XyMTEX (Version 4.02, 4.03) for Typesetting Chemical Structural Formulas. An Extension for Stereochemistry According to PostScript.

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Contents

Chapter 1

Introduction

1.1 History

The history of the XyMTEX system is summarized in Table 1.1:[1]

Table 1.1: Versions of XyMTEX

version	package files and comments
1.00 (1993)	(for LaTeX2.09) See Ref. [1, 2]. aliphat.sty, carom.sty, lowcycle.sty, hetarom.sty, hetaromh.sty, hcycle.sty, chemstr.sty, locant.sty, xymtex.sty
1.01 (1996)	(for LaTeX 2_ε) See Ref. [3]. ccycle.sty, polymers.sty, chemist.sty
1.02 (1998)	(not released) Nested substitution by 'yl'-function.
2.00 (1998)	Enhanced version based on the XyM Notation. See Ref. [4, 5]. 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. [6]
4.00 (2002)	(not released) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00)
4.01 (2004)	PostScript printing and length-variable central atoms
4.02 (2004)	(this version) PostScript printing and wedges bonds for stereochemistry
4.03 (2005)	(this version) PostScript printing and wavy bonds for stereochemistry

As described in the manual for XyMTEX Version 4.01 [7], XyMTEX after version 4.00 provides us with functions for supporting PostScript, where PSTrick [8] is used to generate PostScript codes embedded in a DVI (device-independent) file. After converting the DVI file into a PostScript file by such a converter as dvips, the PostScript file containing XyMTEX structural formulas can be processed by PostScript printer drivers or by the GhostScript interpreter so as to produce printed documents [9]. As a result, the XyMTEX system is now free from the limitations of the LaTeX picture environment. Although the enhanced flexibility of XyMTEX has been accomplished at the expense of portability within TeX/LaTeX, it assures a further expansion of the domain of XyMTEX, where various functions due to PostScript can be used to draw structural formulas.

[1] The description for Version 4.02 in this chapter is also effective to Version 4.03.

One of the most important features of XYMTEX version 4.02 is that new stereochemical functions are supported, where a pair of wedged bonds/hashed dash bonds, a pair of wedged bonds/hashed wedged bonds, and a pair of dash bonds/hashed dash bonds can be switched to draw structural formulas with specified absolute configurations.

1.2 Package Files of XYMTEX Version 4.02

The XYMTEX system (version 4.02) consists of the package files listed in Table 1.2, where the packages xymtx-px.sty and aliphat.sty are enhanced to draw wedged bonds for stereochemistry.

Table 1.2: Package Files of XYMTEX and Related Files

package name	included functions
XYMTEX Files	
aliphat.sty	macros for drawing aliphatic compounds
carom.sty	macros for drawing vertical and horizontal types of carbocyclic compounds
lowcycle.sty	macros for drawing five-or-less-membered carbocycles.
ccycle.sty	macros for drawing bicyclic compounds etc.
hetarom.sty	macros for drawing vertical types of heterocyclic compounds
hetaromh.sty	macros for drawing horizontal types of heterocyclic compounds
hcycle.sty	macros for drawing pyranose and furanose derivatives
chemstr.sty	basic commands for atom- and bond-typesetting
locant.sty	commands for printing locant numbers
polymers.sty	commands for drawing polymers
fusering.sty	commands for drawing units for ring fusion
methylen.sty	commands for drawing zigzag polymethylene chains
sizeredc.sty	commands for size reduction
xymtx-ps.sty	macros for PostScript printing (Version 4.02). These macros are substituted for several macros contained in the chemstr package.
XYMTEX Utilities	
xymtex.sty	a package for calling all package files except xymtx-ps.sty (no PostScript)
xymtexps.sty	a package for calling all package files (PostScript, i.e. with xymtx-ps.sty)
Related Files	
chemist.sty	commands for using 'chem' version and chemical environments
chmst-ps.sty	macros for PostScript printing. These macros are substituted for several macros contained in chemist package.

XYMTEX Version 4.02 works in two modes:

1. TEX/LATEX compatible mode: When xymtex.sty is input, all of the package files of the XYMTEX system except xymtx-ps.sty are loaded. This mode draws β-bonds as thick lines and α-bonds as dotted lines.

```
¥documentclass{article}
¥usepackage{xymtex}
¥begin{document}
(formula)
¥end{document}
```

To reduce formula sizes, epic.sty is automatically loaded.

2. PostScript compatible mode: When xymtexps.sty is input, all of the package files of the XyMTEX system (also xymtx-ps.sty) are loaded. This mode draws β/α-bonds in one format selected from a pair of wedged bonds/hashed dash bonds (default), a pair of wedged bonds/hashed wedged bonds, and a pair of dash bonds/hashed dash bonds.

```
¥documentclass{article}
¥usepackage{xymtexps}
¥begin{document}
(formula)
¥end{document}
```

After compiling these TEX files by the TEX system, the resulting DVI files are converted in the PostScript files, which are printed by PostScript tools.

The TEX file for printing the present manual is written as follows:

```
%xymtx402.tex
%Copyright (C) 2002, 2004, Shinsaku Fujita, All rights reserved.
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%This file is a part of xymtx402.tex that is the manual of the macro
%package 'XyMTeX' for drawing chemical structural formulas.
%This file is not permitted to be translated into Japanese and any other
%languages.
¥typeout{``xymtx402.tex''---
This file is a part of xymtex.tex that is the manual of the macro %
package 'XyMTeX'. 2004/12/20 S. Fujita}
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
¥documentclass[draft]{book}
¥usepackage{xymtexps,chemist,chmst-ps}
¥usepackage{xymman}
¥begin{document}
¥mbox{}
¥thispagestyle{empty}
¥vfill

¥begin{center}
¥LARGE¥bfseries
¥protect¥XyMTeX{} (Version 4.02) for
Typesetting Chemical Structural Formulas.
An Extension for Stereochemistry
According to PostScript.
¥end{center}

¥vspace*{2cm}

¥begin{center}
{¥Large¥bfseries Shinsaku Fujita}

¥vspace*{1cm}
Department of Chemistry and Materials Technology, ¥¥
Kyoto Institute of Technology, ¥¥
Matsugasaki, Sakyoku, Kyoto, 606-8585 Japan
¥par¥vspace*{1cm}
December 20, 2004 (For Version 4.02) ¥copyright ¥¥
¥end{center}
```

```
¥vfill¥mbox{}

¥newpage
¥tableofcontents

% for version 4.02
¥input{xymps402}

% for references
¥input{xym402bib}
¥end{document}
```

Chapter 2

Bonds for Stereochemistry

2.1 Stereochemical Expressions of Bonds

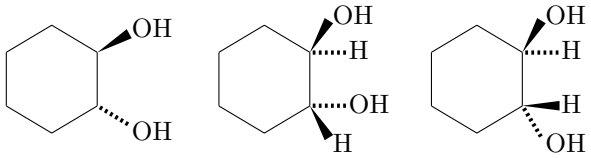
2.1.1 Wedged Bonds and Hashed Dash Bonds

According to "Basic Terminology of Stereochemistry" of IUPAC Recommendations 1996 [10], a bond from an atom in the plane of drawing to an atom above the plane (i.e., so-called β-bond) is shown with a bold wedge, which starts from the atom in the plain at the narrow end of the wedge; and a bond below the plane (i.e., so-called α-bond) is shown with a hashed bold dash (short parallel lines). Hence, the combination of wedges and hashed dashes is selected as a default setting for XyMTEX version 4.02.

For example, the the following codes:

```
¥cyclohexanev{2B==OH;3A==OH}
¥cyclohexanev{2SA==H;2SB==OH;3SA==OH;3SB==H}
¥cyclohexanev{2SA==H;2SB==OH;3Sd==OH;3Su==H}
```

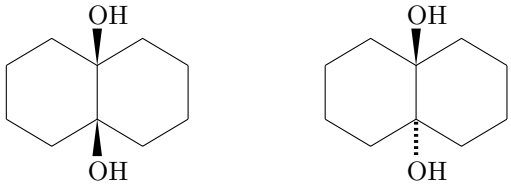
generate formulas represented by:



Codes for drawing *cis*- and *trans*-Decalinediol:

```
¥decaheterov{}{9B==OH;{10}B==OH}
¥decaheterov{}{9A==OH;{10}B==OH}
```

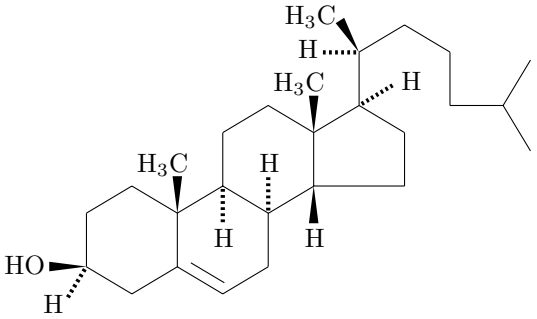
generate the following formulas:



Cholesterol (Cholest-5-en-3β-ol) can be drawn by the following code:

```
¥steroidchain[e]{3Su==HO;3Sd==H;8A==H;9A==H;{{10}B}==¥lmoiety{H$_{3}$C};%
{{13}B}==¥lmoiety{H$_{3}$C};{{14}B}==H;{{17}GA}==H;%
{{20}SB}==¥lmoiety{H$_{3}$C};{{20}SA}==H}
```

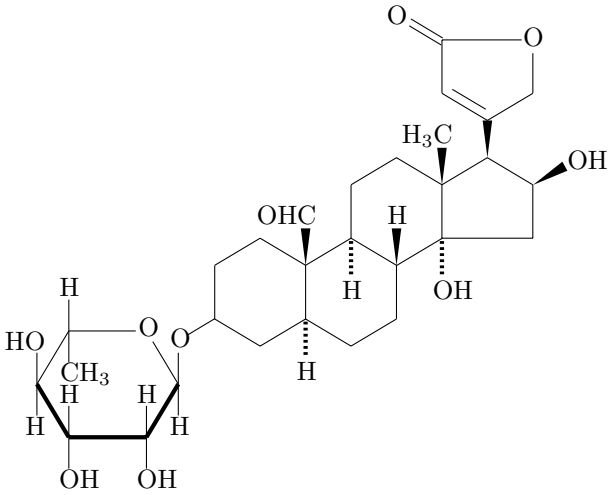
Thereby, we can obtain the following diagram:



The structural formula of adonitoxin, can be drawn by nesting a "yl"-function and a `¥ryl` command, where the pyranose ring is regarded as a mother skeleton. Thus, the code

```
¥pyranose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==CH$_{3}$;%
1Sb==¥ryl(8==O){3==%
¥steroid{3==(yl);5A==H;8B==H;9A==H;{{10}B}==¥lmoiety{OHC};{{14}A}==OH;%
{{13}B}==¥lmoiety{H$_{3}$C};{{16}B}==OH;%
{{17}B}==¥fiveheterov[e]{3==O}{4D==O;1==(yl)}}}}
```

typesets the following formula:

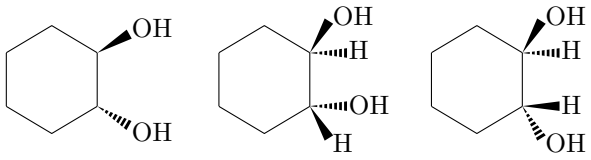


2.1.2 Wedged Bonds and Hashed Wedged Bonds

The use of a wedge of parallel lines (a hashed wedged bond) is not recommended by "Basic Terminology of Stereochemistry" of IUPAC Recommendations 1996 [10]. However, the combination of wedged bonds and hashed wedged bonds is frequently used. By declaring the switching command `¥wedgehashedwedge`, one can draw structural formulas by using the combination. For example, the the following codes:

```
¥wedgehashedwedge
¥cyclohexanev{2B==OH;3A==OH}
¥cyclohexanev{2SA==H;2SB==OH;3SA==OH;3SB==H}
¥cyclohexanev{2SA==H;2SB==OH;3Sd==OH;3Su==H}
```

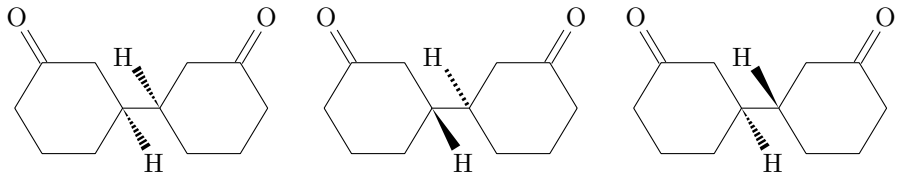
generate formulas represented by:



As found by the inspection of the three formulas depicted above, the β- and α-bonds are drawn by the combination of wedged bonds and hashed wedged bonds after the declaration of `¥wedgehashedwedge`. Thus, a single declaration of `¥wedgehashedwedge` at the top of a document file is sufficient if the combination of wedged bonds and hashed wedged bonds is used throughout the document.

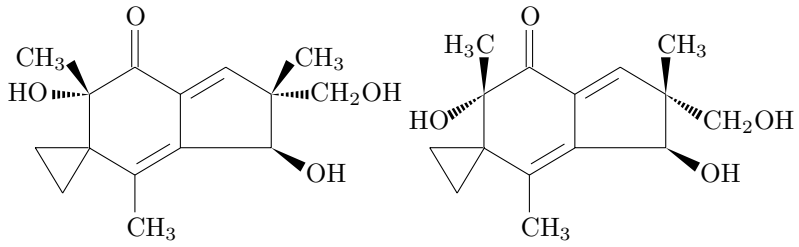
If the switch `¥wedgehasheddash` is declared, the drawing mode is returned to the default mode, as shown in the following examples:

```
¥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}}
```



Illudin S, an anti-tumor antibiotic substance, is drawn in two ways in which the directions of wedges are altered:

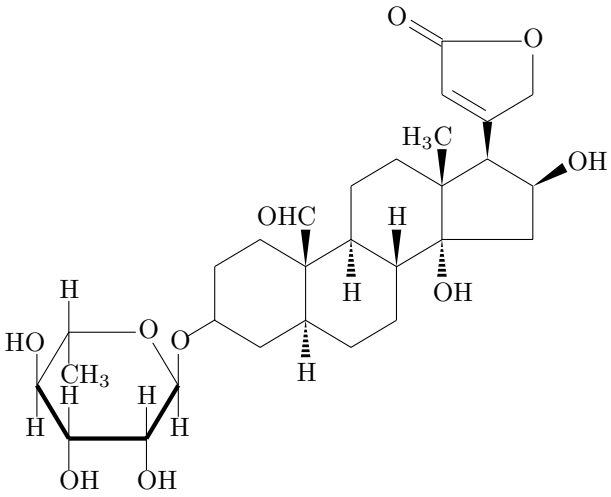
```
¥wedgehashedwedge
¥nonaheterovi[di]{5s==¥cyclopropanev{2==(yl)}}%
{2SB==CH$_{3}$;2SA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;6SB==CH$_{3}$;6SA==HO;7D==O} ¥hskip1cm
¥nonaheterovi[di]{5s==¥cyclopropanev{2==(yl)}}%
{2FB==CH$_{3}$;2GA==CH$_{2}$OH;3B==OH;4==CH$_{3}$;6GB==¥lmoiety{H$_{3}$C};6FA==HO;7D==O}
```



The structural formula of adonitoxin can be drawn in this mode by the code:

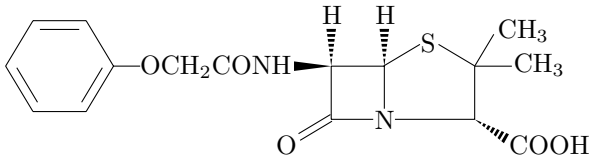
```
¥wedgehashedwedge
¥pyranose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==CH$_{3}$;%
1Sb==¥ryl(8==O){3==%
¥steroid{3==(yl);5A==H;8B==H;9A==H;{{10}B}==¥lmoiety{OHC};{{14}A}==OH;%
{{13}B}==¥lmoiety{H$_{3}$C};{{16}B}==OH;%
{{17}B}==¥fiveheterov[e]{3==O}{4D==O;1==(yl)}}}}
```

which typesets the following formula:



Penicillin V can be drawn as follows:

```
¥wedgehashedwedge
¥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}
```



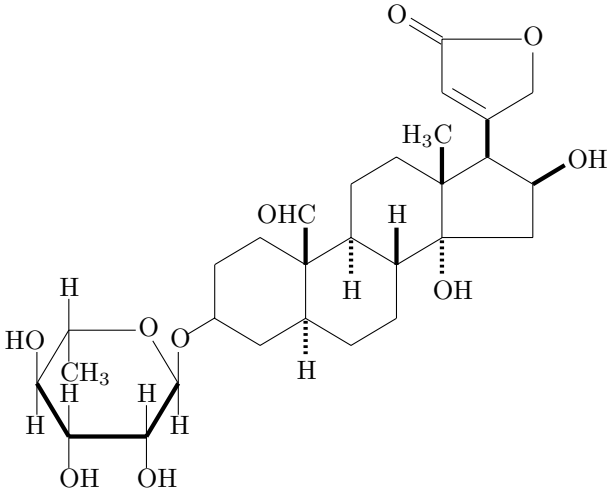
Note that the XyMcompd environment is defined in chemist.sty.

2.1.3 Bold Dash Bonds and Hashed Dash Bonds

A bold dash bond may be used instead of a bold wedged bond according to IUPAC Recommendations 1996 [10]. By declaring the switching command `¥dashhasheddash`, one can draw structural formulas by using the combination of bold dash bonds and hashed dash bonds. In this mode, the code:

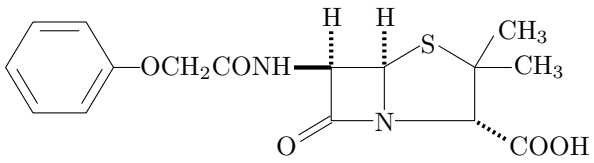
```
¥dashhasheddash
¥pyranose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==CH$_{3}$;%
1Sb==¥ryl(8==O){3==%
¥steroid{3==(yl);5A==H;8B==H;9A==H;{{10}B}==¥lmoiety{OHC};{{14}A}==OH;%
{{13}B}==¥lmoiety{H$_{3}$C};{{16}B}==OH;%
{{17}B}==¥fiveheterov[e]{3==O}{4D==O;1==(yl)}}}}
```

typesets the following formula:



In a similar way, 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}
```



2.2 PostScript Compatible Mode vs. TEX/LATEX Compatible Mode

Three profiles of the PostScript compatible mode are summarized in Fig. 2.1, which also contains structural formulas by the TEX/LATEX compatible mode for comparison. Figure 2.1 is obtained by the following codes:

```
¥begin{tabular}{l}
PostScript compatible mode (wedge and hashed dash): ¥¥
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F} ¥¥
¥noalign{¥vskip10pt}
PostScript compatible mode (wedge and hashed wedge): ¥¥
¥wedgehashedwedge
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F} ¥¥
```

```
¥noalign{¥vskip10pt}
PostScript compatible mode (dash and hashed dash): ¥¥
¥dashhasheddash
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}  ¥¥
¥noalign{¥vskip10pt}
TeX/LaTeX compatible mode: ¥¥
¥reducedsizepicture
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1D==O;4SA==CH$_{3}$;4SB==F} ¥¥
¥end{tabular}
```

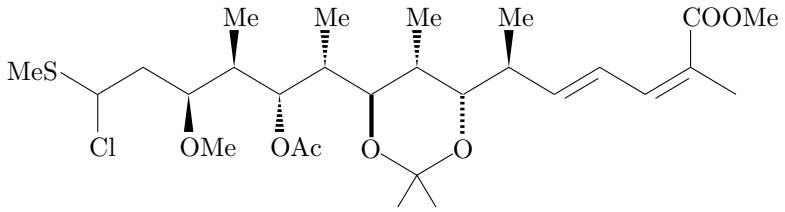
By means of the sizeredc package (distributed after Version 3.00), the original LaTeX picture environment can be used by a switching declaration `¥reducedsizepicture` in order to reduce the sizes of formulas, as shown in the bottom of Fig. 2.1.

2.3 Skeletal Bond Exceptions

Skeletal bonds in a ring system can be drawn in a bold line or a dotted line by using the skeletal list as an optional argument. However, they are not drawn in wedged forms in XyMTEX version 4.02. For example, the code:

```
¥wedgehashedwedge
¥sixheterov({bA}{eB}){3==O;5==O;6s==¥heptamethylene{}
{1W==MeS;1==Cl;3B==OMe;4B==Me;5A==OAc;6A==Me;7==(yl)};%
2s==¥heptamethylene[ce]{}{1==(yl);2B==Me;6==COOMe}}
{1A==Me;4Sa==¥null;4Sb==¥null}
```

draws the following formula:

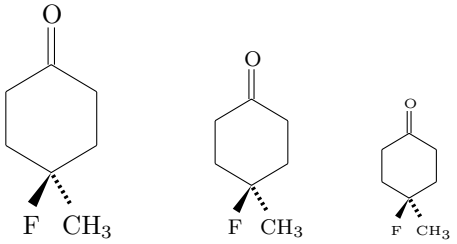


where skeletal bonds are expressed as bold dashes or hashed dashes even if the switching command `¥wedgehashedwedge` is declared.

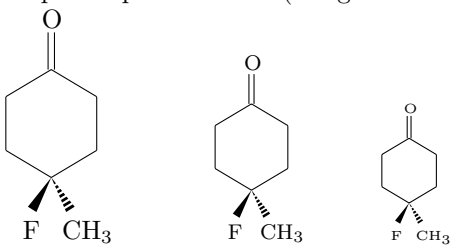
If you change the skeletal bonds into wedges, you should rely on a rather dirty technique. For example, the code:

```
¥wedgehashedwedge
%¥fbox{%
¥begin{XyMcompd}(2800,800)(-1100,150){}{}
¥sixheterov{3==O;5==O;6s==¥heptamethylene{}
{1W==MeS;1==Cl;3B==OMe;4B==Me;5A==OAc;6A==Me;7==(yl);7B==¥null};%
2s==¥heptamethylene[ce]{}{1==(yl);2B==Me;6==COOMe;1A==¥null}}
{1A==Me;4Sa==¥null;4Sb==¥null}[be]
```

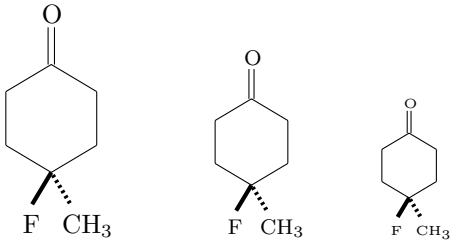
PostScript compatible mode (wedge and hashed dash):



PostScript compatible mode (wedge and hashed wedge):



PostScript compatible mode (dash and hashed dash):



TeX/LaTeX compatible mode:

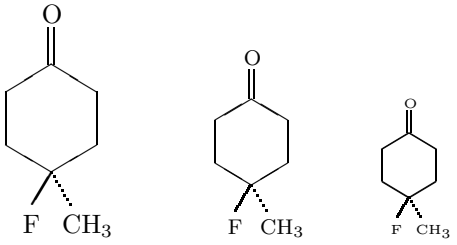
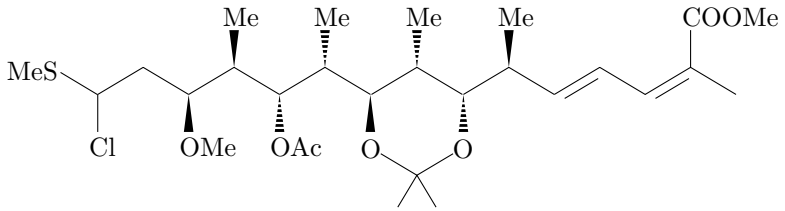


Figure 2.1: PostScript Compatible Mode vs. TEX/LATEXCompatible Mode

```
¥end{XyMcompd}
%}
```

draws the following formula:



The optional argument [be] in the end of this code is the OMITLIST of the `¥sixheterov` command; and the omitted bonds are replaced by a wedge (due to `7B==¥null` in the first `¥heptamethylene` command) and by a hashed wedge (due to `1B==¥null` in the second `¥heptamethylene` command). A more systematic but still dirty approach will be discussed in the next chapter.

Chapter 3

Skeletal Bonds for Stereochemistry

3.1 Skeletal Bonds as Spiro Substituents

The optional argument SKBONDLIST supports bold dash bonds and hashed dash bonds to represent α- and β-bonds for stereochemistry. As shown in the preceding section, such bonds can be changed into wedges and hashed wedges by means of a rather dirty technique. This technique is refined into a more systematic one by defining the following macros:

```
¥WedgeAsSubst(x,y)(x-slope,y-slope){length} %for wedges
¥HashWedgeAsSubst(x,y)(x-slope,y-slope){length} %for hashed wedges
```

where (x,y) represents a starting point, (x-slope,y-slope) represents a slope that is specified in the manner of the LaTeX picture environment, and {length} represents the x-projection of a wedge or hashed wedge. These macros are defined in the package xymtx-ps.sty. For example, the codes:

```
¥wedgehashedwedge
¥sixheteroh({bA}{eB}){3==O;5==O}{1A==Me;2==¥null;6==¥null;4Sa==¥null;4Sb==¥null}¥hskip2cm
¥sixheteroh{3==O;5==O;2s==¥HashWedgeAsSubst(0,0)(1,0){160};%
6s==¥WedgeAsSubst(0,0)(1,0){160}}%
{1A==Me;2==¥null;6==¥null;4Sa==¥null;4Sb==¥null}[be]
```

generate the following structural formulas:

The left formula shows a default expression of skeletal bonds, which is unchanged even if such a switch as ¥wedgehashedwedge is declared. The right formula shows the change of such skeletal bonds by using the macros ¥WedgeAsSubst and ¥HashWedgeAsSubst. It should be noted that these macros are described in the ATOMLIST according to the "atom-derivation" methodology for spiro substituents and that superposed skeletal bonds are omitted by the OMITLIST at the end of the second code ([be]).

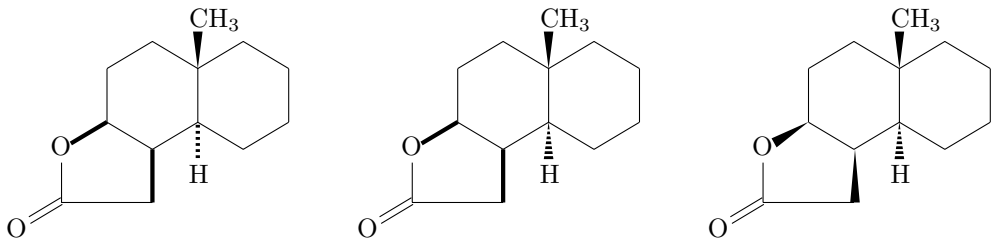
The following examples show three modes of bold skeletal bonds:

```
¥begin{tabular}{lll}
default & ¥verb/¥wedgehashedwedge/ & customized ¥¥
¥decaheterov[%
```

```
{f¥fivefusevi({bB}{eB}){5==O}{4D==O}{A}}]{}{9A==H;{{10}B}==CH$_{3}$} &
¥wedgehashedwedge
¥decaheterov[%
{f¥fivefusevi({bB}{eB}){5==O}{4D==O}{A}}]{}{9A==H;{{10}B}==CH$_{3}$} &
¥wedgehashedwedge
¥decaheterov[%
{f¥fivefusevi{5==O;2s==¥WedgeAsSubst(0,0)(0,-1){200};%
1s==¥WedgeAsSubst(0,0)(-5,-3){130}}{4D==O}{A}[be]}]{}{9A==H;{{10}B}==CH$_{3}$}
¥¥
¥end{tabular}
```

These codes generate structural formulas having various combinations, i.e., default (wedged bonds, hashed dash bonds, and dash skeletal bonds), the `¥wedgehashedwedge` mode (wedged bonds, hashed wedged bonds, and dash skeletal bonds), and a customized mode (wedged bonds, hashed wedged bonds, and wedged skeletal bonds):

default `¥wedgehashedwedge` customized

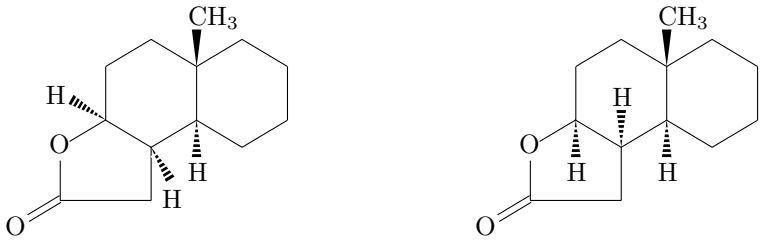


These expressions stress the decaline ring system (6-6) as a template of synthesis so that the five-membered lactone is regarded as a tentative substituent.

If one changes his/her viewpoint, the same molecule may be alternative drawn as follows:

```
¥decaheterov[%
{f¥fivefusevi{5==O}{4D==O}{A}}]{}{9A==H;5SA==H;6GA==H;{{10}B}==CH$_{3}$} ¥hskip2cm
¥decaheterov[%
{f¥fivefusevi{5==O}{4D==O;2FA==H}{A}}]{}{9A==H;6FA==H;{{10}B}==CH$_{3}$}
```

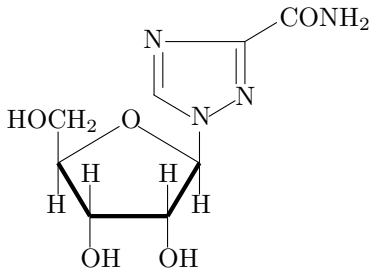
These codes generate such expressions that the tricyclic ring system (6-6-5) is taken into predominant consideration:



3.2 Furanoses

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:

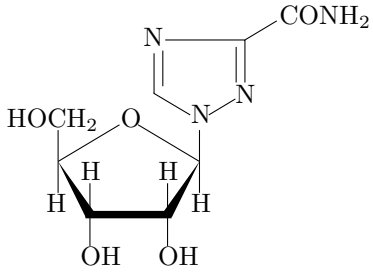
```
¥furanose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H;4Sb==HOC¥rlap{H$_{2}$};
1Sb==¥fiveheterov[bd]{1==N;2==N;4==N}{1==(yl);3==CONH$_{2}$}}
```



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 described above as well as the PSTrick command ¥psline. Thus, the code:

```
¥fivesugarh{5==O;1s==¥WedgeAsSubst(0,0)(-3,-5){120};4s==¥WedgeAsSubst(0,0)(3,-5){120};%
3s==¥psline[linewidth=2.8pt,linestyle=solid,linecolor=black](-17,0)(307,0)%
}{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]
```

generates the following formula:

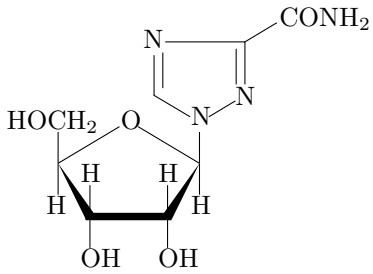


This input code can be simplified by making a tentative macro named ¥myfuranose as follows:

```
¥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==¥psline[linewidth=2.8pt,linestyle=solid,linecolor=black](-17,0)(307,0)}{#2}[abc]}
¥makeatother
```

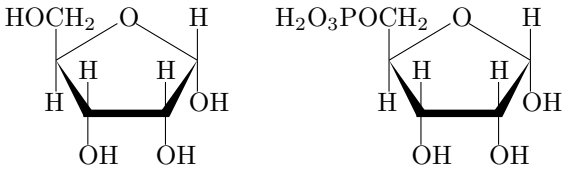
Thereby, the same formula can be typeset by writing a more simplified code:

```
¥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$_{2}$}}
```



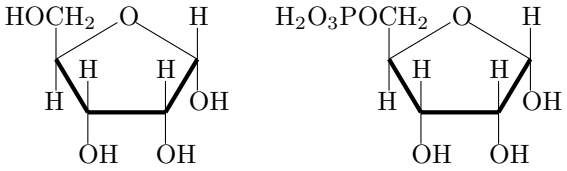
The tentative macro ¥myfuranose is convenient to draw various furanoses, e.g., α-D-ribofuranose and its 5-phosphoric acid:

```
¥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$_{2}$}}
```

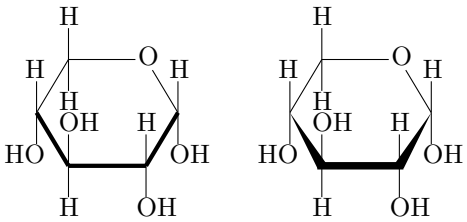


3.3 Pyranoses

The same situations as described for furanose hold true for pyranoses. Thus, two expressions of α-D-xylose are obtained by the following codes:

```
¥pyranose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==OH;3Sa==H;4Sa==HO;4Sb==H;5Sa==H;5Sb==H}
¥sixsugarh{6==O;1s==¥WedgeAsSubst(0,0)(-3,-5){120};4s==¥WedgeAsSubst(0,0)(3,-5){120};%
3s==¥psline[linewidth=2.8pt,linestyle=solid,linecolor=black](-17,0)(307,0)%
}{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==OH;3Sa==H;4Sa==HO;4Sb==H;5Sa==H;5Sb==H}[abc]
```

which generate the following formulas:

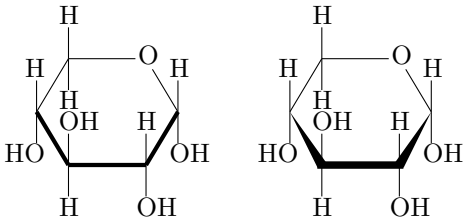


Let us make a macro named ¥mypyranose as follows:

```
¥makeatletter
¥def¥mypyranose{¥@ifnextchar[{¥@mypyranose}{¥@mypyranose[]}}
¥def¥@mypyranose[#1]#2{%
¥sixsugarh[#1]{6==O;1s==¥WedgeAsSubst(0,0)(-3,-5){120};4s==¥WedgeAsSubst(0,0)(3,-5){120};%
3s==¥psline[linewidth=2.8pt,linestyle=solid,linecolor=black](-17,0)(307,0)%
}{#2}[abc]}
¥makeatother
```

Then, the same argument declared in ¥pyranose and ¥mypyranose generates alternative expressions as follows:

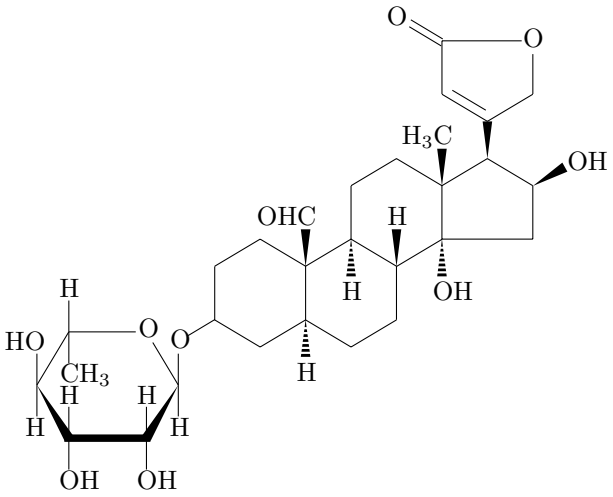
```
¥pyranose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==OH;3Sa==H;4Sa==HO;4Sb==H;5Sa==H;5Sb==H}
¥mypyranose{1Sa==OH;1Sb==H;2Sb==H;2Sa==OH;3Sb==OH;3Sa==H;4Sa==HO;4Sb==H;5Sa==H;5Sb==H}
```



The structural formula of adonitoxin can be drawn by using ¥mypyranose in place of ¥pyranose (cf. the preceding chapter) as follows:

```
¥wedgehashedwedge
¥mypyranose{1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sb==HO;%
4Sa==H;5Sb==H;5Sa==CH$_{3}$;%
1Sb==¥ryl(8==O){3==%
¥steroid{3==(yl);5A==H;8B==H;9A==H;{{10}B}==¥lmoiety{OHC};{{14}A}==OH;%
{{13}B}==¥lmoiety{H$_{3}$C};{{16}B}==OH;%
{{17}B}==¥fiveheterov[e]{3==O}{4D==O;1==(yl)}}}}
```

This code typesets the following formula:

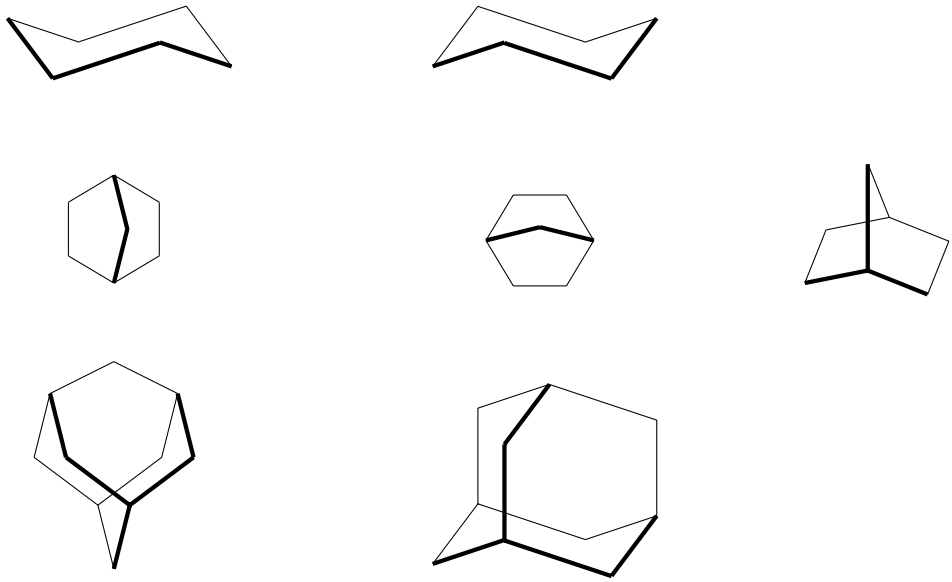


3.4 Skeletal Bonds in Carbocycles

By using the following commands defined in the package ccycle.sty of the X$\mathfrak{Z}$MTEX system, one can draw following carbocycles:

```
¥chair{} ¥chairi{}
¥bicychepv{} ¥bicycheph{} ¥bornane
¥adamantane{} ¥hadamantane{}
```

where the front bonds of each formula are drawn as bold dash bonds.



To convert the bold dash bonds into wedges, the technique described in the preceding section should be applied, although the details are not described in this manual.

Chapter 4

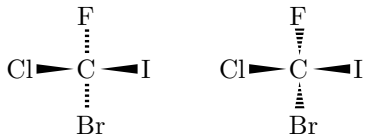
Tetrahedral Units with Wedged Bonds

4.1 Various Tetrahedral Units

In previous versions, the macro `¥tetrahedral` is supported to draw a tetrahedral methane derivative. Because the present version (XƎMTEX version 4.02) is capable of drawing wedged bonds, the codes:

```
¥tetrahedral{0==C;1A==F;2B==Cl;3A==Br;4B==I}
{¥wedgehashedwedge ¥qquad
¥tetrahedral{0==C;1A==F;2B==Cl;3A==Br;4B==I}}
```

now generate the following formulas:



In addition, the XƎMTEX version 4.02 (aliphat.sty) provides us with commands to draw various tetrahedral derivatives with wedged bonds:

```
¥rtetrahedralS[AUXLIST]{SUBSLIST}
¥RtetrahedralS[AUXLIST]{SUBSLIST}
¥ltetrahedralS[AUXLIST]{SUBSLIST}
¥LtetrahedralS[AUXLIST]{SUBSLIST}
¥utetrahedralS[AUXLIST]{SUBSLIST}
¥UtetrahedralS[AUXLIST]{SUBSLIST}
¥dtetrahedralS[AUXLIST]{SUBSLIST}
¥DtetrahedralS[AUXLIST]{SUBSLIST}
¥htetrahedralS[AUXLIST]{SUBSLIST}
```

where the end letter "S" is the abbreviation of the word "stereo". The argument `AUXLIST` designates a character on the central atom of the formula drawn by this macro. It can be used a plus or minus charge on the center:

```
AUXLIST = {0+} :  + charge (or another one chararacter) on the center
```

The SUBSLIST is used to specify a central atom and substituents. Although any bond modifiers can be used, positions 1 and 2 are designed to have no bond modifier (a single thin line), while positions 3 and

4 are considered to take a bond modifier (B or A) so that a bold wedged bond (or bold dash bond) or a hashed wedged bond (or hashed dash bond) is generated. In other words, the positions 1 and 2 and the central atom are coplanar so as to be placed in the plane of a page; the bond to the position 3 is an α-bond; and the bond to the position 4 is a β-bond.

4.1.1 Right- and Left-Types

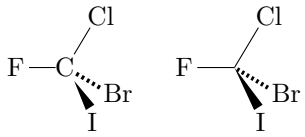
The bond from the central atom to the position 1 of an tetrahedral unit of the right- or left-type is drawn as a horizontal thin line, which shows an east (rightward) or a west (leftward) bond.

¥rtetrahedralS (or \rtetrahedralS)

In a structural formula depicted by the command `¥rtetrahedralS`, position 1, position 2, and the central atom are placed in the plane of a page, where the bond from the central atom to the position 1 is a horizontal west (leftward) bond. For example, the command `¥rtetrahedralS` used in the codes:

```
¥rtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥rtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

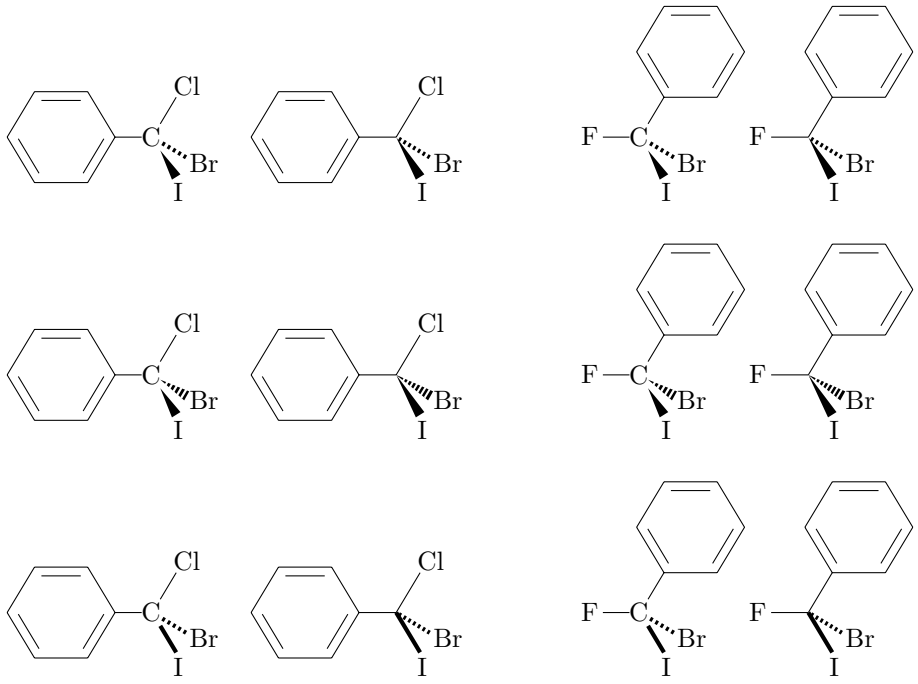
gives the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥rtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{0==C;1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I}
¥rtetrahedralS{1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥rtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{0==C;1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I}
¥rtetrahedralS{1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥rtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥rtetrahedralS{0==C;1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I}
¥rtetrahedralS{1==F;2==¥bzdrh{6==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:



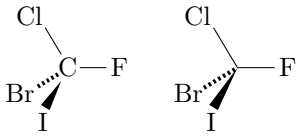
where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

¥ltetrahedralS (or \ltetrahedralS)

In order to draw the mirror-image formulas of those drawn by `¥rtetrahedralS`, we can use the command `¥ltetrahedralS`. In a structural formula depicted by this command, position 1, position 2, and the central atom are placed in the plane of a page, where the bond from the central atom to the position 1 is a horizontal east (rightward) bond. Thus the codes:

```
¥ltetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥ltetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

give the following formulas:

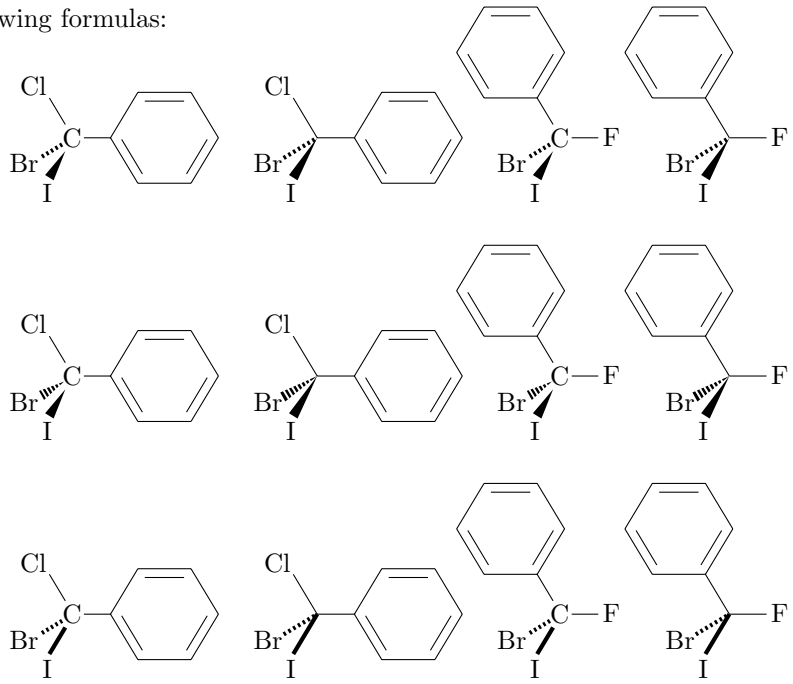


where the presence or absence of `0==C` decides the appearance of generated bonds. In addition, the codes:

```
¥ltetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥ltetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥ltetrahedralS{0==C;1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I}
¥ltetrahedralS{1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥ltetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥ltetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
```

```
¥ltetrahedralS{0==C;1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I}
¥ltetrahedralS{1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥ltetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥ltetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥ltetrahedralS{0==C;1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I}
¥ltetrahedralS{1==F;2==¥bzdrh{5==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:

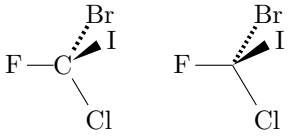


¥RtetrahedralS (or \RtetrahedralS)

A diagram generated by he command `¥RtetrahedralS` is rotated by 180° around the axis through the central carbon and the position 1 so as to give a diagram generated by the command `¥rtetrahedralS`. Thus, the codes:

```
¥RtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥RtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

give the following formulas:

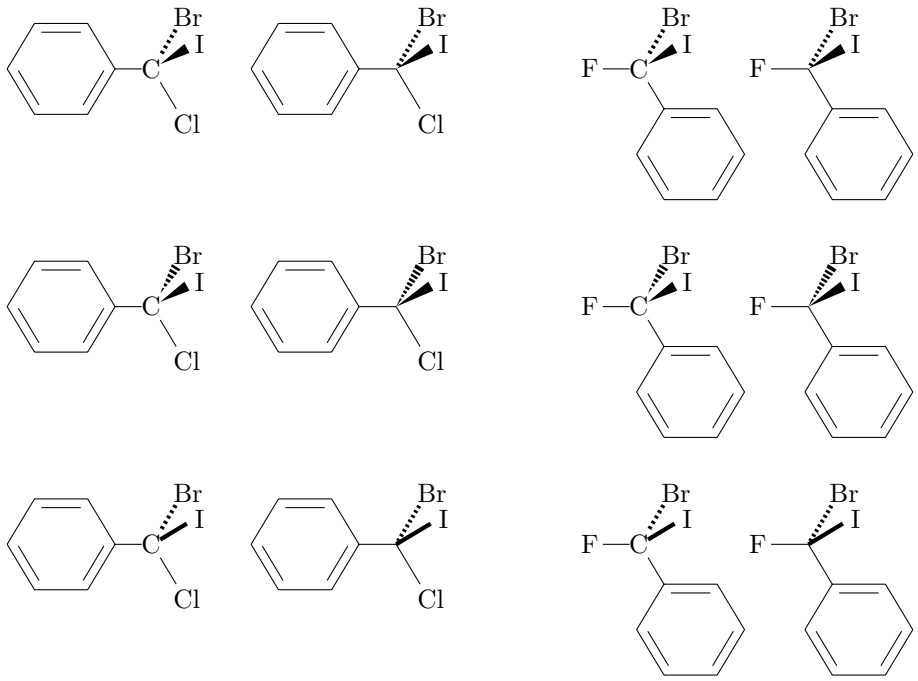


where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥RtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{0==C;1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I}
¥RtetrahedralS{1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I} ¥par
```

```
¥vskip1cm
{¥wedgehashedwedge
¥RtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{0==C;1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I}
¥RtetrahedralS{1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I}} ¥par
¥vskip1cm
{¥dashhasheddash
¥RtetrahedralS{0==C;1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{1==¥bzdrh{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥RtetrahedralS{0==C;1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I}
¥RtetrahedralS{1==F;2==¥bzdrh{2==(yl)};3A==Br;4B==I}} ¥par
```

generate the following formulas:



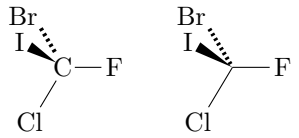
where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

¥LtetrahedralS (or \LtetrahedralS)

In order to draw the mirror-image formulas of those depicted by `¥RtetrahedralS`, we can use the command `¥LtetrahedralS` as follows. Thus the codes:

```
¥LtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥LtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

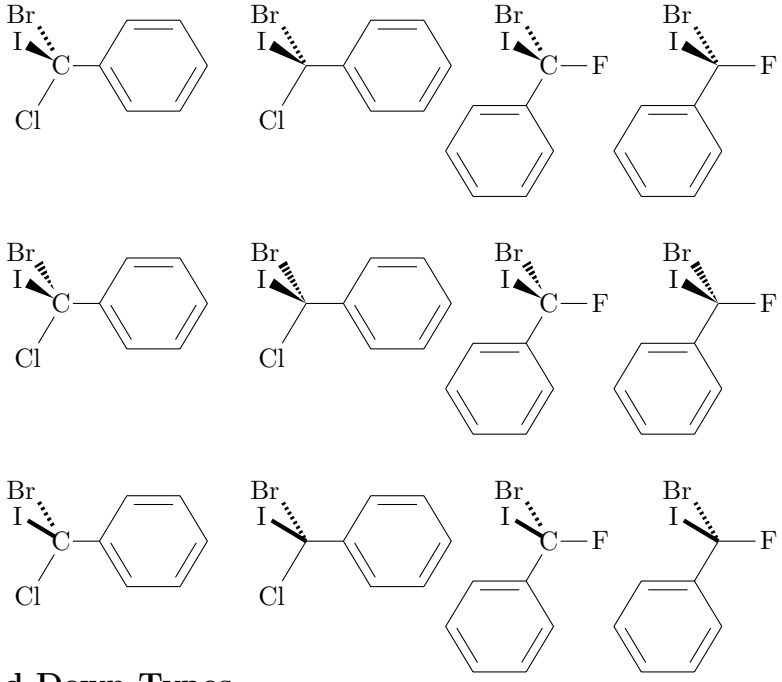
give the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds. In addition, the codes:

```
¥LtetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{0==C;1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I}
¥LtetrahedralS{1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥LtetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{0==C;1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I}
¥LtetrahedralS{1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I}} ¥par
¥vskip1cm
{¥dashhasheddash
¥LtetrahedralS{0==C;1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{1==¥bzdrh{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥LtetrahedralS{0==C;1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I}
¥LtetrahedralS{1==F;2==¥bzdrh{3==(yl)};3A==Br;4B==I}} ¥par
```

generate the following formulas:



4.1.2 Up- and Down-Types

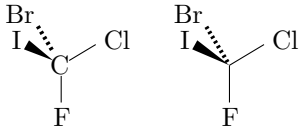
The bond from the central atom to the position 1 of an tetrahedral unit of the up- or down-type is drawn as a vertical thin line, which shows an north (upward) or a south (downward) bond.

¥utetrahedralS (or \utetrahedralS)

The bond to position 1 in a structural formula depicted by `¥utetrahedralS` is a south (downward) bond. For example, the command `¥utetrahedralS` used in the codes:

```
¥utetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥utetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

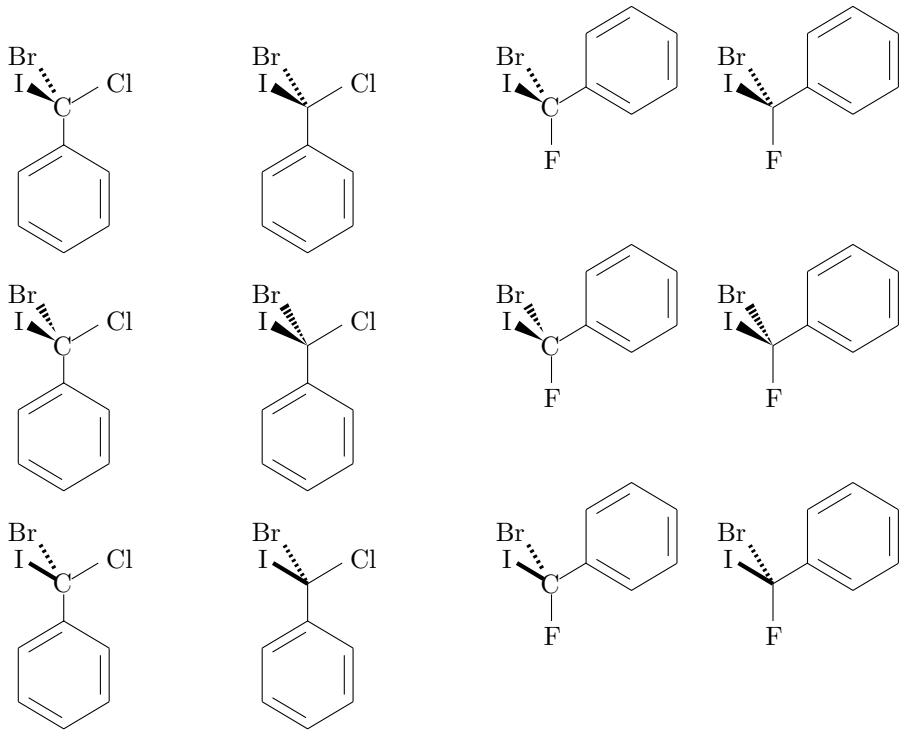
gives the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥utetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{0==C;1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} ¥qquad
¥utetrahedralS{1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥utetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{0==C;1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} ¥qquad
¥utetrahedralS{1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥utetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥utetrahedralS{0==C;1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} ¥qquad
¥utetrahedralS{1==F;2==¥bzdrv{5==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:



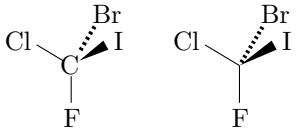
where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

¥UtetrahedralS (or \UtetrahedralS)

The bond to position 1 in a structural formula depicted by `¥UtetrahedralS` is a south (downward) bond. The formula is rotated by 180° around the bond so as to give a formula depicted by `¥utetrahedralS`. For example, `¥UtetrahedralS` used in the codes:

```
¥UtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥UtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

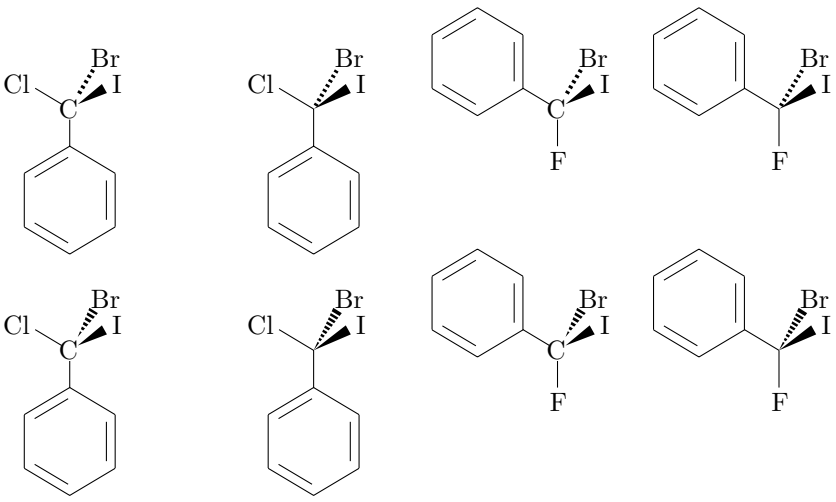
gives the following formulas:

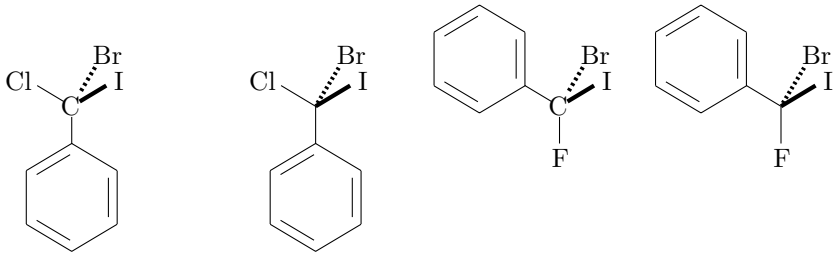


where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥UtetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{0==C;1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} ¥qquad
¥UtetrahedralS{1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥UtetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{0==C;1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} ¥qquad
¥UtetrahedralS{1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥UtetrahedralS{0==C;1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{1==¥bzdrv{1==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥UtetrahedralS{0==C;1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} ¥qquad
¥UtetrahedralS{1==F;2==¥bzdrv{3==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:





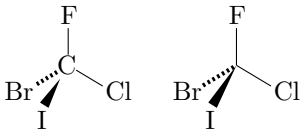
where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

¥dtetrahedralS (or \dtetrahedralS)

The bond to position 1 in a structural formula depicted by `¥dtetrahedralS` is a north (upward) bond. For example, `¥dtetrahedralS` used in the codes:

```
¥dtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥dtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

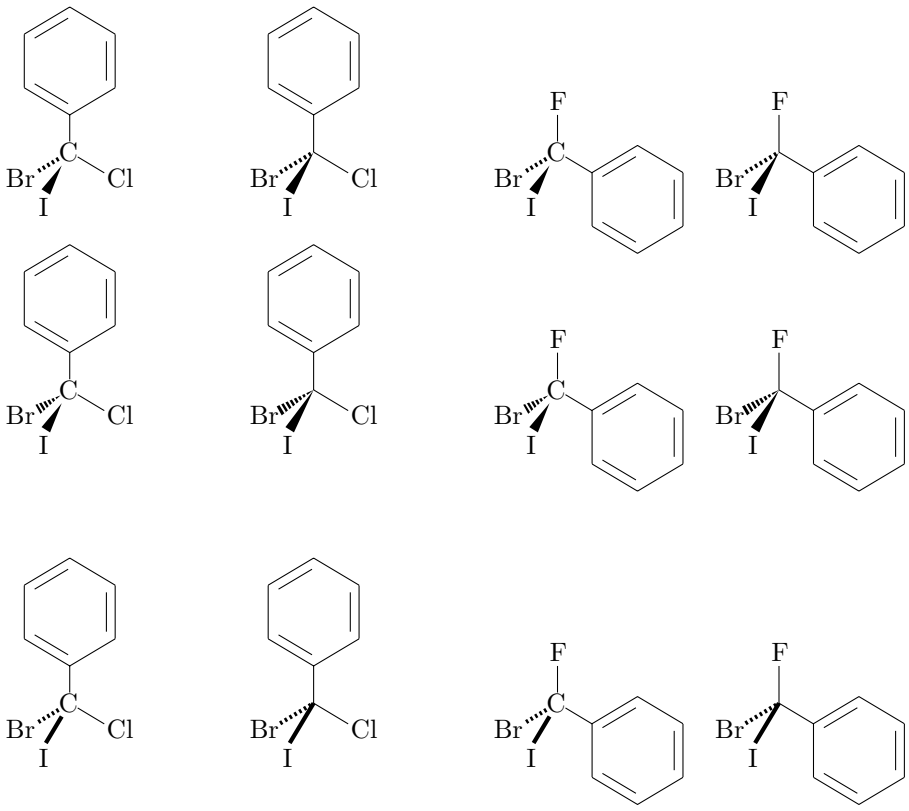
gives the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥dtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥dtetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥dtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥dtetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥dtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥dtetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥dtetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:



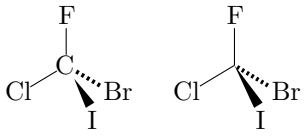
where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

¥DtetrahedralS (or \DtetrahedralS)

The bond to position 1 in a structural formula depicted by `¥DtetrahedralS` is a north (upward) bond. The formula is rotated by 180° around the bond so as to give a formula depicted by `¥dtetrahedralS`. For example, `¥DtetrahedralS` used in the codes:

```
¥DtetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥DtetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

gives the following formulas:

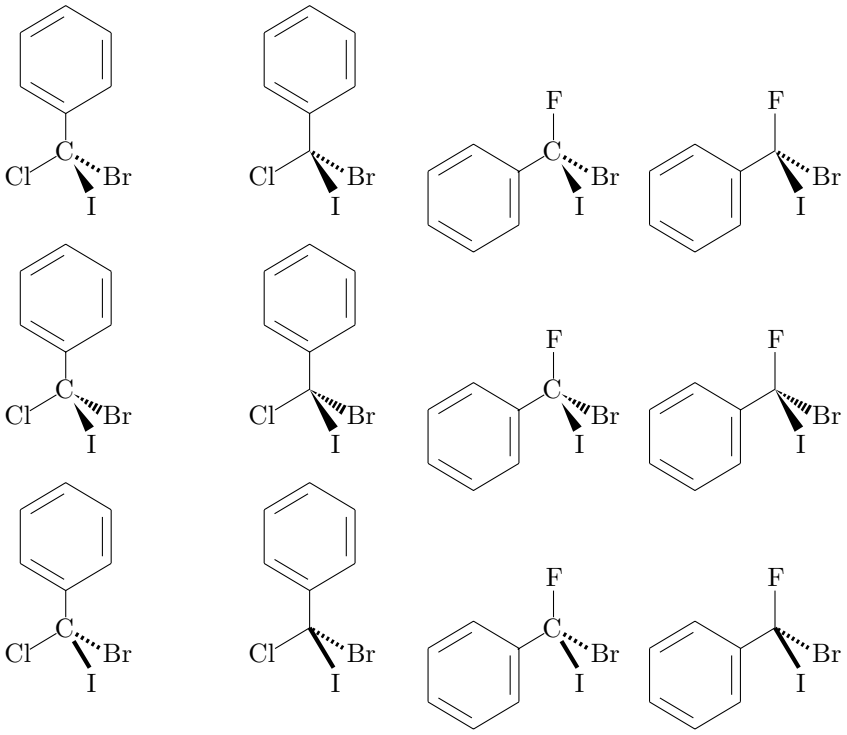


where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥DtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{0==C;1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} ¥qquad
¥DtetrahedralS{1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} ¥par
```

```
¥vskip1cm
{¥wedgehashedwedge
¥DtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{0==C;1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} ¥qquad
¥DtetrahedralS{1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥DtetrahedralS{0==C;1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{1==¥bzdrv{4==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥DtetrahedralS{0==C;1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} ¥qquad
¥DtetrahedralS{1==F;2==¥bzdrv{2==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:



where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

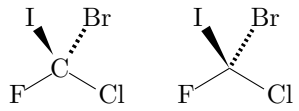
4.1.3 Horizontal-Type

¥htetrahedralS (or \htetrahedralS)

The command `¥htetrahedralS` of horizontal-type draws bonds to positions 1 and 2 to be diagonal thin lines (southeast and southwest bonds). For example, `¥htetrahedralS` used in the codes:

```
¥htetrahedralS{0==C;1==F;2==Cl;3A==Br;4B==I}
¥htetrahedralS{1==F;2==Cl;3A==Br;4B==I}
```

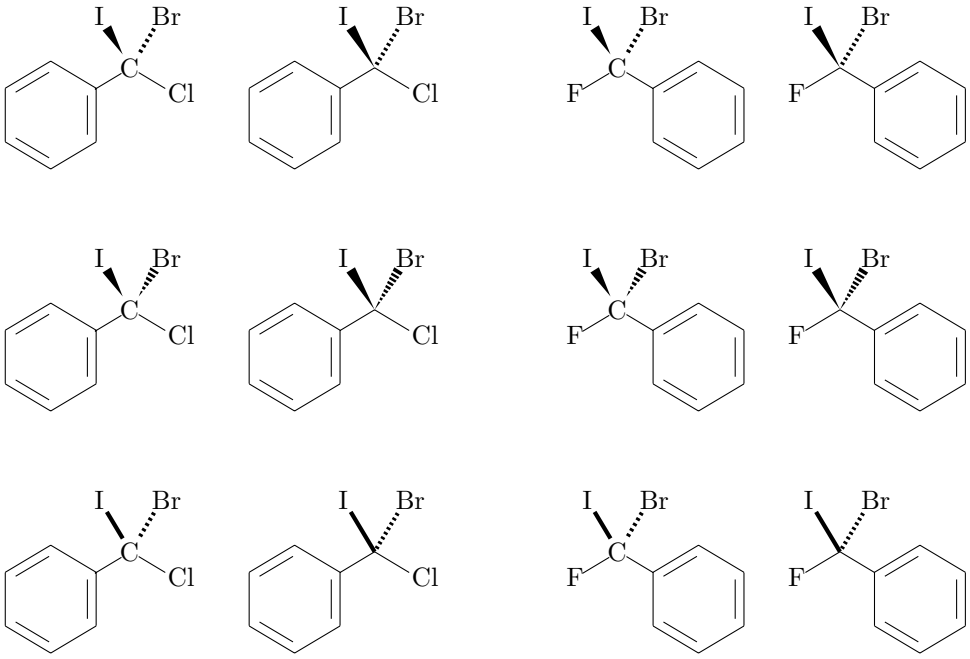
gives the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds. The codes:

```
¥htetrahedralS{0==C;1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥htetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥par
¥vskip1cm
{¥wedgehashedwedge
¥htetrahedralS{0==C;1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥htetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} }¥par
¥vskip1cm
{¥dashhasheddash
¥htetrahedralS{0==C;1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{1==¥bzdrv{2==(yl)};2==Cl;3A==Br;4B==I} ¥hskip1cm
¥htetrahedralS{0==C;1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} ¥qquad
¥htetrahedralS{1==F;2==¥bzdrv{6==(yl)};3A==Br;4B==I} }¥par
```

generate the following formulas:



where structural formulas shown as examples are respectively drawn by the default mode (the top row), the `¥wedgehashedwedge` mode (the middle row), and the `¥dashhasheddash` mode (the bottom row).

4.2 Trigonal Bipyramidal Units

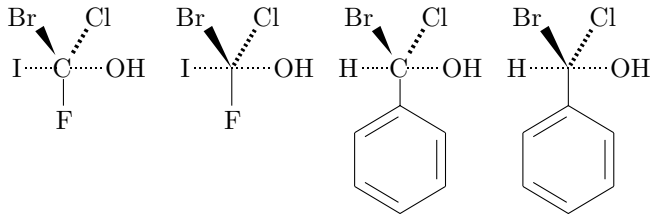
To draw transition states of reactions, we can use trigonal bipyramidal units.

4.2.1 ¥utrigpyramid (or \utrigpyramid)

The bond to position 1 in a structural formula depicted by `¥utrigpyramid` is a south (downward) bond. For example, `¥utrigpyramid` used in the codes:

```
¥utrigpyramid{0==C;1==F;2A==Cl;3B==Br;4A==I;5A==OH}
¥utrigpyramid{1==F;2A==Cl;3B==Br;4A==I;5A==OH}
¥utrigpyramid{0==C;5A==OH;2A==Cl;3B==Br;1==¥bzdrv{1==(yl)};4A==H}
¥utrigpyramid{5A==OH;2A==Cl;3B==Br;1==¥bzdrv{1==(yl)};4A==H}
```

gives the following formulas:



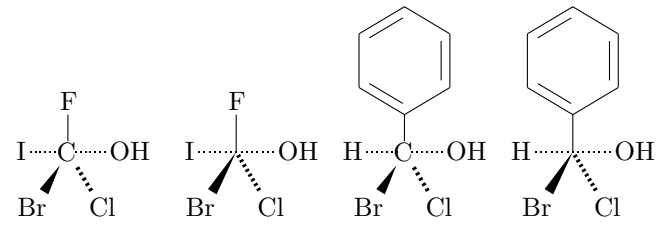
where the presence or absence of `0==C` decides the appearance of generated bonds.

4.2.2 ¥dtrigpyramid (or \dtrigpyramid)

The bond to position 1 in a structural formula depicted by `¥dtrigpyramid` is a north (upward) bond. For example, `¥dtrigpyramid` used in the codes:

```
¥dtrigpyramid{0==C;1==F;2A==Cl;3B==Br;4A==I;5A==OH}
¥dtrigpyramid{1==F;2A==Cl;3B==Br;4A==I;5A==OH}
¥dtrigpyramid{0==C;5A==OH;2A==Cl;3B==Br;1==¥bzdrv{1==(yl)};4A==H}
¥dtrigpyramid{5A==OH;2A==Cl;3B==Br;1==¥bzdrv{1==(yl)};4A==H}
```

gives the following formulas:



where the presence or absence of `0==C` decides the appearance of generated bonds.

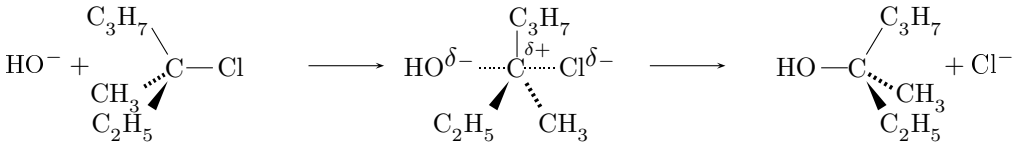
4.3 Applications

4.3.1 Reaction Schemes

By combining two or more commands defined in the present chapter, we can write an reaction scheme containing a transition-state diagram. For example, the code:

```
¥begin{chemeqn}
HO^{-} +
¥raisebox{-28pt}{%
¥ltetrahedralS{0==C;1==Cl;2==C$_{3}$H$_{7}$;3A==CH$_{3}$;4B==C$_{2}$H$_{5}$}}
¥qquad¥reactrarrow{0pt}{1cm}{}{}¥qquad
¥raisebox{-28pt}{%
¥dtrigpyramid[{0{~~$¥delta+$}}]%
{0==C;4A==HO$^{¥delta-}$;5A==Cl$^{¥delta-}$;1==C$_{3}$H$_{7}$;%
2A==CH$_{3}$;3B==C$_{2}$H$_{5}$}}
¥qquad¥reactrarrow{0pt}{1cm}{}{}¥qquad
¥raisebox{-28pt}{%
¥rtetrahedralS{0==C;1==HO;2==C$_{3}$H$_{7}$;3A==CH$_{3}$;4B==C$_{2}$H$_{5}$}}
+ Cl^{-}
¥end{chemeqn}
```

generates the following scheme:

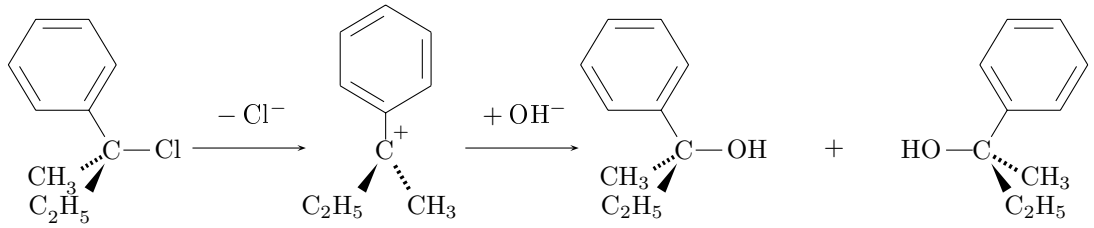


(4.1)

Similarly, the code:

```
¥begin{chemeqn}
¥raisebox{-28pt}{%
¥ltetrahedralS{0==C;1==Cl;2==¥bzdrh{5==(yl)};3A==CH$_{3}$;4B==C$_{2}$H$_{5}$}}
¥reactrarrow{0pt}{1.5cm}{¥chemform{{}-Cl^{-}}}{¥strut}
¥raisebox{-28pt}{%
¥dtrigpyramid[{0{~~$+$}}]%
{0==C;1==¥bzdrv{4==(yl)};2A==CH$_{3}$;3B==C$_{2}$H$_{5}$}}
¥reactrarrow{0pt}{1.5cm}{¥chemform{{}+OH^{-}}}{¥strut}¥quad
¥raisebox{-28pt}{%
¥ltetrahedralS{0==C;1==OH;2==¥bzdrh{5==(yl)};3A==CH$_{3}$;4B==C$_{2}$H$_{5}$}}
¥qquad +¥qquad
¥raisebox{-28pt}{%
¥rtetrahedralS{0==C;1==HO;2==¥bzdrh{6==(yl)};3A==CH$_{3}$;4B==C$_{2}$H$_{5}$}}
¥end{chemeqn}
```

produces the following scheme containing a carbocation intermediate:



(4.2)

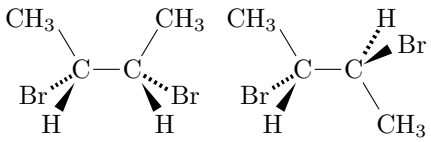
4.3.2 Conformations

An eclipsed conformer and a staggered one are drawn by the codes:

```
¥ltetrahedralS{0==C;1==¥rtetrahedralS{1==(yl);0==C;2==CH$_{3}$;3A==Br;4B==H};%
2==CH$_{3}$;3A==Br;4B==H}
¥qquad
```

```
¥ltetrahedralS{0==C;1==¥RtetrahedralS{1==(yl);0==C;2==CH$_{3}$;3A==H;4B==Br};%
2==CH$_{3}$;3A==Br;4B==H}
```

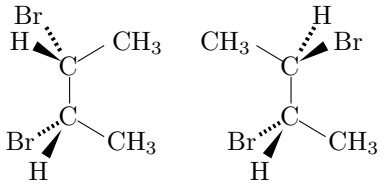
which generate the following formulas:



The corresponding vertical diagrams are drawn by the codes:

```
¥utetrahedralS{0==C;1==¥dtetrahedralS{1==(yl);0==C;2==CH$_{3}$;3A==Br;4B==H};%
2==CH$_{3}$;3A==Br;4B==H}
¥qquad
¥UtetrahedralS{0==C;1==¥dtetrahedralS{1==(yl);0==C;2==CH$_{3}$;3A==Br;4B==H};%
2==CH$_{3}$;3A==H;4B==Br}
```

which generate the following formulas:

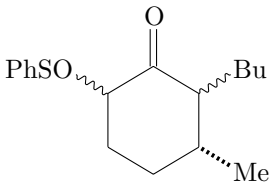


Chapter 5

Wavy Bonds

5.1 Introduction

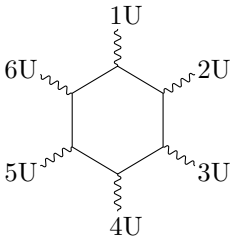
According to the IUPAC Provisional Recommendations 2004, a wavy line can be used to indicate either that the configuration is unknown but only one form is present, or if explained in the text both isomers are present and will be defined when required. In particular, synthetic intermediates are frequently expressed by structural formulas having wavy bonds, e.g.,

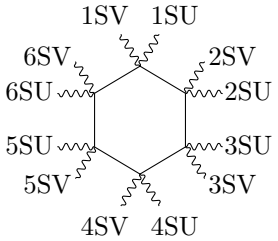


XƎMTEX Version 4.03 supports wavy bonds as additional bond modifiers, i.e., U, SU, SV, FU, and GU. Because the corresponding program codes have been added to chemstr.sty (automatically loaded) and other existing package files, no additional package files have been created in the development of XƎMTEX Version 4.03 in comparison with Version 4.02.

5.2 Bond Modifiers Added for Wavy Bonds

Among the additional bond modifiers, U, SU, and SV have the following specifications for six-membered rings:





These diagrams are drawn by the following codes:

```
¥sixheterov{}{1U==1U;2U==2U;3U==3U;4U==4U;5U==5U;6U==6U}
¥hskip3cm
```

```
¥sixheterov{}{1SU==1SU;2SU==2SU;3SU==3SU;4SU==4SU;5SU==5SU;6SU==6SU;%
1SV==1SV;2SV==2SV;3SV==3SV;4SV==4SV;5SV==5SV;6SV==6SV}
```

The remaining bond modifiers, FU and GU, are inteded to draw bridgehead configurations in fused structures:

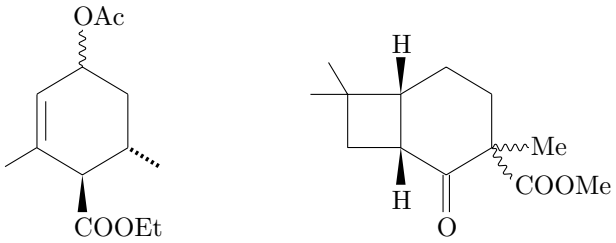
These diagrams are drawn by the following codes:

```
¥sixheterov{}{1FU==1FU;2FU==2FU;3FU==3FU;4FU==4FU;5FU==5FU;6FU==6FU}
¥hskip3cm
¥sixheterov{}{1GU==1GU;2GU==2GU;3GU==3GU;4GU==4GU;5GU==5GU;6GU==6GU}
```

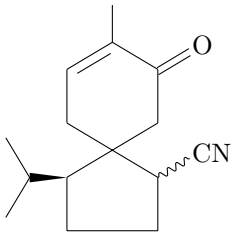
5.3 Examples

5.3.1 Carbocycles

```
¥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}
```

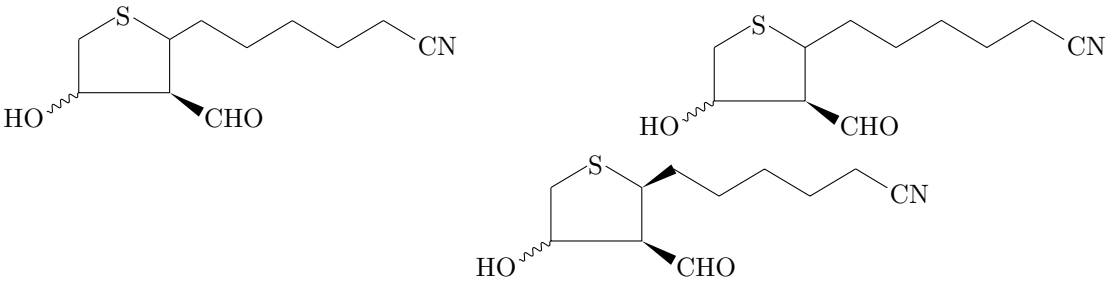



```
¥fiveheterovi{1s==¥sixheterov[f]{}{4==(yl);2D==O;1==}}%
{2U==CN;5Su==¥LtetrahedralS{1==(yl);2==;3==}}
```

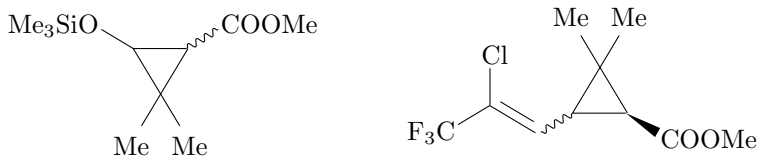



```
¥pentamethylenei{}{%
1W==¥fiveheterovi{1==S}{2==(yl);3B==CHO;4U==HO};5W==CN}
¥hskip4cm
```

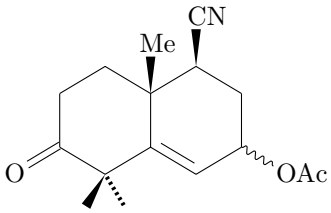
```
¥hexamethylene{1s==¥fiveheterovi{1==S}{2==(yl);3B==CHO;4U==HO}}{6W==CN}
¥¥
¥fiveheterovi{1==S}{3B==CHO;4U==HO;2B==¥pentamethylenei{}{1==(yl);5W==CN}}
```



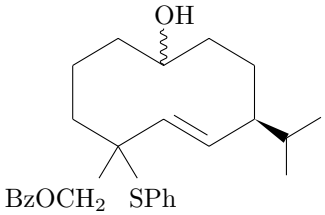

```
¥threeheterov{}{1Sa==Me;1Sb==Me;2U==COOMe;3==Me$_{3}$SiO}
¥hskip3cm
¥threeheterovi{}{1Sa==Me;1Sb==Me;2B==COOMe;%
3U==¥dimethylenei[a]{}{2==(yl);1==Cl;1W==F$_{3}$C}}
```




```
¥decalinev[d]{1B==CN;3U==OAc;5SA==;5SB==;6D==O;{10}B==Me}
```

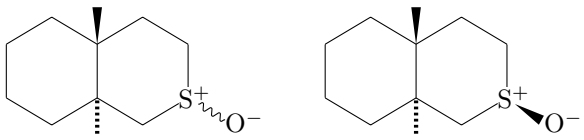



```
¥decaheterov[d]{}{3B==¥UtetrahedralS{2==(yl);1==;4==};%
{10}U==OH;5Sa==SPh;5Sb==BzOCH$_{2}$}[k]
```

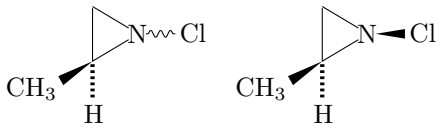


5.3.2 Heterocycles

```
¥decaheterov{3==S$^{+}$}{9A==;{10}B==;3U==O$^{-}$}
¥decaheterov{3==S$^{+}$}{9A==;{10}B==;3B==O$^{-}$}
```

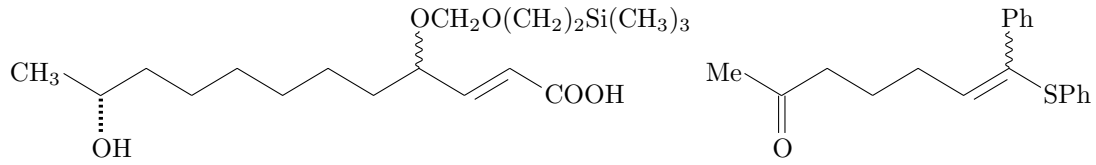



```
¥threeheteroh{1==N}{1U==Cl;2SB==CH$_{3}$;2SA==H}
¥hskip1cm
¥threeheteroh{1==N}{1B==Cl;2SB==CH$_{3}$;2SA==H}
```

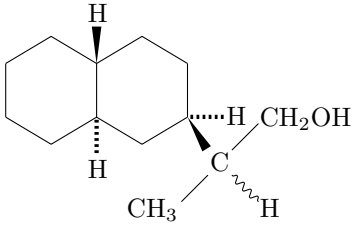


5.3.3 Chains

```
¥decamethylene[i]{}{1W==CH$_{3}$;1A==OH;%
8U==OCH$_{2}$O(CH$_{2}$)$_{2}$Si(CH$_{3}$)$_{3}$;{10}W==COOH}
¥hskip2cm
¥hexamethylene[e]{}{1W==Me;1D==O;6U==Ph;6W==SPh}
```




```
¥decalinev{9A==H;{10}B==H;3SA==H;%
3SB==¥square{4==(yl);0==C;1==CH$_{2}$OH;2U==H;3==CH$_{3}$}}
```



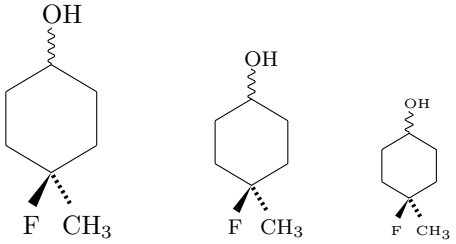
5.4 PostScript Compatible Mode vs. TEX/LATEX Compatible Mode

Wavy bonds can be drawn also in the TEX/LATEX Compatible Mode. Theree types of diagarams in the PostScript compatible mode are summarized in Fig. 5.1, which also contains structural formulas by the TEX/LATEX compatible mode for comparison.

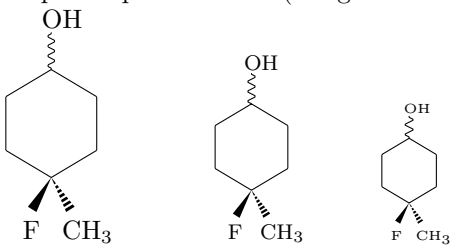
Figure 5.1 is obtained by the following codes:

```
¥begin{tabular}{l}
PostScript compatible mode (wedge and hashed dash): ¥¥
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F} ¥¥
¥noalign{¥vskip10pt}
PostScript compatible mode (wedge and hashed wedge): ¥¥
¥wedgehashedwedge
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F} ¥¥
¥noalign{¥vskip10pt}
PostScript compatible mode (dash and hashed dash): ¥¥
¥dashhasheddash
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}  ¥¥
¥noalign{¥vskip10pt}
TeX/LaTeX compatible mode: ¥¥
¥reducedsizepicture
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.08pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F}
¥changeunitlength{0.06pt}
¥cyclohexanev{1U==OH;4SA==CH$_{3}$;4SB==F} ¥¥
¥end{tabular}
```

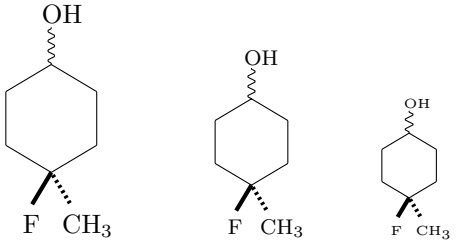
PostScript compatible mode (wedge and hashed dash):



PostScript compatible mode (wedge and hashed wedge):



PostScript compatible mode (dash and hashed dash):



TeX/LaTeX compatible mode:

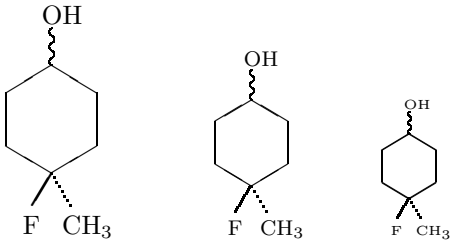


Figure 5.1: PostScript Compatible Mode vs. TEX/LATEXCompatible Mode

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