
\begin{document}
(\XyMTeX{} macros)
\end{document}
```

When you load the utility package xymtexpdf.sty by using `\usepackage`, all the package files listed in XΥMTEX Structural Files (Table 2.1) as well as xymtx-pdf.sty for the PDF-compatible mode of the XΥMTEX system are loaded to draw structural formulas. Note that the utility package xymtexps.sty, on the other hand, loads xymtx-ps.sty for the PostScript-compatible mode as well as all the package files listed in XΥMTEX Structural Files (Table 2.1).

2.2.2 LATEX Processing

For the purpose of LATEX processing, you should type the following command in the command prompt:

```
elatex test1
```

where the extended eTEX version of LATEX is used. In Japanese environment of such an extended eTEX version, type in the command prompt as follows:

```
eplatex test1
```

Thereby, the corresponding dvi file (test1.dvi) is produced.

2.2.3 Conversions by dvipdfm(x)

The dvi file is ready to be processed by the dvipdfm(x) converter by typing the following command in the prompt:

```
dvipdfmx test1
```

which produces a PDF file (named test1.pdf) which contains structural formulas drawn by the XyMTEX system.

2.3 Option "dvips"

2.3.1 LATEX Processing With "dvips" Option

The standard PDF-compatible mode (Subsections 2.2.1 and 2.2.2) produces a dvi file suitable to the subsequent processing by the dvipdfm(x) converter, where the dvi file is converted into a PDF file. The PDF-compatible mode can alternatively produce a dvi file suitable to the dvips converter, which generates a PostScript file.

For the latter purpose, you should use a tex file in accord to the following template (named test2.tex), where xymtexpdf.sty is loaded with the option "dvips":

```
%test2.tex
\documentclass{article}
\usepackage[dvips]{xymtexpdf}
\begin{document}
(\XyMTeX{} macros)
\end{document}
```

For the purpose of LATEX processing, you should type the following command in the command prompt:

```
elatex test2
```

where the extended eTEX version of LATEX is used. In Japanese environment of such an extended eTEX version, type in the command prompt as follows:

```
eplatex test2
```

Thereby, the corresponding dvi file (test2.dvi) is produced. The dvi file is ready to be processed by the dvips converter by typing the following command in the prompt:

```
dvips test2
```

The resulting PostScript file (named test2.ps) contains structural formulas drawn by the XyMTEX system.

Chapter 3

Representative Examples

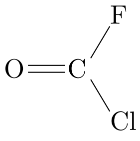
The scope of organic structural formulas to be drawn is common to the three modes of the XΥMTeX system. This chapter is devoted to show that the present PDF mode is also effective to draw representative structural formulas which have been described in the previous documents for the other two modes (the TeX/LaTeXmode and the PostScript-compatible mode).

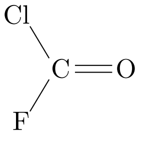
3.1 Acyclic Compounds

To draw acyclic compounds, the codes:

```
\Rtrigonal{0==C;1D==O;2==Cl;3==F}\qquad
\Ltrigonal{0==C;1D==O;2==Cl;3==F}
```

produce the following structures:

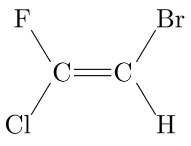


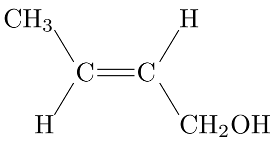


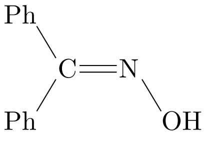
Ethylene derivatives are drawn by the codes:

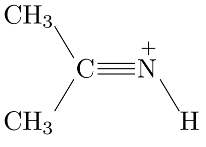
```
\Ethyleneh{1==C;2==C}{1==F;2==Cl;3==H;4==Br}\qquad
\Ethyleneh{1==C;2==C}{1==CH$_{3}$;2==H;3==CH$_{2}$OH;4==H}\par
\Ethyleneh{1==C;2==N}{1==Ph;2==Ph;3==OH}\qquad
\Ethyleneh[t{2+}]{1==C;2==N}{1==CH$_{3}$;2==CH$_{3}$;3==H}
```

which produce the following structures:







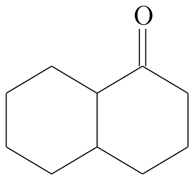


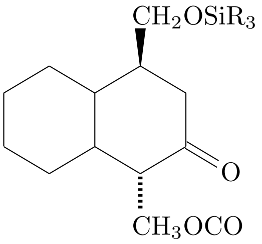
3.2 Carbocyclic Compounds

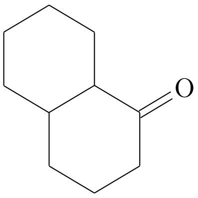
As examples of carbocyclic compounds, decaline skeletons of various directions are drawn by the following codes. Examples:

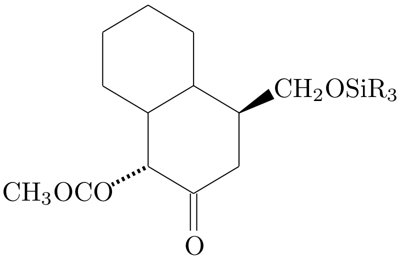
```
\decalinevb{1D==O;0FB==H;0GA==H} \qquad
\decalinevb{1B==CH$_{2}$OSiR$_{3}$;3D==O;4A==CH$_{3}$OCO;%
0FB==CH$_{3}$;0GA==H}
```

These commands produce:







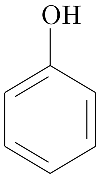


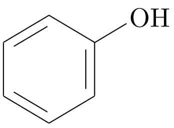
3.3 Aromatic Compounds

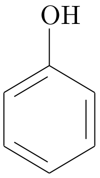
As examples of aromatic compounds, benzene derivatives are drawn by the following codes:

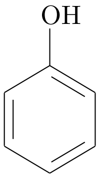
```
\bzdrv{1==OH}
\bzdrv{2==OH}
\bzdrv[r]{1==OH}
\bzdrv[l]{1==OH}
\bzdrv[A]{1==OH}
```

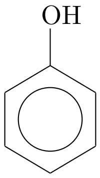
These commands produce:







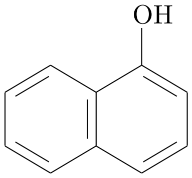


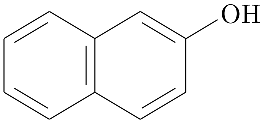


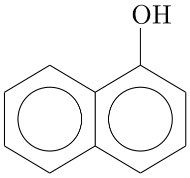
Naphthalene derivatives are drawn by the following codes:

```
\naphdrv{1==OH}
\naphdrv{2==OH}
\naphdrv[A]{1==OH}
```

These commands produce:

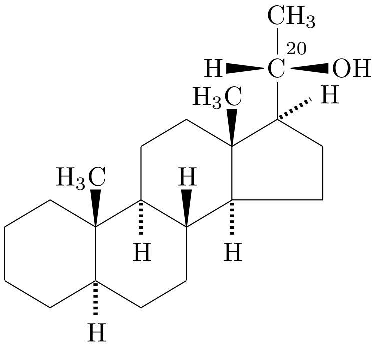






3.4 Steroid Derivatives

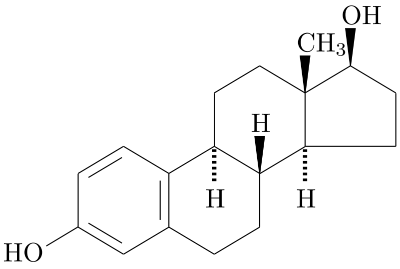
The following example shows a steroid derivative having a side chain drawn by the Newman projection.



5α-pregnan-20α-ol (formerly)
(20S)-5α-pregnan-20-ol

```
\begin{XyMcompd}(1200,1250)(300,150){}{}
\steroid{5A==H;%
{10}B==\lmoiety{H$_{3}$C};8B==H;9A==H;{14}A==H;%
{13}B==\lmoiety{H$_{3}$C};
{17}==\tetrahedral{3==(yl);%
0==C\rlap{\raisebox{5pt}{$^{20}$}};%
2B==H;4B==OH;1==CH$_{3}$};%
{17}GA==H}
\end{XyMcompd}
```

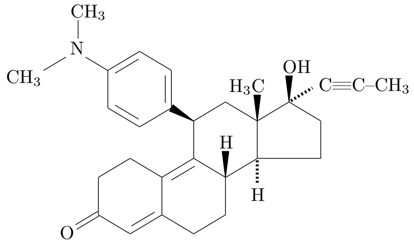
Estradiol, which is a much more potent estrogen than estrone, is drawn by using the command `\steroid` as follows:



estra-1,3,5(10)-triene-3,17β-diol
estradiol

```
\steroid[ack]{3==HO;{17}B==OH;%
8B==H;9A==H;{13}B==CH$_{3}$;{14}A==H}
```

The formula of mifepristone (RU-486), which is a synthetic steroid used as a abortifacient in the first two month of pregnancy, is drawn by using the command `\stereoid`.



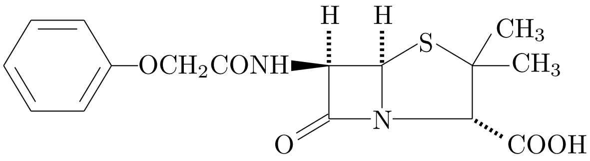
11β-[4-(dimethylamino)phenyl]-17β-hydroxy-
17α-(1-propynyl)estra-4,9-dien-3-one
(RU-486, mifepristone)

```
\begin{XyMcompd}(2000,1300)(-200,200){}{}
\steroid[di]{3D==O;8B==H;%
{11}B==\bzdrv{3==(yl);%
6==\Dtrigonal{0==N;1==CH$_{3}$;%
3==CH$_{3}$;2==(yl)}};%
{13}B==\lmoiety{H$_{3}$C};{14}A==H;%
{17}GA=={C\triplebond C--CH$_{3}$};{17}B==OH}
\end{XyMcompd}
```

3.5 Hetrocyclic Derivatives

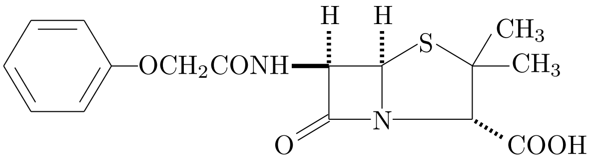
Penicillin V can be drawn as follows:

```
\begin{XyMcompd}(2100,600)(-800,100){}{}
\fourhetero[{b\fivefusevi{1==S;4==\null}{2Sa==CH$_{3}$;2Sb==CH$_{3}$;3A==COOH}{d}}]%
{2==N}{1D==O;3FA==H;4GA==H;4Su==\lyl(4==OCH$_{2}$CONH){4==\bzdrh{4==(yl)}}}
\end{XyMcompd}
```



A bold dash bond may be used instead of a bold wedged bond according to IUPAC Recommendations 1996 [19]. By declaring the switching command `\dashhasheddash`, one can draw structural formulas by using the combination of bold dash bonds and hashed dash bonds. For example, penicillin V can be drawn as follows:

```
\dashhasheddash
\begin{XyMcompd}(2100,600)(-800,100){}{}
\fourhetero[{b\fivefusevi{1==S;4==\null}{2Sa==CH$_{3}$;2Sb==CH$_{3}$;3A==COOH}{d}}]%
{2==N}{1D==O;3FA==H;4GA==H;4Su==\lyl(4==OCH$_{2}$CONH){4==\bzdrh{4==(yl)}}}
\end{XyMcompd}
```



Chapter 4

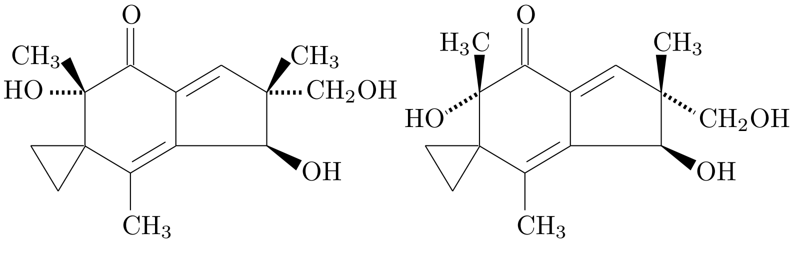
Stereochemistry

In the present PDF-compatible mode (due to `\usepackage{xymtexpdf}`), wedged bonds for stereochemistry are drawn on the basis of the graphics mechanism supported by the `pgf` package. On the other hand, the PostScript-compatible mode (due to `\usepackage{xymtexps}`) has relied on the `pstricks` package. However, each drawing unit in either case is placed on the basis of the LaTeX picture environment, so that appearances of generated structures are not different so much, even if either of the two modes is selected. The following examples show how the PDF-compatible mode produces structural formulas exhibiting similar appearances to the PostScript-compatible mode.

4.1 Wedged Bonds

According to IUPAC Recommendations 1996 [19], the default mode of the XΥMTEX system adopts wedge bonds for representing β bonds and hashed dash bonds for representing α bonds. For example, illudin S, an anti-tumor antibiotic substance, is drawn in two ways in which the directions of wedges are altered:

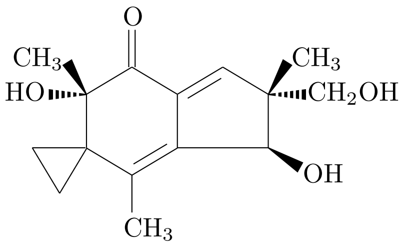
```
\nonaheterovi[di]{5s==\cyclopropanev{2==(yl)}}%
{2SB==CH$_{3}$;2SA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;6SB==CH$_{3}$;6SA==HO;7D==O}
\hskip1cm
\nonaheterovi[di]{5s==\cyclopropanev{2==(yl)}}%
{2FB==CH$_{3}$;2GA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;%
6GB==\lmoiety{H$_{3}$C};6FA==HO;7D==O}
```

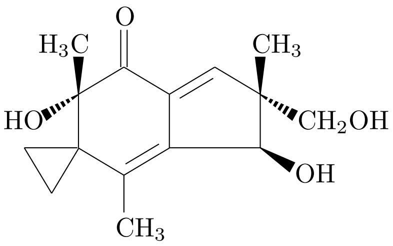


In some cases, hashed wedge bonds are used to designate α-bonds. The XΥMTEX system supports this type of representations, where the `\wedgehashedwedge` command changes dashed bonds into such hashed wedge bonds.

```
\wedgehashedwedge
\nonaheterovi[di]{5s==\cyclopropanev{2==(yl)}}%
{2SB==CH$_{3}$;2SA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;6SB==CH$_{3}$;6SA==HO;7D==O}
\hskip1cm
```

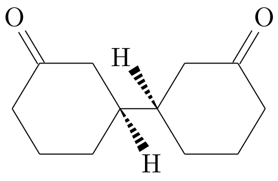
```
\nonaheterovi[di]{5s==\cyclopropanev{2==(yl)}}%
{2FB==CH$_{3}$;2GA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;%
6GB==\lmoiety{H$_{3}$C};6FA==HO;7D==O}
```

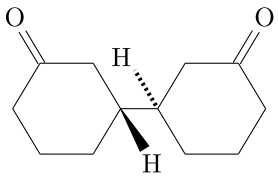


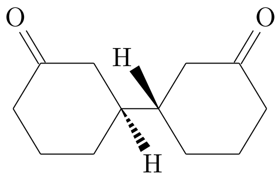


If the switch `\wedgehasheddash` is declared, the drawing mode is returned to the default mode, as shown in the following examples:

```
\wedgehashedwedge
\cyclohexaneh{2D==O;4GA==H;4==\cyclohexaneh{1==(yl);3D==O;1GA==H}}\hskip1cm
\wedgehasheddash%return to the default mode
\cyclohexaneh{2D==O;4GB==H;4==\cyclohexaneh{1==(yl);3D==O;1GA==H}}\hskip1cm
\wedgehashedwedge
\cyclohexaneh{2D==O;4GA==H;4==\cyclohexaneh{1==(yl);3D==O;1GB==H}}
```





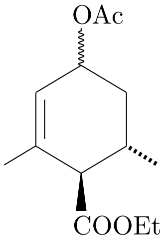


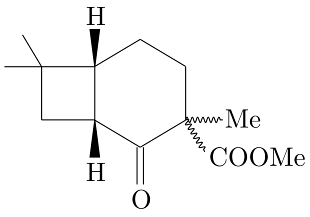
Thus, the central structure is drawn in the default mode.

4.2 Wavy Bonds

Wavy bonds drawn by the PDF mode of the XΥMTEX system are shown in the following examples:

```
\sixheterov[e]{}{1U==OAc;3A==;4B==COOEt;5==}
\hskip2cm
\sixheterov[{e\fourfuse{}{4Sa==;4Sb==}{b}}]{}
{4D==O;3SU==Me;3SV==COOMe;5FB==H;6GB==H}
```

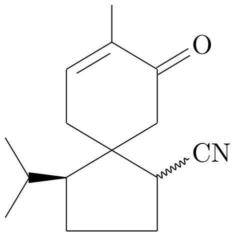




where a bond specifier `U` in such designations as `1U==OAc` is used to draw a wavy line. Note that a ring fusion is realized by writing `\fourfuse` in the BONDLIST of `\sixheterov`.

An additional example is shown as follows:

```
\fiveheterovi{1s==\sixheterov[f]{}{4==(yl);2D==O;1==}}%
{2U==CN;5Su==\LtetrahedralS{1==(yl);2==;3==}}
```



where a bond specifier `U` in such designations as `1U==CN` is used to draw a wavy line. Note that a spiro ring is generated by writing `\sixheterov` in the ATOMLIST of `\fiveheterovi` in a nested fashion.

Chapter 5

Optional Bonds

The graphics mechanism of the `pgf` package can be directly applied to draw extra bonds which cannot be drawn by the standard recipes of the XΥMTEX system. However, direct applications of raw commands of the `pgf` package spoil the compatibility of a tex file containing XΥMTEX codes. For the sake of assuring compatibility, such macros as `\WedgeAsSubst`, `\PutBondLine` and `\PutDashedBond` have been defined to pursue the same purpose conveniently.[1]

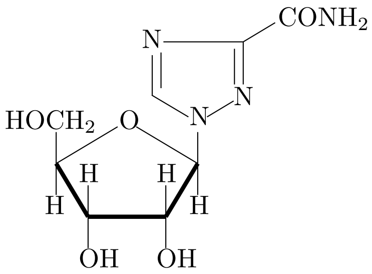
5.1 Bold Bonds of Cyclic Skeletons

5.1.1 Furanoses

This subsection is a rewritten version of Section 3.2 in the on-line manual of XΥMTEX versions 4.02 and 4.03 (xymtx402403.pdf), where the use of the raw command `\psline` of the `pstricks` package is ceased for the same of compatibility to the PDF mode.

The default expression of a furanose skeleton has three front skeletal bonds of bold dashes. For example, the structural formula of ribavirin is drawn by the code:

```
\furanose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;4Sb==HOC\rlap{H$_{2}$};
1Sb==\fiveheterov[bd]{1==N;2==N;4==N}{1==(yl);3==CONH$_{2}$}}
```



Although the quality of the resulting diagram is sufficient to be printed, one may require a more sophisticated format in which the three front bonds are expressed by the combination of wedge–dash–wedge. This type of formats can be drawn by using the command `\WedgeAsSubst` and the `\PutBondLine` command both of which are defined in the `xymtx-pdf` package:

```
\WedgeAsSubst(Starting Point)(Slope){LineLength}
\PutBondLine(Starting Point)(End Point){LineWidth}
```

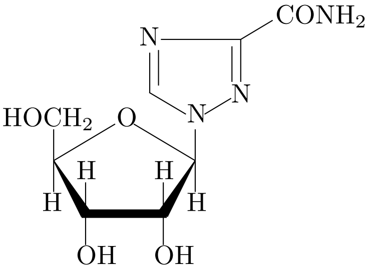
---

[1] The `\PutBondLine` command may be replaced by `\PutPDFLine` in the PDF-compatible mode or by `\PutPSLine` in the PostScript-compatible mode. However, such replacement is not recommended.

Thereby, the code:

```
\begin{XyMcompd}(1200,1000)(100,0){}{}
\fivesugarh{5==O;1s==\WedgeAsSubst(0,0)(-3,-5){120};%
4s==\WedgeAsSubst(0,0)(3,-5){120};%
3s==\PutBondLine(-15,0)(305,0){3.2pt}%
}{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;4Sb==HOC\rlap{H$_{2}$};
1Sb==\fiveheterov[bd]{1==N;2==N;4==N}{1==(yl);3==CONH$_{2}$}%
}[abc]
\end{XyMcompd}
```

generates the following formula:

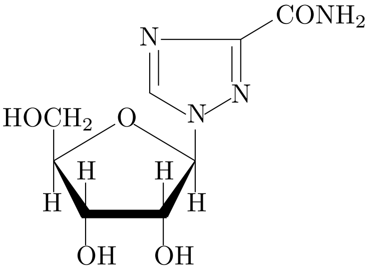


This input code can be simplified by making a tentative macro named `\myfuranose` as follows:

```
\makeatletter
\def\myfuranose{\@ifnextchar[{\@myfuranose}{\@myfuranose[]}}
\def\@myfuranose[#1]#2{%
\fivesugarh[#1]{5==O;1s==\WedgeAsSubst(0,0)(-3,-5){120};%
4s==\WedgeAsSubst(0,0)(3,-5){120};%
3s==\PutBondLine(-15,0)(305,0){3.2pt}}{#2}[abc]}
\makeatother
```

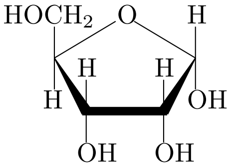
Thereby, the same formula can be typeset by writing a more simplified code:

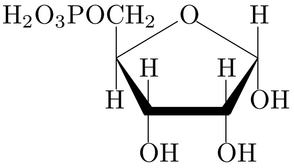
```
\myfuranose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;4Sb==HOC\rlap{H$_{2}$};
1Sb==\fiveheterov[bd]{1==N;2==N;4==N}{1==(yl);3==CONH$_{2}$}}
```



The tentative macro `\myfuranose` is convenient to draw various furanoses, e.g., α-D-ribofuranose and its 5-phosphoric acid:

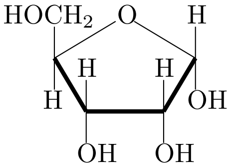
```
\myfuranose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;%
4Sb==HOC\rlap{H$_{2}$}}
\myfuranose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;%
4Sb==H$_{2}$O$_{3}$POC\rlap{H$_{2}$}}
```

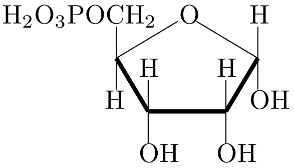




Simply by converting `\myfuranose` into `\furanose`, the corresponding default expressions can be obtained. Thus, the default structural formulas of α-D-ribofuranose and its 5-phosphoric acid are obtained by inputting the following codes:

```
\furanose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;%
4Sb==HOC\rlap{H$_{2}$}}
\furanose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;%
4Sb==H$_{2}$O$_{3}$POC\rlap{H$_{2}$}}
```



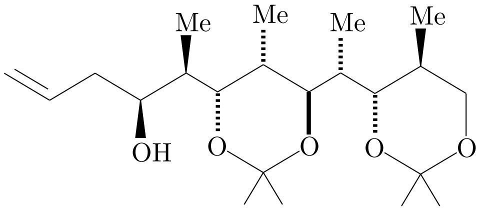


5.1.2 Optional Arguments for Drawing Skeletal Bonds

As found in the on-line manual of XΥMTEX version 2.00 [6], the second argument of the `\ryl` command can accommodate substituents other than a substituent generated by the "yl" function. For example, the inner code `\ryl{0A==Me;...}` in the code,

```
\sixheterov({bB}{eA}){3==O;5==O}{1A==Me;4Sa==\null;4Sb==\null;%
6==\pentamethylenei[a]{}{4B==OH;5B==Me;5==(yl)};%
2==\ryl{0A==Me;5==\sixheterov({eA}){3==O;5==O}{6==(yl);1B==Me;%
4Sa==\null;4Sb==\null}}}
```

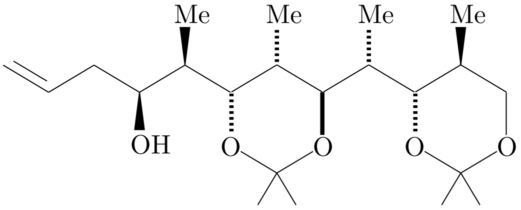
represents a methyl group on a vertex due to the command `\ryl`. Thereby, we have



The optional argument `({bB}{eA})` of `\sixheterov` indicates that bond `b` is a β-bond (a bold bond) and bond `e` is an α-bond (a dashed bond) in the left six-membered ketal.

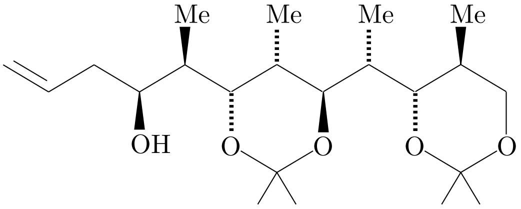
Because three bonds (ring skeletal bonds) in the above structure are shorter than the other polymethylene bonds of standard bond length, they should be lengthened, rigorously speaking. For this purpose, the same compound can be alternatively drawn by a spiro technique, where, for example, the code `6s==\hexamethylenei...` is designated in the atom list of `\shixheterov`.

```
\begin{XyMcompd}(1800,800)(-600,100){}{}
\sixheterov({bB}{eA}){3==O;5==O;%
6s==\hexamethylenei[a]{}{4B==OH;5B==Me;6==(yl)};%
2s==\trimethylene{%
3s==\sixheterov({eA}){3==O;5==O}{6==(yl);1B==Me;%
4Sa==\null;4Sb==\null}
}{1==(yl);2A==Me}}{1A==Me;4Sa==\null;4Sb==\null}
\end{XyMcompd}
```



The skeletal bold bond in the left six-membered ketal can be changed into a wedge bond by using the `\WedgeAsSubst` command as follows:

```
\begin{XyMcompd}(1800,800)(-600,100){}{}
\sixheterov({eA}){3==O;5==O;%
6s==\hexamethylenei[a]{}{4B==OH;5B==Me;6==(yl)};%
2s==\trimethylene{%
3s==\sixheterov({eA}){3==O;5==O}{6==(yl);1B==Me;%
4Sa==\null;4Sb==\null}
}{1==(yl);2A==Me};%
2s==\WedgeAsSubst(0,0)(0,-1){150}%
}{1A==Me;4Sa==\null;4Sb==\null}[b]
\end{XyMcompd}
```



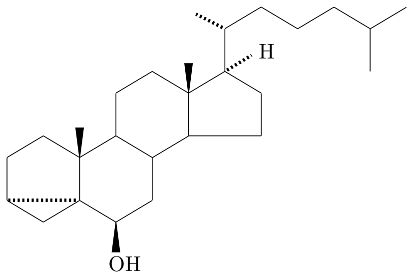
5.2 Linkage Between Non-Adjacent Atoms

This subsection is a partially rewritten version of Subsection 2.4.2 in the on-line manual of XΥMTEX versions 4.04 (xymtx404.pdf), where the use of the raw command `\psline` of the `pstricks` package is ceased for the same of compatibility to the PDF mode.

The linkage between the C-3 and the C-5 results in the formation of a cyclopropane ring as well as a cyclopentane ring. The linking bond is drawn by using `\PutDashedBond`, where the format of arguments is defined as follows:

```
\PutDashedBond(Starting Point)(End Point){LineWidth}
```

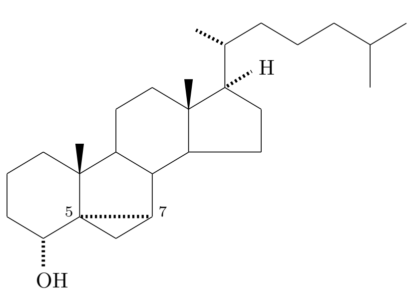
The dimension register `\thickLineWidth` is equal to 1.6pt as a default setting.



3α,5-cyclo-5α-cholestan-6β-ol

```
\steroidChain[{b\null}%dummy
{b{\PutDashedBond(6,0)(336,0)%
{\thickLineWidth}}}]%
{6B==OH;{10}B==\null;{13}B==\null;%
{17}GA==H;{20}A==\null}
```

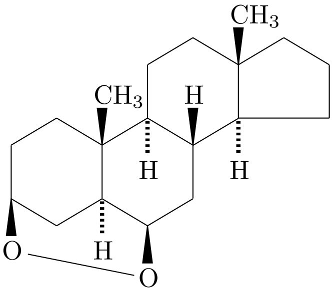
The linkage between the C-5 and the C-7 results in the formation of a cyclopropane ring as well as a cyclopentane ring. The linking bond is also drawn by using `\PutDashedBond`, as shown in the following example.



5,7α-cyclo-5α-cholestan-4α-ol

```
\steroidChain[{b\null}%dummy
{f{\put(30,0){\scriptsize 7}}}%
{d{\put(-70,0){\scriptsize 5}}}%
{d{\PutDashedBond(6,0)(336,0)%
{\thickLineWidth}}}]%
{4A==OH;{10}B==\null;{13}B==\null;%
{17}GA==H;{20}A==\null}
```

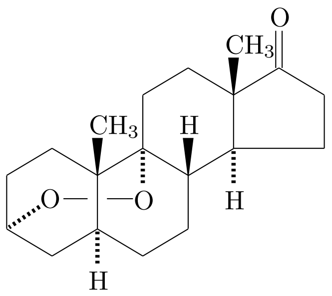
A peroxide bridge between non-adjacent positions of a steroid skeleton cannot be drawn by standard techniques supported by the XΥMTEX system. But optional commands of the PDF mode of the XΥMTEX system can be used in the arguments of XΥMTEX commands. For example, a peroxide bridge can be drawn by means of `\PutBondLine`, where the `\thinLineWidth` (= 0.4pt) specifies the width of a line.



3β,6β-epidioxy-5α-androstane

```
\steroid{5A==H;8B==H;9A==H;{10}B==CH$_{3}$;%
{13}B==CH$_{3}$;{14}A==H;%
3FB==O\put(0,0){%
\PutBondLine(20,20)(420,-60){\thinLineWidth}};6B==O}
```

Drawing a peroxide bridge between the C-3 and the C-9 requires a more complicated set of commands for the PDF mode, i.e., `\PutBondLine` and `\PutDashedBond`, where `\thinLineWidth` is equal to 0.4pt, while `\thickLineWidth` is equal to 1.6pt. Although the `\PutBondLine` and the `\PutDashedBond` are used in the argument of `\put` in the following program, the `\put` can be omitted after appropriate adjustment of output positions.



3α,9-epidioxy-5α-androstan-17-one

```
\steroid{5A==H;{10}B==CH$_{3}$;8B==H;%
{13}B==CH$_{3}$;{14}A==H;{17}D==O;%
9A==O\put(0,0){%
\PutBondLine(-80,40)(-178,40)%
{\thinLineWidth}}%
\put(-171,0){%
\PutBondLine(-80,40)(-171,40)%
{\thinLineWidth}}%
\put(-392,40){\makebox(0,0){O}}%
\put(-392,40){%
\PutDashedBond(-40,-30)(-155,-108)%
{\thickLineWidth}}}
```

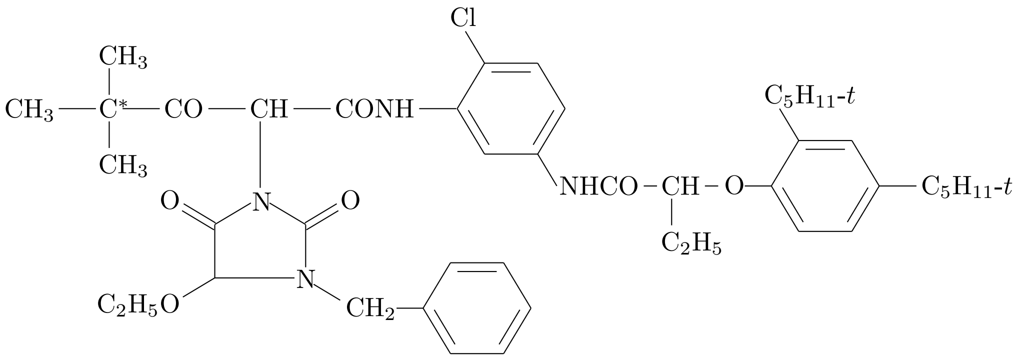
Commands `\PutPDFLine` and `\PutPDFdashed` for the PDF mode (or `\PutPSLine` and `\PutPSdashed` for the PostScript mode) would be used in place of the commands `\PutBondLine` and `\PutDashedBond`. Because they are as local as defined in the xymtx-pdf (or xymtx-ps) package only, as found by the fact that their names contain "PDF" (or "PS"), you should use `\PutBondLine` and `\PutDashedBond` in order to pursue the compatibility to the PDF and the PostScript modes.

5.3 Variable Bond Lengths

The function of variable bond lengths supported by XΥMTEX (Version 4.01 and later) provides us with an elegant solution to draw structures which are crowded around a tetrahedral carbon. Such a structure can be drawn by using the redefined command `\tetrahedral`. Thus, the codes:

```
\bscolorswOFF%no bond coloring
%\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:



1

It should be noted that this drawing is started at the asterisked carbon by using the redefined command `\tetrahedral`. The command `\bscolorswOFF` is a switch for stopping bond coloring. See Chapter 11.

Chapter 6

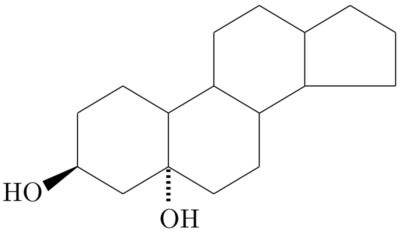
Size Reduction and Enlargement

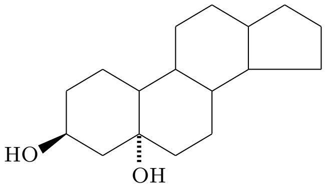
For size reduction and enlargement, see the on-line manual of XΥMTEX version 3.00 (xymtx300.pdf). This chapter is devoted to confirm the fact that the mechanism of size reduction and enlargement is effective to the PDF mode of XΥMTEX version 5.00

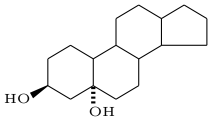
6.1 Utility of XΥMTEX

The XΥMTEX system supports the `\changeunitlength` command for changing sizes of structural formulas, where the unit length defined by `\unitlegth` is changed in XΥMTEX drawing. The following examples show the use of the `\changeunitlength` command in size reductions.

```
\steroid{3B==HO;5A==OH}%default unit length = 0.1pt
{\changeunitlength{0.08pt} \steroid{3B==HO;5A==OH}}
{\changeunitlength{0.05pt} \steroid{3B==HO;5A==OH}}
```

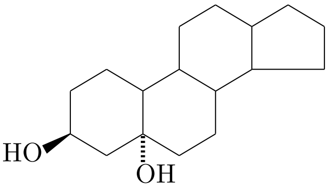


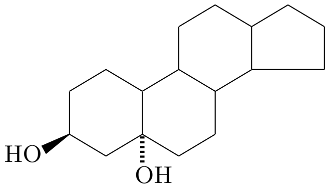


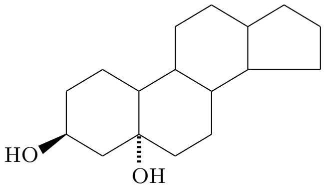


Note that font sizes are also changed during the size reduction. In contrast, the direct change of `\unitlength` causes no change of font sizes. The following examples shows the use of `\substfontsize` for changing font sizes:

```
{\unitlength=0.08pt \steroid{3B==HO;5A==OH}}
{\unitlength=0.08pt \let\substfontsize=\small \steroid{3B==HO;5A==OH}}
{\unitlength=0.08pt \let\substfontsize=\footnotesize \steroid{3B==HO;5A==OH}}
```

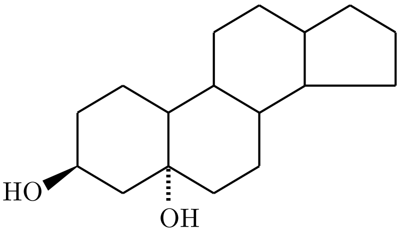


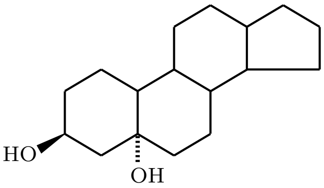


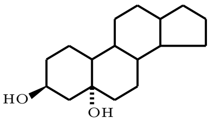


It should be added that the line width of each bond is not changed during size reduction and enlargement. This behavior is amplified by changing a standard line into a thicker one. Because the standard line width is stored in `\thinLineWidth` (0.4pt) as a letter string, it can be changed by its redefinition as follows:

```
\def\thinLineWidth{0.8pt}
\steroid{3B==HO;5A==OH}%default unit length = 0.1pt
{\changeunitlength{0.08pt} \steroid{3B==HO;5A==OH}}
{\changeunitlength{0.05pt} \steroid{3B==HO;5A==OH}}
```





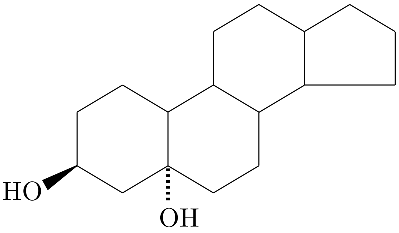


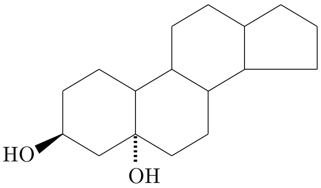
Undoubtedly, the line width of 0.8pt is unchanged in these structural formulas.

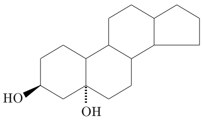
6.2 Utilities Supported by the **graphicx** Package

The `\scalebox` command of the graphicx package can also be used to change the sizes of structural formulas. Thus, essentially equivalent results to those of the preceding subsection can be obtained as follows:

```
\steroid{3B==HO;5A==OH}
\scalebox{0.8}{\steroid{3B==HO;5A==OH}}
\scalebox{0.5}{\steroid{3B==HO;5A==OH}}
```

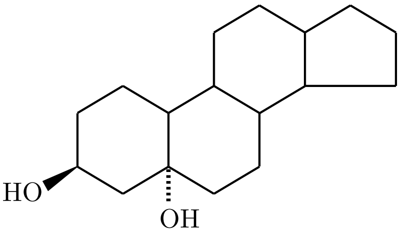


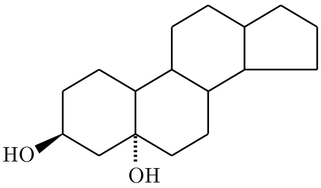


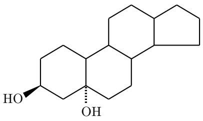


Because the `\scalebox` command causes total size reduction (or enlargement) of a structural formula as an object, bond widths and font sizes are changed simultaneously. This behavior is amplified by changing a standard line into a thicker one, as follows:

```
\def\thinLineWidth{0.8pt}
\steroid{3B==HO;5A==OH}
\scalebox{0.8}{\steroid{3B==HO;5A==OH}}
\scalebox{0.5}{\steroid{3B==HO;5A==OH}}
```



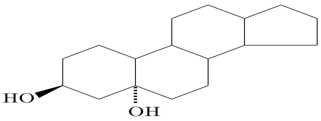


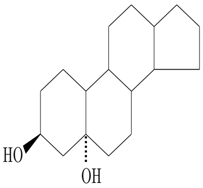


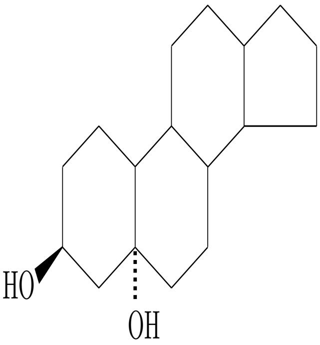
where the initial width (0.8pt) is reduced in accord with a scale factor selected as equal to 0.8 and 0.5.

The `\scalebox` command is capable of taking an optional argument, by which the aspect ratio of a structural formula can be changed, as shown in the following examples:

```
\scalebox{0.8}[0.5]{\steroid{3B==HO;5A==OH}}
\scalebox{0.5}[0.8]{\steroid{3B==HO;5A==OH}}
\scalebox{0.8}[1.5]{\steroid{3B==HO;5A==OH}}
```







Chapter 7

The chmst-pdf Package

The chmst-pdf package based on the LaTeX picture environment and the pgf package is an enhanced version of the chemist package, which provides us with a useful set of utilities for cooperating with the XΥMTeX system. The chmst-pdf package has been designed to be used under the PDF-compatible mode of the XΥMTeX system, which works after reading the xymtexpdf package. Such a set of utilities as supported by the chmst-pdf package is essentially equivalent to that of the chmst-ps based on the LaTeX picture environment and the pstricks package (the PostScript-compatible mode of the XΥMTeX system, which works after reading the xymtexps package).[1]

7.1 Use of the chmst-pdf Package

To use the chmst-pdf package, the file chmst-pdf.sty should be loaded by using the `\usepackage` command after reading xymtexpdf.sty, e.g.,

```
\documentclass{article}
\usepackage{xymtexpdf}%PDF-compatible mode
\usepackage{chmst-pdf}
\begin{document}
(Contents)
\end{document}
```

Subsequent LaTeX processing (Subsection 2.2.2)[2] and dvipdfm(x) conversion (Subsection 2.2.3) produce a PDF file which contains objects due to chmst-pdf package as well as XΥMTeX structural formulas.

7.2 Arrows of Fixed Lengths

Because longer arrows of fixed lengths are frequently used in chemical equations, they are supported by the chemist (chmst-pdf) package.[3] Such commands for drawing longer arrows should be used in an in-text or display math mode (e.g., `$\llongrightarrow$` and `\ChemForm{\llongrightarrow}`), because they are defined as relational operators. The appearances of arrows produced by a command of the same name in chemist and chmst-pdf are different, as summarized in Table 7.1.

---

[1] Because the chmst-ps package and the present chmst-pdf package have the same set of utilities, the on-line manual of the chmst-ps package (xymtx405406B.pdf) is effective to the present chmst-pdf package.

[2] It should be emphasized that the processing requires eLaTeX 2$_\varepsilon$ (an eTeX extended version of LaTeX 2$_\varepsilon$). In particular, arrows of the pgf package would disappear if a usual LaTeX 2$_\varepsilon$ is used.

[3] Arrows and harpoons produced by chemist and chmst-ps packages have been discussed in Sections 2 and 5 of the on-line manual of versions 4.05 and 4.06 (xymtx405406.pdf). If the combination of xymtexps, chemist, and chmst-ps (the PostScript-compatible mode) is replaced by the combination of xymtexpdf, chemist, chmst-pdf (the PDF-compatible mode), the descriptions of the on-line manual for the former combination are applicable to the latter combination.

Table 7.1: Arrows of Fixed Lengths Supported by chemist and chmst-pdf

command	chemist	chmst-pdf	comment
`\llongrightarrow`	$\longrightarrow$	$\longrightarrow$	
`\llongleftarrow`	$\longleftarrow$	$\longleftarrow$	
`\llongleftrightarrow`	$\longleftrightarrow$	$\longleftrightarrow$	
`\Llongrightarrow`	$\Longrightarrow$	$\Longrightarrow$	
`\Llongleftarrow`	$\Longleftarrow$	$\Longleftarrow$	
`\Llongleftrightarrow`	$\Longleftrightarrow$	$\Longleftrightarrow$	
`\llongleftharpoondown`	$\leftharpoondown$	$\leftharpoondown$	
`\llongrightharpoonup`	$\rightharpoonup$	$\rightharpoonup$	
`\llongleftharpoonup`	($\longleftarrow$)	$\leftharpoonup$	not supported by chemist
`\llongrightharpoondown`	($\longrightarrow$)	$\rightharpoondown$	not supported by chemist
`\equilibarrow`	$\rightleftharpoons$	$\rightleftharpoons$	
`\Equilibarrow`	$\rightleftarrows$	$\rightleftarrows$	
`\lllongrightarrow`	$\longrightarrow$	$\longrightarrow$	
`\lllongleftarrow`	$\longleftarrow$	$\longleftarrow$	
`\lllongleftrightarrow`	$\longleftrightarrow$	$\longleftrightarrow$	
`\Lllongrightarrow`	$\Longrightarrow$	$\Longrightarrow$	
`\Lllongleftarrow`	$\Longleftarrow$	$\Longleftarrow$	
`\Lllongleftrightarrow`	$\Longleftrightarrow$	$\Longleftrightarrow$	
`\lllongleftharpoondown`	$\leftharpoondown$	$\leftharpoondown$	
`\lllongrightharpoonup`	$\rightharpoonup$	$\rightharpoonup$	
`\lllongleftharpoonup`	($\longleftarrow$)	$\leftharpoonup$	not supported by chemist
`\lllongrightharpoondown`	($\longrightarrow$)	$\rightharpoondown$	not supported by chemist
`\equiliblongarrow`	$\rightleftharpoons$	$\rightleftharpoons$	
`\Equiliblongarrow`	$\rightleftarrows$	$\rightleftarrows$	

7.3 Arrows for Organic Chemistry

Arrows due to the chemist package have been introduced in Section 12.2 of the manual of XΥMTEX version 2.00 (xymtx200PS.pdf, cf. [5]). The list of arrows of the manual is cited for convenience, as shown in Figure 7.1, where the four arrows for representing equilibriums in the fourth row are new matters in the present version of chemist (chmst-pdf) package.[4] The arrows in the fifth row have been renamed into the present names in order to assign the previous names to the arrows in the fourth row. Note that a combination of left and right arrows is used to represent a forward and reverse reaction, while a combination of left and right harpoons is used to represent an equilibrium.

7.4 TEX/LATEX Mode and PDF-Compatible Mode

The commands for drawing arrows (Table 7.1) can be used in `\ChemForm` as part of a chemical equation. The following list shows several examples, where horizontal spaces before and after each arrow (as a relational operator) are placed automatically.

---

[4] The corresponding summary of chemical arrows produced by chemist and chmst-ps packages have been discussed in Sections 2 and 5 of the on-line manual of versions 4.05 and 4.06 (xymtx405406.pdf).

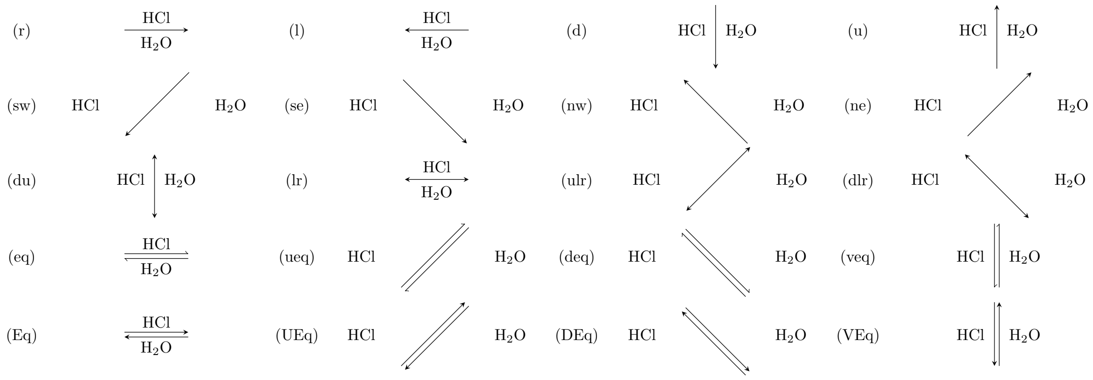


Figure 7.1: Reaction arrows of various types

stoichiometric relationship
`\ChemForm{H_{2}+Br_{2} = 2HBr}` $H_2 + Br_2 = 2HBr$
forward reaction
`\ChemForm{H_{2}+Br_{2} \llongrightarrow 2HBr}` $H_2 + Br_2 \longrightarrow 2HBr$
reverse reaction
`\ChemForm{H_{2}+Br_{2} \llongleftarrow 2HBr}` $H_2 + Br_2 \longleftarrow 2HBr$
equilibrium
`\ChemForm{H_{2}+Br_{2} \equilibarrow 2HBr}` $H_2 + Br_2 \rightleftharpoons 2HBr$
forward and reverse
`\ChemForm{H_{2}+Br_{2} \Equilibarrow 2HBr}` $H_2 + Br_2 \rightleftarrows 2HBr$
resonance
`\ChemForm{H\sbond Br \llongleftrightarrow H^{+} Br^{-}}` $H{-}Br \longleftrightarrow H^{+}Br^{-}$

Because the present document is typeset under the PDF-compatible mode (i.e., the use of the chmst-pdf package), such newly-defined arrows as shown above are drawn by using PDF utilities. If you want to print such arrows according to the embodiment of TEX/LATEX 2ε, you should declare the switching command `\chemistsw` as follows:

`\chemistsw`
stoichiometric relationship
`\ChemForm{H_{2}+Br_{2} = 2HBr}` $H_2 + Br_2 = 2HBr$
forward reaction
`\ChemForm{H_{2}+Br_{2} \llongrightarrow 2HBr}` $H_2 + Br_2 \longrightarrow 2HBr$
reverse reaction
`\ChemForm{H_{2}+Br_{2} \llongleftarrow 2HBr}` $H_2 + Br_2 \longleftarrow 2HBr$
equilibrium
`\ChemForm{H_{2}+Br_{2} \equilibarrow 2HBr}` $H_2 + Br_2 \rightleftharpoons 2HBr$
forward and reverse
`\ChemForm{H_{2}+Br_{2} \Equilibarrow 2HBr}` $H_2 + Br_2 \rightleftarrows 2HBr$
resonance
`\ChemForm{H\sbond Br \llongleftrightarrow H^{+} Br^{-}}` $H{-}Br \longleftrightarrow H^{+}Br^{-}$

Attention should be focused on arrowheads; these appearances of arrows are inherent to the chemist package (without loading the chmst-pdf package). To return to the PDF mode, the switching command should be declared.

`\chmstpspdfsw`
stoichiometric relationship
`\ChemForm{H_{2}+Br_{2} = 2HBr}` $\mathrm{H_2 + Br_2 = 2HBr}$
forward reaction
`\ChemForm{H_{2}+Br_{2} \llongrightarrow 2HBr}` $\mathrm{H_2 + Br_2 \longrightarrow 2HBr}$
(omitted)

7.5 ChemEquation Environment

A `ChemEquation` environment is used to describe a chemical equation, where chemical compounds are printed in upright fonts. The following code is a typical example containing a chemical compound and ionic species. Thus, solid limestone ($\mathrm{CaCO_3}$) is almost water insoluble, but a very small quantity dissolves in water according to the following process:

```
\begin{ChemEquation}
 CaCO_{3(s)} \llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
\end{ChemEquation}
```

$$\mathrm{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{7.1}$$

The molecular formulas are printed in upright fonts, although they are written directly without using the `\mathrm` command. Compare this output with the following one due to an `equation` environment of LaTeX 2ε:

```
\begin{equation}
 CaCO_{3(s)} \llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
\end{equation}
```

$$CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{7.2}$$

where each molecular formula written without using the `\mathrm` command is printed in italic fonts.

Arrows for organic chemistry (Section 7.3) can also be used for outputting objects over or below arrows in inorganic chemical equations. An equivalent result is obtained by using `\reactrarrow`, where `\scriptsize` is declared to adjust the sizes of objects over and below an arrow:

```
\begin{ChemEquation}
Na + Al + 2H_{2}
\reactrarrow{0pt}{3cm}{\scriptsize \ChemForm{THF/140^{\circ}/3\: h}}
{\scriptsize 350~atom}
NaAlH_{4}\quad (99\%~yield)
\end{ChemEquation}
```

$$\mathrm{Na + Al + 2H_2 \xrightarrow[\text{350 atom}]{\text{THF/140°/3 h}} NaAlH_4} \quad \text{(99\% yield)} \tag{7.3}$$

On similar lines, the following set of arrows for organic chemistry (Section 7.3) can be used to draw reaction equations for inorganic chemistry.

`\reactrarrow{0pt}{1cm}{A}{B}` $\xrightarrow[\mathrm{B}]{\mathrm{A}}$

`\reactlarrow{0pt}{1cm}{A}{B}` $\xleftarrow[\mathrm{B}]{\mathrm{A}}$

`\reactlrarrow{0pt}{1cm}{A}{B}` $\xleftrightarrow[\mathrm{B}]{\mathrm{A}}$

`\reacteqarrow{0pt}{1cm}{A}{B}` $\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$

7.6 Round Arrows for Representing Electron Migrations

7.6.1 Round Arrows or Harpoons with Autocalculated Control Points

In order to confirm the compatibility between the PostScript mode and the PDF mode, this subsection is provided as a reproduced version of Section 4.2 of the on-line manual of XΥMTEX version 4.01 (xymtx401.pdf), which has relied on the PostScript mode. The mechanism of drawing round arrows has been improved to be based on Bezier curves, so that it becomes effective to both the PostScript mode and the PDF mode.

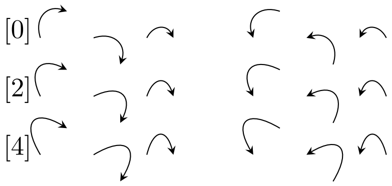
To illustrate the mechanisms of organic reactions, round or curved arrows are used to show electron shift or migration. The macros for drawing such round or curved arrows are defined in the `chmst-ps` package and also in the `chmst-pdf` package: `\electronrshiftarrow` and `\electronlshiftarrow`. Each of these commands takes two pairs of xy-coordinates as arguments (the starting point and the end point), from which two intermediate control points are automatically calculated to draw an arrow.

```
\electronrshiftarrow[Arc Direction](Starting Point)(End Point)
\electronlshiftarrow[Arc Direction](Starting Point)(End Point)
```

The xy-coordinates of the starting and end points are relative values with respect to the origin `(0,0)` (fixed) of the resulting arrow. The automatic calculation of control points postulates that the x-coordinate of the stating point is smaller than the x-coordinate of the end point. Note that `(Starting Point)` and `(End Point)` are not used in a usual meaning (due to the direction of an arrow); thus, an arrow head drawn by `\electronrshiftarrow` appears at the end point, while an arrow head drawn by `\electronlshiftarrow` appears at the starting point. The optional argument `[Arc Direction]` indicates whether a curve (arc) is upward or downward. Even numbers (`[0]` (or default with no designation), `[2]`, and `[4]`; wide to tight) for the optional argument `[Arc Direction]` represent an upward curve, while odd numbers (`[1]`, `[3]`, and `[5]`; wide to tight) for the optional argument `[Arc Direction]` represent a downward curve.

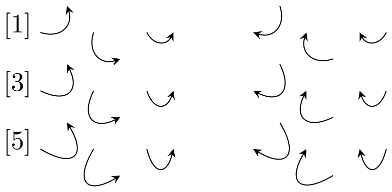
Several upward-curved arrows generated by these commands are shown as examples, where the arrows bend in wide to tight curves as even numbers assigned to the optional argument `[Arc Direction]` become larger.

```
[0]
\electronrshiftarrow(0,0)(100,100)\qquad
\electronrshiftarrow(0,0)(100,-100)\qquad
\electronrshiftarrow(0,0)(100,0)\qquad\qquad
\electronlshiftarrow(0,0)(100,100)\qquad
\electronlshiftarrow(0,0)(100,-100)\qquad
\electronlshiftarrow(0,0)(100,0) \\[10pt]
[2]
\electronrshiftarrow[2](0,0)(100,100)\qquad
\electronrshiftarrow[2](0,0)(100,-100)\qquad
\electronrshiftarrow[2](0,0)(100,0)\qquad\qquad
\electronlshiftarrow[2](0,0)(100,100)\qquad
\electronlshiftarrow[2](0,0)(100,-100)\qquad
\electronlshiftarrow[2](0,0)(100,0) \\[10pt]
[4]
\electronrshiftarrow[4](0,0)(100,100)\qquad
\electronrshiftarrow[4](0,0)(100,-100)\qquad
\electronrshiftarrow[4](0,0)(100,0)\qquad\qquad
\electronlshiftarrow[4](0,0)(100,100)\qquad
\electronlshiftarrow[4](0,0)(100,-100)\qquad
\electronlshiftarrow[4](0,0)(100,0)
```



Several downward-curved arrows generated by these commands are shown as examples, where the arrows bend in wide to tight curves as odd numbers become larger.

```
[1]
\electronrshiftarrow[1](0,0)(100,100)\qquad
\electronrshiftarrow[1](0,0)(100,-100)\qquad
\electronrshiftarrow[1](0,0)(100,0)\qquad\qquad
\electronlshiftarrow[1](0,0)(100,100)\qquad
\electronlshiftarrow[1](0,0)(100,-100)\qquad
\electronlshiftarrow[1](0,0)(100,0) \\[10pt]
[3]
\electronrshiftarrow[3](0,0)(100,100)\qquad
\electronrshiftarrow[3](0,0)(100,-100)\qquad
\electronrshiftarrow[3](0,0)(100,0)\qquad\qquad
\electronlshiftarrow[3](0,0)(100,100)\qquad
\electronlshiftarrow[3](0,0)(100,-100)\qquad
\electronlshiftarrow[3](0,0)(100,0) \\[10pt]
[5]
\electronrshiftarrow[5](0,0)(100,100)\qquad
\electronrshiftarrow[5](0,0)(100,-100)\qquad
\electronrshiftarrow[5](0,0)(100,0)\qquad\qquad
\electronlshiftarrow[5](0,0)(100,100)\qquad
\electronlshiftarrow[5](0,0)(100,-100)\qquad
\electronlshiftarrow[5](0,0)(100,0)
```



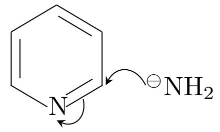
An attack of an amide anion $^{\ominus}$NH$_2$ on the 2-position of pyridine is illustrated as follows. According to the specification of the XΥMTeX system, the code `1==N` should be placed at the last part of the `ATOMLIST` (atom list) of `\sixheterovi`.[5]

```
\sixheterovi[ace]{2==\futuresubst{\kern6pt$^{\ominus}$NH$_{2}$};
2s==\electronlshiftarrow(10,0)(160,0);%
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`.

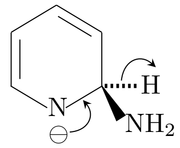
---

[5] Otherwise, the flag for truncating a vertex is deleted so as to print the vertex of the six-membered ring.



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}
```



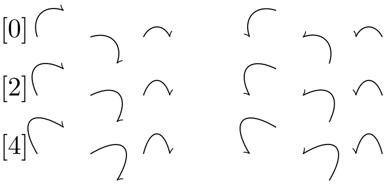
Arrows having an arrow head of harpoon-type are also available. An intermediate keyword in the middle of each command name (e.g., `Hru` in `\electronHrushiftarrow`) represents the feature of the harpoon, i.e., `Hru` (harpoon right upward), `Hrd` (harpoon right downward), `Hlu` (harpoon left upward), or `Hld` (harpoon left downward). The formats of these commands are the same as those of `\electronrshiftarrow` and `\electronlshiftarrow` described above, i.e.,

```
\electronHrushiftarrow[Arc Direction](Starting Point)(End Point)
\electronHrdshiftarrow[Arc Direction](Starting Point)(End Point)
\electronHlushiftarrow[Arc Direction](Starting Point)(End Point)
\electronHldshiftarrow[Arc Direction](Starting Point)(End Point)
```

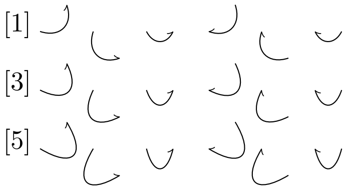
The outputs of these commands are illustrated as follows:

```
[0]
\electronHrushiftarrow(0,0)(100,100)\qquad
\electronHrushiftarrow(0,0)(100,-100)\qquad
\electronHrushiftarrow(0,0)(100,0)\qquad
\electronHlushiftarrow(0,0)(100,100)\qquad
\electronHlushiftarrow(0,0)(100,-100)\qquad
\electronHlushiftarrow(0,0)(100,0) \\[10pt]
[2]
\electronHrushiftarrow[2](0,0)(100,100)\qquad
\electronHrushiftarrow[2](0,0)(100,-100)\qquad
\electronHrushiftarrow[2](0,0)(100,0)\qquad
\electronHlushiftarrow[2](0,0)(100,100)\qquad
\electronHlushiftarrow[2](0,0)(100,-100)\qquad
\electronHlushiftarrow[2](0,0)(100,0) \\[10pt]
[4]
\electronHrushiftarrow[4](0,0)(100,100)\qquad
\electronHrushiftarrow[4](0,0)(100,-100)\qquad
\electronHrushiftarrow[4](0,0)(100,0)\qquad
```

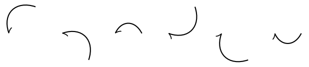
```
\electronHlushiftarrow[4](0,0)(100,100)\qquad
\electronHlushiftarrow[4](0,0)(100,-100)\qquad
\electronHlushiftarrow[4](0,0)(100,0)
```



```
[1]
\electronHrushiftarrow[1](0,0)(100,100)\qquad
\electronHrushiftarrow[1](0,0)(100,-100)\qquad
\electronHrushiftarrow[1](0,0)(100,0) \qquad
\electronHlushiftarrow[1](0,0)(100,100)\qquad
\electronHlushiftarrow[1](0,0)(100,-100)\qquad
\electronHlushiftarrow[1](0,0)(100,0) \\[10pt]
[3]
\electronHrushiftarrow[3](0,0)(100,100)\qquad
\electronHrushiftarrow[3](0,0)(100,-100)\qquad
\electronHrushiftarrow[3](0,0)(100,0) \qquad
\electronHlushiftarrow[3](0,0)(100,100)\qquad
\electronHlushiftarrow[3](0,0)(100,-100)\qquad
\electronHlushiftarrow[3](0,0)(100,0) \\[10pt]
[5]
\electronHrushiftarrow[5](0,0)(100,100)\qquad
\electronHrushiftarrow[5](0,0)(100,-100)\qquad
\electronHrushiftarrow[5](0,0)(100,0) \qquad
\electronHlushiftarrow[5](0,0)(100,100)\qquad
\electronHlushiftarrow[5](0,0)(100,-100)\qquad
\electronHlushiftarrow[5](0,0)(100,0) \\[10pt]
```



```
\electronHrdshiftarrow(0,0)(100,100)\qquad
\electronHrdshiftarrow(0,0)(100,-100)\qquad
\electronHrdshiftarrow(0,0)(100,0)\qquad\qquad
\electronHrdshiftarrow[1](0,0)(100,100)\qquad
\electronHrdshiftarrow[1](0,0)(100,-100)\qquad
\electronHrdshiftarrow[1](0,0)(100,0) \\[20pt]
\electronHldshiftarrow(0,0)(100,100)\qquad
\electronHldshiftarrow(0,0)(100,-100)\qquad
\electronHldshiftarrow(0,0)(100,0)\qquad
\electronHldshiftarrow[1](0,0)(100,100)\qquad
\electronHldshiftarrow[1](0,0)(100,-100)\qquad
\electronHldshiftarrow[1](0,0)(100,0)
```



7.6.2 Round Arrows or Harpoons with Given Control Points

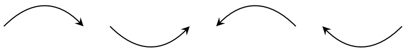
For the purpose of representing electron migration, the chmst-pdf (or chmst-ps) package supports another set of commands for drawing round arrows, i.e., the command `\electronshiftArrowr` for typesetting a right round arrow and the command `\electronshiftArrowl` for typesetting a left round arrow. These commands take one or two additional pairs of xy-coordinates `(Control Points)` to set up control points explicitly:

```
\electronshiftArrowr(Starting Point)(Control Points)(End Point)
\electronshiftArrowl(Starting Point)(Control Points)(End Point)
```

Because control points are given explicitly, such an optional argument as setting up an upward or downward arc is unnecessary. Their behaviors are illustrated in the following examples:

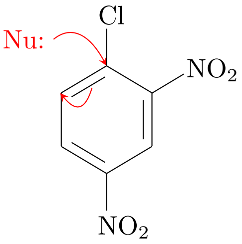
```
\electronshiftArrowr(0,0)(100,100)(200,100)(300,0)\qquad\qquad
\electronshiftArrowr(0,0)(100,-100)(200,-100)(300,0)\qquad\qquad
\electronshiftArrowl(0,0)(100,100)(200,100)(300,0)\qquad\qquad
\electronshiftArrowl(0,0)(100,-100)(200,-100)(300,0)
```

where three or four pairs of xy-coordinates are placed; the first pair of parentheses represents a starting point, the last pair of parentheses represents an end point, and the intermediate one or two pairs designate control point(s). The above codes typeset the following round arrows:



The following example shows round arrows placed at the reaction sites of a benzene ring:

```
\sixheterov[bdf]{%
1s=={\red \electronshiftArrowl(0,0)(-70,130)(-140,150)(-200,100)};%
1s==\put(-200,100){\makebox(0,0)[rc]{\red Nu:~}};%
6s=={\red \electronshiftArrowl(0,0)(50,-60)(90,-80)(120,20)}%
}{1==Cl;2==NO$_{2}$;4==NO$_{2}$}
```

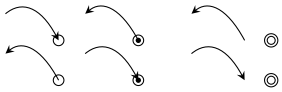


The pairs of xy-coordinates for the first `\electronshiftArrowl` command are designated inversely, so that the arrow head of the first arrow appears to be irregular. However, the behavior obeys a rule, because the suffix `l` indicates that an arrow head appears at the position of the first pair of xy-coordinates among the pairs of xy-coordinates, e.g., `(0,0)` among `(0,0)(-70,130)(-140,150)(-200,100)`. On a similar line, the arrow head of the second arrow drawn by `\electronshiftArrowl` appears at the position `(0,0)` among `(0,0)(50,-60)(90,-80)(120,20)`.

On the other hand, the suffix `r` of `\electronshiftArrowr` indicates that an arrow head appears at the position of the last pair of xy-coordinates among the pairs of xy-coordinates, e.g., `(-200,100)` among `(0,0)(-70,130)(-140,150)(-200,100)`.

It should be emphasized that the origin of each arrow (having no dimensions) is always located at the position `(0,0)`, so that the origin `(0,0)` of the arrow is superposed on a substitution position designated in a structural formula. Note that the origin of an arrow is not always identical with the starting point (or the end point) of the arrow. The following examples illustrate how the origin of an arrow is placed at a substitution position, where such a substitution position is tentatively given as a circle (or as a double circle) by the `\put` command in the LaTeX picture environment.

```
\begin{picture}(1000,300)(-200,0)
%origins of arrows (0,0) on (0,0) or (0,150)
\put(0,0){\circle{40}}
\put(0,0){\electronshiftArrowr(0,0)(-70,130)(-140,150)(-200,100)}
\put(0,150){\circle{40}}
\put(0,150){\electronshiftArrowl(0,0)(-70,130)(-140,150)(-200,100)}
%origins of arrows (0,0) on (300,0) or (300,150)
\put(300,0){\circle{40}}\put(300,0){\circle*{20}}
\put(300,0){\electronshiftArrowr(-200,100)(-140,150)(-70,130)(0,0)}
\put(300,150){\circle{40}}\put(300,150){\circle*{20}}
\put(300,150){\electronshiftArrowl(-200,100)(-140,150)(-70,130)(0,0)}
%origins of arrows (0,0) on (800,0) or (800,150)
\put(800,0){\circle{50}}\put(800,0){\circle{30}}
\put(800,0){\electronshiftArrowr(-300,100)(-240,150)(-170,130)(-100,0)}
\put(800,150){\circle{50}}\put(800,150){\circle{30}}
\put(800,150){\electronshiftArrowl(-300,100)(-240,150)(-170,130)(-100,0)}
\end{picture}
```



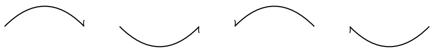
On the other hand, one-electron migration is represented by a round arrow with a harpoon-type arrow head:

```
\electronshiftHru(Starting Point)(Control Points)(End Point)
\electronshiftHrd(Starting Point)(Control Points)(End Point)
\electronshiftHlu(Starting Point)(Control Points)(End Point)
\electronshiftHld(Starting Point)(Control Points)(End Point)
```

where the formats of arguments are designed to be the same as those of `\electronshiftArrowr` and `\electronshiftArrowl` described above.

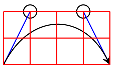
The following examples shows harpoons drawn by these commands:

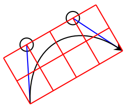
```
\electronshiftHru(0,0)(100,100)(200,100)(300,0) \qquad\qquad
\electronshiftHrd(0,0)(100,-100)(200,-100)(300,0) \qquad\qquad
\electronshiftHlu(0,0)(100,100)(200,100)(300,0) \qquad\qquad
\electronshiftHld(0,0)(100,-100)(200,-100)(300,0)
```



7.6.3 Notes on Control Points

The autocalculation of control points for `\electronrshiftarrow` etc. (Subsection 7.6.1) is based on a simple model as follows:





where two circles represent control points. For example, when the starting point `(0,0)` and the end point `(400,0)` are given for an arrow, two control points are calculated to be `(100,200)` and `(300,200)`. Hence, `\electronrshiftarrow` (Subsection 7.6.1) and `\electronshiftArrowr` (Subsection 7.6.2) give equivalent results, when the following codes are written:

```
\electronrshiftarrow(0,0)(400,0)
\hskip50pt
\electronshiftArrowr(0,0)(100,200)(300,200)(400,0)
```

Thereby, we obtain the following arrows:

Chapter 8

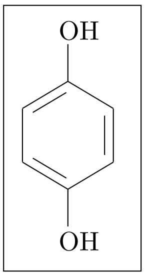
EPS Files Containing X^ΥMTEX Formulas

8.1 LaTeX Documents with X^ΥMTEX Codes

As shown in Section 2.2, a LaTeX document with X^ΥMTEX codes can be directly processed by the PDF-compatible mode. For example, the X^ΥMTEX code placed in the present LaTeX document (named xymtx500.tex as a tex file):

```
\fbox{%
\begin{XyMcompd}(300,900)(250,0){}{}
\bzdrv{1==OH;4==OH}
\end{XyMcompd}
}
```

produces the following structural formula:



where the bounding box of the formula is specified by using the `XyMcompd` environment defined in the chemist package.

Another route for incorporating X^ΥMTEX formulas is to use LaTeX documents with EPS files of X^ΥMTEX structures produced by separate procedures. The present chapter is devoted to describe know-how of making and manipulating EPS files.

8.2 Incorporation of X^ΥMTEX Formulas as EPS Files

8.2.1 Making a Single-Page PostScriptFile with X^ΥMTEX Formulas

As shown in Section 2.3, the option "dvips" of the xymtexpdf package (loaded by means of the declaration: `\usepackage[dvips]{xymtexpdf}`) results in the generation of a PostScript file, which can be converted into the corresponding EPS file. For the purpose of accomplishing smooth conversion, a PostScript file should be of a single page, which contains a set of XΥMTEX structures to be bundled. For example, the following tex file (named eps-test1.tex) shows a typical format for producing a single-page PostScript file.

```
%eps-test1.tex
\documentclass{article}
\usepackage[dvips]{xymtexpdf}
\usepackage{chmst-pdf}
\pagestyle{empty}
\begin{document}

\begin{XyMcompd}(300,900)(250,0){}{}
\bzdrv{1==OH;4==OH}
\end{XyMcompd}

\end{document}
```

Note that the declaration `\pagestyle{empty}` is important to obtain a correct bounding box. In addition, the declaration `\usepackage[dvips]{xymtexpdf}` contains an optional argument `[dvips]`.

According to the procedures of Section 2.3, the eLaTeX processing of the tex file (eps-test1.tex):

```
elatex eps-test1
```

and the subsequent processing by dvips:

```
dvips eps-test1
```

produce the corresponding PostScript file (eps-test1.ps), which can be browsed by GSview coupled with Ghostscript.

8.2.2 EPS Files with Correct Bounding Boxes

Conversion of PostScript Files to EPS Files

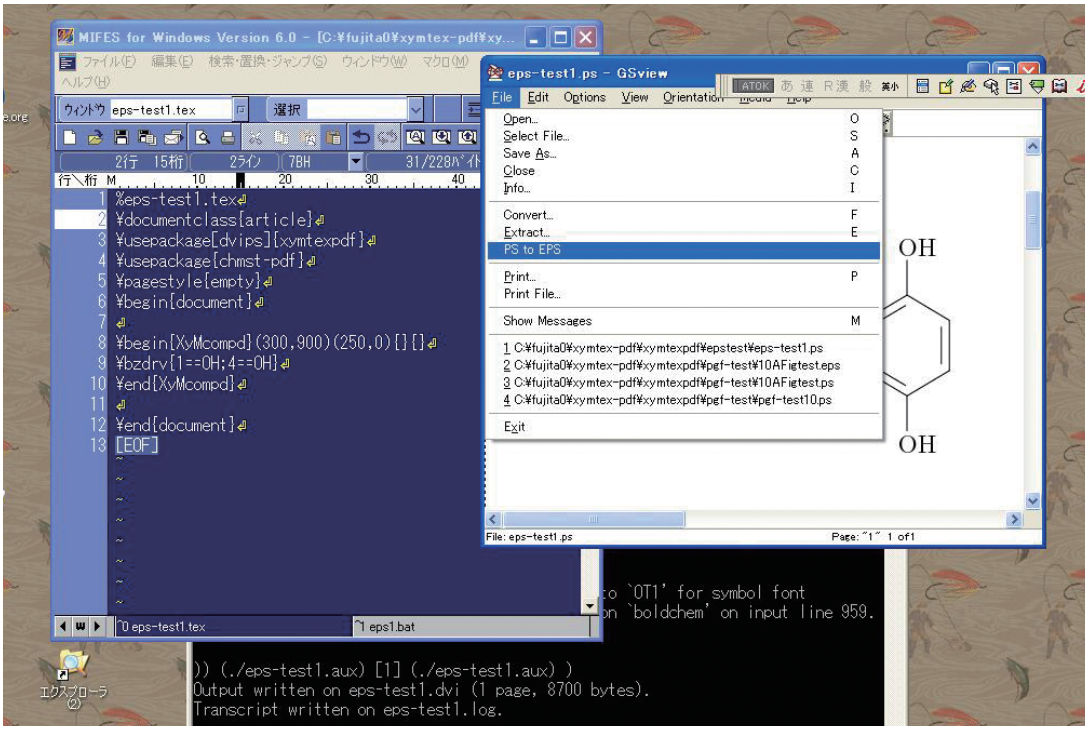
In order to convert PostScript file (eps-test1.ps) into an EPS file, the following procedure is typical:

1. The PostScript file (eps-test1.ps) is browsed by GSview (coupled with Ghostscript), where the button “File” is clicked to show its menu (Figure 8.1).
2. The button “PS to EPS” in the menu (Figure 8.1) is selected to result in the appearance of a confirmation box (Figure 8.2), in which the button “yes” is clicked after checking “automatically calculated Bounding Box”.
3. Thereby, there appears an input box (Figure 8.3), from which the resulting eps file is stored after inputting an appropriate name (here “eps-test1Figr.eps”). Note that the “保存” button in Japanese means “store”.
4. The resulting file (eps-test1Figr.eps) can be browsed by GSview as shown in Figure 8.4, where the XΥMTEX structure is surrounded by a dotted frame showing the corresponding bounding box.

Conversion of DVI Files to EPS Files

The dvips converter can produce EPS files directly from dvi files when the option -E is added to the command line, e.g.,

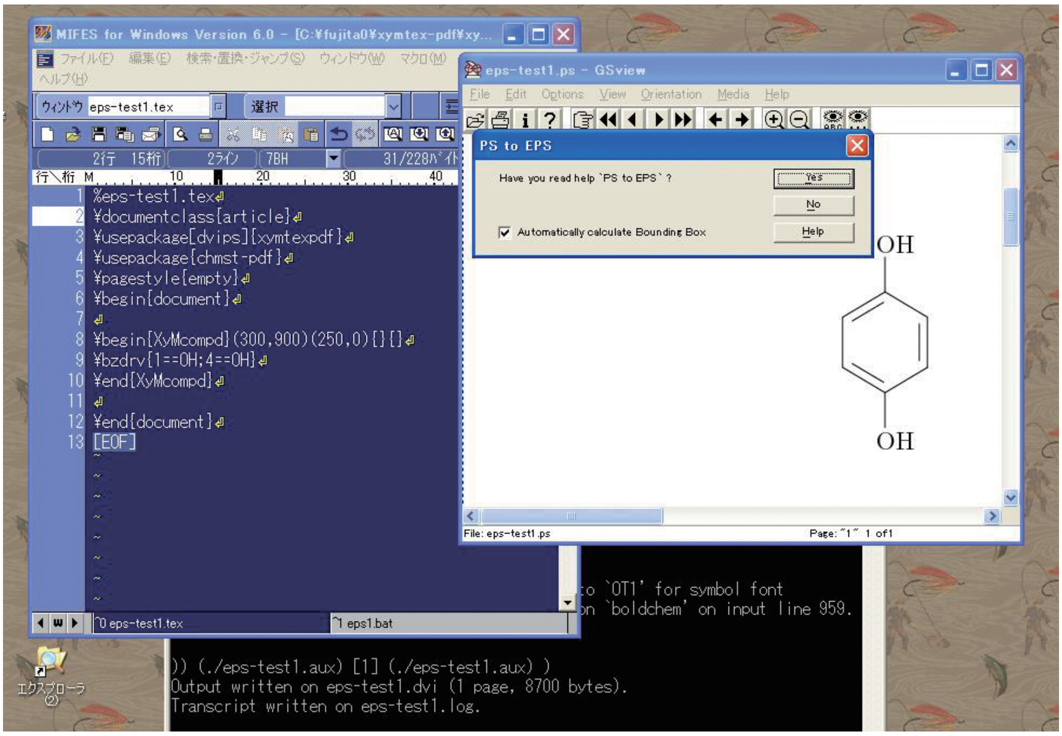
```
dvipsk -E -D2400 -Pdl -p1 -n1 eps-test1.dvi -o eps-test1FigA.eps
```



```
%eps-test1.tex
¥documentclass{article}
¥usepackage[dvips]{xymtexpdf}
¥usepackage{chmst-pdf}
¥pagestyle{empty}
¥begin{document}

¥begin{XyMcompd}(300,900)(250,0){}{}
¥bzdrv{1==OH;4==OH}
¥end{XyMcompd}

¥end{document}
[EOF]
```

```
o `OT1' for symbol font
on `boldchem' on input line 959.

)) (./eps-test1.aux) [1] (./eps-test1.aux) )
Output written on eps-test1.dvi (1 page, 8700 bytes).
Transcript written on eps-test1.log.
```

Figure 8.1: Making EPS files of structural formulas. “EP to EPS” button



```
%eps-test1.tex
¥documentclass{article}
¥usepackage[dvips]{xymtexpdf}
¥usepackage{chmst-pdf}
¥pagestyle{empty}
¥begin{document}

¥begin{XyMcompd}(300,900)(250,0){}{}
¥bzdrv{1==OH;4==OH}
¥end{XyMcompd}

¥end{document}
[EOF]
```

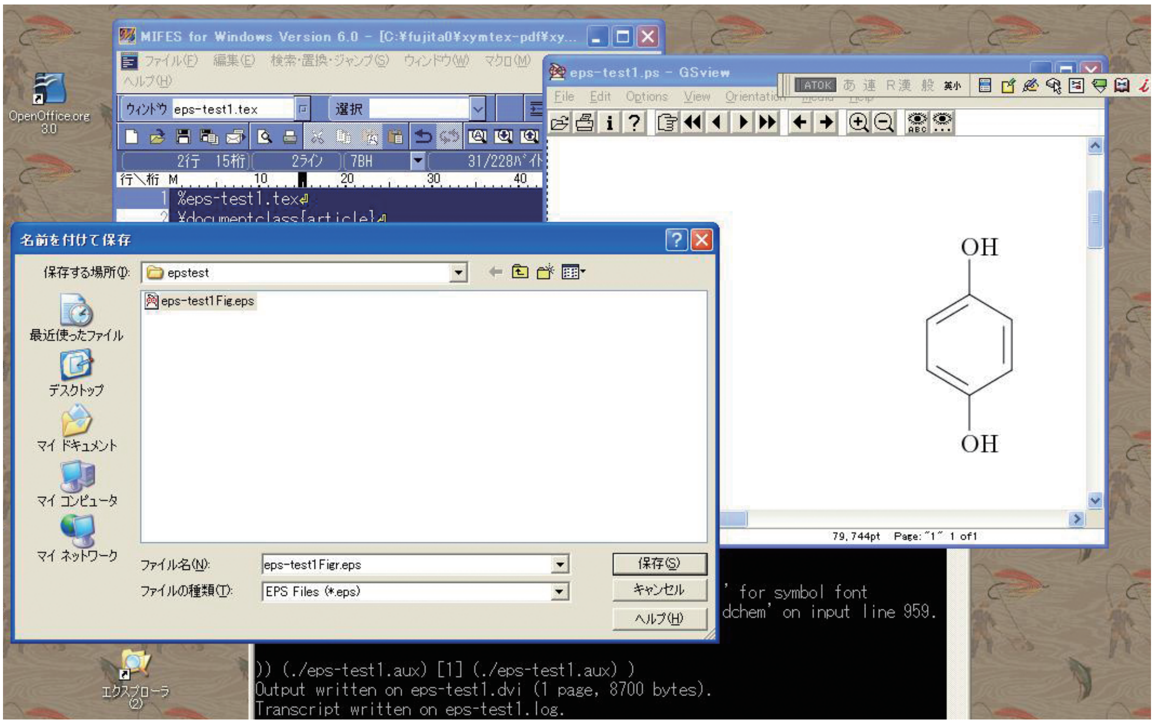
```
o `OT1' for symbol font
on `boldchem' on input line 959.

)) (./eps-test1.aux) [1] (./eps-test1.aux) )
Output written on eps-test1.dvi (1 page, 8700 bytes).
Transcript written on eps-test1.log.
```

PS to EPS

Have you read help `PS to EPS` ?

☑ Automatically calculate Bounding Box

Figure 8.2: Making EPS files of structural formulas. Confirmation box



```
%eps-test1.tex
¥documentclass[article]
```

保存する場所(I): epstest

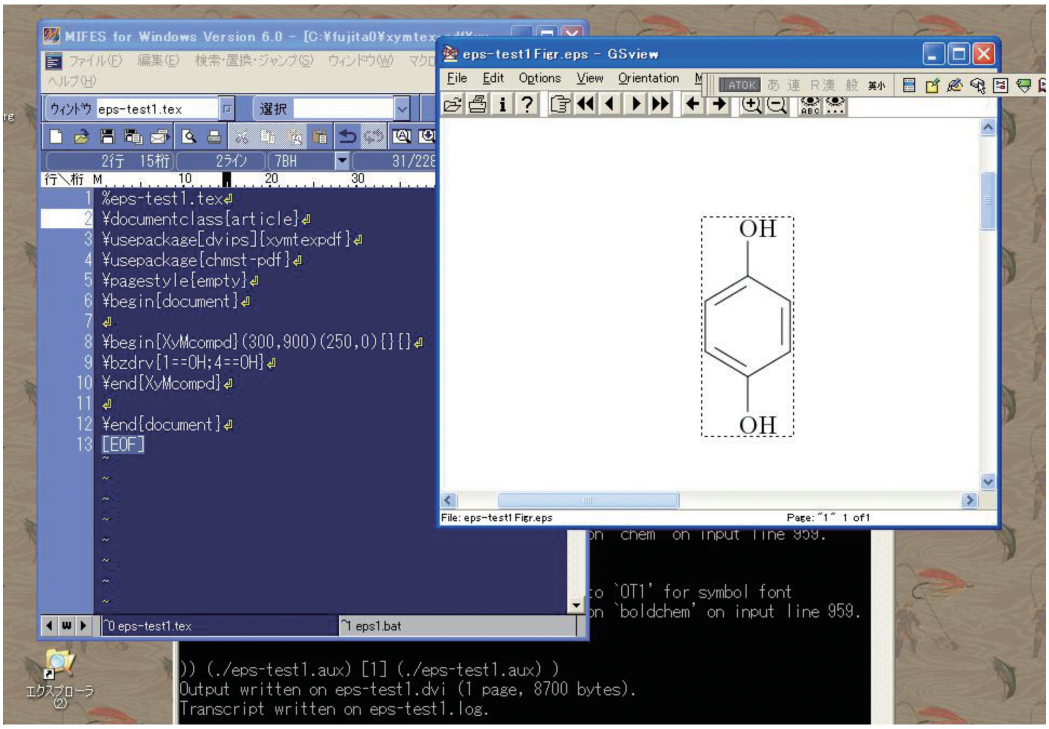
eps-test1Fig.eps

ファイル名(N): eps-test1Figr.eps

ファイルの種類(T): EPS Files (*.eps)

```
' for symbol font
dchem' on input line 959.

)) (./eps-test1.aux) [1] (./eps-test1.aux) )
Output written on eps-test1.dvi (1 page, 8700 bytes).
Transcript written on eps-test1.log.
```

Figure 8.3: Making EPS files of structural formulas. Naming and storing an EPS file



```
%eps-test1.tex
¥documentclass[article]
¥usepackage[dvips][xymtexpdf]
¥usepackage{chmst-pdf}
¥pagestyle{empty}
¥begin{document}

¥begin{XyMcompd}(300,900)(250,0){}{}
¥bzdrv{1==OH;4==OH}
¥end{XyMcompd}

¥end{document}
[EOF]
```

```
on  chem  on input line 959.

to `OT1' for symbol font
on `boldchem' on input line 959.

)) (./eps-test1.aux) [1] (./eps-test1.aux) )
Output written on eps-test1.dvi (1 page, 8700 bytes).
Transcript written on eps-test1.log.
```

Figure 8.4: Making EPS files of structural formulas. EPS file with a bounding box

However, the resulting EPS files sometimes exhibit incorrect bounding boxes.

To calculate correct bounding boxes, the resulting EPS files (e.g., eps-test1FigA.eps) are opened by GSview and processed according to Figures 8.1 to 8.4. Thereby, new EPS files with a recalculated bounding box are generated.

8.2.3 Incorporation of EPS Files in LaTeX Documents

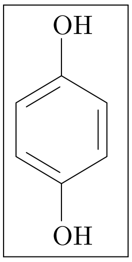
The following tex file (eps-test2.tex) is prepared to incorporate the file (eps-test1Figr.eps) described above. Because the command `\usepackage{xymtexpdf}` has no optional argument, the resulting dvi file is processed by the dvipdfm(x) converter so as to generate the corresponding PDF file (eps-test2.pdf) directly. The command `\includegraphics` is supported by the graphicx package. Note that the xymtexpdf package automatically loads the pgf package, which in turn loads the graphicx package automatically.

```
%eps-test2.tex
\documentclass{article}
\usepackage{xymtexpdf}
\usepackage{chmst-pdf}
%\pagestyle{empty}
\begin{document}

\fbox{%
\includegraphics{eps-test1Figr.eps}
}

\end{document}
```

To simulate the processing of eps-test2.tex, the same code for the XΥMTEX structure is written here in the present document:

```
\fbox{%
\includegraphics{eps-test1Figr.eps}
}
```

which generates the following structural formula:



The bounding box of the EPS file (eps-test1Figr.eps) can be checked by an appropriate editor, where it contains the following line:

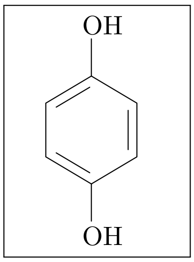
```
%%BoundingBox: 151 627 188 715
```

where the set of four integers represents a boundary box as a rectangle. Thus, `(151 627)` represents the xy-coordinates of the left bottom point of the bounding box, while `(188 715)` represents the xy-coordinates of the right upper point.

The bounding box can be changed directly by replacing these four integers by others, because the EPS file can be edited freely by the editor. The bounding box can alternatively be changed by setting up an optional argument `[bb=...]` of `\includegraphics` as follows:

```
\fbox{%
\includegraphics[bb=140 627 200 715]{eps-test1Figr.eps}
}
```

This change gives a figure with a slightly wider bonding box.



Chapter 9

Mathversion Utilities

All of the functions of the chmst-ps package (on-line manual: xymtx405406B.pdf) are also supported by the chmst-pdf package. A part of the chmst-pdf package has been already discussed in Chapter 7. This section is a rewritten version of mathversion utilities described in Section 1.2 of the on-line manual ("Use of chemist and chmst-ps Packages" in xymtx405406B.pdf), where the previous chmst-ps package is replaced by the present chmst-pdf package.

9.1 Mathversions of the **chmst-pdf** Packages

9.1.1 **chemist**, **chmst-ps**, and **chmst-pdf**

According to the three modes of the XΥMTEX system, there are three sets of mathversion utilities. The following templates are ready to switch the three sets.

1. **TEX/LATEX mode**: The chemist package is read by a command `\usepackage` declared in the preamble of a tex file, as shown in the following template:

```
\documentclass{article}
\usepackage{xymtex}
\usepackage{chemist}
\begin{document}
(text)%default (normal)

\mathversion{bold}
(text)

\mathversion{chem}
(text)

\mathversion{boldchem}
(text)

\mathversion{normal}
(text)%return to the default
\end{document}
```

2. **PostScript-compatible mode**: Alternatively, the chmst-ps package is read to meet PostScript requirements, where the chemist package is automatically loaded. See the on-line manual of

XΥMTEX versions 4.05 and 4.06 (xymtx405406B.pdf). Note that the xymtexps package provides the PostScript-compatible mode of the XΥMTEX system.

```
\documentclass{article}
\usepackage{xymtexps}
\usepackage{chmst-ps}%%\usepackage{chemist,chmst-ps}
\begin{document}
(text)%default (normal)

\mathversion{bold}
(text)

\mathversion{chem}
(text)

\mathversion{boldchem}
(text)

\mathversion{normal}
(text)%return to the default
\end{document}
```

3. **PDF-compatible mode**: In the present extension, the chmst-pdf package is read to meet PDF requirements, where the chemist package is automatically loaded.

```
\documentclass{article}
\usepackage{xymtexpdf}
\usepackage{chmst-pdf}%%\usepackage{chemist,chmst-pdf}
\begin{document}
(text)%default (normal)

\mathversion{bold}
(text)

\mathversion{chem}
(text)

\mathversion{boldchem}
(text)

\mathversion{normal}
(text)%return to the default
\end{document}
```

The xymtexpdf package provides the PDF-compatible mode of the XΥMTEX system. Hence, the resulting dvi file should be converted into a PDF file by means of an appropriate converter (e.g., dvipdfm(x)). The resulting PDF file can be browsed by Adobe Reader. See Section 2.2. For an alternative browsing method, see Section 2.3.

9.2 New Mathverstions

There are two mathversions (“normal” and “bold”) for mathematical usage in LaTeX 2ε. The chemist (chmst-pdf or chmst-ps) package provides additional two mathversions (“chem” and “boldchem”) for chemical usage. The latter two mathversions have already been introduced in Chapter 17 of the manual of XΥMTEX version 1.01 (xymtex.pdf).

If a mathversion command is not explicitly declared, the mathversion "normal" is effective so as to provide usual (default) typesetting inherent in the math mode of LATEX 2ε, where letters etc. are typeset by using *italic* fonts. When `\mathversion{bold}` command is declared, the LATEX 2ε typesetting is conducted under the mathversion "bold", where letters etc. are typeset by using ***boldfaced italic*** fonts. The chemist package (chmst-pdf or chmst-ps) provides us with two additional mathversions, i.e., "chem" and "boldchem", where letters etc. are typeset by using usual or boldfaced **upright** fonts, which mainly aim at the output of chemical elements or compounds (such as $\mathrm{H_2}$ and $\mathrm{H_2O}$).

This section is devoted to add further comments with examples, where the chemical environments discussed in Chapter 7 are tested under the respective mathversions.

9.2.1 Mathversion "normal"

The mathversion "normal" gives outputs of default mode, which are inherent in LATEX 2εwithout any declaration or with declaring `\mathversion{normal}`.

Default Outputs

To show such standard outputs, the listing command `\testmathversion` (Output A) is defined as follows:

```
\def\testmathversion{%for Output A
\[abcdefghijklmnopqrstuvwxyz\imath \jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ\]
\[\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda
\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega
\varepsilon\vartheta\varpi\varrho\varsigma\varphi
\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega\]
\[1234567890\]
\[\mathnormal{1234567890}\]
\[\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}\]
\[\int \sum \prod \coprod \bigcup \bigcap
\bigodot \bigoplus \biguplus \bigotimes \]
\[(, ), [, ], ?, !, \{, \}, =, > (\mathgreater), < (\mathless),
\leftharpoonup, \leftharpoondown, \rightharpoonup, \rightharpoondown,
\ell, \wp, \partial, \flat, \natural, \sharp, \triangleleft, \triangleright,
\smile, \frown, \star\]
\[\check{x}, \breve{x}, \dot{x}, \vec{x},
\acute{x}, \grave{x}, \ddot{x},  \bar{x},
\tilde{x}, \hat{x}, \widetilde{x}, \widehat{x}\]}
```

Thereby, the following code using `\testmathversion`:

```
{\def\tboxtitle{\bf Output A due to ‘‘normal’’}
\begin{tboxscreen}
\testmathversion
\end{tboxscreen}}
```

is described in a `tboxtitle` environment (supported by the chemist package) so as to produce:

Output A due to “normal”

$abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ$

$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}$

1234567890

1234567890

$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

$$\int\sum\prod\coprod\bigcup\bigcap\bigodot\bigoplus\biguplus\bigotimes$$

$(,), [,], ?, !, \{, \}, =, > (>), < (<), \leftharpoonup, \leftharpoondown, \rightharpoonup, \rightharpoondown, \ell, \wp, \partial, \flat, \natural, \sharp, \triangleleft, \triangleright, \smile, \frown, \star$

$\check{x}, \breve{x}, \dot{x}, \vec{x}, \acute{x}, \grave{x}, \ddot{x}, \bar{x}, \tilde{x}, \hat{x}, \widetilde{x}, \widehat{x}$

To test `equation` and `eqnarray` environments, the command `\testequation` (Output B) is defined as follows:

```
\def\testequation{%%for Output B
Euler's summation:
\begin{equation}
\sum_{a\leq k < b}f(k)  =  \int_{a}^{b}f(x)\mathrm{d}x
+ \sum_{k=1}^{m}\frac{B_{k}}{k!}f^{(k-1)}(x)\Big|_{a}^{b} + R_{m}.
\end{equation}
The term \(R_{m}\) is represented as follows:
\begin{eqnarray}
R_{m} & = & (-1)^{m+1}\int_{a}^{b}
\frac{B_{m}(\{x\})}{m!}f^{(m)}(x)\mathrm{d}x, \\
      &   &  a\leq b \mbox{~and~} m\geq 1, \nonumber
\end{eqnarray}
where the symbols $a$, $b$, and $m$ represent integers.
}
```

Thereby, the output produced by `\testequation` shows default outputs of `equation` and `eqnarray` environments in the present mathversion “normal” as follows:

Output B due to “normal”

Euler’s summation:

$$\sum_{a\leq k<b} f(k) = \int_{a}^{b} f(x)\mathrm{d}x + \sum_{k=1}^{m}\frac{B_k}{k!}f^{(k-1)}(x)\Big|_{a}^{b} + R_m. \tag{9.1}$$

The term R_m is represented as follows:

$$\begin{aligned} R_m \quad &= \quad (-1)^{m+1}\int_{a}^{b}\frac{B_m(\{x\})}{m!}f^{(m)}(x)\mathrm{d}x, \\ & \quad\quad a\leq b \text{ and } m\geq 1, \end{aligned} \tag{9.2}$$

where the symbols a, b, and m represent integers.

Convenient Environments for Chemical Equations

To test `equation` and `eqnarray` environments containing chemical formulas, the following test command `\testequationforchemistry` (Output C) is defined as follows:

```
\def\testequationforchemistry{%%for Output C
An equation enviroment:
\begin{equation}
2H_2 + O_2  \rightarrow  2H_2O
\end{equation}
An eqnarray environment:
\begin{eqnarray}
C + O_2 & \rightarrow & CO_2 \\
Na^{+} + Cl^{-} & \rightarrow & NaCl\downarrow
\end{eqnarray}
}%
```

Under the mathversion “normal”, alphabets in a math mode (such as an equation or eqnarray environment) are typeset by using italic fonts, which do not meet chemical requirements. Thus the test command `\testequationforchemistry` defined above gives the following output.

Output C due to “normal”

An equation environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{9.3}$$

An eqnarray environment:

$$C + O_2 \quad \rightarrow \quad CO_2 \tag{9.4}$$

$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow \tag{9.5}$$

The chemist (chmst-ps or chmst-pdf) package defines `chemeqn` and `chemeqnarray` environments in order to support chemical requirements. (cf. Subsection 17.1 of the manual of XΥMTEX version 1.01 (xymtex.pdf)). The following `\testchemequation` command (Output D) is defined to test the functions of the `chemeqn` and `chemeqnarray` environments and related commands.

```
\def\testchemequation{%%for Output D
A chemeqn enviroment:
\begin{chemeqn}
2H_2 + O_2  \rightarrow  2H_2O
\end{chemeqn}
\begin{chemeqn}
abcdefghijklmnopqrstuvwxyz\imath \jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ
\end{chemeqn}
\begin{chemeqn}
\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda
\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega
\varepsilon\vartheta\varpi\varrho\varsigma\varphi
\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega
\end{chemeqn}
A chemeqnarray environment:
\begin{chemeqnarray}
C + O_2 & \rightarrow & CO_2 \\
Na^{+} + Cl^{-} & \rightarrow & NaCl\downarrow
```

```
\end{chemeqnarray}
A chemeqnarray$*$ environment:
\begin{chemeqnarray*}
C + O_2 & \rightarrow & CO_2 \\
Na^{+} + Cl^{-} & \rightarrow & NaCl\downarrow
\end{chemeqnarray*}
In-text chemical formulas: \chemform{2H_2 + O_2  \rightarrow  2H_2O}
and \chemform{C + O_2 \rightarrow CO_2}
}%
```

Under the mathversion “normal”, alphabets in a chemeqn environment etc. are typeset by using upright fonts. Thus the test command `\testchemequation` defined above gives the following output.

Output D due to “normal”

A chemeqn environment:

$$\mathrm{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.6}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.7}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.8}$$

A chemeqnarray environment:

$$\begin{align} \mathrm{C + O_2} &\rightarrow \mathrm{CO_2} \tag{9.9}\\ \mathrm{Na^{+} + Cl^{-}} &\rightarrow \mathrm{NaCl}\downarrow \tag{9.10} \end{align}$$

A chemeqnarray∗ environment:

$$\begin{aligned} \mathrm{C + O_2} &\rightarrow \mathrm{CO_2}\\ \mathrm{Na^{+} + Cl^{-}} &\rightarrow \mathrm{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $\mathrm{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathrm{C + O_2 \rightarrow CO_2}$

In addition to the `chemeqn` and `chemeqnarray` environments (cf. Subsection 17.1 of the manual of XΥMTEX version 1.01 (xymtex.pdf)), the latest version of the chemist (chmst-ps or chmst-pdf) package provides another set of commands for chemical requirements, i.e., `ChemEquation`, `ChemEqnarray`, and `ChemEqnarray`∗ environments as well as `\ChemForm` command. The following `\testChemEquation` command (Output E) is defined to test the functions of these newly-defined commands.

```
\def\testChemEquation{%%for Output E
A ChemEquation enviroment:
\begin{ChemEquation}
2H_2 + O_2  \rightarrow  2H_2O
\end{ChemEquation}
\begin{ChemEquation}
abcdefghijklmnopqrstuvwxyz\imath \jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ
\end{ChemEquation}
\begin{ChemEquation}
\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda
\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega
\varepsilon\vartheta\varpi\varrho\varsigma\varphi
\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega
\end{ChemEquation}
A ChemEqnarray environment:
```

```
\begin{ChemEqnarray}
C + O_2 & \rightarrow & CO_2 \\
Na^{+} + Cl^{-} & \rightarrow & NaCl\downarrow
\end{ChemEqnarray}
A ChemEqnarray$*$ environment:
\begin{ChemEqnarray*}
C + O_2 & \rightarrow & CO_2 \\
Na^{+} + Cl^{-} & \rightarrow & NaCl\downarrow
\end{ChemEqnarray*}
In-text chemical formulas: \ChemForm{2H_2 + O_2  \rightarrow  2H_2O}
and \ChemForm{C + O_2 \rightarrow CO_2}
}%
```

Under the mathversion "normal", alphabets in a `ChemEquation` etc. are typeset also by using upright fonts. Thus the test command `\testChemEquation` defined above gives the following output.

Output E due to "normal"

A ChemEquation environment:

$$\mathrm{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.11}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.12}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.13}$$

A ChemEqnarray environment:

$$\mathrm{C + O_2} \quad \rightarrow \quad \mathrm{CO_2} \tag{9.14}$$

$$\mathrm{Na^{+} + Cl^{-}} \quad \rightarrow \quad \mathrm{NaCl}\downarrow \tag{9.15}$$

A ChemEqnarray$*$ environment:

$$\begin{array}{rcl}
\mathrm{C + O_2} & \rightarrow & \mathrm{CO_2} \\
\mathrm{Na^{+} + Cl^{-}} & \rightarrow & \mathrm{NaCl}\downarrow
\end{array}$$

In-text chemical formulas: $\mathrm{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathrm{C + O_2 \rightarrow CO_2}$

9.2.2 Mathversion "bold"

The mathversion "bold" gives outputs of boldfaced fonts, when the switching command `\mathversion` is explicitly declared. An alternative (rather old) method to enter the mathversion "bold" is the declaration of `\boldmath`. For example, `{\boldmath $x_{i}$}` produces $\boldsymbol{x_i}$ according to LaTeX2.09. This section is typeset after the declaration of

```
\mathversion{bold}
```

according to LaTeX 2ε.

Outputs under Mathversion "bold"

The mathversion "bold" gives outputs of "bold" mode, which are inherent in LaTeX 2ε. To show such outputs, the listing command `\testmathversion` defined above is used after the declaration of `\mathversion{bold}`. The result is shown as follows:

Output A due to “bold”

$$\boldsymbol{abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}}$$

$$\mathbf{1234567890}$$

$$\oldstylenums{1234567890}$$

$$\boldsymbol{\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}}$$

$$\int\sum\prod\coprod\bigcup\bigcap\bigodot\bigoplus\biguplus\bigotimes$$

$$\boldsymbol{(,), [,], ?, !, \{, \}, =, > (>), < (<), \leftharpoonup, \leftharpoondown, \rightharpoonup, \rightharpoondown, \ell, \wp, \partial, \flat, \natural, \sharp, \triangleleft, \triangleright, \smile, \frown, \star}$$

$$\boldsymbol{\check{x}, \breve{x}, \dot{x}, \vec{x}, \acute{x}, \grave{x}, \ddot{x}, \bar{x}, \tilde{x}, \hat{x}, \widetilde{x}, \widehat{x}}$$

To test `equation` and `eqnarray` environments under the mathversion “bold”, the above-defined command `\testequation` is again used here so as to give the following output:

Output B due to “bold”

Euler’s summation:

$$\boldsymbol{\sum_{a\leq k<b} f(k) = \int_a^b f(x)\mathrm{d}x + \sum_{k=1}^{m} \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m.} \tag{9.16}$$

The term $\boldsymbol{R_m}$ is represented as follows:

$$\boldsymbol{\begin{aligned} R_m &= (-1)^{m+1}\int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)\mathrm{d}x, \\ & a \leq b \text{ and } m \geq 1, \end{aligned}} \tag{9.17}$$

where the symbols $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{m}$ represent integers.

Environments and Commands for Chemistry

Under the mathversion “bold”, alphabets in a math mode (such as an equation or eqnarray environment) are typeset by using boldfaced italic fonts. Thus the test command `\testequationforchemistry` defined above gives the following output, which does not meet chemical requirements.

Output C due to “bold”

An equation environment:

$$\boldsymbol{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.18}$$

An eqnarray environment:

$$\boldsymbol{C + O_2 \rightarrow CO_2} \tag{9.19}$$

$$\boldsymbol{Na^+ + Cl^- \rightarrow NaCl\downarrow} \tag{9.20}$$

Even under the mathversion “bold”, alphabets in a chemeqn environment etc. are typeset by using upright fonts. Thus the test command `\testchemequation` defined above gives the following output, which is equivalent to the above output of the mathversion “normal”.

Output D due to “bold”

A chemeqn environment:

$$\mathrm{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.21}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.22}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.23}$$

A chemeqnarray environment:

$$\mathrm{C + O_2} \;\rightarrow\; \mathrm{CO_2} \tag{9.24}$$

$$\mathrm{Na^+ + Cl^-} \;\rightarrow\; \mathrm{NaCl}\downarrow \tag{9.25}$$

A chemeqnarray$*$ environment:

$$\begin{aligned} \mathrm{C + O_2} &\;\rightarrow\; \mathrm{CO_2} \\ \mathrm{Na^+ + Cl^-} &\;\rightarrow\; \mathrm{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $\mathrm{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathrm{C + O_2 \rightarrow CO_2}$

In contrast, `ChemEquation`, `ChemEqnarray`, and `ChemEqnarray*` environments as well as a `\ChemForm` command typeset boldfaced alphabets of upright shape under the mathversion “bold”. Thus the test command `\testChemEquation` defined above gives the following output, which is different from the corresponding output of the mathversion “normal”.

Output E due to “bold”

A ChemEquation environment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.26}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\boldsymbol{\imath\jmath}\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.27}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}} \tag{9.28}$$

A ChemEqnarray environment:

$$\mathbf{C + O_2} \;\rightarrow\; \mathbf{CO_2} \tag{9.29}$$

$$\mathbf{Na^+ + Cl^-} \;\rightarrow\; \mathbf{NaCl}\downarrow \tag{9.30}$$

A ChemEqnarray$*$ environment:

$$\begin{aligned} \mathbf{C + O_2} &\;\rightarrow\; \mathbf{CO_2} \\ \mathbf{Na^+ + Cl^-} &\;\rightarrow\; \mathbf{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $\mathbf{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathbf{C + O_2 \rightarrow CO_2}$

9.2.3 Mathversion “chem”

Subsection 17.1 of the manual of XΥMTEX version 1.01 (xymtex.pdf) has discussed the original version of the mathversion “chem”, which involved some irregular outputs of letters. The latest version of the chemist (chmst-ps or chmst-pdf) package gives more sufficient results with respect to letter outputs.

This section is typeset after the declaration of

```
\mathversion{chem}
```

Outputs under Mathversion “chem”

The mathversion “chem” gives outputs of “chem” mode, which aim at upright letters for chemical formulas. To show such outputs, the listing command `\testmathversion` defined above is used after the declaration of `\mathversion{chem}`. The result is shown as follows:

Output A due to “chem”

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}$$

$$1234567890$$

$$1234567890$$

$$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\int\sum\prod\coprod\bigcup\bigcap\bigodot\bigoplus\biguplus\bigotimes$$

$$(,), [,], ?, !, \{, \}, =, \text{¿}\ (>), \text{¡}\ (<), \leftharpoonup, \leftharpoondown, \rightharpoonup, \rightharpoondown, \ell, \wp, \partial, \flat, \natural, \sharp, \triangleleft, \triangleright, \smile, \frown, \star$$

$$\check{\mathrm{x}}, \breve{\mathrm{x}}, \dot{\mathrm{x}}, \vec{\mathrm{x}}, \acute{\mathrm{x}}, \grave{\mathrm{x}}, \ddot{\mathrm{x}}, \bar{\mathrm{x}}, \tilde{\mathrm{x}}, \hat{\mathrm{x}}, \widetilde{\mathrm{x}}, \widehat{\mathrm{x}}$$

As found in the first line of Output A due to “chem”, lowercase and uppercase alphabets are typeset upright except $\imath$ and $\jmath$.

Note that the symbols < and > are not properly typeset if they are input directly. The commands `$\mathless$` and `$\mathgreater$` should be used to give correct printing.

To test equation and eqnarray environments under the mathversion “chem”, the above-defined command `\testequation` is again used here, although the resulting output is contrary to mathematical conventions:

Output B due to “chem”

Euler’s summation:

$$\sum_{\mathrm{a}\leq \mathrm{k}\text{¡}\mathrm{b}} \mathrm{f(k)} = \int_{\mathrm{a}}^{\mathrm{b}} \mathrm{f(x)dx} + \sum_{\mathrm{k}=1}^{\mathrm{m}} \frac{\mathrm{B_k}}{\mathrm{k!}} \mathrm{f}^{(\mathrm{k}-1)}(\mathrm{x})\Big|_{\mathrm{a}}^{\mathrm{b}} + \mathrm{R_m}. \tag{9.31}$$

The term $\mathrm{R_m}$ is represented as follows:

$$\begin{aligned} \mathrm{R_m} \quad &= \quad (-1)^{\mathrm{m}+1} \int_{\mathrm{a}}^{\mathrm{b}} \frac{\mathrm{B_m}(\{\mathrm{x}\})}{\mathrm{m!}} \mathrm{f}^{(\mathrm{m})}(\mathrm{x})\mathrm{dx}, \\ & \quad\quad \mathrm{a} \leq \mathrm{b} \text{ and } \mathrm{m} \geq 1, \end{aligned} \tag{9.32}$$

where the symbols a, b, and m represent integers.

Note that the symbols < and > are not properly typeset if they are input directly. Thus, the symbol < in the lower limit of the above summation is erroneously replaced by the symbol ¡. The commands `$\mathless$` and `$\mathgreater$` should be used to give correct printing. For example, the code:

```
\[\sum_{a\leq k \mbox{\scriptsize $\mathless$} b}f(k)\]
```

gives the following output:

$$\sum_{\mathrm{a}\leq \mathrm{k}<\mathrm{b}} \mathrm{f(k)}$$

Because this output does not meet mathematical conventions, it should be written as follows:

```
{\mathversion{normal}
```

```
\[\sum_{a\leq k < b}f(k)\]
}
```

which gives the following output:

$$\sum_{a\leq k<b} f(k)$$

Environments and Commands for Chemistry

Under the mathversion “chem”, alphabets in a math mode (such as an `equation` or `eqnarray` environment) are typeset by using upright fonts. Thus the test command `\testequationforchemistry` defined above gives the following output, which meets chemical requirements.

Output C due to “chem”

An equation environment:

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O} \tag{9.33}$$

An eqnarray environment:

$$\begin{align} \mathrm{C} + \mathrm{O}_2 &\rightarrow \mathrm{CO}_2 \tag{9.34}\\ \mathrm{Na}^+ + \mathrm{Cl}^- &\rightarrow \mathrm{NaCl}\downarrow \tag{9.35}\end{align}$$

Under the mathversion “chem”, alphabets in a `chemeqn` environment etc. are also typeset by using upright fonts. Thus the test command `\testchemequation` defined above gives the following output, which is equivalent to the above output of the mathversion “normal”.

Output D due to “chem”

A chemeqn environment:

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O} \tag{9.36}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.37}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.38}$$

A chemeqnarray environment:

$$\begin{align} \mathrm{C} + \mathrm{O}_2 &\rightarrow \mathrm{CO}_2 \tag{9.39}\\ \mathrm{Na}^+ + \mathrm{Cl}^- &\rightarrow \mathrm{NaCl}\downarrow \tag{9.40}\end{align}$$

A chemeqnarray$*$ environment:

$$\begin{aligned} \mathrm{C} + \mathrm{O}_2 &\rightarrow \mathrm{CO}_2\\ \mathrm{Na}^+ + \mathrm{Cl}^- &\rightarrow \mathrm{NaCl}\downarrow\end{aligned}$$

In-text chemical formulas: $2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O}$ and $\mathrm{C} + \mathrm{O}_2 \rightarrow \mathrm{CO}_2$

On the same line, `ChemEquation`, `ChemEqnarray`, and `ChemEqnarray∗` environments as well as a `\ChemForm` command typeset alphabets of upright shape under the mathversion “chem”. Thus the test command `\testChemEquation` defined above gives the following output, which is different from the corresponding output of the mathversion “bold” but equivalent to the corresponding output of the mathversion “normal”.

Output E due to "chem"

A ChemEquation environment:

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O} \tag{9.41}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.42}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.43}$$

A ChemEqnarray environment:

$$\mathrm{C} + \mathrm{O}_2 \quad \rightarrow \quad \mathrm{CO}_2 \tag{9.44}$$

$$\mathrm{Na}^+ + \mathrm{Cl}^- \quad \rightarrow \quad \mathrm{NaCl}\downarrow \tag{9.45}$$

A ChemEqnarray∗ environment:

$$\begin{aligned} \mathrm{C} + \mathrm{O}_2 &\quad \rightarrow \quad \mathrm{CO}_2 \\ \mathrm{Na}^+ + \mathrm{Cl}^- &\quad \rightarrow \quad \mathrm{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O}$ and $\mathrm{C} + \mathrm{O}_2 \rightarrow \mathrm{CO}_2$

9.2.4 Mathversion "boldchem"

In addition to the mathversion "chem" supported by the original version of the chemist (chmst-ps or chmst-pdf) package (cf. Subsection 17.1 of the manual of X͡ΥMTEX version 1.01 (xymtex.pdf)), the latest version of the chemist package packed in X͡ΥMTEX version 4.05 supports the mathversion "boldchem".

This section is typeset after the declaration of

```
\mathversion{boldchem}
```

Outputs under Mathversion "boldchem"

The mathversion "boldchem" gives outputs of "boldchem" mode, which aim at upright letters for chemical formulas. To show such outputs, the listing command `\testmathversion` defined above is used after the declaration of `\mathversion{boldchem}`. The result is shown as follows:

Output A due to "boldchem"

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\boldsymbol{\imath\jmath}\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}}$$

$$\mathbf{1234567890}$$

$$\mathbf{1234567890}$$

$$\boldsymbol{\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}}$$

$$\int\sum\prod\coprod\bigcup\bigcap\bigodot\bigoplus\biguplus\bigotimes$$

$$(,), [,], ?, !, \{, \}, =, ¿\ (>), ¡\ (<), \leftharpoonup, \leftharpoondown, \rightharpoonup, \rightharpoondown, \ell, \wp, \partial, \flat, \natural, \sharp, \triangleleft, \triangleright, \smile, \frown, \star$$

$$\check{\mathbf{x}}, \breve{\mathbf{x}}, \dot{\mathbf{x}}, \vec{\mathbf{x}}, \acute{\mathbf{x}}, \grave{\mathbf{x}}, \ddot{\mathbf{x}}, \bar{\mathbf{x}}, \tilde{\mathbf{x}}, \hat{\mathbf{x}}, \widetilde{\mathbf{x}}, \widehat{\mathbf{x}}$$

As found in the first line of Output A due to "boldchem", lowercase and uppercase alphabets are typeset in boldfaced upright fonts except $\imath$ and $\jmath$.

Note that the symbols $<$ and $>$ are not properly typeset if they are input directly. The commands `$\mathless$` and `$\mathgreater$` should be used to give correct printing.

To test `equation` and `eqnarray` environments under the mathversion “boldchem”, the above-defined command `\testequation` is again used here, although the resulting output is contrary to mathematical conventions:

Output B due to “boldchem”

Euler’s summation:

$$\sum_{\mathbf{a}\leq\mathbf{k}\text{¡}\mathbf{b}} \mathbf{f(k)} = \int_{\mathbf{a}}^{\mathbf{b}} \mathbf{f(x)dx} + \sum_{\mathbf{k}=1}^{\mathbf{m}} \frac{\mathbf{B_k}}{\mathbf{k!}}\mathbf{f^{(k-1)}(x)}\Big|_{\mathbf{a}}^{\mathbf{b}} + \mathbf{R_m}. \tag{9.46}$$

The term $\mathbf{R_m}$ is represented as follows:

$$\begin{aligned} \mathbf{R_m} &= (-1)^{\mathbf{m}+1}\int_{\mathbf{a}}^{\mathbf{b}} \frac{\mathbf{B_m(\{x\})}}{\mathbf{m!}}\mathbf{f^{(m)}(x)dx}, \\ &\quad \mathbf{a} \leq \mathbf{b} \text{ and } \mathbf{m} \geq \mathbf{1}, \end{aligned} \tag{9.47}$$

where the symbols **a**, **b**, and **m** represent integers.

Note that the symbols $<$ and $>$ are not properly typeset if they are input directly. Thus, the symbol $<$ in the lower limit of the above summation is erroneously replaced by the symbol **¡**. The commands `$\mathless$` and `$\mathgreater$` should be used to give correct printing. For example, the code:

```
\[\sum_{a\leq k \mbox{\scriptsize $\mathless$} b}f(k)\]
```

gives the following output:

$$\sum_{\mathbf{a}\leq\mathbf{k}<\mathbf{b}} \mathbf{f(k)}$$

Because this output does not meet mathematical conventions, it should be written as follows:

```
{\mathversion{bold}
\[\sum_{a\leq k < b}f(k)\]
}
```

which gives the following output:

$$\boldsymbol{\sum_{a\leq k<b} f(k)}$$

Environments and Commands for Chemistry

Under the mathversion “boldchem”, alphabets in a math mode (such as an `equation` or `eqnarray` environment) are typeset by using upright fonts. Thus the test command `\testequationforchemistry` defined above gives the following output, which meets chemical requirements.

Output C due to “boldchem”

An equation environment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.48}$$

An eqnarray environment:

$$\mathbf{C + O_2} \quad \rightarrow \quad \mathbf{CO_2} \tag{9.49}$$

$$\mathbf{Na^+ + Cl^-} \quad \rightarrow \quad \mathbf{NaCl} \downarrow \tag{9.50}$$

Under the mathversion “boldchem”, alphabets in a `chemeqn` environment etc. are typeset by using upright fonts (not boldfaced). Thus the test command `\testchemequation` defined above gives the following output, which is equivalent to the above output of the mathversion “chem”.

Output D due to “boldchem”

A chemeqn environment:

$$\mathrm{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.51}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.52}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{9.53}$$

A chemeqnarray environment:

$$\begin{align} \mathrm{C + O_2} &\rightarrow \mathrm{CO_2} \tag{9.54}\\ \mathrm{Na^+ + Cl^-} &\rightarrow \mathrm{NaCl}\downarrow \tag{9.55} \end{align}$$

A chemeqnarray∗ environment:

$$\begin{aligned} \mathrm{C + O_2} &\rightarrow \mathrm{CO_2}\\ \mathrm{Na^+ + Cl^-} &\rightarrow \mathrm{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $\mathrm{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathrm{C + O_2 \rightarrow CO_2}$

In contrast, `ChemEquation`, `ChemEqnarray`, and `ChemEqnarray*` environments as well as a `\ChemForm` command typeset boldfaced alphabets of upright shape under the mathversion “boldchem”. Thus the test command `\testChemEquation` defined above gives the following output, which is equivalent to the corresponding output of the mathversion “bold’.

Output E due to “boldchem”

A ChemEquation environment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{9.56}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\boldsymbol{\imath\jmath}\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{9.57}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}} \tag{9.58}$$

A ChemEqnarray environment:

$$\begin{align} \mathbf{C + O_2} &\rightarrow \mathbf{CO_2} \tag{9.59}\\ \mathbf{Na^+ + Cl^-} &\rightarrow \mathbf{NaCl}\downarrow \tag{9.60} \end{align}$$

A ChemEqnarray∗ environment:

$$\begin{aligned} \mathbf{C + O_2} &\rightarrow \mathbf{CO_2}\\ \mathbf{Na^+ + Cl^-} &\rightarrow \mathbf{NaCl}\downarrow \end{aligned}$$

In-text chemical formulas: $\mathbf{2H_2 + O_2 \rightarrow 2H_2O}$ and $\mathbf{C + O_2 \rightarrow CO_2}$

Chapter 10

Cooperative Use of the **amsmath** Package

On a similar line to the chmst-ps packages (on-line manual: xymtx405406B.pdf), the chmst-pdf package supports cooperative use of the amsmath package, where new chemical equation environments akin to the standard `ChemEquation` and `ChemEqnarray` environments are created to be in harmony with the methodology of the amsmath package. This section is a reproduced version of Section 2.3 of the on-line manual ("Creation of New Environments for Chemical Equations" in xymtx405406B.pdf), where the previous chmst-ps package is replaced by the present chmst-pdf package.

10.1 Creation of New Environments for Chemical Equations

When the amsmath package is loaded, several environments for printing multiline display equations are available. These mathematical environments can be converted into chemical versions by using the `\newchemenvironment` command supported by the present chmst-pdf package. [1]

format: `\newchemenvironment{New Chem Environment}{Original Math Environment}`

10.1.1 Creation of the `chemmultline` Environment

The `multline` environment of the amsmath package provides us with a mathematical tool for folding a long display equation into a multiline display equation in accord with the text width to be set up:

```
\begin{minipage}{0.6\textwidth}
\begin{multline}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{multline}
{\mathversion{chem}
\begin{multline}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{multline}}
\end{minipage}
```

---

[1] The chemst or chmst-ps package is also effective for this purpose. See the on-line manual (xymtx405406B.pdf).

$$Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\ Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq) \quad (10.1)$$

$$\mathrm{Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} \rightarrow \\ \mathrm{Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq)} \quad (10.2)$$

Note that the `minipage` environment reduces the text width to emphasize the function of the `multiline` environment. Each molecular formula in the `multline` environment is printed in italic fonts on a similar line to `equation` and like environments of LaTeX 2ε. The latter example shows that the declaration of `\mathversion{chem}` changes the appearance of the `multiline` environment.

We can create a chemical version of the `multline` environment of the `amsmath` package by declaring

```
\newchemenvironment{chemmultline}{multline}
```

Thereby, the newly-defined `chemmultline` environment is substituted for the `multline` environment shown above so as to give the following result:

```
\newchemenvironment{chemmultline}{multline}
\begin{minipage}{0.6\textwidth}
\begin{chemmultline}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{chemmultline}
{\mathversion{boldchem}
\begin{chemmultline}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{chemmultline}}
\end{minipage}
```

$$\mathrm{Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} \rightarrow \\ \mathrm{Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq)} \quad (10.3)$$

$$\mathbf{Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} \rightarrow \\ \mathbf{Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq)} \quad (10.4)$$

The latter example shows the declaration of `\mathversion{boldchem}` changes the appearance of the `chemmultiline` environment.

On a similar line, the `multiline*` environment of the `amsmath` package can be converted into a chemical version named `chemmultiline*`. The newly-defined `chemmultiline*` environment is used in place of the `chemmultiline` environment so as to give the following result without printing equation numbers:

```
\newchemenvironment{chemmultline*}{multline*}
\begin{minipage}{0.6\textwidth}
\begin{chemmultline*}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{chemmultline*}
\end{minipage}
```

$$\begin{multline*}\mathrm{Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} \rightarrow \\ \mathrm{Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)}\end{multline*}$$

Environments created by `\newchemenvironment` have properties equivalent to `ChemEquation` and like environments, which are originally supported by the chmst-pdf (chmst-ps) package. Hence, fonts used in such newly-defined environments can be changed by declaring `\let\ChemEqFont=\sf` etc. After the declaration `\let\ChemEqFont=\sf`, the same code as shown above gives following result:

```
\let\ChemEqFont=\sf
\begin{minipage}{0.6\textwidth}
\begin{chemmultline*}
Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow \\
Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)
\end{chemmultline*}
\end{minipage}
```

$$\begin{multline*}\mathsf{Cu^{2+}(aq) + SO_{4}^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} \rightarrow \\ \mathsf{Cu(OH)_{2}(s) + 2Li^{+}(aq) + SO_{4}^{2-}(aq)}\end{multline*}$$

10.1.2 Creation of the `chemgather` Environment

The `chemgather` environment as a chemical version of the `gather` environment of the amsmath package can be created on a similar line by using `\newchemenvironment`. A typical example is shown as follows:

```
\newchemenvironment{chemgather}{gather}
\begin{chemgather}
Bi(NO_{3})_{3}\cdot 5H_{2}O \overset{50-60^{\circ}}{\lllongrightarrow}
[Bi_{6}O_{6}]_{2}(NO_{3})_{11}(OH)\cdot 6H_{2}O
\overset{77-130^{\circ}}{\lllongrightarrow} \notag \\
[Bi_{6}O_{6}](NO_{3})_{6}(OH)\cdot 3H_{2}O
\overset{400-450^{\circ}}{\lllongrightarrow}
\alpha\mbox{-}Bi_{2}O_{3} \\
Bi(NO_{3})_{3}\cdot N_{2}O_{4}
\overset{200^{\circ}}{\lllongrightarrow}
Bi_{2}O(NO_{3})_{4}
\overset{415^{\circ}}{\lllongrightarrow}
Bi_{4}O_{5}(NO_{3})_{2}
\end{chemgather}
```

$$\mathrm{Bi(NO_{3})_{3}\cdot 5H_{2}O} \xrightarrow{50-60^{\circ}} \mathrm{[Bi_{6}O_{6}]_{2}(NO_{3})_{11}(OH)\cdot 6H_{2}O} \xrightarrow{77-130^{\circ}}$$

$$\mathrm{[Bi_{6}O_{6}](NO_{3})_{6}(OH)\cdot 3H_{2}O} \xrightarrow{400-450^{\circ}} \alpha\text{-}\mathrm{Bi_{2}O_{3}} \tag{10.5}$$

$$\mathrm{Bi(NO_{3})_{3}\cdot N_{2}O_{4}} \xrightarrow{200^{\circ}} \mathrm{Bi_{2}O(NO_{3})_{4}} \xrightarrow{415^{\circ}} \mathrm{Bi_{4}O_{5}(NO_{3})_{2}} \tag{10.6}$$

where the equation number of the first line is suppressed by declaring `\notag`.

10.1.3 Creation of the `chemalign` Environment

The `chemalign` environment can be created as a chemical version of the `align` environment of the `amsmath` package. What you have to do is only to declare `\newchemenvironment{chemalign}{align}`. Just as the `align` environment of the `amsmath` package is based on the alignment mechanism of TEX, the present `chemalign` environment succeeds in functions due to the alignment mechanism. Hence, such commands as `\noalign` can be used in the `chemalign` environment so as to give the following output:

```
\newchemenvironment{chemalign}{align}
\begin{chemalign}
5Fe^{2+} & \llongrightarrow 5Fe^{3+} + 5e^{-} \notag \\
MnO_{4}^{-} + 5e^{-} + 8H^{+} & \llongrightarrow Mn^{2+} + 4H_{2}O \notag \\
\noalign{\vskip-8pt}
\noalign{\hfil\hbox to9cm{\hrulefill\kern0.5cm}\hfil}
\noalign{\vskip-4pt}
MnO_{4}^{-} + 5Fe^{2+} + 8H^{+} & \llongrightarrow Mn^{2+} + 5Fe^{3+} + 4H_{2}O
\end{chemalign}
```

$$\begin{array}{rl}
5\mathrm{Fe}^{2+} & \longrightarrow 5\mathrm{Fe}^{3+} + 5\mathrm{e}^{-} \\
\mathrm{MnO}_4^{-} + 5\mathrm{e}^{-} + 8\mathrm{H}^{+} & \longrightarrow \mathrm{Mn}^{2+} + 4\mathrm{H}_2\mathrm{O} \\
\hline
\mathrm{MnO}_4^{-} + 5\mathrm{Fe}^{2+} + 8\mathrm{H}^{+} & \longrightarrow \mathrm{Mn}^{2+} + 5\mathrm{Fe}^{3+} + 4\mathrm{H}_2\mathrm{O}
\end{array} \tag{10.7}$$

On a similar line, the `chemalign*` environment corresponding to the `align*` environment of the `amsmath` package can be created by declaring `\newchemenvironment{chemalign*}{align*}`.

```
\newchemenvironment{chemalign*}{align*}
\begin{chemalign*}
Co(CN)_{6}^{4-} & \equilibarrow Co(CN)_{6}^{3-} + e^{-} \\
Fe(CN)_{6}^{4-} & \equilibarrow Co(CN)_{6}^{3-} + e^{-}
\end{chemalign*}
```

$$\begin{aligned}
\mathrm{Co(CN)}_6^{4-} & \rightleftharpoons \mathrm{Co(CN)}_6^{3-} + \mathrm{e}^{-} \\
\mathrm{Fe(CN)}_6^{4-} & \rightleftharpoons \mathrm{Co(CN)}_6^{3-} + \mathrm{e}^{-}
\end{aligned}$$

10.1.4 Creation of the `chemalignat` Environment

The `chemalignat` environment can be created as a chemical version of the `alignat` environment of the `amsmath` package by declaring `\newchemenvironment{chemalignat}{alignat}`. The usage of the newly-defined `chemalignat` environment is exemplified as follows:

```
\newchemenvironment{chemalignat}{alignat}
\begin{chemalignat}{4}
\mbox{Solution of zinc oxide:} \qquad
& ZnO + 2H^{+}  & \llongrightarrow\quad & Zn^{2+} + H_{2}O \\
\mbox{Cathode reaction:} \qquad
& Zn^{2+} + 2e^{-} &\llongrightarrow\quad & Zn \\
\mbox{Anode reaction:} \qquad
& H_{2}O  & \llongrightarrow\quad & {\textstyle\frac{1}{2}}O_{2} + 2H^{+} + 2e^{-} \\
\mbox{Over-all reaction:} \qquad
& ZnO  & \llongrightarrow\quad  & Zn + {\textstyle\frac{1}{2}}O_{2}
\end{chemalignat}
```

$$\begin{aligned}
&\text{Solution of zinc oxide:} && \mathrm{ZnO} + 2\mathrm{H}^{+} \longrightarrow && \mathrm{Zn}^{2+} + \mathrm{H}_2\mathrm{O} && (10.8)\\
&\text{Cathode reaction:} && \mathrm{Zn}^{2+} + 2\mathrm{e}^{-} \longrightarrow && \mathrm{Zn} && (10.9)\\
&\text{Anode reaction:} && \mathrm{H}_2\mathrm{O} \longrightarrow && \tfrac{1}{2}\mathrm{O}_2 + 2\mathrm{H}^{+} + 2\mathrm{e}^{-} && (10.10)\\
&\text{Over-all reaction:} && \mathrm{ZnO} \longrightarrow && \mathrm{Zn} + \tfrac{1}{2}\mathrm{O}_2 && (10.11)
\end{aligned}$$

10.1.5 The Use of the `split` Environment

The `split` environment supported by the amsmath package is originally used in combination with `equation` (redefined in amsmath), `gather`, etc. Because the `ChemEquation` environment of the present chmst-pdf package has been tuned to the setting of the amsmath package, it can be used in combination with the split environment:

```
\begin{ChemEquation}
\begin{split}
 [(\eta^{5}\mbox{-}C_{5}H_{5})(CO)_{2}MnSbPhI_{2}]
& + [(\eta^{5}\mbox{-}C_{5}H_{5})Mn(CO)_{2}]\cdot THF \\
& \reactrarrow{0pt}{3cm}{\scriptsize K/THF}{\scriptsize [18]crown-6}
[PhSb\{Mn(CO)_{2}(\eta^{5}\mbox{-}C_{5}H_{5})\}_{2}] + 2KI + \cdots \\
& \mbox{and further lines}
\end{split}
\end{ChemEquation}
```

$$\begin{split}
[(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})(\mathrm{CO})_{2}\mathrm{MnSbPhI}_{2}] & + [(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})\mathrm{Mn(CO)}_{2}]\cdot \mathrm{THF} \\
& \xrightarrow[\text{[18]crown-6}]{\text{K/THF}} [\mathrm{PhSb}\{\mathrm{Mn(CO)}_{2}(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})\}_{2}] + 2\mathrm{KI} + \cdots \\
& \text{and further lines}
\end{split} \tag{10.12}$$

where an ampersand is used to mark an alignment point.

Note that the equation number is centered vertically on the height of the split environment. To print the equation number at the end of the display equation, the switching command `\ctagsplit@false` is declared as follows:

```
{\makeatletter
\ctagsplit@false
\begin{ChemEquation}
\begin{split}
 [(\eta^{5}\mbox{-}C_{5}H_{5})(CO)_{2}MnSbPhI_{2}]
& + [(\eta^{5}\mbox{-}C_{5}H_{5})Mn(CO)_{2}]\cdot THF \\
& \reactrarrow{0pt}{3cm}{\scriptsize K/THF}{\scriptsize [18]crown-6}
[PhSb\{Mn(CO)_{2}(\eta^{5}\mbox{-}C_{5}H_{5})\}_{2}] + 2KI + \cdots \\
& \mbox{and further lines}
\end{split}
\end{ChemEquation}
\makeatother
}
```

$$\begin{aligned}
[(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})(\mathrm{CO})_{2}\mathrm{MnSbPhI}_{2}] & + [(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})\mathrm{Mn(CO)}_{2}]\cdot \mathrm{THF} \\
& \xrightarrow[\text{[18]crown-6}]{\text{K/THF}} [\mathrm{PhSb}\{\mathrm{Mn(CO)}_{2}(\eta^{5}\text{-}\mathrm{C}_{5}\mathrm{H}_{5})\}_{2}] + 2\mathrm{KI} + \cdots \\
& \text{and further lines} \qquad (10.13)
\end{aligned}$$

The `chemalign` environment defined by `\newchemenvironment{chemalign}{align}` can be combined with the `split` environment.

```
\begin{chemalign}
\begin{split}
H_{2}O + H_{2}SO_{4} & \equilibarrow  H_{3}O^{+} + HSO_{4}^{-}; \\
& \mathit{K}_{H_{2}O}(25^{\circ}) = \frac{[H_{3}O^{+}][HSO_{4}^{-}]}{[H_{2}O]} \sim 1
\end{split} \\
SO_{3} + H_{2}SO_{4} & \equilibarrow  H_{2}S_{2}O_{7} \\
\begin{split}
H_{2}S_{2}O_{7} + H_{2}SO_{4} & \equilibarrow  H_{3}SO_{4}^{+} + HS_{2}O_{7}^{-}; \\
& \mathit{K}_{H_{2}S_{2}O_{7}}(25^{\circ})
= \frac{[H_{3}SO_{4}^{+}][HS_{2}O_{7}^{-}]}{[H_{2}S_{2}O_{7}]} = 1.4 \times 10^{-2}
\end{split}
\end{chemalign}
```

$$\begin{split} H_2O + H_2SO_4 &\rightleftharpoons H_3O^+ + HSO_4^-; \\ &K_{H_2O}(25^\circ) = \frac{[H_3O^+][HSO_4^-]}{[H_2O]} \sim 1 \end{split} \tag{10.14}$$

$$SO_3 + H_2SO_4 \rightleftharpoons H_2S_2O_7 \tag{10.15}$$

$$\begin{split} H_2S_2O_7 + H_2SO_4 &\rightleftharpoons H_3SO_4^+ + HS_2O_7^-; \\ &K_{H_2S_2O_7}(25^\circ) = \frac{[H_3SO_4^+][HS_2O_7^-]}{[H_2S_2O_7]} = 1.4 \times 10^{-2} \end{split} \tag{10.16}$$

The `chemgather` environment defined above is capable of containing the `split` environment (the amsmath package) and the `chemalign*` environment (defined above) at the same time. The following example exemplifies such a nested specification of chemical equations:

```
\begin{chemgather}
\begin{split}
[Cr(CO)_{6}] & \overset{A}{\llongrightarrow}
\underset{yellow}{[Cr(CO)_{5}(AsPhH_{2})]} \overset{B}{\llongrightarrow} \\
& \underset{orange}{[Cr(CO)_{5}(AsPhLi_{2})]} \overset{C}{\llongrightarrow}
\underset{\text{dark violet}~(mp~104^{\circ})}{[\{Cr(CO)_{5}\}_{2}AsPh]}
\end{split} \\
\begin{chemalign*}
A:\qquad & PhAsH_{2} \\
B:\qquad & LiBu \\
C:\qquad & \text{cyclohexyl-}NCl_{2}
\end{chemalign*}
\end{chemgather}
```

$$\begin{split} [Cr(CO)_6] &\xrightarrow{\text{A}} \underset{\text{yellow}}{[Cr(CO)_5(AsPhH_2)]} \xrightarrow{\text{B}} \\ &\underset{\text{orange}}{[Cr(CO)_5(AsPhLi_2)]} \xrightarrow{\text{C}} \underset{\text{dark violet (mp } 104^\circ)}{[\{Cr(CO)_5\}_2AsPh]} \end{split} \tag{10.17}$$

$$\begin{aligned} A:\qquad & PhAsH_2 \\ B:\qquad & LiBu \\ C:\qquad & \text{cyclohexyl-}NCl_2 \end{aligned}$$

10.2 Objects Placed Over or Under Arrows

10.2.1 Combination of Commands

The command `\overset` of the `amsmath` package is applicable to place an object over an arrow:

```
\begin{ChemEquation}
CCl_{4} + HF \overset{SbFCl_{4}}{\lllongrightarrow}
CFCl_{3} + HCl
\end{ChemEquation}
```

$$\mathrm{CCl_4 + HF \xrightarrow{SbFCl_4} CFCl_3 + HCl} \tag{10.18}$$

The command `\stackrel` of LaTeX 2ε can be also applied to a similar target as follows:

```
\begin{ChemEquation}
CFCl_{3} + HF
\stackrel{SbFCl_{4}}{\lllongrightarrow}
CF_{2}Cl_{2} + HCl
\end{ChemEquation}
```

$$\mathrm{CFCl_3 + HF \xrightarrow{SbFCl_4} CF_2Cl_2 + HCl} \tag{10.19}$$

A nested usage of `\underset` and `\overset` comes out well in placing objects under and over an arrow.

```
\begin{ChemEquation}
Na + Al + 2H_{2}
\underset{350~atom}{\overset{THF/140^{\circ}/3\: h}{\lllongrightarrow}}
NaAlH_{4}\quad (99\%~yield)
\end{ChemEquation}
```

$$\mathrm{Na + Al + 2H_2 \underset{350~atom}{\overset{THF/140^{\circ}/3\: h}{\longrightarrow}} NaAlH_4}\quad (99\%\ \text{yield}) \tag{10.20}$$

Chapter 11

Coloring Substituents and Substitution Bonds

One of main improvements of the XΥMTEX system Version 5.00 (both the PostScript-compatible mode and the PDF-compatible mode) is a newly-developed set of enhanced functions for drawing colored structural formulas. The chapters after this chapter are devoted to explain such enhanced functions for coloring.

11.1 Commands for Colors

Because the PostScript-compatible mode of the XΥMTEX system (called by the xymtexps) is based on the pstricks package, such commands as `\red`, `\green`, and `\blue` are defined to generated colored objects. These commands are not defined in the PDF-compatible mode of the XΥMTEX system (called by the xymtexpdf), because the pgf package used as a graphical tool calls the xcolor package internally as a coloring tool. Instead of these commands, the `\color` command is used in the PDF mode. For example, the code `{\color{red} Red}` generates Red.

For the sake of compatibility, the XΥMTEX system supports a set of control sequences of declaration-type, i.e., `\red`, `\green`, `blue`, `\cyan`, `\magenta`, `\yellow`, `white`, and `\black`, which are differently defined according to a mode selected. Thereby, the codes `{\red Red},{\green Green},and {\blue Blue}` in the PDF-compatible mode generate colored objects such as Red, Green, and Blue in a parallel way to the PostScript-compatible mode.

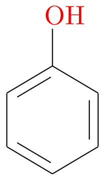
Further, the XΥMTEX system supports another set of control sequences of command-type, i.e., `\redx`, `\greenx`, `bluex`, `\cyanx`, `\magentax`, `\yellowx`, `whitex`, and `\blackx`, which are differently defined according to a mode selected. Thereby, the codes `\redx{Red},\greenx{Green},and \bluex{Blue}` in the PDF-compatible mode as well as in the PostScript-compatible mode generate colored objects such as Red, Green, and Blue.

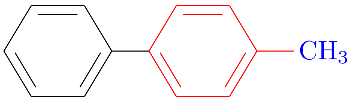
11.2 Coloring Substituents

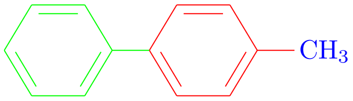
To color a substituent, the substituent is designated in a `SUBSTLIST` (substitution list) by adding an appropriate command of coloring. For example, the codes:

```
\bzdrv{1=={\red OH}}
\bzdrh{4=={\red \bzdrh{1==(yl);4=={\blue CH$_{3}$}}}} \hskip60pt
{\green \bzdrh{4=={\red \bzdrh{1==(yl);4=={\blue CH$_{3}$}}}}}
```

produce the following structures:





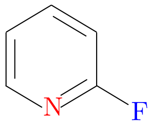


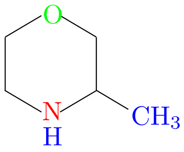
where the phenyl group designated by a (yl) function is regarded as a substituent to be colored.

A hetero atom in a heterocycle can be colored by adding an appropriate command of coloring to the `ATOMLIST` (atom list) of the command for drawing the heterocycle. For example, the codes:

```
\sixheterovi[ace]{1=={\red N}}{2=={\blue F}}
\sixheterovi{1==\downnobond{\red N}{\blue H};4=={\green O}}{2=={\blue CH$_{3}$}}
```

produce the following structures:

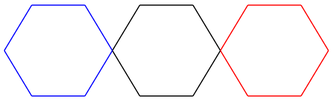




Parts of a spiro ring can be colored by adding appropriate commands of coloring in the `ATOMLIST`. For example, the code:

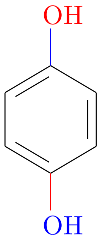
```
\sixheteroh{4s=={\red \sixheteroh{}{1==(yl)}};1s=={\blue \sixheteroh{}{4==(yl)}}}{}
```

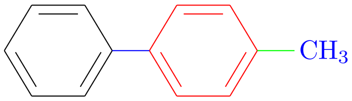
produces the following structure:

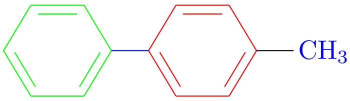


In most cases, the color of a substitution bond can be differentiated from the color of the corresponding substituent by using the `\aftergroup` command of TeX primitive. The formulas drawn above are modified by this technique as follows:

```
\bzdrv{1=={\red\aftergroup\blue OH};4=={\blue\aftergroup\red OH}}
\bzdrh{4=={\red\aftergroup\blue \bzdrh{1==(yl);%
4=={\blue\aftergroup\green CH$_{3}$}}}} \hskip60pt
{\green \bzdrh{4=={\red\aftergroup\blue \bzdrh{1==(yl);%
4=={\blue\aftergroup\black CH$_{3}$}}}}}
```



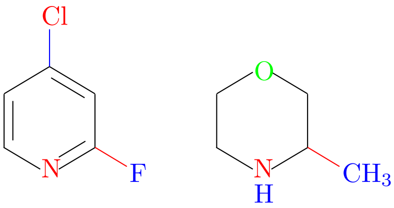




On the same line, we obtain the following printing of structural formulas, where the color of a substitution bond is differentiated from that of the corresponding substituent. The codes:

```
\sixheterovi[ace]{1=={\red N}}{2=={\blue\aftergroup\red F};%
4=={\red\aftergroup\blue Cl}}
\sixheterovi{1==\downnobond{\red N}{\blue H};4=={\green O}}%
{2=={\blue\aftergroup\red CH$_{3}$}}
```

produce the following structures:



Note

The use of `dvipdfmx` in processing the resulting dvi files containing these coloring codes may result in the appearance of a warning:

```
** WARNING ** Color stack underflow. Just ignore.
```

In spite of this warning, we can obtain the correct printing of structural formulas. So we just ignore this warning in the preceding examples.
The warning can be avoided by using control sequences of command type such as `\redx` in place of control sequances of declaration type such as `\red`. Hereafter we will use the former type as far as possible.

11.3 Coloring Substitution Bonds

11.3.1 Systematic Method for Coloring Substitution Bonds

The bondcolor package of the XΥMTEX version 5.00 supports the function of coloring substitution bonds. The command `\addbscolor` is defined to specify the color of a substitution bond. It has a format represented by

```
\addbscolor{COLOR}{SUBSTITUENT}
```

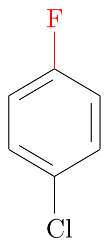
The argument `COLOR` is a command for specifying color (`\red`)[1] and the second argument `SUBSTITUENT` is a text or a set of commands for drawing a substituent. For example, the codes:

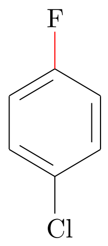
```
\bzdrv{1==\addbscolor{\red}{F};4==Cl}
\bzdrv{1==\addbscolor{\red}{\blackx{F}};4==Cl}
\bzdrv{1==\addbscolor{\red}{\bluex{F}};4==Cl}
\bzdrv{1==\bluex{F};4==Cl}
```

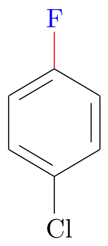
generate the following structural formulas:

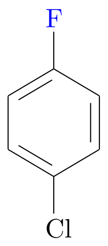
---

[1] This command can be used in the PDF mode (as well as in the PostScript mode), because it has been defined for representing `\color{red}`.









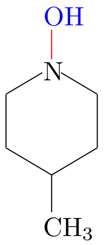
The `\addbscolor` command changes the color of a substitution bond as well as that of a substitution, as shown in the first example. If a substitution bond is desired to be solely changed, `{\black F}` should be declared as the second argument `SUBSTITUENT`, as shown in the second example. The third example shows the separate change of the colors of a substitution bond and a substituent.

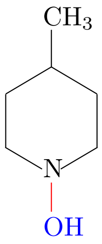
11.3.2 Examples

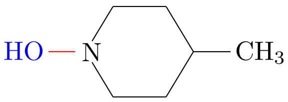
Other commands defined by the carom package are also colored by the systematic methods. More low-level commands defined by the hetarom and hetaromh packages can be colored similarly. For example, a six-membered hydroxylamine is drawn in different ways by the codes:

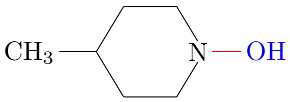
```
\sixheterov{1==N}{1==\addbscolor{\red}{\bluex{OH}};4==CH$_{3}$} \qquad
\sixheterovi{1==N}{1==\addbscolor{\red}{\bluex{OH}};4==CH$_{3}$} \qquad
\sixheteroh{1==N}{1==\addbscolor{\red}{\bluex{HO}};4==CH$_{3}$} \qquad\qquad
\sixheterohi{1==N}{1==\addbscolor{\red}{\bluex{OH}};4==CH$_{3}$}
```

which generate the following structures:



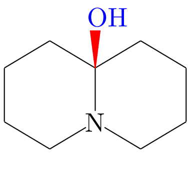


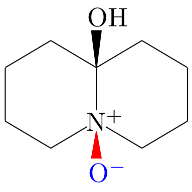


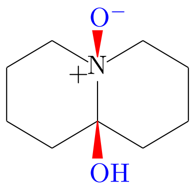


Substitution bonds in fused rings can be colored by the systematic method as follows:

```
\decaheterov{9==N}{{10}B==\addbscolor{\red}{\bluex{OH}}}
\decaheterov{9==N\rlap{$^{+}$}}{9B==\addbscolor{\red}{\bluex{O$^{-}$}};{10}B==OH}
\decaheterov[{{10}+}]{{{10}}==N}{9B==\addbscolor{\red}{\bluex{OH}};
{10}B==\addbscolor{\red}{\bluex{O{\normalsize $^{-}$}}}}
```

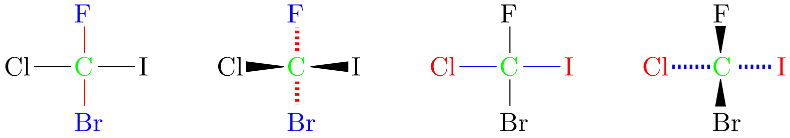






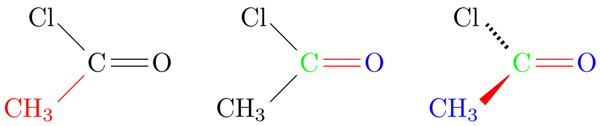
Commands defined by the aliphat package are also colored by the systematic methods. The following examples illustrate colored structural formulas produced by using the `\addbscolor` command variously in the `\tetrahedral` command.

```
\tetrahedral{0==\greenx{C};
1==\addbscolor{\red}{\bluex{F}};%
2==Cl;3==\addbscolor{\red}{\bluex{Br}};4==I} \qquad
\tetrahedral{0==\greenx{C};
1A==\addbscolor{\red}{\bluex{F}};%
2B==Cl;3A==\addbscolor{\red}{\bluex{Br}};4B==I} \qquad
\tetrahedral{0==\greenx{C};1==F;%
2==\addbscolor{\blue}{\redx{Cl}};
3==Br;4==\addbscolor{\blue}{\redx{I}}} \qquad
\tetrahedral{0==\greenx{C};1B==F;%
2A==\addbscolor{\blue}{\redx{Cl}};
3B==Br;4A==\addbscolor{\blue}{\redx{I}}}
```



The following examples show colored structures produced by using the `\addbscolor` command in the `\ltrigonal` command.

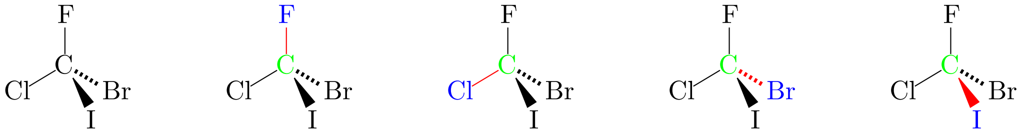
```
\ltrigonal{0==C;1D==O;2==Cl;3==\addbscolor{\red}{CH$_{3}$}}\qquad
\ltrigonal{0==\greenx{C};1D==\addbscolor{\red}{\bluex{O}};2==Cl;3==CH$_{3}$}\qquad
\ltrigonal{0==\greenx{C};1D==\addbscolor{\red}{\bluex{O}};2A==Cl;%
3B==\addbscolor{\red}{\bluex{CH$_{3}$}}}
```



Wedged and dashed bonds for stereochemistry can be colored by the systematic way. For example, the codes:

```
\DtetrahedralS{0==C;1==F;
2==Cl;3A==Br;4B==I} \qquad
\DtetrahedralS{0==\green{C};
1==\addbscolor{\red}{\bluex{F}};
2==Cl;3A==Br;4B==I} \qquad
\DtetrahedralS{0==\greenx{C};1==F;
2==\addbscolor{\red}{\bluex{Cl}};3A==Br;4B==I} \qquad
\DtetrahedralS{0==\greenx{C};1==F;
2==Cl;3A==\addbscolor{\red}{\bluex{Br}};4B==I} \qquad
\DtetrahedralS{0==\greenx{C};1==F;
2==Cl;3A==Br;4B==\addbscolor{\red}{\bluex{I}}}
```

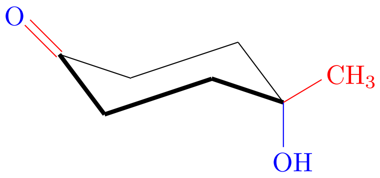
produce the following colored structures:

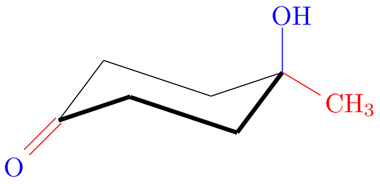


The commands `\chair` and `\chairi` defined in the ccycle package of the XΥMTEX system have been modified to support a systematic method of coloring substitution bonds. For example, the following codes:

```
\chair{1D==\addbscolor{\red}{\bluex{O}};%
4Se==\addbscolor{\red}{CH$_{3}$};4Sa==\addbscolor{\blue}{OH}}\qquad
\chairi{1D==\addbscolor{\red}{\bluex{O}};%
4Se==\addbscolor{\red}{CH$_{3}$};4Sa==\addbscolor{\blue}{OH}}
```

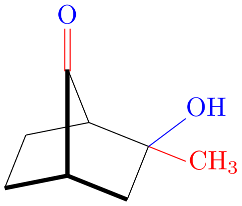
produce colored structural formulas:

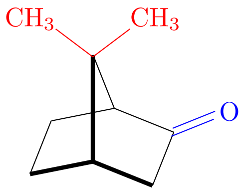




The command `\bornane` defined in the ccycle package of the XΥMTEX system has been also modified to support a systematic method of coloring substitution bonds.

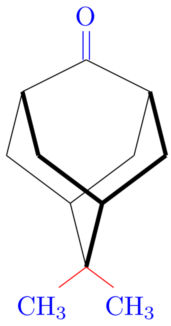
```
\bornane{7D==\addbscolor{\red}{\bluex{O}};%
2Sa==\addbscolor{\red}{CH$_{3}$};2Sb==\addbscolor{\blue}{OH}}\qquad
\bornane{7Sa==\addbscolor{\red}{CH$_{3}$};7Sb==\addbscolor{\red}{CH$_{3}$};%
2D==\addbscolor{\blue}{O}}
```

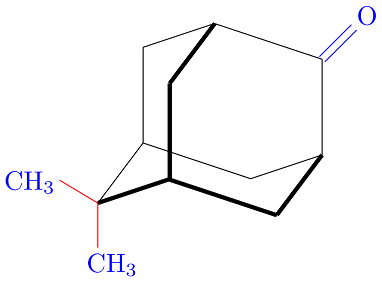




The following examples show the coloring of substitution bonds by using the `\addbscolor` command in the arguments of the commands `\adamantane` and `\hadamantane`, the definitions of which have been modified in the ccycle package of the XΥMTEX system for the purpose of supporting a systematic mechanism of coloring.

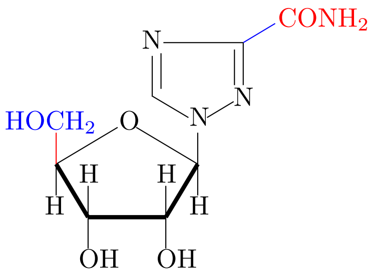
```
\adamantane{2D==\addbscolor{\blue}{O};%
6a==\addbscolor{\red}{\bluex{CH$_{3}$}};6b==\addbscolor{\red}{\bluex{CH$_{3}$}}} \qquad
\hadamantane{2D==\addbscolor{\blue}{O};%
6a==\addbscolor{\red}{\bluex{CH$_{3}$}};6b==\addbscolor{\red}{\bluex{CH$_{3}$}}}
```





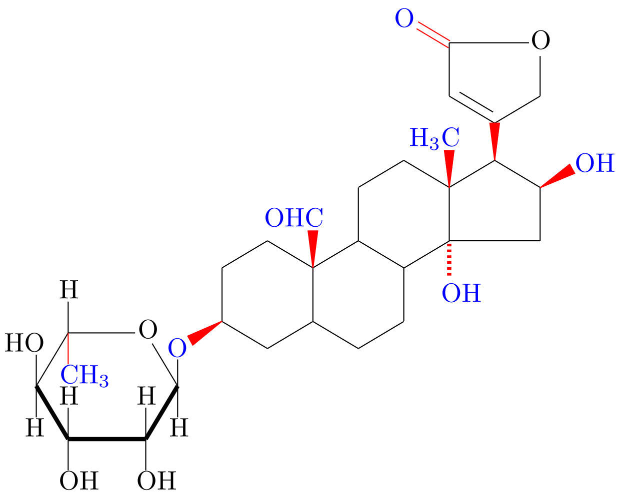
Substitution bonds in a furanose derivative drawn by the command `\furanose` (defined in the hcycle package of the XΥMTEX system) can be colored by using the `\addbscolor` command. By applying the method to the example shown in Subsection 5.1.1, substitution bonds in the structural formula of ribavirin can be colored, as found in the following result:

```
\begin{XyMcompd}(1200,1000)(100,0){}{}
\furanose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;%
4Sb==\addbscolor{\red}{\bluex{HOC\rlap{H$_{2}$}}};
1Sb==\fiveheterov[bd]{1==N;2==N;4==N}{1==(yl);
3==\addbscolor{\blue}{\redx{CONH$_{2}$}}}}
\end{XyMcompd}
```



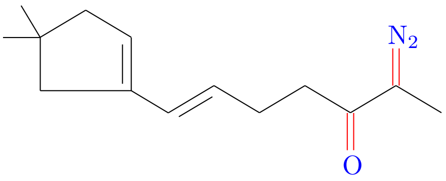
The command `\pyranose` defined in the hcycle package of the XΥMTEX system has been modified to support a systematic method of coloring substitution bonds. The following example shows the use of `\black` in the second argument of the `\addbscolor` command in order to avoid the coloring of a furan skeleton due to `\fiveheterov` and to avoid the coloring of a pyranose skeleton due to `\pyranose`. Note that the furan skeleton and the pyranose skeleton are regarded as substituents of the steroid skeleton in the following code:

```
\begin{XyMcompd}(2100,1800)(-500,-280){}{}
\steroid{{10}B==\addbscolor{\red}{\bluex{\lmoiety{OHC}}};%
{14}A==\addbscolor{\red}{\bluex{OH}};%
{13}B==\addbscolor{\red}{\bluex{\lmoiety{H$_{3}$C}}};%
{16}B==\addbscolor{\red}{\bluex{OH}};%
{17}B==\addbscolor{\red}{\blackx{%
\fiveheterov[e]{3==O}{4D==\addbscolor{\red}{\bluex{O}};1==(yl)}}};%
3B==\addbscolor{\red}{\blackx{\lyl(3==\bluex{O}){8==%
\pyranose{1Sb==(yl);1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==\addbscolor{\red}{\bluex{CH$_{3}$}}}}}}}
\end{XyMcompd}
```



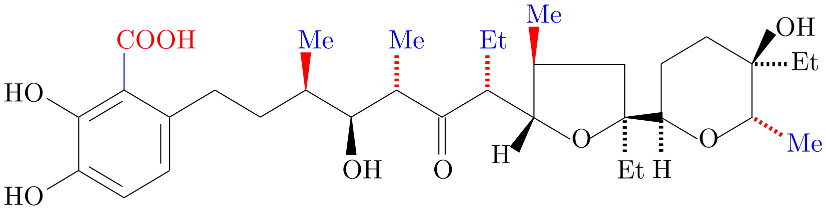
Substitution bonds of polymethylene units defined in the methylene package are now capable of being colored by means of the `\addbscolor` command. The following structure is drawn by this technique applied to the command `\heptamethylene`.

```
\heptamethylene[a]{}{1W==\cyclopentanevi[b]{3==(yl);5Sa==\null;5Sb==\null};%
5D==\addbscolor{\red}{\bluex{O}};6D==\addbscolor{\red}{\bluex{N$_{2}$}}}
```



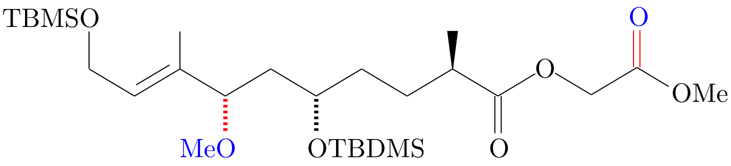
On a similar line, this technique applied to the command `\nonamethylene` draws the following structure with colored bonds and substituents.

```
\nonamethylene{%
1s==\bzdrv{1==\addbscolor{\blue}{\redx{COOH}};2==(yl);5==HO;6==HO};%
9s==\fiveheterov{1==O}{5==(yl);5SB==H;%
4GB==\addbscolor{\red}{\bluex{Me}};2GA==Et;%
2Su==\sixheterovi{1==O}{6==(yl);6FA==H;3SB==OH;3SA==Et;%
2A==\addbscolor{\red}{\bluex{Me}}}}}%
{4B==\addbscolor{\red}{\bluex{Me}};5B==OH;%
6A==\addbscolor{\red}{\bluex{Me}};7D==O;8A==\addbscolor{\red}{\bluex{Et}}}
```



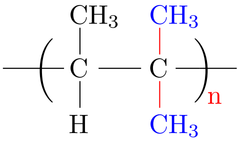
Further, the following structure is drawn by applying this technique to the `\decamethylenei` command.

```
\decamethylenei[b]{}{1==\lmoiety{TBMSO};3==\null;%
4A==\addbscolor{\red}{\bluex{\lmoiety{MeO}}};6A==OTBDMS;%
9B==\null;{10}D==O;%
{10}W==\trimethylenei{1==O}{1==(yl);%
3D==\addbscolor{\red}{\bluex{O}};3W==OMe}}
```



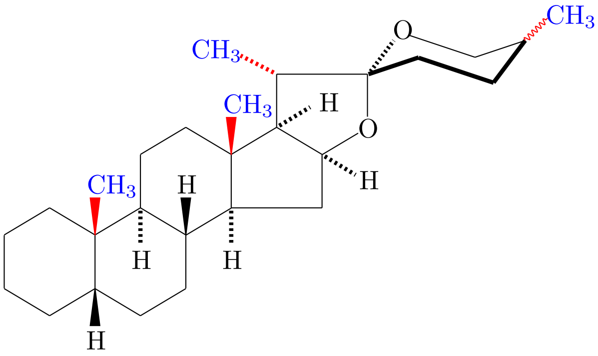
The command `\polyethylene` defined in the polymers package has been also modified to support this technique of bond coloring, as shown in the following example:

```
\polyethylene{1==C;2==C}%
{1==CH$_{3}$;2==;3==H;4==\addbscolor{\red}{\bluex{CH$_{3}$}};%
5==;6==\addbscolor{\red}{\bluex{CH$_{3}$}};0=={\redx{n}}}
```



Substitution bonds in a spiro pyranose ring due to `\pyranoseChairi` (defined in the steroid package) as well as in a fused furan ring due to `\fivefusev` are now capable of being colored by means of the `\addbscolor` command, as found in the following example. Note that the bond coloring technique applied to these commands works well even when these are designated as a fusing unit or a more-nested spiro unit in the `BONDLIST` (bond list) argument of the command `steroid`.

```
\begin{XyMcompd}(2200,1350)(200,150){}{}
\steroid[%
{s{\fivefusev{2==O;%
3s==\mbox{\changeunitlength{0.07pt}%
\pyranoseChairi{1==(yl);%
4U==\addbscolor{\red}{\bluex{\normalsize CH$_{3}$}}}}}%
{4A==\addbscolor{\red}{\bluex{CH$_{3}$}}}{e}%
}}]{5B==H;{10}B==\addbscolor{\red}{\bluex{CH$_{3}$}};
8B==H;9A==H;{13}B==\addbscolor{\red}{\bluex{CH$_{3}$}};
{14}A==H;{17}GA==H;{16}GA==H}
\end{XyMcompd}
```

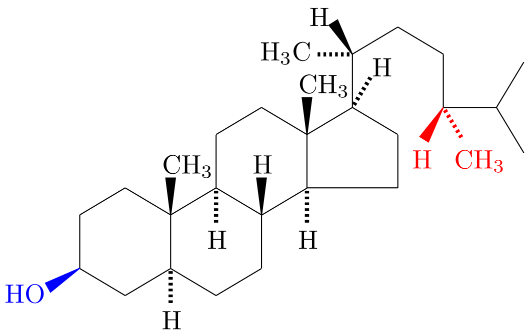


It should be emphasized that wedged bonds, dashed bold bonds, and wavy bonds for stereochemistry are colored by the same technique of bond coloring due to the `\addbscolor` command.

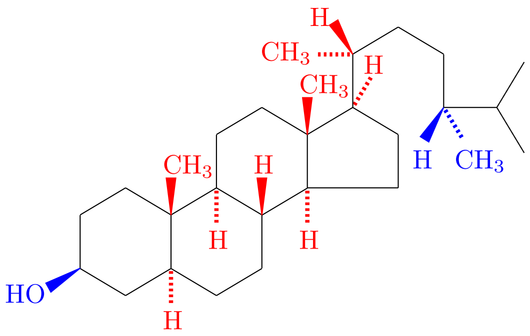
Commands of high level have a fixed set of substituents, which are not changed by the systematic method described here. For the purpose of coloring the fixed set, you should use the corresponding commands of low level. For example, the high-level command `\cholestanealpha` is compared with the low-level command `\steroidchain` as follows:

```
\begin{tabular}{ll}
high-level macro: & low-level macro: \\
\cholestanealpha{3B==\addbscolor{\blue}{HO};
{24}SA==\addbscolor{\red}{CH$_{3}$};{24}SB==\addbscolor{\red}{H}}
&
\steroidchain{3B==\addbscolor{\blue}{HO};
{24}SA==\addbscolor{\blue}{CH$_{3}$};{24}SB==\addbscolor{\blue}{H};
5A==\addbscolor{\red}{H};
8B==\addbscolor{\red}{H};
9A==\addbscolor{\red}{H};
{10}B==\addbscolor{\red}{CH$_{3}$};
{13}B==\addbscolor{\red}{CH$_{3}$};
{14}A==\addbscolor{\red}{H};
{17}SA==\addbscolor{\red}{\raisebox{-3pt}{H}};
{20}SA==\addbscolor{\red}{CH$_{3}$};{20}SB==\addbscolor{\red}{H}}
\\
\end{tabular}
```

high-level macro:



low-level macro



Note that the black bonds in the left structure (or the red bonds in the right structure) indicate the fixed set of substituents for the `\cholestanealpha` command of high level.

11.3.3 Switches for Coloring Substitution Bonds

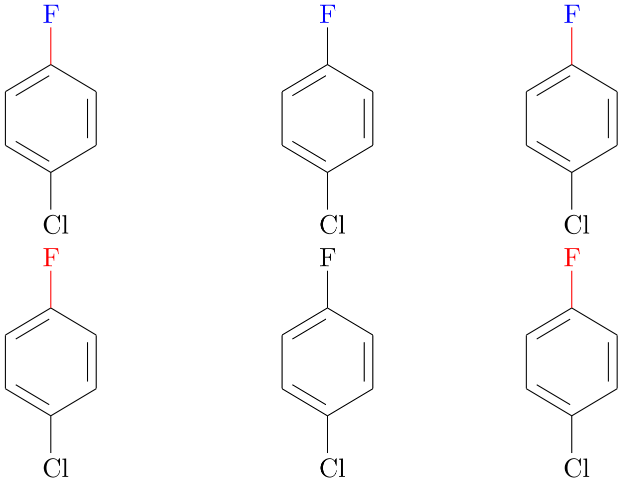
The mechanism for coloring substitution bonds relies on a one-by-one procedure of testing whether or not the designation of each substituent contains the `\addbscolor` command. Because this mechanism works even if the `\addbscolor` command is not contained, there are accidental cases which require prolonged processing times. In particular, multiple nesting of substituents causes such prolongation, as exemplified in the structure shown in Page 29.[2] For the purpose of skipping such prolonged bond coloring, the switch `\bscolorswOFF` is defined. The switch `\bscolorswON` is ready to return to the default mode of coloring.

---

[2] In fact, the deletion of the `\bscolorswOFF` in the example of Page 29 results in such prolonged processing.

```
\begin{tabular}{ccc}
default (\verb/\bscolorswON/) & \verb/\bscolorswOFF/ & \verb/\bscolorswON/ \\
\bzdrv{1==\addbscolor{\red}{\bluex{F}};4==Cl} &
\bscolorswOFF \bzdrv{1==\addbscolor{\red}{\bluex{F}};4==Cl} &
\bscolorswON \bzdrv{1==\addbscolor{\red}{\bluex{F}};4==Cl} \\
\bzdrv{1==\addbscolor{\red}{F};4==Cl} &
\bscolorswOFF \bzdrv{1==\addbscolor{\red}{F};4==Cl} &
\bscolorswON \bzdrv{1==\addbscolor{\red}{F};4==Cl} \\
\end{tabular}
```

default (`\bscolorswON`) `\bscolorswOFF` `\bscolorswON`



It should be noted that the designation of each colored substituent (`{\blue F}`) shown in the first row of structures results in the same effect during such switching of coloring.

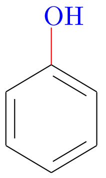
11.4 Dirty Techniques for Coloring Substitution Bonds

If no systematic routes to color substitution bonds have been defined with respect to your target command for drawing structures, rather dirty (but versatile) techniques should be tested case by case. For example, the `\PutBondLine` command is used to place a substitution bond (Page 23), which is colored by adding an appropriate command of coloring.

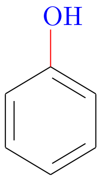
For the simplicity of explanation about such dirty techniques, let us use again the examples described above for the systematic technique. For example, the codes:

```
\sixheterov[ace]{1s==\redx{\PutBondLine(0,0)(0,140){\thinLineWidth}};%
1s==\bluex{\put(-30,150){OH}}}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov[ace]{}{1==\addbscolor{\red}{\bluex{OH}}}
```

generate the following structures:



Compare with

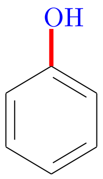


where the `ATOMLIST` (atom list) is used in place of the `SUBSLIST` (substituent list) in order to place the substitution bond at position 1. Compare the left formula with the right formula drawn by the systematic method of bond coloring.

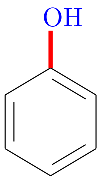
By replacing `\thinLineWidth` by `\thickLineWidth` in the last argument of `\PutBondLine`, the substitution bond appears as a bold-line bond. The same effect can be brought about locally by the first argument `{\red\dashhasheddash\thicklines}` of the `\addbscolor` command. Compare between the codes:

```
\sixheterov[ace]{1s==\redx{\PutBondLine(0,0)(0,140){\thickLineWidth}};%
1s==\bluex{\put(-30,150){OH}}}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov[ace]{}{1==\addbscolor{\red
\dashhasheddash
\thicklines}{\bluex{OH}}}
```

which generate the following structures:



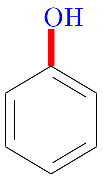
Compare with



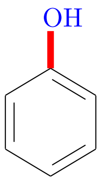
It should be pointed out again that the last argument of `\PutBondLine` is capable of accommodating a direct designation of a bond width, as found in the following example (left). Note that `\thinLineWidth` is equal to 0.4pt and `\thickLineWidth` is equal to 1.6pt.

The following example (left) shows a thicker substitution bond (2.5pt), which is given directly to the last argument of `\PutBondLine`. The same effect is accomplished by designating the first argument of `\addbscolor` as being `{\red\dashhasheddash \def\thickLineWidth{2.5pt} \thicklines}`, as shown in the right example.

```
\sixheterov[ace]{1s=={\red \PutBondLine(0,0)(0,140){2.5pt}};%
1s=={\blue \put(-30,150){OH}}}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov[ace]{}{1==\addbscolor{\red
\dashhasheddash\def\thickLineWidth{2.5pt}%
\thicklines}{\bluex{OH}}}
```



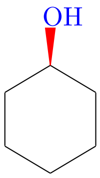
Compare with



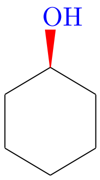
The `\WedgeAsSubst` command is used to draw a substitution bond of wedge type (Page 23), which is colored by adding an appropriate command of coloring. The systematic way of bond coloring supports this case as a standard usage. The codes:

```
\sixheterov{1s==\redx{\WedgeAsSubst(0,0)(0,1){140}};%
1s==\bluex{\put(-30,150){OH}}}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov{}{1B==\addbscolor{\red}{\bluex{OH}}}
```

generate the following structures:



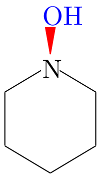
Compare with



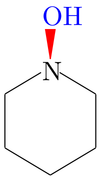
A nitrogen atom at position 1 can be typeset by placing the designation `1==N` in the `ATOMLIST` (atom list) after setting up the substitution bond and the substituent. This position of the designation is important to restore a flag of truncation at the position 1, as shown in the following code:

```
\sixheterov{1s==\redx{\WedgeAsSubst(0,40)(0,1){100}};%
1s==\bluex{\put(-30,150){OH}};1==N}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov{1==N}{1B==\addbscolor{\red}{\bluex{OH}}}
```

The code and a comparison code of a systematic way generate the following structures:

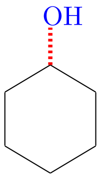


Compare with

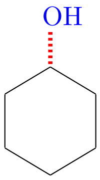


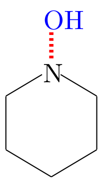
The `\PutDashedBond` command (Page 26) is used to draw a dashed bond, as found in the following examples:

```
\sixheterov{1s==\redx{\PutDashedBond(0,0)(0,140){\thickLineWidth}};%
1s==\bluex{\put(-30,150){OH}}}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov{}{1A==\addbscolor{\red}{\bluex{OH}}} \par
\sixheterov{1s==\redx{\PutDashedBond(0,40)(0,140){\thickLineWidth}};%
1s=={\blue \put(-30,150){OH}};1==N}{}
\qquad \raisebox{45pt}{Compare with}
\sixheterov{1==N}{1A==\addbscolor{\red}{\bluex{OH}}}
```

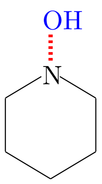


Compare with





Compare with



11.5 Substitution Bonds of Unnatural Directions

Usual substitution bonds drawn by the XΥMTEX system have natural directions intrinsic to the attached positions of a skeleton. In some cases, however, substitution bonds of unnatural directions are necessary to draw special structural formulas. To do this task along with bond coloring, the commands `\RightAtomBond` and `\LeftAtomBond` are defined in the `bondcolor` package.

11.5.1 Commands for Use of Atom Lists

The `\RightAtomBond` Command

The macro `\RightAtomBond` is defined to color substitution bonds (and substituents), when it is to be designated in an `ATOMLIST` (atom list) or in a `BONDLIST` (bond list) of a command for drawing a structural formula.

```
\RightAtomBond(x,y)[COLOR]<CLIPPING>{SUBSTLIST}
```

The first optional argument `(x,y)` is a set of increments of xy-coordinates, if some adjustment is necessary when a spiro function (`1s==...`) is not supported. The default value is `(0,0)`. The second optional argument `[COLOR]` is a command of coloring (e.g., `\red`). The default value is `\black`. The third optional argument `<CLIPPING>` accommodates `<s>` for non-clipping; and a vacant or omitted argument represents a clipping (truncation) of a corner. The default value is a vacant value. The fourth argument is a `SUBSLIST` (substituent list), in which a substitution number 1–8 represents a bond slope to be drawn. Slopes to cover a right-handed half circle are numbered on a similar line to those of the `\ryl` macro, as follows:

```
SLOPE

  0       : (0,1)
  1       : (3,5)
  2       : (1,1)
  3       : (5,3)
  4       : (1,0)
  5       : (5,-3)
  6       : (1,-1)
  7       : (3,-5)
  8       : (0,-1)
```

As for the format of the `SUBSLIST`, see the specification of the `\ryl` command (Chapter 4 of xymtx200.pdf [6]). When the number of a slope (n) and a bond specifier (M) are to be considered, designations in the `SUBSLIST` are given as being `nM==...` etc. For example, the designation `0B==Cl` for drawing a bond and a substituent corresponds to a slope 0 (`(0,1)`), a bond specifier B (β bond) and a substituent Cl (a chlorine atom). Figure 11.1 shows directions of substitution bonds drawn by `\RightAtomBond`, where each number corresponds to the direction listed above.

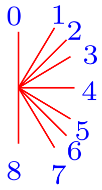
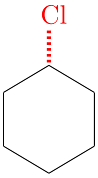


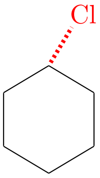
Figure 11.1: Directions of substitution bonds drawn by `\RightAtomBond`

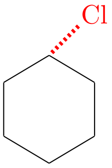
Natural and unnatural directions of substitution bonds depend on respective substitution positions of a skeleton. For example, the top position (position 1) of a six-membered ring drawn by the `\sixheterov` command is substituted by a bond (a dashed bond) due to a `\RightAtomBond` command, whose ATOMLIST (`0A==Cl` etc.) indicates a direction selected as being 1 to 8.

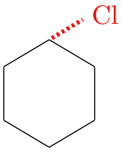
```
\textbf{Bonds of natural directions}: \\[10pt]
\sixheterov{1s==\RightAtomBond[\red]{0A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{1A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{2A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{3A==Cl}}{} \par
\textbf{Bonds of unnatural directions}: \\
\sixheterov{1s==\RightAtomBond[\red]{4A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{5A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{6A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{7A==Cl}}{}
\sixheterov{1s==\RightAtomBond[\red]{8A==Cl}}{}
```

Bonds of natural directions:

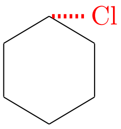


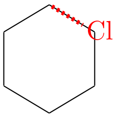


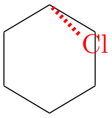


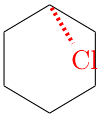


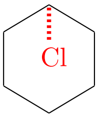
Bonds of unnatural directions:









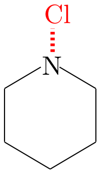


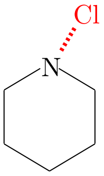
The four structures in the first row show natural directions, while the five structures in the second row show unnatural directions, because the latter five contain a bond situated within the domain of the six-membered ring.

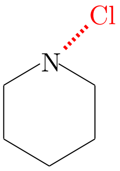
The following examples shows the placement of a nitrogen atom on the position 1 and the substitution due to `\RightAtomBond`, where the designation `1s==` is replaced by `1==N;1==` in the ATOMLIST of each `\sixheterov` command. Thereby, a clipping mechanism at the position 1 is realized.

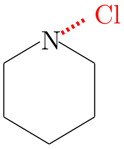
```
\textbf{Bonds of natural directions}: \\[10pt]
\sixheterov{1==N;1==\RightAtomBond[\red]{0A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{1A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{2A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{3A==Cl}}{} \par
\textbf{Bonds of unnatural directions}: \\
\sixheterov{1==N;1==\RightAtomBond[\red]{4A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{5A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{6A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{7A==Cl}}{}
\sixheterov{1==N;1==\RightAtomBond[\red]{8A==Cl}}{}
```

Bonds of natural directions:

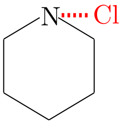


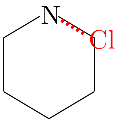


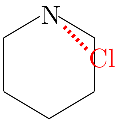


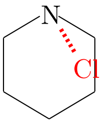


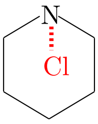
Bonds of unnatural directions:







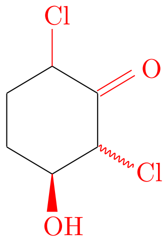


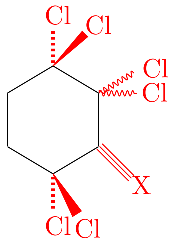


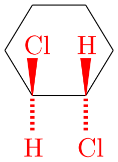
The SUBSTLIST of the `\RightAtomBond` command has a similar format to the SUBSTLIST of commands for drawing structural formulas, where bond specifiers such as `A` (α-bonds), `B` (β-bonds), `U` (wavy bonds), `D` (exocyclic double bonds), and `T` (exocyclic triple bonds) can be declared. Random use of these bond specifiers is illustrated in the following examples:

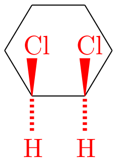
```
\sixheterov{%
1s==\RightAtomBond[\red]{0==Cl};%
2s==\RightAtomBond[\red]{3D==O};%
3s==\RightAtomBond[\red]{5U==Cl};%
4s==\RightAtomBond[\red]{8B==OH};%
}{}
\sixheterov{%
1s==\RightAtomBond[\red]{0A==Cl;2B==Cl};%
2s==\RightAtomBond[\red]{3U==Cl;4U==Cl};%
3s==\RightAtomBond[\red]{6T==X};%
4s==\RightAtomBond[\red]{7B==Cl;8A==Cl};%
}{}
\sixheteroh{%
5s==\RightAtomBond[\red]{0B==H;8A==Cl};%
6s==\RightAtomBond[\red]{0B==Cl;8A==H}%
}{}
\sixheteroh{%
```

```
5s==\RightAtomBond[\red]{0B==Cl;8A==H};%
6s==\RightAtomBond[\red]{0B==Cl;8A==H}%
}{}
```









The `\LeftAtomBond` Command

On a similar way, the macro `\LeftAtomBond` is defined to color substitution bonds (and substituents) in a left-handed half circle. The macro is to be designated in a `ATOMLIST` or in a `BONDLIST` of a command for drawing a structural formula. The format of specifying arguments for `\LeftAtomBond` is parallel to that of the `\RightAtomBond` command, as shown in the following scheme:

```
\LeftAtomBond(x,y)[COLOR]<CLIPPING>{SUBSTLIST}
```

The first optional argument `(x,y)`, the first optional argument `[COLOR]`, and the third optional argument `<CLIPPING>` are parallel to those of `\RightAtomBond`. The fourth argument is a `SUBSLIST`, in which a substitution number 1–8 represents a bond slope to be drawn. Slopes to cover a left-handed half circle are numbered on a similar line to those of the `\lyl` macro, as follows:

```
SLOPE

 0     : (0,1)
 1     : (-3,5)
 2     : (-1,1)
 3     : (-5,3)
 4     : (-1,0)
 5     : (-5,-3)
 6     : (-1,-1)
 7     : (-3,-5)
 8     : (-0,-1)
```

As for the format of the `SUBSLIST`, see the specification of the `\lyl` command (Chapter 4 of xymtx200.pdf [6]). Figure 11.2 shows directions of substitution bonds drawn by `\LightAtomBond`, where each number corresponds to the direction listed above.

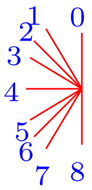
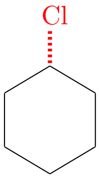


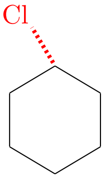
Figure 11.2: Directions of substitution bonds drawn by `\LeftAtomBond`

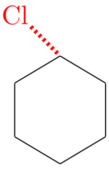
The following examples show natural and unnatural directions of substitution bonds, where modes of depending on respective substitution positions of a skeleton are illustrated by using the `\LeftAtomBond` command.

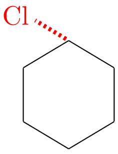
```
\textbf{Bonds of natural directions}: \\[10pt]
\sixheterov{1s==\LeftAtomBond[\red]{0A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{1A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{2A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{3A==Cl}}{}\par
\textbf{Bonds of unnatural directions}: \\
\sixheterov{1s==\LeftAtomBond[\red]{4A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{5A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{6A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{7A==Cl}}{}
\sixheterov{1s==\LeftAtomBond[\red]{8A==Cl}}{}
```

Bonds of natural directions:

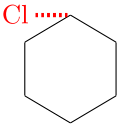


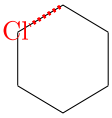


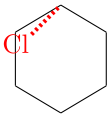


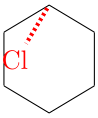


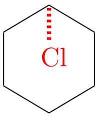
Bonds of unnatural directions:







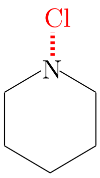


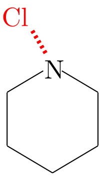


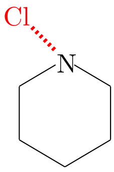
The `\LeftAtomBond` command supports a function for permitting the placement of a hetero atom (e.g., a nitrogen atom) at the substitution position (e.g., the position 1), where the designation `1s==` is replaced by `1==N;1==` in the ATOMLIST of each `\sixheterov` command.

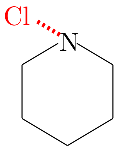
```
\textbf{Bonds of natural directions}: \\[10pt]
\sixheterov{1==N;1==\LeftAtomBond[\red]{0A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{1A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{2A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{3A==Cl}}{} \par
\textbf{Bonds of unnatural directions}: \\
\sixheterov{1==N;1==\LeftAtomBond[\red]{4A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{5A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{6A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{7A==Cl}}{}
\sixheterov{1==N;1==\LeftAtomBond[\red]{8A==Cl}}{}
```

Bonds of natural directions:

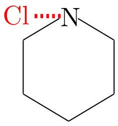


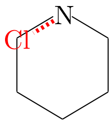


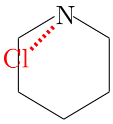


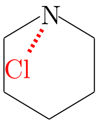


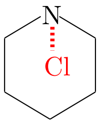
Bonds of unnatural directions:







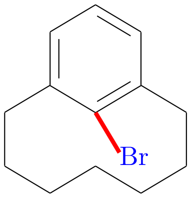


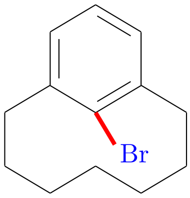


Unnatural Directions of Substitution Bonds

13-Bromo-(2,6)metacyclophane (cf. Section 13.4 of the on-line document of XΥMTEX version 1.01 (xymtex.pdf)) is printed by the following code, where the `\RightAtomBond` command is used to draw a bromine substituent.

```
\sixheterov[ace%
{c{\sixfusev{}{}{F}[ef]}}%
{d{\sixfusev{}{}{A}[ab]}}%
]{4s==\RightAtomBond[\red\def\thinLineWidth{1.6pt}]%
{7==\kern0.1em\raise1ex\hbox{\blue Br}}}{}
\sixheterov[ace%
{c{\sixfusev{}{}{F}[ef]}}%
{d{\sixfusev{}{}{A}[ab]}}%
]{}{4Sa==\addbscolor{\red\def\thinLineWidth{1.6pt}}%
{\kern.5em\raise1ex\hbox{\blue Br}}}
```

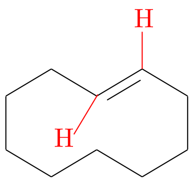


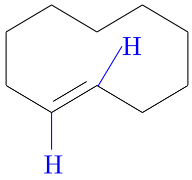


This case can be drawn as a natural direction as shown in the right structure, where the bromine substituent is regarded as a substituent of the benzene ring.

Unnatural directions of substitution bonds are illustrated by *trans*-cyclododecene, where structures of different positions of double bonds are drawn as follows by using `\RightAtomBond` and `\LeftAtomBond`.

```
\decaheterov[j]{%
{10}s==\LeftAtomBond(-32,30)[\red]{7==\raise1ex\hbox{H}\kern0.1em}}%
{1==\addbscolor{\red}{H}}[k]
\decaheterov[e]{%
9s==\RightAtomBond(-32,35)[\blue]{1==\kern0.1em\lower1ex\hbox{H}}}%
{5==\addbscolor{\blue}{H}}[k]
```

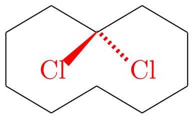


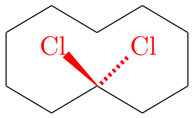


These formulas are drawn by using `\decaheterov`, where each central bond is erased by using the optional argument `[k]` placed at the end of the command. Because the spiro mechanism of the XΥMTEX system is not supported for the bridgehead positions of `\decaheterov`,[3] the optional argument `(x,y)` should be used to adjust the joint positions of substitution bonds. The values of `(x,y)` are decided in a trial-and-error fashion.

Further examples for illustrating unnatural directions of substitution bonds are shown as follows:

```
\decaheterov{%
{10}s==\RightAtomBond(-32,30)[\red]{6A==Cl};%
{10}s==\LeftAtomBond(-32,30)[\red]{6B==Cl}}{}[k]
\decaheterov{%
9s==\RightAtomBond(-32,35)[\red]{2A==Cl};%
9s==\LeftAtomBond(-32,35)[\red]{2B==Cl}}{}[k]
```





Because these formulas are drawn by using `\decaheterov`, similar situations to *trans*-cyclododecene hold true for these cases, so that the optional argument `(x,y)` is inserted to adjust the joint positions of substitution bonds.

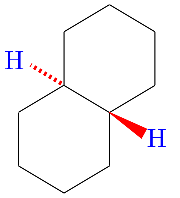
Further additional examples for illustrating natural and unnatural directions of substitution bonds are shown by using `\decaheterovt`:

```
\begin{center}
\begin{tabular}{cc}
Natural directions & Unnatural directions \\[10pt]
\decaheterovt{}{9B==\addbscolor{\red}{\bluex{H}};%
{10}A==\addbscolor{\red}{\bluex{H}}}
&
\decaheterovt{9s==\RightAtomBond(35,29)[\red]{0B==\bluex{H}};%
{10}s==\RightAtomBond(-31,48)[\red]{8A==\bluex{H}}}{} \\
\end{tabular}
\end{center}
```

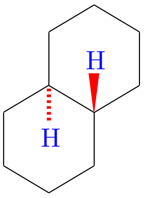
---

[3] In spite of no support of the spiro mechanism, the specifier `s` of the designation `9s==` or `{10}s==` is necessary to assure the correct behavior of the `\RightAtomBond` or `\LeftAtomBond` command.

Natural directions



Unnatural directions

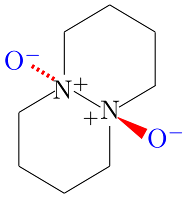


The `\decaheterovt` command takes the same format as `\decaheterov`. Hence, similar situations described above hold true for these cases, so that the optional argument `(x,y)` is inserted to adjust the joint positions of substitution bonds.

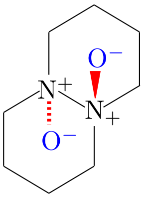
Hetero atoms and substitution bonds at the bridgehead positions of `\decaheterovt` are illustrated in the following examples:

```
\begin{center}
\begin{tabular}{cc}
Natural directions & Unnatural directions \\[10pt]
\decaheterovt{9==\llap{$_{+}$}N;{{10}}==N\rlap{$^{+}$}}
{9B==\addbscolor{\red}{\bluex{O$^{-}$}};%
{10}A==\addbscolor{\red}{\bluex{O\rlap{$^{-}$}}}}
&
\decaheterovt{9==N\rlap{$_{+}$};%
9==\RightAtomBond[\red]{0B==\bluex{O$^{-}$}};%
{{10}}==N\rlap{$^{+}$};%
{{10}}==\RightAtomBond(-70,0)[\red]{8A==\bluex{O$^{-}$}}}{} \\
\end{tabular}
\end{center}
```

Natural directions



Unnatural directions



11.5.2 Commands for Use of Bond Lists

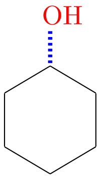
The `\RightAtomBond` and `\LeftAtomBond` Commands in Bond Lists

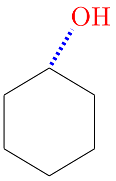
The commands `\RightAtomBond` and `\LeftAtomBond` described above are also capable of being declared in the `BONDLIST`. Hence, they are effective to commands which do not support the `ATOMLIST`.

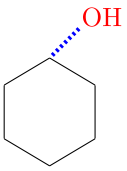
Examples shown in Page 89 (in `ATOMLIST`) can be obtained by the present method using `BONDLIST`, where the optional argument `<s>` is used to assure correct behaviors of the command `\RightAtomBond`.

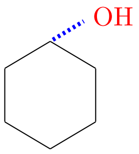
```
\sixheterov[{a{\RightAtomBond[\blue]<s>{0A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{1A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{2A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{3A=={\red OH}}}}]{}{}\par
```

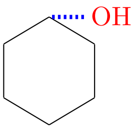
```
\sixheterov[{a{\RightAtomBond[\blue]<s>{4A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{5A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{6A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{7A=={\red OH}}}}]{}{}
\sixheterov[{a{\RightAtomBond[\blue]<s>{8A=={\red OH}}}}]{}{}
```

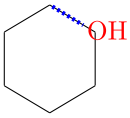


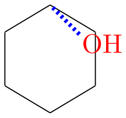


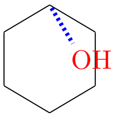


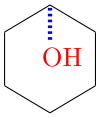






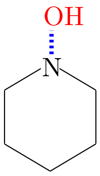


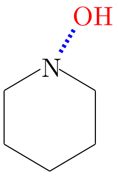


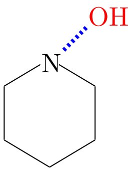


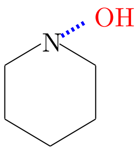
Examples shown in Page 90 (in `ATOMLIST`) can be also obtained by the present method using `BONDLIST`.

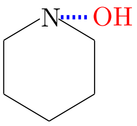
```
\sixheterov[{a{\RightAtomBond[\blue]{0A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{1A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{2A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{3A=={\red OH}}}}]{1==N}{}\par
\sixheterov[{a{\RightAtomBond[\blue]{4A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{5A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{6A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{7A=={\red OH}}}}]{1==N}{}
\sixheterov[{a{\RightAtomBond[\blue]{8A=={\red OH}}}}]{1==N}{}
```

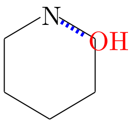


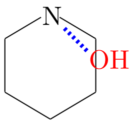


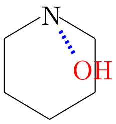


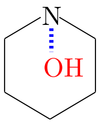










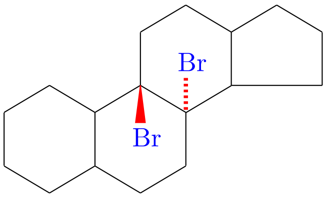


Unnatural Directions of Substitution Bonds

By using `\steroid` of the XΥMTEX system, a substitution bond at the position 8 or 9 (a bridgehead position) is drawn as an endocyclic bond of the resulting steroid ring. Thus, the structure drawn by the code:

```
\steroid{8A==\addbscolor{\red}{\bluex{Br}};9B==\addbscolor{\red}{\bluex{Br}}}
```

has endocyclic substitution bonds, as shown in the resulting formula:

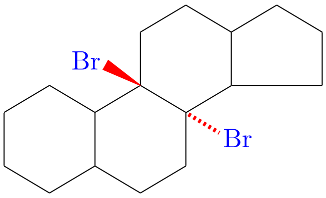


Hence, the direction appearing in the above structure is regarded as being natural in the X͡ΥMTEX system.

Exocyclic substitution bonds may be required in some situation. Because the `\steroid` command lacks an ATOMLIST but has a BONDLIST, the present technique is effective to draw such exocyclic substitution bonds. For example, the code:

```
\steroid[{g{\RightAtomBond[\red]<s>{5A==\bluex{Br}}}}%
{h{\LeftAtomBond[\red]<s>{3B==\bluex{Br}}}}]{}
```

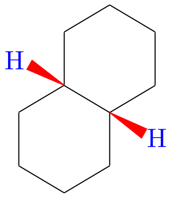
generates the following structural formula:

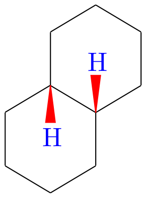


where unnatural exocyclic substitution bonds are available.

In bicyclic systems such as decalines, being natural and being unnatural are inverted as compared with steroids. When we use the `\decalinevt` command in place of `\decaheterovt` (cf. Page 94), we should use the `\RightAtomBond` or `\LeftAtomBond` command in its BONDLIST. The following examples compares natural and unnatural directions:

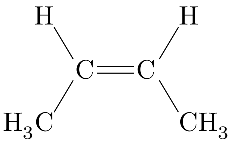
```
\decalinevt{9B==\addbscolor{\red}{\bluex{H}};%
{10}B==\addbscolor{\red}{\bluex{H}}}
\decalinevt[%
{e{\RightAtomBond[\red]<s>{0B==\bluex{H}}}}
{j{\RightAtomBond[\red]<s>{8B==\bluex{H}}}}]{}
```

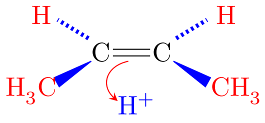


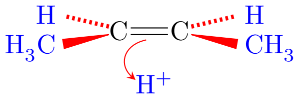


11.5.3 Other Unnatural Directions of Substitution Bonds

The `\Ethylene` command draws a planar ethylene derivative, as shown in the left-hand structure of the following examples. The substitution bonds in this structure are regarded as being in natural directions.







On the other hand, an electrophilic addition to an olefinic double bond requires a stereochemical representation, as shown usually in the middle structure or more extremely in the right-hand structure.

These three structural formulas are drawn by the following codes:

```
\Ethylene{}{1==H;2==\ChemForm{H_3C};3==\ChemForm{CH_3};4==H} \hskip50pt
\Ethylene{%
1s==\LeftAtomBond[\blue]{5B==\redx{\ChemForm{H_3C}}};%
1s==\LeftAtomBond(0,80)[\blue]{3A=={\red H}};1==C;%
2s==\RightAtomBond(80,0)[\blue]{5B==\redx{\ChemForm{CH_3}}};
2s==\RightAtomBond(80,80)[\blue]{3A==\redx{H}};2==C;
1==\put(100,-200){\bluex{H$^{+}$}};
1=={\red \electronrshiftarrow(140,0)(100,-150)}}{} \hskip50pt
\Ethylene{%
1=={\red \WedgeAsSubst(0,20)(-5,-1){171}};%
1==\put(-200,-50){\llap{\bluex{\ChemForm{H_3C}}}};%
1=={\red \PutDashedBond(0,50)(-171,90){\thickLineWidth}};%
1==\put(-200,60){\llap{\bluex{H}}};%
1==C;%
2=={\red \WedgeAsSubst(80,20)(5,-1){171}};%
2==\put(280,-50){\rlap{\bluex{\ChemForm{CH_3}}}};%
2=={\red \PutDashedBond(80,50)(251,90){\thickLineWidth}};%
2==\put(280,60){\rlap{\bluex{H}}};%
2==C;%
1==\put(100,-200){\bluex{H$^{+}$}};%
1==\redx{\electronrshiftarrow(140,0)(100,-150)}}{}
```

The middle structure is drawn by using `\RightAtomBond` and `\LeftAtomBond` defined in this section. On the other hand, the right-hand structure is drawn by using `\WedgeAsSubst` and `\PutDashedBond` according to Section 11.4.

The position number 1 of the designation `1==\put(-200,-50)...` in the `SUBSLIST` of the `\Ethylene` command (for drawing the right-hand formula) indicates that the origin is located at the lowerleft corner of C_1 (the left carbon) of ethylene and that the command `\put` places an object (e.g., `{\llap{\blue \ChemForm{H_3C}}}`) just as the origin of the object is superposed on the origin decided by the C_1 of ethylene. Thereby, the object appears at the position separated from the origin `(0,0)` by the xy-coordinate `(-200,-50)`.

Chapter 12

Coloring Skeletal Bonds and Double Bonds

12.1 Coloring Skeletal Bonds

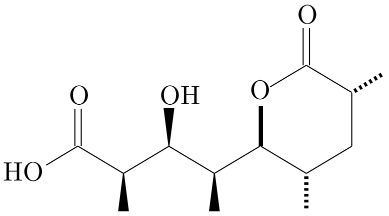
12.1.1 Systematic Method for Coloring Skeletal Bonds

Low-level commands (`\genCOM`) such as `\sixheterov` have an optional argument `(SKBONDLIST)` (cf. Section 10.1 of the on-line manual of XΥMTEX version 2.00 (xymtx200.pdf)) as follows:

```
\genCOM(SKBONDLIST)[BONDLIST]{ATOMLIST}{SUBSLIST}[OMIT]
```

The optional argument `(SKBONDLIST)` is originally designed to change a skeletal bond into a bold bond (β bond) or a dashed bond (α bond), e.g.,

```
\sixheterov({eB}){6==O;%
5s==\pentamethylenei{}{1W==HO;1D==O;2B==\null;3B==OH;4B==\null;5==(yl)}%
}{1D==O;2A==\null;4A==\null}
```



where the designation `({eB})` indicates that the skeletal bond `e` of a six-membered ring is changed into a bold bond (β bond).

This mechanism of changing a skeletal bond is extended to be suitable to coloring the skeletal bond. According to this guideline, the bondcolor package of the XΥMTEX version 5.00 has been developed to support the function of coloring skeletal bonds.

The command `\addskbcolor` is defined to specify the color of a skeletal bond, where it has a format represented by

```
\addskbcolor{COMMAND-TYPE}{COLOR}
```

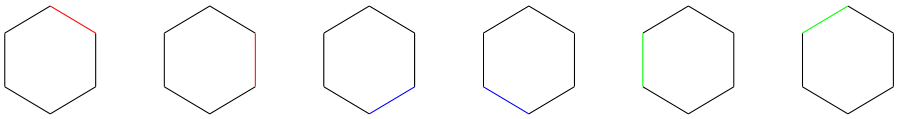
where the first argument `COMMAND-TYPE` is used to specify the vertical or horizontal type of a command. The vacant argument is the same thing as `v` for corresponding to commands of vertical types (suffix `v`) or of inverse vertical type (suffix `vi`). The second argument `COLOR` is a command for specifying color (e.g.,

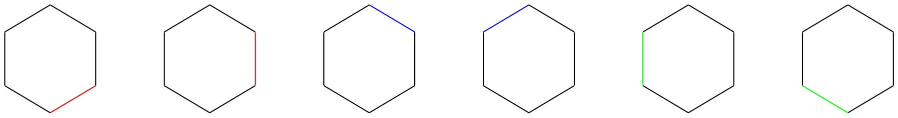
`\red` or `\color{red}`). The `\addskbcolor` command is designated in the `(SKBONDLIST)` (skeletal-bond list) of each command for drawing a skeleton.

For example, the codes:

```
\sixheterov({a{\addskbcolor{}{\red}}}){}{}\hskip-20pt
\sixheterov({b{\addskbcolor{}{\red}}}){}{}\hskip-20pt
\sixheterov({c{\addskbcolor{}{\blue}}}){}{}\hskip-20pt
\sixheterov({d{\addskbcolor{}{\blue}}}){}{}\hskip-20pt
\sixheterov({e{\addskbcolor{}{\green}}}){}{}\hskip-20pt
\sixheterov({f{\addskbcolor{}{\green}}}){}{} \par
\sixheterovi({a{\addskbcolor{}{\red}}}){}{}\hskip-20pt
\sixheterovi({b{\addskbcolor{}{\red}}}){}{}\hskip-20pt
\sixheterovi({c{\addskbcolor{}{\blue}}}){}{}\hskip-20pt
\sixheterovi({d{\addskbcolor{}{\blue}}}){}{}\hskip-20pt
\sixheterovi({e{\addskbcolor{}{\green}}}){}{}\hskip-20pt
\sixheterovi({f{\addskbcolor{}{\green}}}){}{}
```

show the use of the `\addskbcolor` command in `\sixheterov` (vertical type) and `\sixheterovi` (inverse vertical type), which generate the following structures:

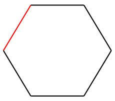
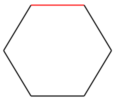
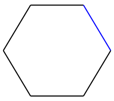
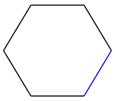
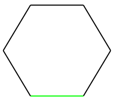
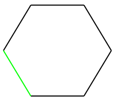


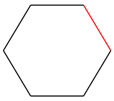
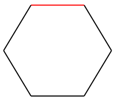
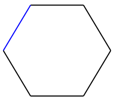
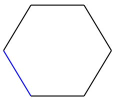
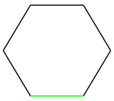
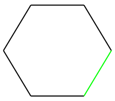


The use of the `\addskbcolor` command in `\sixheteroh` (horizontal type) and `\sixheterohi` (inverse horizontal type) is illustrated by the following codes:

```
\sixheteroh({a{\addskbcolor{h}{\red}}}){}{}\hskip-20pt
\sixheteroh({b{\addskbcolor{h}{\red}}}){}{}\hskip-20pt
\sixheteroh({c{\addskbcolor{h}{\blue}}}){}{}\hskip-20pt
\sixheteroh({d{\addskbcolor{h}{\blue}}}){}{}\hskip-20pt
\sixheteroh({e{\addskbcolor{h}{\green}}}){}{}\hskip-20pt
\sixheteroh({f{\addskbcolor{h}{\green}}}){}{} \par
\sixheterohi({a{\addskbcolor{h}{\red}}}){}{}\hskip-20pt
\sixheterohi({b{\addskbcolor{h}{\red}}}){}{}\hskip-20pt
\sixheterohi({c{\addskbcolor{h}{\blue}}}){}{}\hskip-20pt
\sixheterohi({d{\addskbcolor{h}{\blue}}}){}{}\hskip-20pt
\sixheterohi({e{\addskbcolor{h}{\green}}}){}{}\hskip-20pt
\sixheterohi({f{\addskbcolor{h}{\green}}}){}{}
```

where the first argument `{h}` of `\addskbcolor` corresponds to horizontal type or horizontal inverse type. These codes generate structural formulas with colored skeletal bonds:

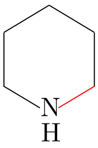







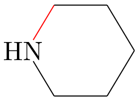







The presence of a ring atom results in bond shortening, where such a shortened bond can be also colored by the use of the `\addskbcolor` command. Thus the codes:

```
\sixheterovi({a{\addskbcolor{v}{\red}}}){1==\downnobond{N}{H}}{}
\sixheteroh({a{\addskbcolor{h}{\red}}}){1==HN}{}
```

generate structural formulas with colored shortened bonds:

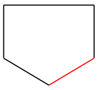
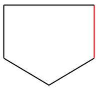
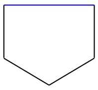
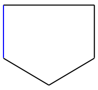
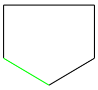


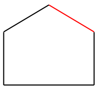


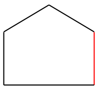
The use of the `\addskbcolor` command in `\fiveheterov` (vertical type) and `\fiveheterovi` (inverse vertical type) as shown in the codes:

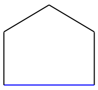
```
\fiveheterov({a{\addskbcolor{}{\red}}}){}{}
\fiveheterov({b{\addskbcolor{}{\red}}}){}{}
\fiveheterov({c{\addskbcolor{}{\blue}}}){}{}
\fiveheterov({d{\addskbcolor{}{\blue}}}){}{}
\fiveheterov({e{\addskbcolor{}{\green}}}){}{} \par
\fiveheterovi({a{\addskbcolor{}{\red}}}){}{}
\fiveheterovi({b{\addskbcolor{}{\red}}}){}{}
\fiveheterovi({c{\addskbcolor{}{\blue}}}){}{}
\fiveheterovi({d{\addskbcolor{}{\blue}}}){}{}
\fiveheterovi({e{\addskbcolor{}{\green}}}){}{}
```

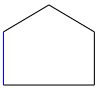
generates the following structures:

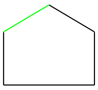










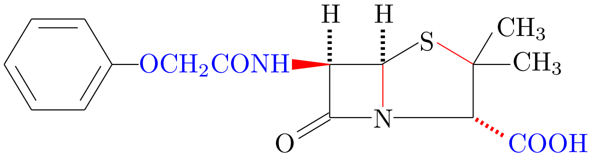






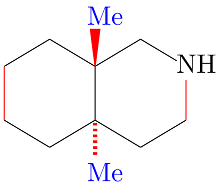
Other commands which support a skeletal bond list can use the `\addskbcolor` command. The following structure is drawn by using `\addskbcolor` commands in `\fourhetero` and `\fivefusevi`.

```
\begin{XyMcompd}(2100,600)(-800,100){}{}
\fourhetero({b{\addskbcolor{}{\red}}})%
[{b\fivefusevi({a{\addskbcolor{}{\red}}})%
{1==S;4==\null}{2Sa==CH$_{3}$;2Sb==CH$_{3}$;%
3A==\addbscolor{\red}{\bluex{COOH}}}{d}}]%
{2==N}{1D==O;3FA==H;4GA==H;%
4Su==\addbscolor{\red}{\blackx{%
\lyl(4=={\blue OCH$_{2}$CONH}){4==\bzdrh{4==(yl)}}}}}
\end{XyMcompd}
```



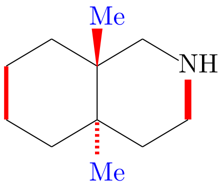
The following structure is drawn by using `\addskbcolor` commands in `\decaheterov`.

```
\decaheterov({b{\addskbcolor{v}{\red}}}%
{g{\addskbcolor{v}{\red}}}){2==NH}%
{9A==\addbscolor{\red}{\bluex{Me}};{10}B==\addbscolor{\red}{\bluex{Me}}}
```



The line width of a skeletal bond drawn by an `\addskbcolor` command can be changed by the first argument `{\red\thicklines}`. Such a line width can be reset by redefining the line width stored by `\thickLineWidth`, e.g., `\def\thickLineWidth{2.5pt}`.

```
\decaheterov({b{\addskbcolor{v}{\red\def\thickLineWidth{2.5pt}\thicklines}}}%
{g{\addskbcolor{v}{\red\thicklines}}}){2==NH}%
{9A==\addbscolor{\red}{\bluex{Me}};{10}B==\addbscolor{\red}{\bluex{Me}}}
```



12.1.2 Dirty Techniques for Coloring Skeletal Bonds

The technique base on `\addskbcolor` cannot be applied to commands which have no skeletal bond list (`SKBONDLIST`), e.g., `\steroid`. Because an original object can be erased by overwriting a white object in the PDF mode (also in the PostScript mode), the macro `\addPDFLine` (or `\addPSLine`) is defined tentatively to draw a colored skeletal bond.

The `\addPSLine` command for the PostScript mode is defined as follows:

```
\makeatletter
\def\white{\color{white}}
\def\addPSLine{%
\@ifnextchar[{\@ddPSLine}{\@ddPSLine[\thinLineWidth]}}
\def\@ddPSLine[#1](#2,#3)(#4,#5)#6{%
\psline[unit=\unitlength,linewidth=#1,linecolor=white](#2,#3)(#4,#5)%
\put(0,0){#6\PutBondLine(#2,#3)(#4,#5){#1}}}%
\makeatother
```

The optional argument can be applied to change a bond width and the last argument is used to designate a color.

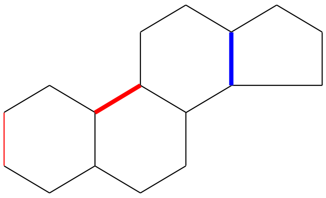
On the other hand, the `\addPDFLine` command for the PDF mode is defined as follows:

```
\makeatletter
\def\white{\color{white}}
\def\addPDFLine{%
\@ifnextchar[{\@ddPDFLine}{\@ddPDFLine[\thinLineWidth]}}
\def\@ddPDFLine[#1](#2,#3)(#4,#5)#6{%
\put(0,0){\white\PutBondLine(#2,#3)(#4,#5){1.6pt}}%
\put(0,0){#6\PutBondLine(#2,#3)(#4,#5){#1}}}%
\makeatother
```

The optional argument can be applied to change a bond width and the last argument is used to designate a color.

Because this document is typeset in the PDF mode, the macro `\addPDFLine` is written in a bond list, as shown in the following example:

```
\steroid[{b{\addPDFLine(0,0)(0,200){\red}}}%
{i{\addPDFLine[1.6pt](0,0)(171,103){\red}}}%
{o{\addPDFLine[1.6pt](0,0)(0,-200){\blue}}}]{}
```



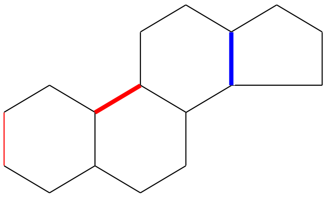
It should be noted that the macro `\addPDFLine` is so local as defined in the PDF mode, because the inner macro `\PutBondLine` depends upon the selected mode. The macro `\addPSLine` for the PostScript mode can be used by replacing `\addPDFLine` by `\addPSLine`.

The command `\replaceSKbond` is defined in the `bondcolor` package in order to color skeletal bonds in the PDF mode as well as in the PostScript mode, where a line to be colored is designated by specifying its starting point, slope, and length (as the x-axis projection):

```
\replaceSKbond[BONDWIDTH](Starting Point)(SLOPE){LENGTH}{COLOR}
```

The last argument `COLOR` of the `\replaceSKbond` command is set for a bond color. The first optional argument `[BONDWIDTH]` specifies the bond width to be drawn, as found in the following example:

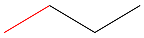
```
\steroid[{b{\replaceSKbond(0,0)(0,1){200}{\red}}}%
{i{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{o{\replaceSKbond[1.6pt](0,0)(0,-1){200}{\blue}}}]{}
```

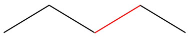
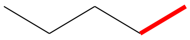


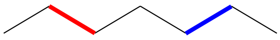
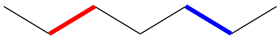
The command `\replaceSKbond` is effective to color skeletal bonds of polymethylenes, as found in the following list of examples:

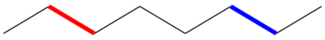
```
\tetramethylene[{a{\replaceSKbond(0,0)(5,3){171}{\red}}}]{}{}
\tetramethylenei[{b{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}]{}{}
\pentamethylene[{c{\replaceSKbond(0,0)(5,3){171}{\red}}}]{}{}
\pentamethylenei[{d{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}]{}{} \par
\hexamethylene[{c{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{e{\replaceSKbond[1.6pt](0,0)(5,3){171}{\blue}}}]{}{}
\hexamethylenei[{c{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{e{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\blue}}}]{}{} \par
\heptamethylene[{b{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{e{\replaceSKbond[1.6pt](0,0)(5,3){171}{\blue}}}]{}{}
\heptamethylenei[{b{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
```

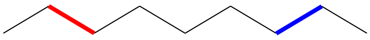
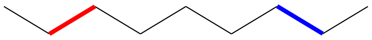
```
{e{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\blue}}}]{}{} \par
\octamethylene[{b{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{f{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\blue}}}]{}{}
\octamethylenei[{b{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{f{\replaceSKbond[1.6pt](0,0)(5,3){171}{\blue}}}]{}{} \par
\nonamethylene[{b{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{g{\replaceSKbond[1.6pt](0,0)(5,3){171}{\blue}}}]{}{}
\nonamethylenei[{b{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{g{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\blue}}}]{}{} \par
\decamethylene[{b{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{h{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\blue}}}]{}{}
\decamethylenei[{b{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{h{\replaceSKbond[1.6pt](0,0)(5,3){171}{\blue}}}]{}{} \par
```

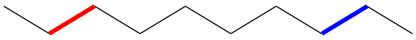


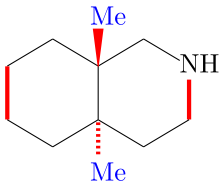


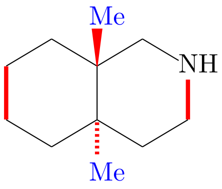




The colored structure shown in Page 102 can be alternatively drawn by using the `\replaceSKbond` command. Note that the pair of bond specifiers ‘`b/B`’ or ‘`g/G`’ designates the alternative terminals of a bond to be selected as starting points. With respect to the pair ‘`b/B`’ or ‘`g/G`’, check the slope `(0,1)` or `(0,-1)` specified as the argument of `\replaceSKbond`.

```
\decaheterov[{b{\replaceSKbond[1.6pt](0,-50)(0,-1){150}{\red}}}%
{g{\replaceSKbond[1.6pt](0,0)(0,1){200}{\red}}}]%
{2==NH}%
{9A==\addbscolor{\red}{\bluex{Me}};{10}B==\addbscolor{\red}{\bluex{Me}}}
\decaheterov[{B{\replaceSKbond[1.6pt](0,0)(0,1){150}{\red}}}%
{G{\replaceSKbond[1.6pt](0,0)(0,-1){200}{\red}}}]%
{2==NH}%
{9A==\addbscolor{\red}{\bluex{Me}};{10}B==\addbscolor{\red}{\bluex{Me}}}
```





12.2 Coloring Double Bonds

12.2.1 A Systematic Way

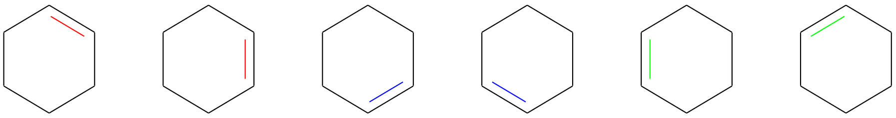
The bondcolor package of the XΥMTEX version 5.00 supports the function of coloring double bonds.[1] The command `\adddbcolor` is defined to specify the color of a double bond, where it has a format represented by

```
\adddbcolor{COMMAND-TYPE}{COLOR}
```

where the first argument `COMMAND-TYPE` is used to specify the vertical or horizontal type of a command, such as `v` for commands of vertical types (suffix `v`), `vi` for commands of inverse vertical types (suffix `vi`), and so on. The second argument `COLOR` is a command for specifying color (e.g., `\red` or `\color{red}`). The `\adddbcolor` command is designated in the `BONDLIST` (bond list) of each command for drawing a double bond. For example, the codes:

```
\sixheterov[{a{\adddbcolor{v}{\red}}}]{}{}\hskip-20pt
\sixheterov[{b{\adddbcolor{v}{\red}}}]{}{}\hskip-20pt
\sixheterov[{c{\adddbcolor{v}{\blue}}}]{}{}\hskip-20pt
\sixheterov[{d{\adddbcolor{v}{\blue}}}]{}{}\hskip-20pt
\sixheterov[{e{\adddbcolor{v}{\green}}}]{}{}\hskip-20pt
\sixheterov[{f{\adddbcolor{v}{\green}}}]{}{}\par
\sixheterovi[{a{\adddbcolor{vi}{\red}}}]{}{}\hskip-20pt
\sixheterovi[{b{\adddbcolor{vi}{\red}}}]{}{}\hskip-20pt
\sixheterovi[{c{\adddbcolor{vi}{\blue}}}]{}{}\hskip-20pt
\sixheterovi[{d{\adddbcolor{vi}{\blue}}}]{}{}\hskip-20pt
\sixheterovi[{e{\adddbcolor{vi}{\green}}}]{}{}\hskip-20pt
\sixheterovi[{f{\adddbcolor{vi}{\green}}}]{}{}\par
```

generate the following structures with colored double bonds:



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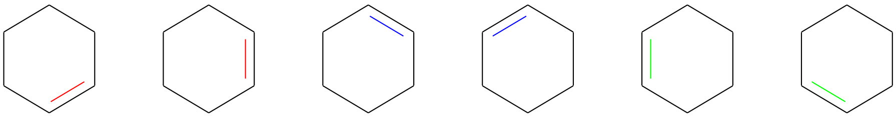
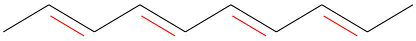
[1] According to the terminology of the XΥMTEX system, one bond of a double bond is regarded as a skeletal bond, while the other bond is regarded as a double bond to be added by an optional designation in `BONDLIST`.



Double bonds in polymethylene chains drawn by the macros of the methylen package can be colored by using the `\adddbcolor` command. For commands of normal type (e.g., `\decamethylene`), the first argument of `\adddbcolor` is set to be vacant. Lowercase bond specifiers `a` to `i` are used in the following examples:

```
\decamethylene[%
{a{\adddbcolor{}{\red}}}%
{c{\adddbcolor{}{\red}}}%
{e{\adddbcolor{}{\red}}}%
{g{\adddbcolor{}{\red}}}%
{i{\adddbcolor{}{\red}}}%
]{}{}
\decamethylene[%
{b{\adddbcolor{}{\red}}}%
{d{\adddbcolor{}{\red}}}%
{f{\adddbcolor{}{\red}}}%
{h{\adddbcolor{}{\red}}}%
]{}{}
```

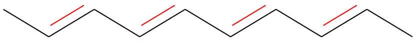


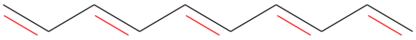
Uppercase bond specifiers `A` to `I` are used to draw double bonds at the opposite sides in comparison with bond specifiers `a` to `i`.

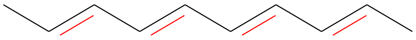
```
\decamethylene[%
{A{\adddbcolor{}{\red}}}%
{C{\adddbcolor{}{\red}}}%
{E{\adddbcolor{}{\red}}}%
{G{\adddbcolor{}{\red}}}%
{I{\adddbcolor{}{\red}}}%
]{}{}
\decamethylene[%
{B{\adddbcolor{}{\red}}}%
{D{\adddbcolor{}{\red}}}%
{F{\adddbcolor{}{\red}}}%
{H{\adddbcolor{}{\red}}}%
]{}{}
```

For commands of inverse type (e.g., `\decamethylenei`), on the other hand, the first argument of `\adddbcolor` is set to be `i`. Lowercase (`a` to `i`) and uppercase bond specifiers (`A` to `I`) are tested as follows by using the `\decamethylenei` command.

```
\decamethylenei[%
{a{\adddbcolor{i}{\red}}}{c{\adddbcolor{i}{\red}}}%
{e{\adddbcolor{i}{\red}}}{g{\adddbcolor{i}{\red}}}%
{i{\adddbcolor{i}{\red}}}%
]{}{}
\decamethylenei[%
{b{\adddbcolor{i}{\red}}}{d{\adddbcolor{i}{\red}}}%
{f{\adddbcolor{i}{\red}}}{h{\adddbcolor{i}{\red}}}%
]{}{} \par
\decamethylenei[%
{A{\adddbcolor{i}{\red}}}{C{\adddbcolor{i}{\red}}}%
{E{\adddbcolor{i}{\red}}}{G{\adddbcolor{i}{\red}}}%
{I{\adddbcolor{i}{\red}}}%
]{}{}
\decamethylenei[%
{B{\adddbcolor{i}{\red}}}{D{\adddbcolor{i}{\red}}}%
{F{\adddbcolor{i}{\red}}}{H{\adddbcolor{i}{\red}}}%
]{}{}
```

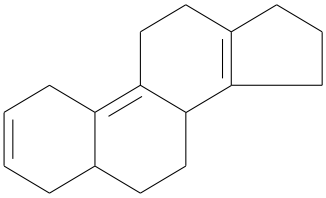


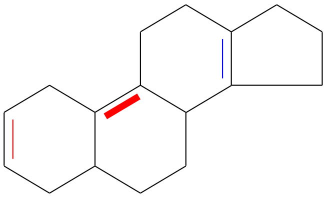




The following examples show the comparison between a non-color version and a colored version of the same structure.

```
\steroid[bio]{}
\steroid[{b{\adddbcolor{v}{\red}}}%
{i{\adddbcolor{v}{\red
\dashhasheddash\def\thickLineWidth{2.5pt}%
\thicklines}}}%
{o{\adddbcolor{v}{\blue}}}]{}
```

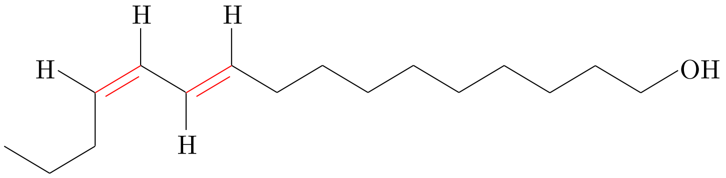


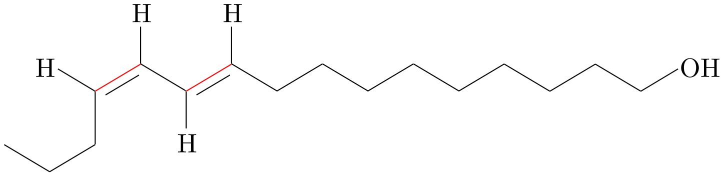


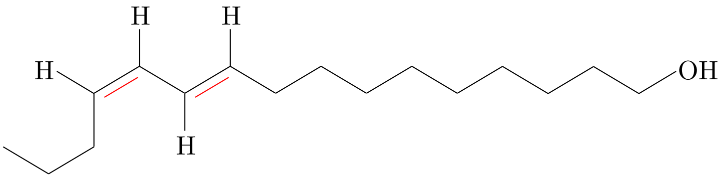
12.3 Coloring Both Skeletal and Double Bonds

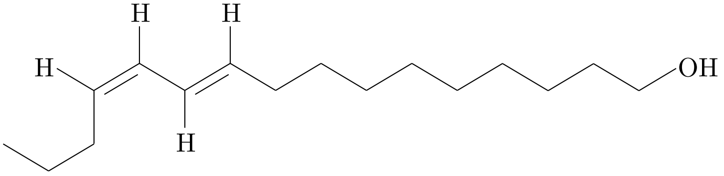
The techniques for coloring skeletal bonds (Section 12.1) can be used simultaneously with those for coloring double bonds (Section 12.2). Double bonds in bombykol (an insect pheromone of a silkworm moth) are colored in three different versions as follows. The last structure is a non-color version.

```
\begin{XyMcompd}(2600,600)(-100,-100){}{}
\decamethylene[%
{a{\adddbcolor{}{\red}}}%
{c{\adddbcolor{}{\red}}}%
{a{\replaceSKbond(0,0)(5,3){171}{\red}}}%
{c{\replaceSKbond(0,0)(5,3){171}{\red}}}%
]{%
{10}s==\tetramethylenei{}{1==(yl);4W==OH};%
1s==\sixheterov{}{2==(yl)}[aef]%
}{1W==H;2==H;3==H;4==H}
\end{XyMcompd}\par
\begin{XyMcompd}(2600,600)(-100,-100){}{}
\decamethylene[ac%
{a{\replaceSKbond(0,0)(5,3){171}{\red}}}%
{c{\replaceSKbond(0,0)(5,3){171}{\red}}}%
]{%
{10}s==\tetramethylenei{}{1==(yl);4W==OH};%
1s==\sixheterov{}{2==(yl)}[aef]%
}{1W==H;2==H;3==H;4==H}
\end{XyMcompd}\par
\begin{XyMcompd}(2600,600)(-100,-100){}{}
\decamethylene[%
{a{\adddbcolor{}{\red}}}%
{c{\adddbcolor{}{\red}}}%
]{%
{10}s==\tetramethylenei{}{1==(yl);4W==OH};%
1s==\sixheterov{}{2==(yl)}[aef]%
}{1W==H;2==H;3==H;4==H}
\end{XyMcompd}\par
\begin{XyMcompd}(2600,600)(-100,-100){}{}
\decamethylene[ac]{%
{10}s==\tetramethylenei{}{1==(yl);4W==OH};%
1s==\sixheterov{}{2==(yl)}[aef]%
}{1W==H;2==H;3==H;4==H}
\end{XyMcompd}
```





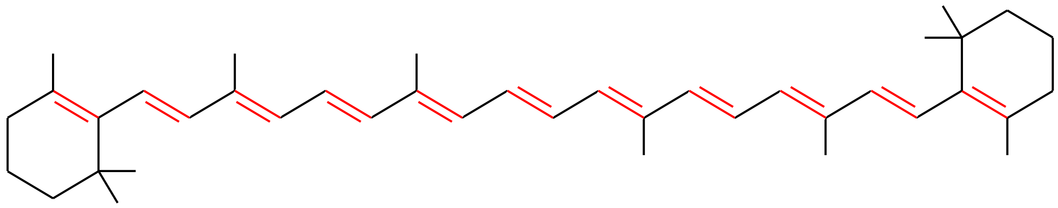


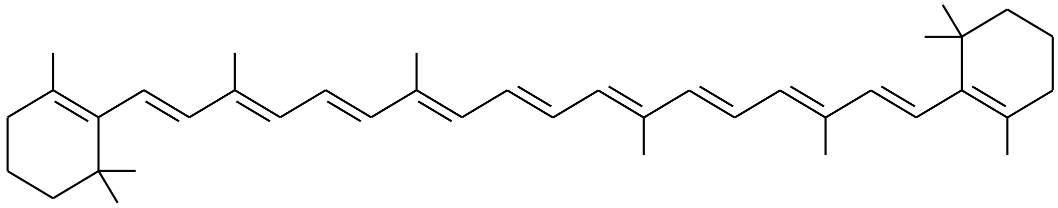


Colored and non-colored structures of β-Carotene are drawn by the following codes:

```
%%%%%%%%%%%%%%%
%color version %
%%%%%%%%%%%%%%%
{\def\thinLineWidth{0.8pt}
\begin{XyMcompd}(3850,800)(-100,-150){}{}
\decamethylene[%bdfh
{b{\adddbcolor{}{\red}}}%
{d{\adddbcolor{}{\red}}}%
{f{\adddbcolor{}{\red}}}%
{h{\adddbcolor{}{\red}}}%
{b{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{d{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{f{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{h{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
]
{1s==\sixheterov(%
{a{\addskbcolor{v}{\red}}}%
)[%a
{a{\adddbcolor{v}{\red}}}%
]{}{2==(yl);1==\null;3Sa==\null;3Sb==\null};
{10}s==\decamethylenei[%acegi
{a{\adddbcolor{i}{\red}}}%
{c{\adddbcolor{i}{\red}}}%
{e{\adddbcolor{i}{\red}}}%
{g{\adddbcolor{i}{\red}}}%
{i{\adddbcolor{i}{\red}}}%
{a{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{c{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{e{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{g{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
{i{\replaceSKbond[0.8pt](0,0)(5,-3){171}{\red}}}%
]{{10}s==\dimethylene{%
2s==\sixheterov(%
{d{\addskbcolor{v}{\red}}}%
)[%d
{d{\adddbcolor{v}{\red}}}%
]{}{5==(yl);4==\null;6Sa==\null;6Sb==\null}
}{1==(yl)}}{1==(yl);4==\null;8==\null}}{4==\null;8==\null}
\end{XyMcompd}\par
```

```
%%%%%%%%%%%%%%%%%%%%%%
%non-colored version %
%%%%%%%%%%%%%%%%%%%%%%
\begin{XyMcompd}(3850,800)(-100,-150){}{}
\decamethylene[bdfh]
{1s==\sixheterov[a]{}{2==(yl);1==\null;3Sa==\null;3Sb==\null};
{10}s==\decamethylenei[acegi]{{10}s==\dimethylene{%
2s==\sixheterov[d]{}{5==(yl);4==\null;6Sa==\null;6Sb==\null}
}{1==(yl)}}{1==(yl);4==\null;8==\null}}{4==\null;8==\null}
\end{XyMcompd}
}
```





The top declaration `\def\thinLineWidth{0.8pt}` results in printing bold bonds. In accord with this declaration, the command `\replaceSKbond` should take an optional argument `[0.8pt]`.

12.4 Background Colors

Commands for coloring skeletal and double bonds are summarized as follows:

Skeletal bonds	`\replaceSKbond`	in a bond list [...]
	`\addskbcolor`	in a skeletal bond list (...)
Double bonds	`\adddbcolor`	in a bond list [...]

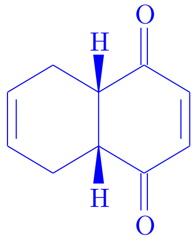
The three techniques can be combined freely, as well as in combination with `\addbscolor` for coloring substitution bonds and substituents. The following examples illustrate a combined use of `\addskbcolor`, `\adddbcolor` and `\addbscolor` in the arguments of the `\decaheterov` command.

```
\begin{tabular}{ccc}
Background: blue & Background: blue & Background: green \\
\bluex{%
\decaheterov[bg]{}{9B==H;{10}B==H;1D==O;4D==O}}
&
\bluex{%
\decaheterov(%SKBONDLIST
{f{\addskbcolor{v}{\red}}}%
{g{\addskbcolor{v}{\red}}}%
{h{\addskbcolor{v}{\red}}}%
)[b%BONDLIST
```

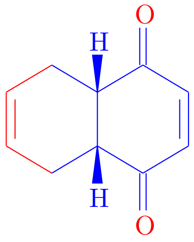
```
{g{\adddbcolor{v}{\red}}}%
]{}{%SUBSTLIST
9B==\bluex{H};{10}B==\bluex{H};%\blue is necessary
1D==\redx{O};4D==\redx{O}}}
&
\greenx{%
\decaheterov(%SKBONDLIST
{e{\addskbcolor{v}{\blue}}}%
{f{\addskbcolor{v}{\red}}}%
{g{\addskbcolor{v}{\red}}}%
{h{\addskbcolor{v}{\red}}}%
{i{\addskbcolor{v}{\blue}}}%
{k{\addskbcolor{v}{\blue}}}%
)[b%BONDLIST
{g{\adddbcolor{v}{\red}}}%
]{}{%SUBSTLIST
1D==\addbscolor{\blue}{\redx{O}};4D==\addbscolor{\blue}{\redx{O}};%
9B==\addbscolor{\blue}{H};{10}B==\addbscolor{\blue}{H}}} \\
\end{tabular}
```

The background color of a structural formula can be changed from a default black into any color, where explicit designations of bond colors due to the present techniques are maintained during the change of the background color.

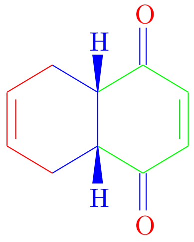
Background: blue



Background: blue



Background: green



Chapter 13

Coloring Chemical Schemes

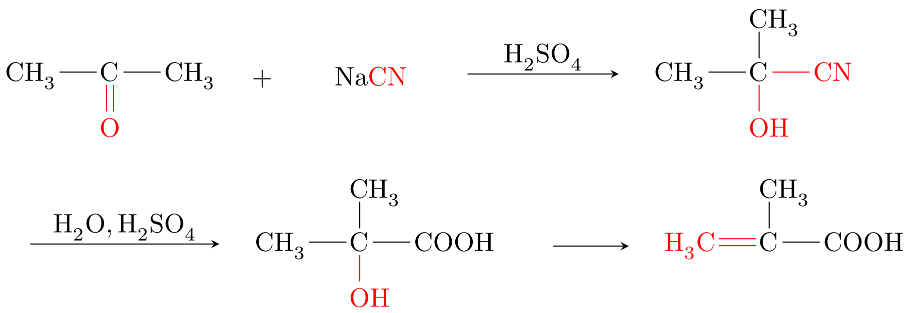
The techniques for coloring bonds and substituents (Chapters 11 and 12) can be combined freely. This chapter is devoted to show that combined techniques are effective to draw chemical schemes which contain colored structural formulas.

13.1 Formation of Cyanohydrins

Formation of cyanohydrin is represented by using the `ChemEqnarray` environment (defined in the chemist package), as found in the following code:

```
\begin{ChemEqnarray}
&&
\tetrahedral{0==C;2==\ChemForm{CH_3};3D==\addbscolor{\red}{O};%
4==\ChemForm{CH_3}}
\qquad \raisebox{25pt}{ + \qquad Na{\red CN}} \qquad
\reactrarrow{25pt}{2cm}{\ChemForm{H_2SO_4}}{\strut} \qquad
\tetrahedral{0==C;2==\ChemForm{CH_3};3==\addbscolor{\red}{OH};%
1==\ChemForm{CH_3};4==\addbscolor{\red}{CN}} \nonumber \\
&&
\reactrarrow{25pt}{2.5cm}{\ChemForm{H_2O, H_2SO_4}}{\strut} \qquad
\tetrahedral{0==C;2==\ChemForm{CH_3};3==\addbscolor{\red}{OH};%
1==\ChemForm{CH_3};4==COOH} \qquad\qquad
\reactrarrow{25pt}{1cm}{\strut}{\strut} \qquad
\tetrahedral{0==C;2D==\addbscolor{\red}{\ChemForm{H_3C}};%
1==\ChemForm{CH_3};4==COOH} \label{eq:cyanohydrin}
\end{ChemEqnarray}
```

By means of the `ChemEqnarry` environment (not by means of the `eqnarray` environment of LaTeX 2$_\varepsilon$), the compound NaCN is printed out in upright format (cf. Section 7.5 and Subsection 9.2.1). The participating compounds are drawn by using the `\tetrahedral` command, where substituents and substitution bonds are colored by using the `\addbscolor` command. The reaction arrows are drawn by means of the `\reactrarrow` command, which is defined in the chemist (chmst-pdf or chmst-ps) package.



(13.1)

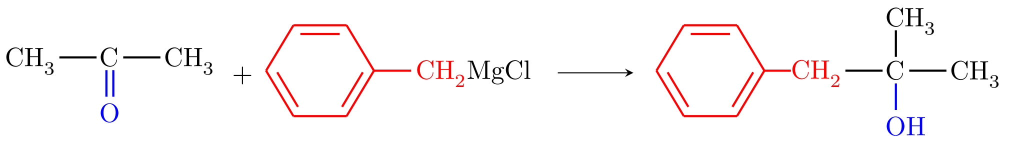
It should be noted that subscripts due to the `\ChemForm` command are printed to show the same depth, even if they coexist with superscripts. Compare the subscripts appearing in $H_2SO_4^{--}$ (due to `\ChemForm{H_2  SO_4^{--}}`) with those appearing in $H_2SO_4^{--}$ (due to `H$_2$SO$_4^{--}$`). Thus, the subscripts 2 and 4 printed by `\ChemForm` appear at the positions of the same depth, while the counterparts printed by `$...$` appear at the positions of different depths.

13.2 Grignard Reactions

A Grignard reagent derived from benzyl chloride reacts with actone so as to give a *tert*-alcohol, as shown in the following scheme due to the `ChemEquation` environment defined by the `chemist` package. The code:

```
\begin{ChemEquation}
\def\thinLineWidth{0.8pt}
\begin{XyMcompd}(600,300)(0,100){}{}
\tetrahedral{0==C;2==\ChemForm{CH_3};3D==\addbscolor{\blue}{O};%
4==\ChemForm{CH_3}}
\end{XyMcompd}
\quad \raisebox{0pt}{+} \quad
\begin{XyMcompd}(800,300)(350,250){}{}
\redx{\bzdrh{4==\ChemForm{CH_2{\blackx{MgCl}}}}}
\end{XyMcompd}
\quad \reactrarrow{0pt}{1cm}{\strut}{\strut} \quad
\begin{XyMcompd}(1100,500)(-500,50){}{}
\tetrahedral{0==C;1==\ChemForm{CH_3};3==\addbscolor{\blue}{OH};%
2==\redx{\lyl(4==\ChemForm{CH_2}){4==\bzdrh{4==(yl)}}};%
4==\ChemForm{CH_3}}
\end{XyMcompd}
\end{ChemEquation}
```

generates the following equation containing structures with colored bonds and moieties:

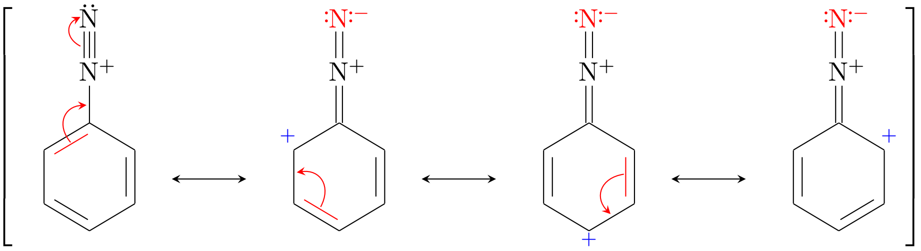


(13.2)

The declaration `\def\thinLineWidth{0.8pt}` just after the beginning of the `ChemEquation` environment indicates that the line width of each bond is changed from the standard width (0.4pt) to a thicker one (0.8pt).

13.3 Resonance Structures

A versatile convention in organic chemistry is based on resonance structures, which represent electron shift in an intuitive way. For example, a benzenediazonium ion is represented by a set of resonance structures shown below:



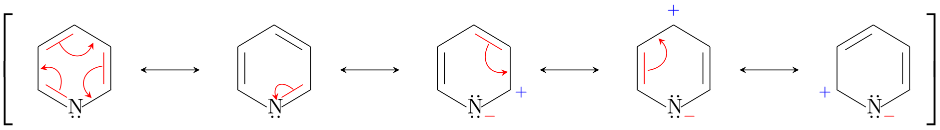
(13.3)

Equation 13.3 is drawn by the following code. Curved arrows for representing electron shifts in resonance structures are drawn by using such commands as `\electronrshiftarrow`, which have been defined in the chemist (chmst-pdf or chmst-ps) package (cf. Subsection 7.6.1). Lone pairs on a nitrogen atom are drawn by using `\lonepairA`, which has been defined in the lewisstruc package of the XΥMTEX system (cf. Chapter 2.1 of the on-line manual for XΥMTEX version 4.05, i.e., xymtx405A.pdf).

```
\begin{ChemEquation}
\left[%
\begin{tabular}{ccccccc}
\begin{XyMcompd}(300,900)(230,200){}{}
\sixheterov[bd{f{\adddbcolor{v}{\red}}}%
{f{\redx{\electronrshiftarrow(100,30)(160,170)}}}]%
{}{1==\tetrahedral{3==(yl);0==N\rlap{$^{+}$};%
0==\redx{\electronrshiftarrow[1](-30,130)(-30,240)};%
1T==\lonepairA[1]{N}}}
\end{XyMcompd}
&\raisebox{-20pt}{$\llongleftrightarrow$}&
\begin{XyMcompd}(300,900)(230,200){}{}
\sixheterov[b%
{d{\adddbcolor{v}{\red}}}%
{d{\red\electronlshiftarrow(-160,220)(-70,90)}}
]%
{6s=={\blue$^{+}\!$}}{1D==\tetrahedral{3==(yl);0==N\rlap{$^{+}$};%
1D==\redx{\lonepairA[24]{N\rlap{\,$^{-}$}}}}}
\end{XyMcompd}
&\raisebox{-20pt}{$\llongleftrightarrow$}&
\begin{XyMcompd}(300,900)(230,200){}{}
\sixheterov[e%
{b{\adddbcolor{v}{\red}}}%
{b{\red\electronrshiftarrow(-40,-90)(-90,-240)}}
]%
{4==\lower.4em\hbox{\blue\scriptsize$+$};4s==\null}%
{1D==\tetrahedral{3==(yl);0==N\rlap{$^{+}$};%
1D==\redx{\lonepairA[24]{N\rlap{$\,^{-}$}}}}}
\end{XyMcompd}
&\raisebox{-20pt}{$\llongleftrightarrow$}&
\begin{XyMcompd}(300,900)(230,200){}{}
\sixheterov[ce]%
{2s==\bluex{$\!^{+}$}}{1D==\tetrahedral{3==(yl);0==N\rlap{$^{+}$};%
```

```
1D==\redx{\lonepairA[24]{N\rlap{$\,^{-}$}}}}}
\end{XyMcompd}
\\
\end{tabular}
\right]
\label{eq:diazonium}
\end{ChemEquation}
```

On a similar line, pyridine is represented by a set of resonance structures shown below.



(13.4)

Equation 13.4 is drawn by the following code.

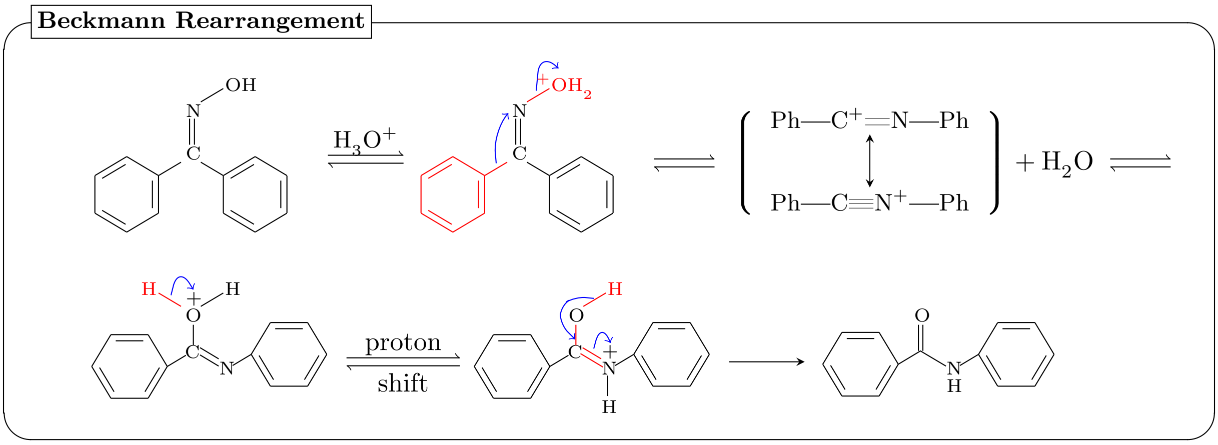
```
\begin{ChemEquation}
\left[%
\scalebox{0.8}{%
\begin{tabular}{ccccccccc}
\begin{XyMcompd}(300,500)(230,200){}{}
\sixheterov[%
{b{\adddbcolor{v}{\red}}}%
{b{\red\electronrshiftarrow(-40,-90)(-90,-240)}}
{d{\adddbcolor{v}{\red}}}%
{d{\red\electronlshiftarrow(-160,200)(-70,100)}}
{f{\adddbcolor{v}{\red}}}%
{f{\red\electronrshiftarrow[1](100,20)(260,20)}}%
]%
{4==\lonepairA[3]{N}}{}
\end{XyMcompd}
&$\llongleftrightarrow$&
\begin{XyMcompd}(300,500)(230,200){}{}
\sixheterov[ae%
{c{\adddbcolor{v}{\red}}}%
{c{\red\electronlshiftarrow[2](-160,-50)(-80,0)}}
]%
{4==\lonepairA[3]{N}}{}
\end{XyMcompd}
&$\llongleftrightarrow$&
\begin{XyMcompd}(300,500)(230,200){}{}
\sixheterov[e%
{a{\adddbcolor{v}{\red}}}%
{a{\red\electronrshiftarrow[1](70,-90)(160,-220)}}
]%
{4==\lonepairA[13]{N}\rlap{\red $_{-}$};3s=={\blue$\,_{+}$}
}{}
\end{XyMcompd}
&$\llongleftrightarrow$&
\begin{XyMcompd}(300,500)(230,200){}{}
\sixheterov[b%
{e{\adddbcolor{v}{\red}}}%
{e{\red\electronrshiftarrow[1](50,90)(100,240)}}
```

```
]%
{4==\lonepairA[13]{N}\rlap{\red $_{-}$};%
1==\raise1em\hbox{\blue\scriptsize$+$};1s==\null
}{}
\end{XyMcompd}
&$\llongleftrightarrow$&
\begin{XyMcompd}(300,500)(230,200){}{}
\sixheterov[bf%
]%
{4==\lonepairA[13]{N}\rlap{\red $_{-}$};5s=={\blue$_{+}\!$}
}{}
\end{XyMcompd}
\\
\end{tabular}}
\right]
\label{eq:pyridine}
\end{ChemEquation}
```

13.4 Beckmann Rearrangement

The following scheme concerning a Beckmann rearrangement is a color version of the reaction scheme drawn in Section 4.5 of the on-line manual of XΥMTEX versions 4.05 and 4.06 (xymtx405406B.pdf).

Beckmann Rearrangement



This scheme is drawn by the following code:

```
\begingroup
\def\tboxtitle{\bf Beckmann Rearrangement}
\begin{tboxscreen}
\changeunitlength{0.07pt}
\begin{ChemEqnarray*}
&&
\begin{XyMcompd}(1000,850)(-150,-150){}{}
\Ethylenev{1==C;2==N}{3==OH;2==\bzdrv{6==(yl)};1==\bzdrv{2==(yl)}}
\end{XyMcompd}
\mskip6mu \reacteqarrow{0pt}{1cm}{\small H$_{3}$O$^{+}$}{\strut} \mskip6mu
\begin{XyMcompd}(1000,850)(-150,-150){}{}
\Ethylenev{1==C;2==N;%
1=={\blue \putRoundArrow{(-85,-20)(-100,150)(-20,250)}};%
```

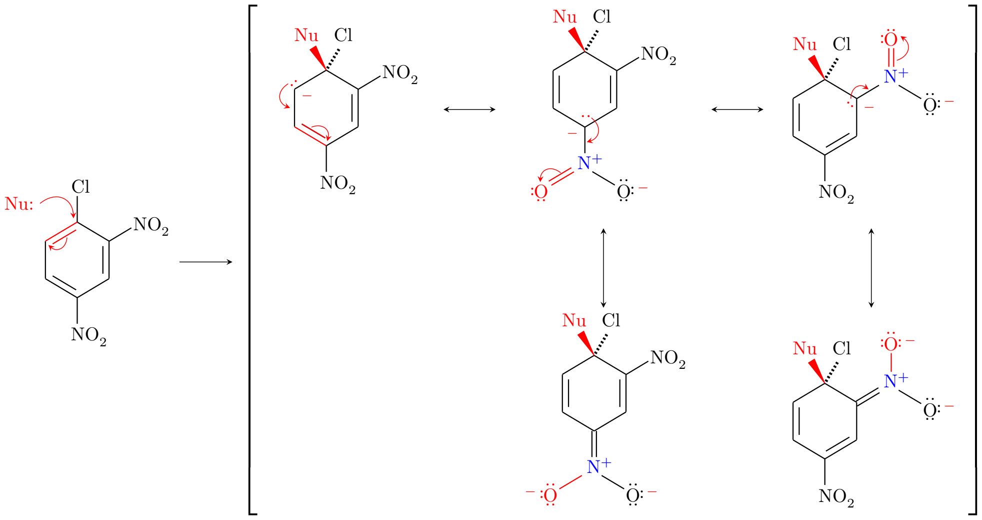
```
2=={\blue \putRoundArrow{(130,140)(150,350)(250,260)}}%
%%%PostScript Mode only%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%1==\pscurve[unit=\unitlength,linewidth=0.4pt]{->}%
%(-85,-20)(-100,150)(-20,250);%                   %
%2==\pscurve[unit=\unitlength,linewidth=0.4pt]{->}%
%(130,140)(150,350)(250,280)%                     %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
}{3==\addbscolor{\red}{\llap{$^{+}$}OH$_{2}$};%
2==\bzdrv{6==(yl)};1==\addbscolor{\red}{\bzdrv{2==(yl)}}}
\end{XyMcompd}
\mskip6mu \reacteqarrow{0pt}{0.8cm}{}{} \mskip6mu
\left\lgroup
\begin{tabular}{c}
\small Ph\sbond C$^{+}$\dbond N\sbond Ph \\[-8pt]
\reactduarrow{0pt}{20pt}{}{} \\
\small Ph\sbond C\tbond N$^{+}$\sbond Ph \\
\end{tabular}
\right\rgroup
+ H_{2}O
\mskip6mu \reacteqarrow{0pt}{0.8cm}{}{}
\\ \noalign{\vskip20pt}
& &
\begin{XyMcompd}(1100,500)(-400,0){}{}
\dimethylenei[a]{1==C;2==N}{2W==\bzdrh{1==(yl)};1W==\bzdrh{4==(yl)};%
1==\Utrigonal{1==(yl);0==\upnobond{O}{+};2==H;3==\addbscolor{\red}{H};%
0=={\blue \putRoundArrow{(-80,140)(-40,300)(40,170)}
}}}
\end{XyMcompd}
\mskip6mu \reacteqarrow{0pt}{1.5cm}{proton}{shift} \mskip6mu
\begin{XyMcompd}(1100,500)(-400,0){}{}
\dimethylenei[%
{a{\replaceSKbond(25,-15)(5,-3){120}{\red}}}%
{a{\adddbcolor{i}{\red}}}%
]{1==C;2==\upnobond{N}{+};%
1=={\blue \putRoundArrow[<-]{(-40,100)(-120,180)(-120,280)(-40,330)(60,320)}};%
1=={\blue \putRoundArrow{(60,50)(100,200)(150,80)}}%
%%%PostScript Mode only%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%1==\pscurve[unit=\unitlength,linewidth=0.4pt]{<-}%
%(-40,100)(-120,180)(-120,280)(-40,330)(60,320);% %
%1==\pscurve[unit=\unitlength,linewidth=0.4pt]{->}%
%(60,50)(100,200)(150,80)%                        %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
}%
{2==H;2W==\bzdrh{1==(yl)};1W==\bzdrh{4==(yl)};%
1==\addbscolor{\red}{\Utrigonal{0=={\black O};2==H;1==(yl)}}}
\end{XyMcompd}
\mskip6mu \reactrarrow{0pt}{1cm}{}{} \mskip6mu
\begin{XyMcompd}(1100,500)(-400,0){}{}
\dimethylenei{2==\downnobond{N}{H}}{2W==\bzdrh{1==(yl)};1W==\bzdrh{4==(yl)};1D==O}
\end{XyMcompd}
\end{ChemEqnarray*}
\end{tboxscreen}
```

```
\endgroup
```

Skeletal and double bonds participating in the Beckman reaction are colored by using `\replaceSKbond` (skeletal bonds) and `\adddbcolor` (double bonds). Although round arrows have been drawn by using `\psline` (defined in the `pstricks` package) in Section 4.5 of xymtx405406.pdf, they are now drawn by using the newly-defined command `\putRoundArrow`, which is compatible to the PDF mode as well as to the PS mode of the XΥMTEX system. Because the old designations due to `\psline` are commented out, the comparison between `\putRoundArrow` and `\psline` shows their correspondence.[1] Compare these commands with another set of commands for drawing round arrows described Section 13.3.

13.5 Nucleophilic Substitutions

The chlorine atom of 1-cloro-2,4-dinitrobenzene is reactive to a nucleophilic reagent (Nu:), where its intermediate (a Meisenheimer complex) is delocalized by the two nitro groups, as shown in the following scheme:



(13.5)

This scheme (eq. 13.5) is drawn by the following code:

```
\begin{ChemEquation}\def\thinLineWidth{0.6pt}
\scalebox{0.7}{%
\begin{XyMcompd}(800,900)(50,0){}{}
\sixheterov({f{\addskbcolor{v}{\red}}})[bd{f{\adddbcolor{v}{\red}}}]{%
1s=={\red \electronrshiftarrow(-200,100)(-20,20)};%
1s==\put(-200,100){\makebox(0,0)[rc]{\red Nu:~}};%
6s=={\red \electronlshiftarrow[1](20,-20)(120,20)}%
}{1==Cl;2==NO$_{2}$;4==NO$_{2}$}
\end{XyMcompd}}
\mathrel{\scalebox{0.7}{\reactrarrow{0pt}{1cm}{}{}}}
\left[%
\scalebox{0.7}{%
\begin{tabular}{ccccc}
```

---

[1] The mechanism of drawing curves by the `pgf` package (used in the PDF-compatible mode of the XΥMTEX system is different from the corresponding mechanism by the `pstricks` package (used in the PostScript-compatible mode). Hence, the same argument of `\putRoundArrow` of the two modes results in different outputs.

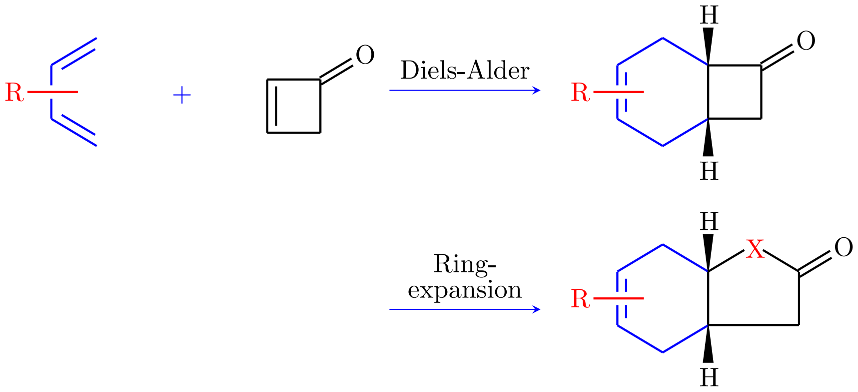
```
\begin{XyMcompd}(700,900)(150,0){}{}
\sixheterov({d{\addskbcolor{v}{\red}}})[bd{d{\adddbcolor{v}{\red}}}]{%
6=={\red \lonepairB[4]{\phantom{c}\rlap{$_{-}$}}};%
6s=={\red \electronrshiftarrow[1](-30,30)(-20,-100)};%
4s=={\red \electronrshiftarrow(-80,100)(5,25)}%
}{1SA==Cl;1SB==\addbscolor{\red}{Nu};2==NO$_{2}$;4==NO$_{2}$}
\end{XyMcompd}
& $\llongleftrightarrow$ &
\begin{XyMcompd}(700,1100)(150,-200){}{}
\sixheterov[be]{%
4==\lower0.5em\hbox{\red \lonepairA[1]{\llap{$_{-}$}\phantom{C}}};%
4s=={\red \electronrshiftarrow[1](35,50)(10,-80)}%
}{1SA==Cl;1SB==\addbscolor{\red}{Nu};2==NO$_{2}$;
4==\Dtrigonal{1==(yl);0=={\blue N\rlap{$^{+}$}};%
0=={\red \electronlshiftarrow(-200,-70)(-90,-20)};%
2==\lonepairA[123]{O\rlap{\red $\,\,^{-}$}};3D==\addbscolor{\red}{\lonepairA[34]{O}}}}
\end{XyMcompd}
& $\llongleftrightarrow$ &
\begin{XyMcompd}(800,1000)(250,0){}{}
\sixheterov[ce]{%
2==\lower0.1em\hbox{\red \lonepairB[3]{\phantom{C}\rlap{$_{-}$}}};%
2s=={\red \electronrshiftarrow(-35,0)(60,50)}%
}{1SA==Cl;1SB==\addbscolor{\red}{Nu};
4==NO$_{2}$;%
2==\Dtrigonal{3==(yl);0=={\blue N\rlap{$^{+}$}};%
0=={\red \electronrshiftarrow[1](70,120)(90,250)};%
2==\lonepairA[123]{O\rlap{\red $\,\,^{-}$}};%
1D==\addbscolor{\red}{\lonepairA[14]{O}}}}
\end{XyMcompd}
\\
& & \reactduarrow{0pt}{1.5cm}{}{} & & \reactduarrow{0pt}{1.5cm}{}{} \\
&&
\begin{XyMcompd}(800,1100)(50,-200){}{}
\sixheterov[be]{%
}{1SA==Cl;1SB==\addbscolor{\red}{Nu};2==NO$_{2}$;
4D==\Dtrigonal{1==(yl);0=={\blue N\rlap{$^{+}$}};%
%0=={\red \electronlshiftarrow(-200,-70)(-90,-20)};%
2==\lonepairA[123]{O\rlap{\red $\,\,^{-}$}};%
3==\addbscolor{\red}{\lonepairA[134]{\llap{$^{-}\,\,$}O}}}}
\end{XyMcompd}
& &
\begin{XyMcompd}(800,1000)(250,0){}{}
\sixheterov[ce]{%
}{1SA==Cl;1SB==\addbscolor{\red}{Nu};
4==NO$_{2}$;%
2D==\Dtrigonal{3==(yl);0=={\blue N\rlap{$^{+}$}};%
2==\lonepairA[123]{O\rlap{\red $\,\,^{-}$}};%
1==\addbscolor{\red}{\lonepairA[124]{O\rlap{$\,\,^{-}$}}}}}
\end{XyMcompd}
\\
\end{tabular}}
\right] \label{eq:Nucl-Subs}
```

```
\end{ChemEquation}
```

In this code, a set of round arrows `\electronrshiftarrow` and `\electronlshiftarrow` (Subsection 7.6.1) is used to indicate electron shifts on a similar line to Section 13.3. Compare these commands with another set of commands for drawing round arrows described Section 13.4. The scheme of delocalization surrounded by a pair of brackets is typeset by using the `tabular` environment, the size of which is reduced by using the `\scalebox` command. The total scheme (eq. 13.5) is typeset by using the `ChemEquation` environment, which is supported by the `chemist` (or `chmst-pdf` or `chmst-ps`) package.

13.6 A New Diels-Alder Bulding Block

The following scheme (eq. 13.6) is cited from a short article "Diels-Alder Bulding Block Debuts" published in *Chem. & Eng. News*, August 9 (2010) pages 30–31.



(13.6)

R = various group; X = CH_2, O, or NH

This scheme is drawn by writing the following code:

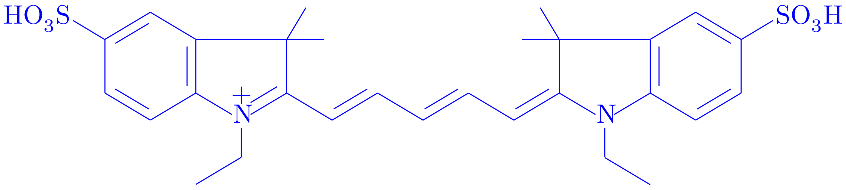
```
\def\markashR(#1,#2){%
\ifPSmode
{\put(#1,#2){\tetrahedral{4==(yl);%
2==\addbscolor{\psset{linecolor=white}\def\thinLineWidth{5pt}}{\null};%
2==R\kern-5pt}}}%
\else
{\put(#1,#2){\tetrahedral{4==(yl);%
2==\addbscolor{\white\def\thinLineWidth{5pt}}{\null};%
2==R\kern-5pt}}}\fi%
}
{\blue \def\thinLineWidth{0.8pt}
\begin{ChemEqnarray}
\begin{XyMcompd}(300,600)(100,150){}{}
{\blue \sixheterov[df{e{\red\markashR(100,100)}}]{}{}[abc]}
\end{XyMcompd}
\qquad + \qquad
\begin{XyMcompd}(300,400)(400,200){}{}\black
\fourhetero[d]{}{3D==O}
\end{XyMcompd}
& \reactrarrow{0pt}{2cm}{\black Diels-Alder}{\strut}
```

```
&
\begin{XyMcompd}(900,600)(100,150){}{}
\sixheterov({b{\addskbcolor{v}{\black}}})
[e{e{\red\markashR(100,100)}}%
{b{\black \fourfuse{}{3D==O;1FB==H;4GB==H}{d}}}]{}{}
\end{XyMcompd}
\nonumber \\
\noalign{\vskip10pt}
& \reactrarrow{0pt}{2cm}{\black Ring-expansion}{\strut}
&
\begin{XyMcompd}(900,600)(100,150){}{}
\sixheterov({b{\addskbcolor{v}{\black}}})
[e{e{\red\markashR(100,100)}}%
{b{\black \fivefusevi{1=={\red X}}{2D==O;4FB==H;5GB==H}{D}}}%
]{}{}
\end{XyMcompd}
\label{eq:Diels-Alder} \\
\noalign{\black\centering {\red R} = various group;
{\red X} = \ChemForm{CH_2}, O, or NH} \nonumber
\end{ChemEqnarray}
}
```

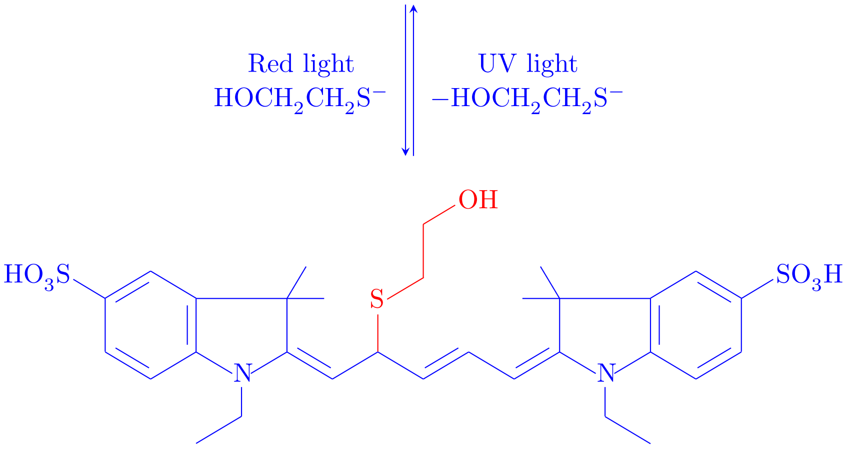
The newly-defined command `\markashR` is to put a Markash-type substituent on a specific bond of a structural formula. The white line due to the code,
`2==\addbscolor{\white\def\thinLineWidth{5pt}}{\null}`,
erases a part of the single bond to be substituted in a Markash way. By declaring the code, `\blue \def\thinLineWidth{0.8pt}`, just before `\begin{ChemEqnarray}`, the whole domain derived by the `ChemEqnarray` environment is colored in blue and typeset with using bold-lined bonds.

13.7 Thiols and Cyanine Dyes

The following scheme (eq. 13.7) is cited from a short article "How Thiols Photoswitch Cyanine Dyes" published in *Chem. & Eng. News*, December 14 (2009) page 34. Photoswitching of cyanine dyes is a key to super-resolution fluorescence microscopy techniques used for biological imaging. Red laser light switches a dye from a fluorescent to a dark state, where a thiol attacks the polymethine unit to give an adduct. Inversely, ultraviolet illumination stimulates the release of the thiol unit from the adduct so as to turn the fluorescence back on.



Fluorescent



Dark

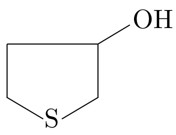
This scheme is drawn by writing the following code:

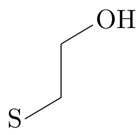
```
{\blue
\begin{ChemEqnarray*}
&
%\fbox{
\begin{XyMcompd}(3000,700)(-800,-50){}{}
\heptamethylenei[bdf]{%
1s==\nonaheterov[aegj{1+}]{1==N}{2==(yl);1==\dimethylene{}{2==(yl)};%
3Sa==\null;3Sb==\null;5==\ChemForm{HO_{3}S}};%
7s==\fiveheterov[{b{\sixfusev[ace]{}{2==\ChemForm{SO_{3}H}}{e}}}]%
{1==N}{5==(yl);1==\dimethylenei{}{1==(yl)};4Sa==\null;4Sb==\null}}{}
\end{XyMcompd}
%}
& \nonumber \\
\noalign{\centering\black Fluorecent}\\
\noalign{\vskip10pt}
&
\reactVEqarrow{0pt}{2cm}%
{\shortstack{Red light \\ \ChemForm{HOCH_2CH_2S^-}}}
{\shortstack{UV light \\ \ChemForm{- HOCH_2CH_2S^-}}}
& \nonumber\\
&
%\fbox{
\begin{XyMcompd}(3000,1000)(-800,-50){}{}
\heptamethylenei[adf]{%
1s==\nonaheterov[egj]{1==N}{2==(yl);1==\dimethylene{}{2==(yl)};%
3Sa==\null;3Sb==\null;5==\ChemForm{HO_{3}S}};%
7s==\fiveheterov[{b{\sixfusev[ace]{}{2==\ChemForm{SO_{3}H}}{e}}}]%
{1==N}{5==(yl);1==\dimethylenei{}{1==(yl)};4Sa==\null;4Sb==\null}}%
{3==\addbscolor{\red}{\fiveheterov{1==S}{1==(yl);3==OH}[cde]}}
\end{XyMcompd}
%}
```

```
& \label{eq:cyaninedye} \\
\noalign{\centering\black Dark}
\end{ChemEqnarray*}
}
```

The left indole (benzopyrrole) moiety is drawn by using a ready-made command `\nonaheterov`, while the right indole (benzopyrrole) moiety is drawn by a ring-fusion technique of the `\fiveheterov` and `\sixfusev` commands. It should be noted that the SCH_2CH_2OH unit of the adduct is drawn by using the `\fiveheterov` command, where an optional deletion list `[cde]` is used to designate skeletal bonds to be erased. Compare the following two structures drawn by using the `\fiveheterov` command.

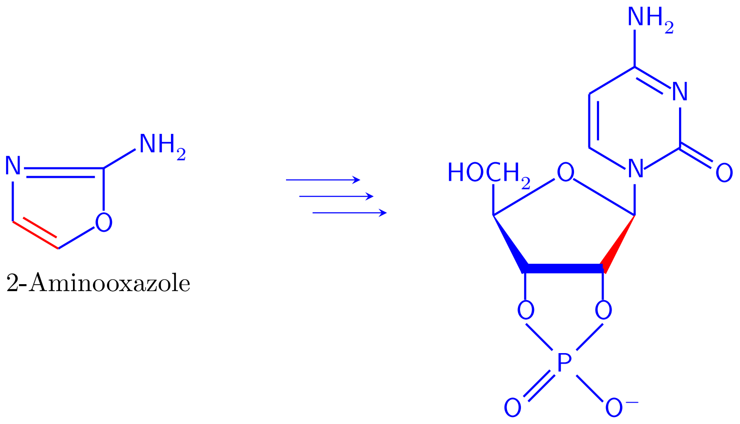
```
\fiveheterov{1==S}{3==OH}
\fiveheterov{1==S}{3==OH}[cde]
```





13.8 RNA Derived by a Counterintuitive Start

The following scheme (eq. 13.7) is cited from “Chemical Year in Review 2009” published in *Chem. & Eng. News*, December219 (2009) page 37 (entitled “DNA May Have Had a Counterintuitive Start”).



2-Aminooxazole

(13.7)

This scheme is drawn by writing the following code:

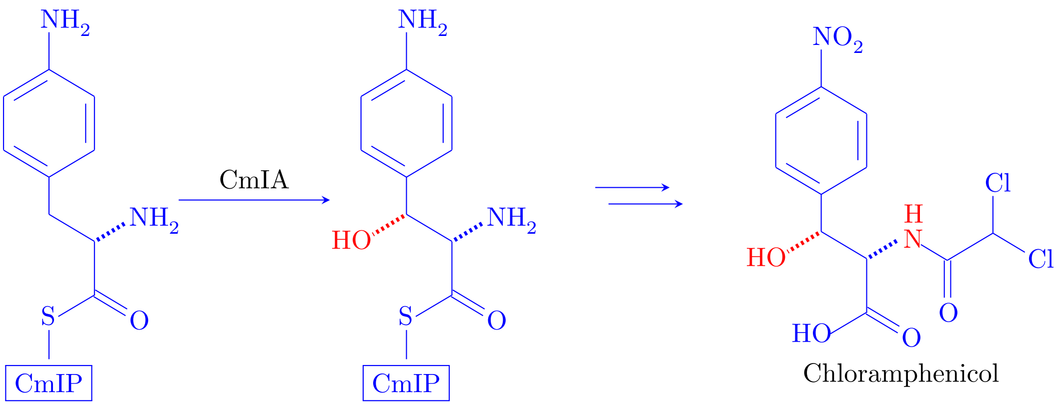
```
{\blue \def\thinLineWidth{0.8pt}
\let\substfont=\sffamily
\begin{ChemEquation}
\begin{tabular}{c}
\begin{XyMcompd}(500,500)(300,200){}{}
\fiveheterov({e{\addskbcolor{v}{\red}}})%
[c{e{\adddbcolor{i}{\red}}}]{2==O;4==N}{3==NH$_{2}$}
\end{XyMcompd}\\
\black 2-Aminooxazole
```

```
\end{tabular}
\qquad
\shortstack{$\llongrightarrow$ \\
\kern10pt$\llongrightarrow$ \\
\kern20pt$\llongrightarrow$}
\qquad
\begin{XyMcompd}(1000,1550)(100,-350){}{}
\fivesugarh{5==O;1s=={\red \WedgeAsSubst(0,0)(-3,-5){125}};%
4s==\WedgeAsSubst(0,0)(3,-5){125};%
3s==\PutBondLine(-15,0)(292,0){3.6pt}%
}{2Sa==O\put(-171,-190){\squareplanar{1==(yl);0==P;2==O$^{-}$;3D==O;1==;4==}};
%OH;
3Sa==O;4Sb==HOC\rlap{H$_{2}$};
1Sb==\sixheterov[ae]{2==N;4==N}{4==(yl);3D==O;1==NH$_{2}$}%
}[abc]
\end{XyMcompd}
\label{eq:DNA}
\end{ChemEquation}
}
```

For drawing furanose derivatives having bold skeletal bonds, see Page 24. The cyclic phosphate group is drawn by using the `\squareplanar` command. The declaration `\let\substfont=\sffamily` changes the font for printing substituents.

13.9 Hydroxylations

The following scheme (eq. 13.8) is cited from a short article "Diiron Enzymes Spark Hydroxylations" published in *Chem. & Eng. News*, August 23 (2010) page 33, which is concerned with a step in the biosynthesis of the antibiotic chloramphenicol.



Chloramphenicol

(13.8)

This scheme is drawn by writing the following code:

```
\begin{ChemEquation}\blue
\begin{XyMcompd}(500,1500)(300,-50){}{}
\sixheterov{4==S}{1==\bzdrv{4==(yl);1==NH$_{2}$};%
3D==O;2A==NH$_{2}$;4==\makebox(0,0){\kern6pt\fbox{CmIP}}}[def]
\end{XyMcompd}
\reactrarrow{0pt}{2cm}{\black CmIA}{\strut}
```

```
\begin{XyMcompd}(600,1500)(200,-50){}{}
\sixheterov{4==S;1s==\LeftAtomBond[\red]{5A=={HO}}
}{1==\bzdrv{4==(yl);1==NH$_{2}$};%
3D==O;2A==NH$_{2}$;4==\makebox(0,0){\kern6pt\fbox{CmIP}}}[def]
\end{XyMcompd}
\qquad
\shortstack{$\llongrightarrow$ \\
\kern10pt$\llongrightarrow$}
\qquad
\begin{tabular}{c}
\begin{XyMcompd}(1000,1200)(200,250){}{}
\sixheterov
{1s==\LeftAtomBond[\red]{5A=={HO}};4==\lmoiety{HO}}
{1==\bzdrv{4==(yl);1==NO$_{2}$};3D==O;%
2A==\bluex{\ryl(4=={\red \upnobond{N}{H}}){%
5==\dimethylene{}{1==(yl);1D==O;2==Cl;2W==Cl}}}}[def]
\end{XyMcompd}\\
\noalign{\vskip5pt}
{\black Chloramphenicol}
\end{tabular}
\label{eq:CmIA}
\end{ChemEquation}
```

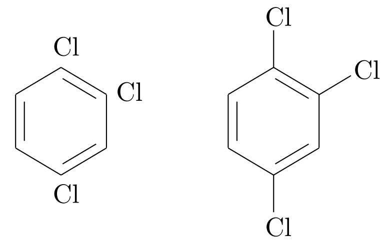
For the command `\LeftAtomBond`, see Subsection 11.5.1.

13.10 Friedel-Crafts Acylation

As found in several textbooks, substitution bonds of aromatic rings are omitted so that substituents link to ring positions directly. Although the XΥMTEX system does not support structural formulas of this type, a rather dirty technique is available by combining utilities supported by XΥMTEX. For example, the codes:

```
\sixheterov[ace]{%
1==\upnobond{}{Cl};1s==\null;%
2==\phantom{C}Cl;2s==\null;%
4==\downnobond{}{Cl};4s==\null%
}{}
\sixheterov[ace]{}{1==Cl;2==Cl;4==Cl}
```

generate the following structural formulas:



where the latter shows a structural formula due to a standard drawing of XΥMTEX. Note that the substituents of the former structure are designated in the ATOMLIST (the atom list) of `\sixheterov`, while those of the latter structure are designated in the the SUBSLIST (the substituent list) of `\sixheterov`.

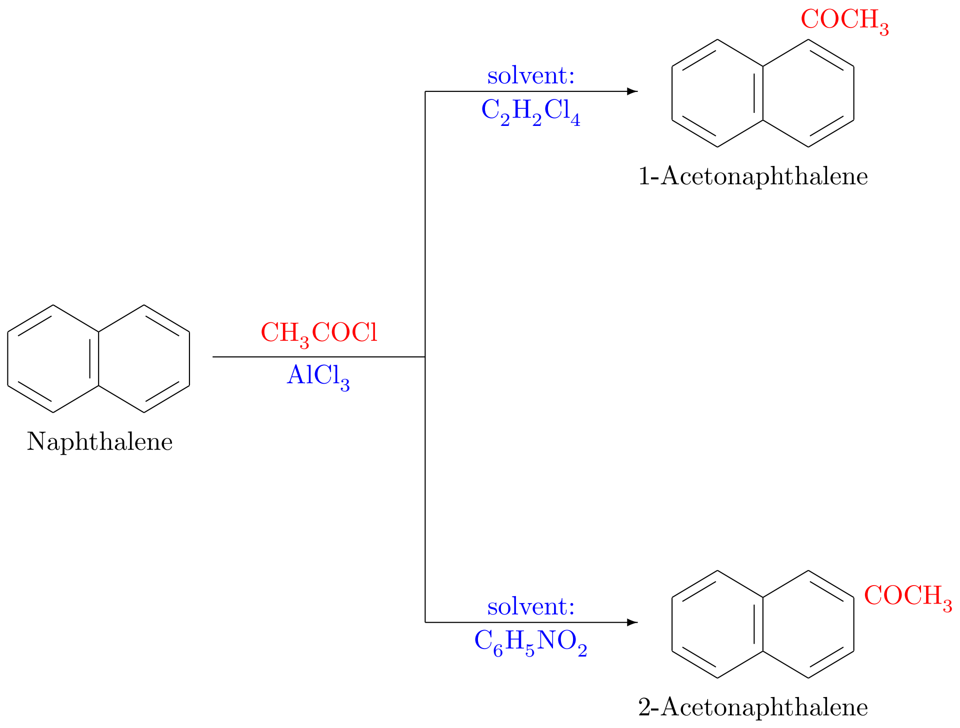


Figure 13.1: Friedel-Crafts acylation of naphthalene

The designation `1s==\null` in the former code redraws erased lines at a corner position, which have been brought about as a result of a designation placed just before (e.g., `\upnobond{}{Cl}`).

This technique is applicable to draw a reaction scheme of the Friedel-Crafts acylation of naphthalene, as shown in Figure 13.1. Coloring portions of formulas is realized by a usual technique of coloring.

Figure 13.1 has been drawn by the following code, where XΥMTEX codes are written in a `picture` environment supported by LATEX 2$_\varepsilon$. It should be noted that `\unitlength` (=0.1pt) of XΥMTEX codes is common to the the `picture` environment.

```
\begin{picture}(4000,3000)(0,0)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Structural formulas and their names%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\put(0,1000){\decaheterov[acfhk]{}{}}
\put(300,1100){Naphthalene}
\put(2500,2000){%
\decaheterov[acfhk]{1==\upnobond{}{\red\ChemForm{COCH_3}};1s==\null}{}}
\put(2600,2100){1-Acetonaphthalene}
\put(2500,0){%
\decaheterov[acfhk]{2=={\red \phantom{C}\ChemForm{COCH_3}};2s==\null}{}}
\put(2600,100){2-Acetonaphthalene}
%%%%%%%%%%%%%%%%%%%
%Lines and arrows%
%%%%%%%%%%%%%%%%%%%
```

```
\put(1000,1450){\line(1,0){800}}
\put(1800,450){\line(0,1){2000}}
\put(1800,2450){\vector(1,0){800}}
\put(1800,450){\vector(1,0){800}}
%%%%%%%%%%%%%%%%%%%%
%Reaction conditions%
%%%%%%%%%%%%%%%%%%%%
\put(1000,1480){\makebox(800,0)[bc]{\red \ChemForm{CH_3 COCl}}}
\put(1000,1420){\makebox(800,0)[tc]{\blue \ChemForm{AlCl_3}}}
\put(1800,2480){\makebox(800,0)[bc]{\blue solvent:}}
\put(1800,2420){\makebox(800,0)[tc]{\blue \ChemForm{C_2 H_2 Cl_4}}}
\put(1800,480){\makebox(800,0)[bc]{\blue solvent:}}
\put(1800,420){\makebox(800,0)[tc]{\blue \ChemForm{C_6 H_5 NO_2}}}
\end{picture}
```

Chemical formulas such as $C_6H_5NO_2$ are typeset by such designations as `\ChemForm{C_6␣H_5␣NO_2}` in this code, where a space (␣) is inserted to differentiate every units for the same of readability. The same chemical formulas can be obtain by writing `\ChemForm{C_6H_5NO_2}`, `\ChemForm{C_{6}H_{5}NO_{2}}`, and `C$_{6}$H$_{5}$NO$_{2}$`.

The two steps of Figure 13.1 can be numbered by using the `ChemEqnarray` environment, which is supported by the `chemist` package. To do this task, the command `\FrCrArrows` is first defined to draw an arrow unit which appears in Figure 13.1, as follows:

```
\def\FrCrArrows{%
%\fbox{
%\begin{picture}(1600,2600)(1000,0)%totally surrounding box
\begin{picture}(1600,0)(1000,1450)%surrounding box of height zero
%%%%%%%%%%%%%%%%%
%Lines and arrows%
%%%%%%%%%%%%%%%%%
\put(1000,1450){\line(1,0){800}}
\put(1800,450){\line(0,1){2000}}
\put(1800,2450){\vector(1,0){800}}
\put(1800,450){\vector(1,0){800}}
%%%%%%%%%%%%%%%%%%%%
%Reaction conditions%
%%%%%%%%%%%%%%%%%%%%
\put(1000,1480){\makebox(800,0)[bc]{\red \ChemForm{CH_3 COCl}}}
\put(1000,1420){\makebox(800,0)[tc]{\blue \ChemForm{AlCl_3}}}
\put(1800,2480){\makebox(800,0)[bc]{\blue solvent:}}
\put(1800,2420){\makebox(800,0)[tc]{\blue \ChemForm{C_2 H_2 Cl_4}}}
\put(1800,480){\makebox(800,0)[bc]{\blue solvent:}}
\put(1800,420){\makebox(800,0)[tc]{\blue \ChemForm{C_6 H_5 NO_2}}}
\end{picture}%}
}
```

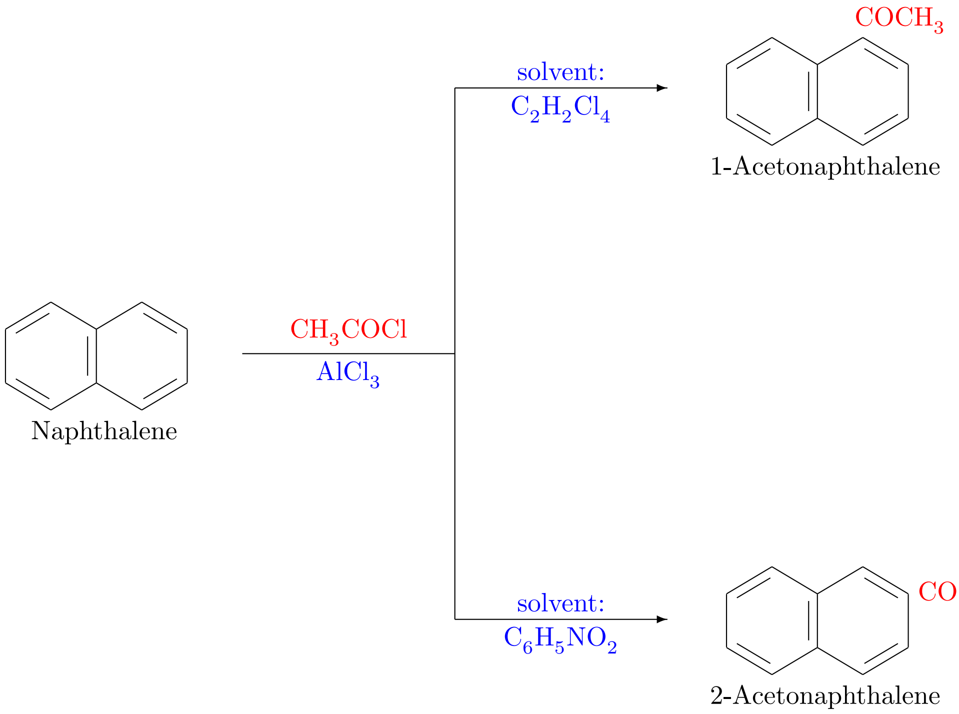
where the designation `\begin{picture}(1600,0)(1000,1450)` is a key to decide a surrounding box; i.e., its height is equal to zero and its width is equal to the domain of the resulting arrow unit.

Then the following code based on the `ChemEqnarray` environment is written:

```
\begin{ChemEqnarray}
&&
\begin{tabular}{c}
```

```
\begin{XyMcompd}(600,450)(300,250){}{}
\decaheterov[acfhk]{1==\upnobond{}{\red\ChemForm{COCH_3}};1s==\null}{}
\end{XyMcompd} \\
1-Acetonaphthalene \\
\end{tabular}
\label{eq:FrCr1} \\
\noalign{\vskip35pt}%vertical space adjustment
\begin{tabular}{c}
\begin{XyMcompd}(600,450)(300,250){}{}
\decaheterov[acfhk]{}{}
\end{XyMcompd} \\
Naphthalene \\
\end{tabular}
& \raisebox{8pt}{\FrCrArrows} & \nonumber \\
\noalign{\vskip35pt}%vertical space adjustment
&&
\begin{tabular}{c}
\begin{XyMcompd}(600,450)(300,250){}{}
\decaheterov[acfhk]{2=={\red \phantom{C}\ChemForm{COCH_3}};2s==\null}{}
\end{XyMcompd} \\
2-Acetonaphthalene \\
\end{tabular}
\label{eq:FrCr2}
\end{ChemEqnarray}
```

Thereby, we are able to obtain the following scheme, each step of which is numbered sequentially. The reaction-step numbers (eqs. 13.9 and 13.10) are cited by the `\label` and `\ref` mechanism of LaTeX 2ε.



(13.9)

(13.10)

13.11 Vitamin D_2

This is a color version of the reaction scheme drawn in Section 2.5 of the on-line manual of XΥMTEX version 4.04 (xymtx404.pdf), where skeletal and double bonds participating photochemical and thermochemical reactions are colored by using `\replaceSKbond` (skeletal bonds) and `\adddbcolor` (double bonds).

Irradiation of ergosterol (and lumisterol) causes the opening of the B ring to produce previtamin D_2 having a conjugated triene, which is a precursor of vitamin D_2 (ergocalciferol), as shown in Figure 13.2. The double bonds of each intermediate are colored by the present technique of coloring double bonds.

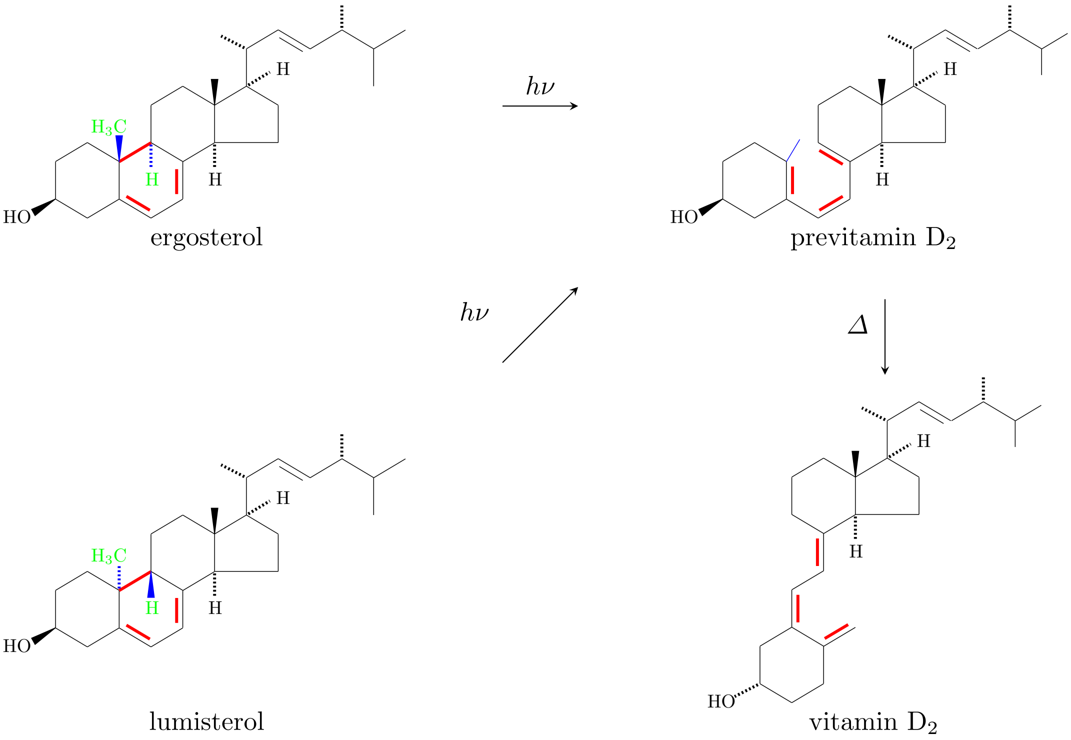


Figure 13.2: Photochemistry of ergosterol and lumisterol

To draw the intermediates contained in Figure 13.2, macros for drawing them are defined by applying the systematic way of coloring double bonds, i.e., `\lumisterol` for drawing limisterol, `\ergosterol` for drawing ergosterol, `\previtaminD` for drawing previtamin D, and `\vitaminDii` for drawing vitamin D_2.

```
%lumisterol
\def\lumisterol{%
\begin{XyMcompd}(2050,1150)(0,250){}{}
\steroidChain[{Zc}%
{i{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{e{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{g{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
]%
{3B==HO;9B==\addbscolor{\blue}{\greenx{H}};%
{10}A==\addbscolor{\blue}{\greenx{\lmoiety{H$_{3}$C}}};%
{13}B==\null;{14}A==H;{17}GA==H;%
{20}A==\null;{24}A==\null}
\end{XyMcompd}
```

```
}

%ergosterol
\def\ergosterol{%
\begin{XyMcompd}(2050,1150)(0,250){}{}
\steroidChain[{Zc}%
{i{\replaceSKbond[1.6pt](0,0)(5,3){171}{\red}}}%
{e{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{g{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
]%
{3B==HO;9A==\addbscolor{\blue}{\greenx{H}};%
{10}B==\addbscolor{\blue}{\greenx{\lmoiety{H$_{3}$C}}};%
{13}B==\null;{14}A==H;{17}GA==H;%
{20}A==\null;{24}A==\null}
\end{XyMcompd}
}

%previtamin D
\def\previtaminD{%
\begin{XyMcompd}(2050,1150)(0,250){}{}
\sixheterov[%
{b{\sixfusev[%
{a{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{c{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{e{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{a{\sixfusev[%
{b{\fivefusevi[%
{a{\sixfusev[a]{%
2s==\trimethylene{}{1==(yl);2A==\null;3==\null;3W==\null}
}{6A==\null}{D}[bc]}}
]{}{1GA==H}{D}}}
]{}{2FB==\null;3GA==H}{D}}}
]{}{}{E}[f]}}]
{}{2Sb==\addbscolor{\blue}{\null};5B==HO}
\end{XyMcompd}
}

%vitamin D$_{2}$ (ergocalciferol)
\def\vitaminDii{%
\begin{XyMcompd}(1650,1750)(0,250){}{}
\sixheterov[%
{a{\sixfusev[%
{c{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{e{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{f{\sixfusev[%b%
{b{\adddbcolor{v}{\red\def\thinLineWidth{1.6pt}}}}%
{a{\sixfusev[%
{b{\fivefusevi[
{a{\sixfusev[a]{%
2s==\trimethylene{}{1==(yl);2A==\null;3==\null;3W==\null}
}{6A==\null}{D}[bc]}}
]{}{1GA==H}{D}}}
]{}{2FB==\null;3GA==H}{D}%
```

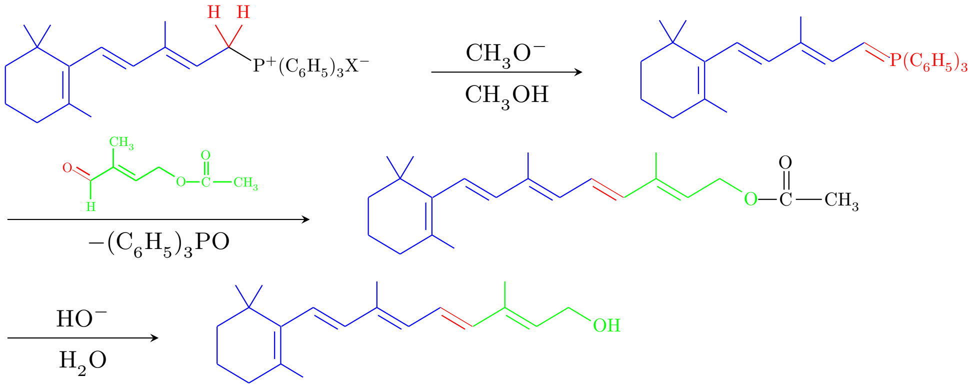
```
}}]{}{}{C}[def]}}]{}{}{D}[ab]}}]{}{5A==HO}
\end{XyMcompd}
}
```

By using these macros, Figure 13.2 is drawn by the following code:

```
\begin{figure}[h]
\begin{center}
\begin{tabular}{ccc}
\scalebox{0.7}{\ergosterol} &
\reactrarrow{0pt}{1cm}{$h\nu$}{\strut} & \scalebox{0.7}{\previtaminD} \\
ergosterol & & previtamin D$_{2}$ \\[10pt]
& \reactnearrow{0pt}{1cm}{\raisebox{10pt}{\rlap{$h\nu$}}}{\strut} &
\reactdarrow{0pt}{1cm}{$\Delta$}{\strut}  \\
\scalebox{0.7}{\lumisterol} && \scalebox{0.7}{\vitaminDii} \\
lumisterol & & vitamin D$_{2}$
\end{tabular}
\end{center}
\caption{Photochemistry of ergosterol and lumisterol}
\label{ff:PEL}
\end{figure}
```

13.12 Vitamin A_1

Vitamin A_1 is synthesized industrially by using a Wittig reaction, as shown in the following scheme (eq. 13.11), where a phosphorus ylide is an important intermediate.



Vitamin A_1 (13.11)

This scheme (eq. 13.11) is obtained by the following code due to the `ChemEqnarray` environment of the chemist package (or the chmst-pdf or chmst-ps package):

```
{\def\thinLineWidth{0.6pt}
\begin{ChemEqnarray}
&&
\scalebox{0.7}{\VitaminAiIntA}\qquad
\reactrarrow{-5pt}{2cm}{\small \ChemForm{CH_3O^{-}}}{\small \ChemForm{CH_3OH}}\qquad
\scalebox{0.7}{\VitaminAiIntB} \nonumber \\
&&
```

```
\reactrarrow{0pt}{4cm}{\def\thinLineWidth{1pt}
\scalebox{0.5}{\VitaminAiIntC}\\[5pt]}{\small \ChemForm{-(C_6H_5)_3PO}}\qquad
\scalebox{0.7}{\VitaminAiEster} \nonumber \\
&&
\reactrarrow{25pt}{2cm}{\small \ChemForm{HO^{-}}}{\small \ChemForm{H_2O}}\qquad
\shortstack{\scalebox{0.7}{\VitaminAi} \\ Vitamin A$_{1}$}
\end{ChemEqnarray}}
```

where respective intermediates (A–C and a Vitamin A_1 ester) and the final product (Vitamin A_1) are drawn after we define such commands as:

`\VitaminAiIntA`, `\VitaminAiIntB`, `\VitaminAiIntC`, `\VitaminAiEster`, and `\VitaminAi`.

The top declaration `\def\thinLineWidth{0.6pt}` is placed to make bonds thicker, so that the narrowing effects of size reduction (`\scalebox`) are cancelled out.

The intermediate A (the right intermediate in the first row of eq. 13.11 is drawn by the command `\VitaminAiIntA`, which is defined as follows:

```
\def\VitaminAiIntA{%
\begin{XyMcompd}(1800,650)(300,250){}{}\blue
\sixheterov[b]{%
2s==\hexamethylene[bd]{}{1==(yl);4==\null;%
6W==\addbscolor{\black}{\ChemForm{P^{+}(C_6H_5)_3X^{-}}};%
6Sa==\addbscolor{\red}{H};6Sb==\addbscolor{\red}{H}}}
{1Sa==\null;1Sb==\null;3==\null}
\end{XyMcompd}
}
```

where `\addbscolor` commands are used to color substituents and substitution bonds. Although the whole structure of `\VitaminAiIntA` is colored blue by declaring `\blue` globally, the local declarations of `\red` and `\black` overwrite respective colored objects over the blue backbone of the structure.

The intermediate B (the left intermediate in the first row of eq. 13.11) is a Wittig reagent (a phosphorus ylide), which is drawn by the macro `\VitaminAiIntB`. The macro is defined as follows:

```
\def\VitaminAiIntB{%
\begin{XyMcompd}(1800,600)(300,250){}{}\blue
\sixheterov[b]{%
2s==\heptamethylene[bd
{f{\adddbcolor{}{\red}}}%
{f{\replaceSKbond(0,0)(5,-3){130}{\red}}}%
]{7==\redx{\ChemForm{P(C_6H_5)_3}}
}{1==(yl);4==\null}}
{1Sa==\null;1Sb==\null;3==\null}
\end{XyMcompd}
}
```

where the `\adddbcolor` command is used to color a double bond and the `\replaceSKbond` command is used to color a skeletal bond.

The intermediate C above the reaction arrow in the second row of eq. eq. 13.11 is an aldehyde intermediate, which is drawn by the command `\VitaminAiIntC`. The macro for drawing the intermediate C is defined as follows:

```
\def\VitaminAiIntC{%
\begin{XyMcompd}(1300,500)(250,0){}{}\green
\pentamethylenei[c%
```

```
{a{\adddbcolor{i}{\red}}}%
{a{\replaceSKbond(171,-103)(-5,3){135}{\red}}}%
]{1==\redx{O}}%
{2==H;3==\ChemForm{CH_3};%
5W==\ryl(2==O){4==\tetrahedral{2==(yl);0==C;1D==O;4==\ChemForm{CH_3}}}}
\end{XyMcompd}
}
```

where the `\adddbcolor` command is used to color a double bond and the `\replaceSKbond` command is used to color a skeletal bond. Note that the local declaration of `\red` partially cancels the global coloring of the intermediate C by `\green`.

The right intermediate in the second row of eq. 13.11 is a Vitamin A_1 ester, which is drawn by the macro `\VitaminAiEster` defined as follows:

```
\def\VitaminAiEster{%
\begin{XyMcompd}(2500,600)(300,250){}{}\blue
\sixheterov[b]{%
2s==\heptamethylene[bd
{f{\adddbcolor{}{\red}}}%
{f{\replaceSKbond(0,0)(5,-3){171}{\red}}}%
]{%
7s==\greenx{\tetramethylene[b]{}%
{1==(yl);2==\null;%
4W==\blackx{\ryl(2==\greenx{O}){%
4==\tetrahedral{2==(yl);0==C;1D==O;4==\ChemForm{CH_3}}}}}}
}{1==(yl);4==\null}}
{1Sa==\null;1Sb==\null;3==\null}
\end{XyMcompd}
}
```

where the left moiety (due to the Wittig reagent) and the right moiety (due to the aldehyde intermediate) are differentiated by colors (blue and green). Moreover, the resulting olefinic function is emphasized by drawing in red. The terminal acetyl group is differentiated from other portions by drawing in black, because it participates in a subsequent hydrolysis.

The final product, Vitamin A_1, in the third row of eq. 13.11 is drawn by the following code:

```
\def\VitaminAi{%
\begin{XyMcompd}(2000,600)(300,250){}{}\blue
\sixheterov[b]{%
2s==\heptamethylene[bd%
{f{\adddbcolor{}{\red}}}%
{f{\replaceSKbond(0,0)(5,-3){171}{\red}}}]
{7s==\greenx{\tetramethylene[b]{}%
{1==(yl);2==\null;4W==OH}}}%
{1==(yl);4==\null}}%
{1Sa==\null;1Sb==\null;3==\null}
\end{XyMcompd}
}
```

where a newly introduced double bond is differentiated by red color.

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