X͡ΥMTEX: A Macro Package for Typesetting Chemical Structural Formulas

Shinsaku Fujita

Ashigara Research Laboratories, Fuji Photo Film Co., Ltd.,
Minami-Ashigara, Kanagawa, 250-01 Japan

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Chapter 1

Introduction

1.1 Backgrounds

The text formatter TEX developed by Knuth [4] is widely used in preparing manuscripts of scientific papers and in the typesetting processes of several scientific journals and books (for a recent example, see [4]). In particular, LATEX, a TEX macro package that was released by Lamport [4], has expanded the society of TEX users because of plainness.

Since the beginning of its history, TEX (LATEX) places special emphasis on mathematics typesetting. Hence, it has been accepted by scientists who have to write mathematic equations. In contrast, the TEX/LATEX typesetting is less popular in chemistry than in mathematics and other fields. One of the reasons is that there are few TEX/LATEX utilities for typesetting chemical structural diagrams.

Although LATEX provides us with a picture enviroment for drawing simple figures, its original commands are so primitive as to be directly applied to the drawing of structural formulas. Hence, the commands should be combined to produce more convenient macros.

Pioneering works by Haas and O'Kane [4] and by Ramek [4] have provided such macros that allow us to typeset structural formulas. The macros of the former approach are available in the public domain, being named ChemTEX. Although they are easier to use than the original picture environment of LATEX, they still have some items to be improved. The most inconvenient item is the incapability of accommodating 10 or more substituents. It stems from the fact that one argument is used to assign one substituent (or one object) in each of the macros of Haas-O'kane's approach. Note that the direct usage of arguments enables us only to assign 9 or less substituents, because a macro in TEX/LATEX is capable of taking 9 or less arguments.

For example, the `\steroid` macro reported for typesetting a steroid skeleton takes 9 arguments [4]:

```
\steroid{A1}{A2}{A3}{A4}{A5}{A6}{A7}{A8}{A9}
```

where Argument 1 (`A1`) can take 'D' (a second bond between positions 1 and 2), 'Q' (no action), or 'R^{11}' (a substituent on position 11 and the corresponding double bond); Argument 2 (`A2`) can take 'D' (a second bond between positions 3 and 4), 'Q' (no action), or 'R^{3}' (a substituent on position 3 and the corresponding double bond); Argument 3 (`A3`) can take 'Q' (no action), or 'R^{3}' (a substituent on position 3 and the corresponding single bond); and so on. Through the total statement of arguments, only six substituents are specified, while the skeleton have 20 or more substitution positions to be considered.

Moreover, the specification of the arguments is not systematic, since so many functions are included into the macro within the restriction of the direct usage of arguments.

1. One argument (Argument 2) specifies objects of two different categories *e.g.,* inner double bonds and outer double bonds.

2. Arguments 2 and 3 specify a substituent attaching to the same position (position 3).

3. It is difficult without a reference manual to differentiate between one argument for specifying bonds and another argument for specifying substituents.

4. The argument 'Q' is selected to show no modification because this character is hardly ever found in a chemical structure formula. However, the use of this character may become necessary in future. Such explicit description of 'no action' should be avoided.

As a result, the formats and contents of arguments are different from one argument to another and from one macro to another such that a typical TEX user, a secretary or a chemist author, may give up to memorize such macros. Hence, more systematic and convenient macros are desirable in order to spread the typesetting of chemical structures with TEX/LATEX.

The present package XΥMTEX involves convenient macros for typesetting chemical structural formulas [4]. These macros are based on techniques in which inner bonds, substituents and hetero-atoms on a skeleton are separately assigned without such limitation of numbers. The package XΥMTEX[1] will be a more versatile tool if it is coupled with the macros which the author has released in a book [4].

1.2 The Name of the Package

The word 'chemistry' stems from an Arabian root 'alchemy', which is, in turn, considered to come from Greek, $\chi\upsilon\mu\epsilon\acute{\iota}\bar{\alpha}$. The XΥM of the name XΥMTEX is an uppercase form of $\chi\upsilon\mu$. This conforms to a rule of coinage, because the name TEX is also a word of Greek origin ($\tau\epsilon\chi$).

The pronuncialtion of XΥMTEX is recommended to be 'khýmtekh', in which the 'kh' sound may be a Russian 'kh' or more simply an English 'k' and the symbol 'y' is expected to be pronounced like a German 'ü'.

The logo XΥMTEX is defined as being either of the following statements. The second one has been adopted throughout the present manual.[2]

```
%%%XyMTeX Logo: Definition 1%%%
\newcount\TestCount
\def\XyM{\ifnum\fam=-1\relax\fam=0\relax\fi\TestCount=\fam%
X\kern-.30em\smash{\raise.50ex\hbox{$\fam\TestCount\Upsilon$}}%
\kern-.30em{M}}
\def\XyMTeX{\XyM\kern-.1em\TeX}

%%%XyMTeX Logo: Definition 2%%%
\def\UPSILON{\char'7}
\def\XyM{X\kern-.30em\smash{\raise.50ex\hbox{\UPSILON}}\kern-.30em{M}}
\def\XyMTeX{\XyM\kern-.1em\TeX}
```

When such a raised Greek letter as the 'Υ' is not available, XΥMTEX may be referred to by typing '`XyMTeX`'.

1.3 Requirements

The macro package XΥMTEX runs within LATEX, since it is based on the picture environment of LATEX. BigLATEX should be used because XΥMTEX requires a considerable resource of memory.

It also requires an option file 'epic.sty' developed by Podar [4], because the `\dottedline` command of epic is used in the macros. For example, a manuscript file should begin with such a statement as follows:

```
\documentstyle[epic,carom,hetarom]{article}
```

wherein 'carom' and 'hetarom' are style files contained in the package XΥMTEX.

[1] The present manual on XΥMTEX is not permitted to be translated into Japanese and any other languages.

[2] Definition 2 is adopted in the manual because of simplicity. The methodology used in Definition 1 is applicable to a wide variety of cases in which font sizes have to be changed.

Chapter 2

The Construction of XΥMTEX

2.1 Overview

XΥMTEX contains style files listed in Table 2.1 and their documents. The style file 'chemstr.sty' is the basic file that is automatically read within any other style file of XΥMTEX. It contains macros for internal use, *e.g.*, common commands for bond-setting and atom-setting. The other style files contain macros for users.

Table 2.1: Style Files of XΥMTEX

style name	included functions
aliphat.sty	macros for drawing aliphatic compounds
carom.sty	macros for drawing vertical and horizontal types of carbocyclic compounds
lowcycle.sty	macros for drawing five-or-less-membered carbocyles.
ccycle.sty	macros for drawing bicyclic compounds etc.
hetarom.sty	macros for drawing vertical types of heterocyclic compounds
hetaromh.sty	macros for drawing horizontal types of heterocyclic compounds
hcycle.sty	macros for drawing pyranose and furanose derivatives
chemstr.sty	basic commands for atom- and bond-typesetting
locant.sty	commands for printing locant numeres

These files are designed to be option style files used within LaTEX. The complete list of the XΥMTEX commands is shown in Appendix A.

2.2 General Conventions

2.2.1 User Commands for Specified Use and for General Use

XΥMTEX user commands are classified into two types, *i.e.*, commands for specified use and those for general use.

Specified user commands of XΥMTEX are used to draw a narrow range of structures. More precisely speaking, they are short-cut commands of general user commands with a specific bond pattern for drawing carbocycles or with a specific pattern of skeletal hetero-atoms for drawing heterocycles. They take such general forms as follows:

`\Sformb[OPT]{SUBSLIST}`	for drawing carbocycles
`\Sformd[BONDLIST]{SUBSLIST}`	for drawing heterocycles

where `\Sformb` and `\Sformd` may be approriate command names. These are selected from chemical names that represent the compound-group names to be typeset. In accord with LATEX conventions, an argument in brackets is an option.

The command `\Sformb` typesets a carbocyclic compound with a specific bond pattern which may be altered by the optional argument OPT. The command `\Sformd` prints a heterocyclic compound with a specific atom pattern on its skeleton.[1]

For example, `\bzdrv[OPT]{SUBSLIST}` is a command for the specified use of drawing benzene derivatives, where the stem '`\bzdr` without a suffix 'v' is an abbreviation of 'benzene derivative'. The command `pyridinev[BONDLIST]{SUBSLIST}` is a command for drawing pyridine derivatives, in which the nitrogen atom on the pyridine ring is automatically typeset.

On the other hand, more elaborate commands for general use can be used within XΥMTEX. They are designed to have a variable set of skeletal heteroatoms in accord with our designation so that they cover a wide range of structures. They have general formats as follows.

`\Sforma[BONDLIST]{SUBSLIST}`	for drawing carbocycles
`\Sformc[BONDLIST]{ATOMLIST}{SUBSLIST}`	for drawing heterocycles

where `\Sforma` and `\Sformc` may be approriate command names.

The command `\Sforma` for general use generates a carbocyclic structure, in which its individual bonds can be independently altered by means of BONDLIST. The command `\Sformd` prints a heterocyclic compound so that individual atoms on its skeleton can be independently typeset through ATOMLIST.

For example, `\cyclohexanev[BONDLIST]{SUBSLIST}` is a command for the general use of drawing cyclohexane derivatives, by which six-membered carbocyles of any unsaturation level can be typeset. The command `sixheterov[BONDLIST]{ATOMLIST}{SUBSLIST}` is a command for drawing six-membered heterocyclic compounds, which may have any set of skeletal hetero-atoms (ATOMLIST) and any set of unsaturation (BONDLIST).

2.2.2 Suffix and Arguments

Most user commands of XΥMTEX are suffixed with 'v', 'vi', 'h' and 'hi'. The suffix 'v' means that the command prints a structural formula of vertical form. The suffix 'h' means that the command typesets a structural formula of horizontal form. When alternative orientations are possible, XΥMTEX commands are differentiated by an additional suffix 'i'.

The specification of each argument in a XΥMTEXcommand is based on list-treating macros [4]. Thus, items to be specified are listed sequentially with or without appropriate delimeters.

The argument SUBSLIST lists substituents with bonds. The argument {1==Cl;3D==O;...}, for example, means that position 1 takes a chlorine atom (Cl) through a single bond, position 3 takes an oxygen atom (O) through a double bond, and so on. Thus, a character string before every semicolon represents a mode of substitution, where a locant number with a bond modifier is separated from a substituent by means of a double equality symbol (==). Each bond modifier consists of one or two characters listed in Table 2.2. The diagrams below Table 2.2 illustrate these bond modifiers by using a cyclohexane skeleton (`\cyclohexanev`).

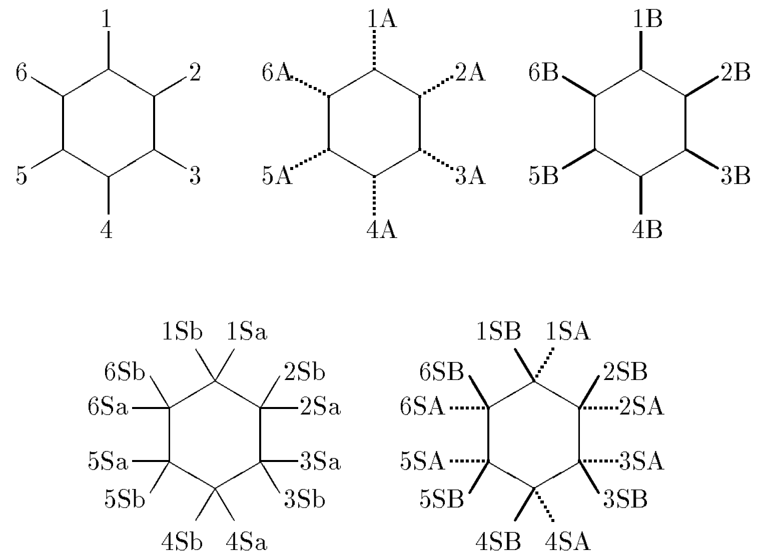
The optional argument OPT of `\Sformb` contains a string of one or two characters for giving a pattern of double bonds (*e.g.*, 'r' for a right-hand set of aromatic double bonds 'l' for a left-hand set of aromatic double bonds, and 'c' for an aromatic circle for the macro `\bzdrv`). Since the argument OPT is an option, a default set of bonds is used when omitted.

The optional argument BONDLIST contains a character string, each character of which is used for assigning a specific inner double bond (*e.g.*, 'a', 'b', ... for the double bonds of a given bond-numbering).

[1] If we take a strictly systematic approach, the `\Sformd` should be designed to take an option argument OPT instead of the BONDLIST. However, a simple format of the OPT cannot be designed because heterocyclic compounds take a wide variety of bond patterns.

Table 2.2: Locant numbering and bond modifiers for SUBSLIST

Bond Modifiers	Printed structures
*n*D	exocyclic double bond at *n*-atom
n or *n*S	exocyclic single bond at *n*-atom
*n*A	alpha single bond at *n*-atom
*n*B	beta single bond at *n*-atom
*n*SA	alpha single bond at *n*-atom (dotted line)
*n*SB	beta single bond at *n*-atom (boldface)
*n*Sa	alpha (not specified) single bond at *n*-atom
*n*Sb	beta (not specified) single bond at *n*-atom



Since the argument BONDLIST is an option, a default is used when omitted: the commands `\Sformd` and `\Sformc` (for drawing heterocycles) typeset default sets of bonds, while most `Sforma` commands (for drawing carbocycles) print fully saturated skeletons.

The argument ATOMLIST (*e.g.*, {1==O;4==O}) contains hetero atoms and their positions on the ring structure to be printed: this example argument produces a dioxane skeleton, when used in command `\sixheterov`.

Chapter 3

Six-Membered Carbocycles

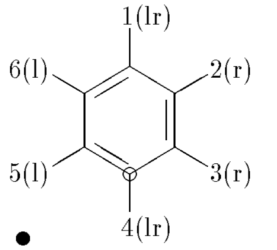
3.1 Drawing Benzene Derivatives

3.1.1 Vertical Forms of Benzene Derivatives

The macro `\bzdrv` is used to draw benzene derivatives of vertical type (carom.sty). The format of this command is as follows:

```
\bzdrv[OPT]{SUBSLIST}
```

The name and arguments of this command conform to the general conventions described in the preceding chapter. Locant numbers for designating substitution positions in the SUBSLIST are represented by the following diagram:



○: (400,240)
•: (0,0)

in which a character set in parentheses represent the handedness of each position. In accord with the default definitons of the macro `bzdrv`, each of the right-handed positions (2 and 3) is designed to take only a right-handed substituent, while each of the left-handed positions (5 and 6) is to take only a left-handed substituent. Such positions (designated with the letter 'r' or 'l') are referred to as 'oriented' positions in this manual. In contrast, the top (and also the bottom) position of a benzene ring (designated with the string 'lr') can accommodate a substituent of both handedness. It is referred to as a 'double-sided' position in this manual. Although the default definition is to put a right-handed moiety, a left-handed substituent can be printed by means of the macro `\lmoiety`.

The symbols • and ○ in the diagram respectively represent the reference point and the inner origin of the macro. These will be described in detail in Chapter 14.

The optional argument OPT specifying a bond pattern are shown in Table 3.1. Thereby, a wide variety of bond patterns (such as two patterns of benzene double bonds as well as an aromatic circle) can be depicted.

The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 6. For example, the statements,

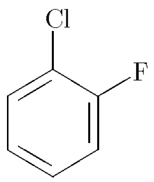
```
\bzdrv{1==Cl;2==F}
```

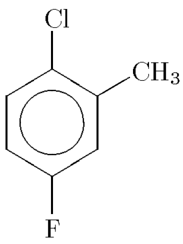
Table 3.1: Argument OPT for commands \ **bzdrv** and \ **bzdrh**

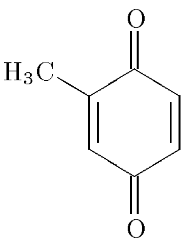
Character	Printed structure
none or r	right-handed set of double bonds
l	left-handed set of double bonds
c	aromatic circle
p or pa	*p*-benzoquinone (A) (Oxygen atomes at 1,4-positions)
pb	*p*-benzoquinone (B) (Oxygen atomes at 2,5-positions)
pc	*p*-benzoquinone (C) (Oxygen atomes at 3,6-positions)
o or oa	*o*-benzoquinone (A) (Oxygen atomes at 1,2-positions)
ob	*o*-benzoquinone (B) (Oxygen atomes at 2,3-positions)
oc	*o*-benzoquinone (C) (Oxygen atomes at 3,4-positions)
od	*o*-benzoquinone (D) (Oxygen atomes at 4,5-positions)
oe	*o*-benzoquinone (E) (Oxygen atomes at 5,6-positions)
of	*o*-benzoquinone (F) (Oxygen atomes at 1,6-positions)

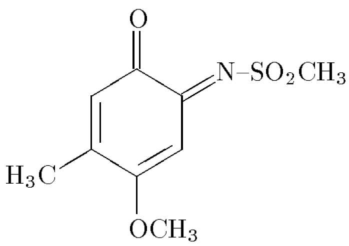
```
\bzdrv[c]{1==Cl;4==F;2==CH$_{3}$}\qquad
\bzdrv[pa]{1D==O;4D==O;6==H$_{3}$C}
\bzdrv[oa]{1D==O;2D==N--SO$_{2}$CH$_{3}$;4==OCH$_{3}$;5==H$_{3}$C}
```

produce the following structures:





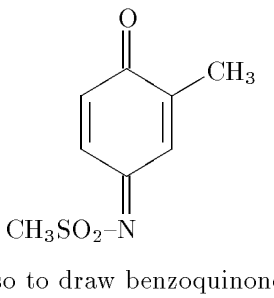


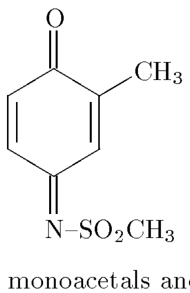


In order to designate the handedness of a substituent explicitly, you can use **\rmoiety** or **\lmoiety** commands. Thus, the statements,

```
\bzdrv[pa]{1D==O;4D==\lmoiety{CH$_{3}$SO$_{2}$--N};2==CH$_{3}$}
\bzdrv[pa]{1D==\rmoiety{O};4D==\rmoiety{N--SO$_{2}$CH$_{3}$};2==CH$_{3}$}
```

produce the following structures with left-handed and right-handed methanesulfonimido groups.

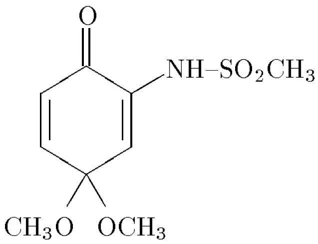


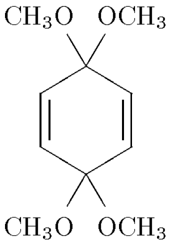


The macro **bzdrv** is used also to draw benzoquinone monoacetals and diacetals. The handedness of a substituent attached at such a tetrahedral position is determined in the light of chemical conventions. For example,

```
\bzdrv[pa]{1D==O;4Sb==CH$_{3}$O;4Sa==OCH$_{3}$;2==NH--SO$_{2}$CH$_{3}$}
\qquad \qquad
\bzdrv[pa]{1Sb==CH$_{3}$O;1Sa==OCH$_{3}$;4Sb==CH$_{3}$O;4Sa==OCH$_{3}$}
```

produce the following structures.



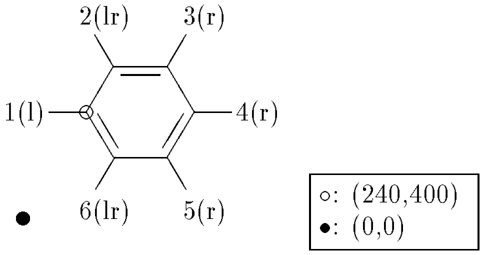


3.1.2 Horizontal Forms of Benzene Derivatives

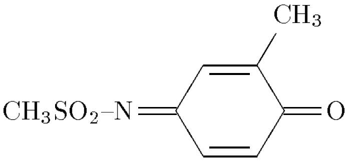
You can use the macro `\bzdrh` to draw benzene derivatives of horizontal type (carom.sty). The format of this command is as follows:

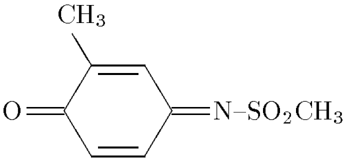
```
\bzdrh[OPT]{SUBSLIST}
```

The formats of the arguments are the same as those of `\bzdrv` (Tables 2.2 and 3.1). The locant numbering and the handedness of substitution are designed as follows:



For example, the diagrams:





are typeset by inputting the statements:

```
\bzdrh[pa]{4D==O;1D==CH$_{3}$SO$_{2}$--N;3==CH$_{3}$} \qquad
\bzdrh[pa]{1D==O;4D==N--SO$_{2}$CH$_{3}$;2==CH$_{3}$}
```

It should be noted the the commands `\bzdrv` and `\bzdrh` are based respectively on the commands `\cyclohexanev` and `\cyclohexaneh` that will be described in the next section. Hence, structures drawn with the former set of commands can be also drawn with the latter set of commands.

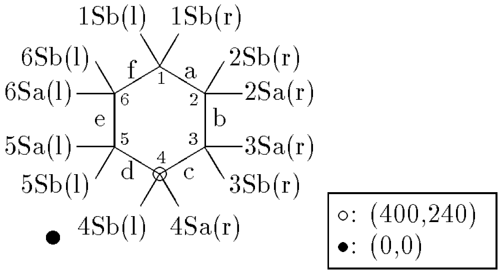
3.2 Drawing Cyclohexane Derivatives

3.2.1 Vertical Forms of Cyclohexane Derivatives

The macro `\cyclohexanev` is used to draw cyclohexane derivatives of vertical type (carom.sty). The format of this command is as follows:

```
\cyclohexanev[BONDLIST]{SUBSLIST}
```

Locant numbers (1–6) for designating substitution positions and characters (a–f) for showing bonds to be doubled are represented by the following diagram:



Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character. The bond-correspondence is rather arbitrary in some cases but conforms to chemical conventions as faithfully as possible if such conventions are presence (Table 3.2).

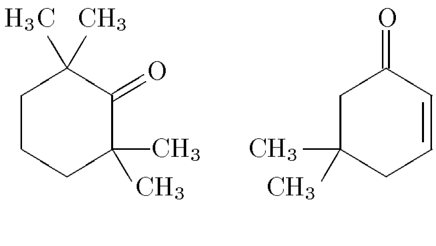
Table 3.2: Argument BONDLIST for commands `\cyclohexanev` and `\cyclohexaneh`

Character	Printed structure
none	cyclohexane
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond
A	aromatic circle

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used. Suppose you input the commands:

```
\cyclohexanev{2D==O;1Sb==H$_{3}$C;1Sa==CH$_{3}$;%
3Sb==CH$_{3}$;3Sa==CH$_{3}$} \qquad\qquad
\cyclohexanev[b]{1D==O;5Sb==CH$_{3}$;5Sa==CH$_{3}$}
```

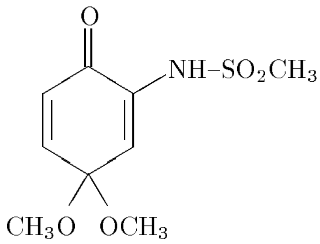
The first example illustrates the case that `\cyclohexanev` accompanies no optional argument. On the other hand, the second one take [b] as an optional BONDLIST, which prints an inner bond between 2 and 3 positions. Thus, you can obtain the following diagrams:

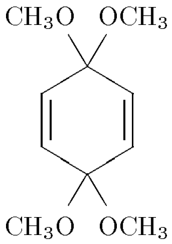


Since the macro `\cyclohexanev` is the basis of the macro `\bzdrv`, structural formulas depicted with the latter command can also be written by the former one. For example, the quinone acetals described above are also typeset by the following statements.

```
\cyclohexanev[be]{1D==O;4Sb==CH$_{3}$O;4Sa==OCH$_{3}$;2==NH--SO$_{2}$CH$_{3}$}
\qquad \qquad
\cyclohexanev[be]{1Sb==CH$_{3}$O;1Sa==OCH$_{3}$;4Sb==CH$_{3}$O;4Sa==OCH$_{3}$}
```

These commands are completely equivalent to those describe above and produce the following structures.

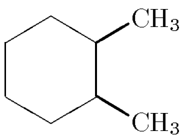


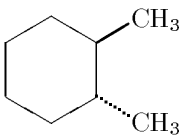


For the purpose of depicting the stereochemisty of a cyclohexane ring, input the following:

```
\cyclohexanev{2B==CH$_{3}$;3B==CH$_{3}$}\qquad\qquad
\cyclohexanev{2B==CH$_{3}$;3A==CH$_{3}$}
```

Thereby, you can obtain:



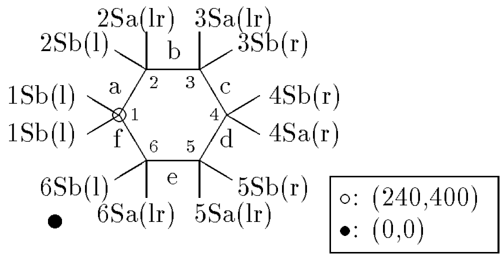


3.2.2 Horizontal Forms of Cyclohexane Derivatives

The macro `\cyclohexaneh` is used to draw cyclohexane derivatives of horizontal type (carom.sty). The format of this command is as follows:

```
\cyclohexaneh[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:

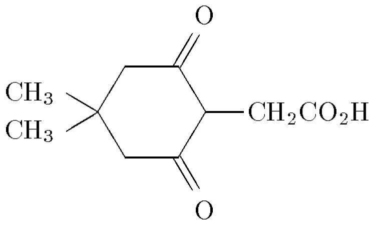


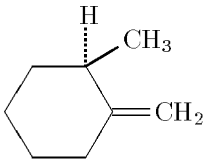
Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros. The SUBSLIST and the BONDLIST format are shown in Table 2.2 and 3.2, respectively.

Example:

```
\cyclohexaneh{3D==O;5D==O;1Sb==CH$_{3}$;1Sa==CH$_{3}$;%
4==CH$_{2}$CO$_{2}$H}\qquad\qquad
\cyclohexaneh{4D==CH$_{2}$;3SB==CH$_{3}$;3SA==H}
```

These commands produce:





Chapter 4

Carbocycles with Fused Six-Membered Rings

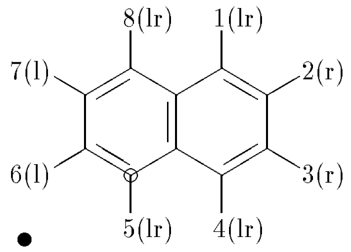
4.1 Drawing Naphthalene Derivatives

4.1.1 Vertical Forms of Naphthalene Derivatives

The macro **\naphdrv** is used to draw naphthalene derivatives of vertical type (carom.sty) as well as various naphthoquinone derivatives. The format of this command is as follows:

```
\naphdrv[OPT]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:



○: (400,240)
●: (0,0)

The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument OPT is used to specify a bond pattern as shown in Table 4.1. The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 8.

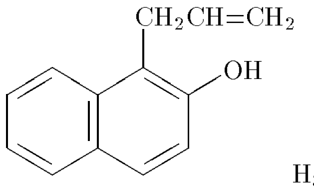
Example:

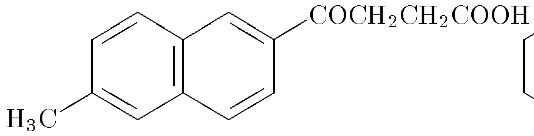
```
\naphdrv{1==CH$_{2}$CH=CH$_{2}$;2==OH} \qquad
\naphdrv{6==H$_{3}$C;2==COCH$_{2}$CH$_{2}$COOH} \hskip1.5cm
\naphdrv[o]{1Sb==Cl;1Sa==Cl;2D==O}
```

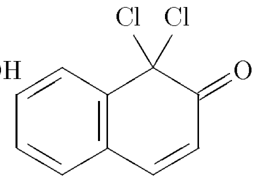
These commands produce:

Table 4.1: Argument OPT for commands `\naphdrv` and `\naphdrh`

Character	Printed structure
none	naphthalene
A	aromatic circle
p or pa	1,4-quinone (A) left aromatic, right quinone
pb	1,4-quinone (B) right aromatic, left quinone
o or oa	*o*-quinone (A) (Oxygen atomes at 1,2-positions)
ob	*o*-quinone (B) (Oxygen atomes at 2,3-positions)
oc	*o*-quinone (C) (Oxygen atomes at 3,4-positions)
od	*o*-quinone (D) (Oxygen atomes at 4,5-positions)
oe	*o*-quinone (E) (Oxygen atomes at 5,6-positions)
of	*o*-quinone (F) (Oxygen atomes at 1,6-positions)
q or qa	2,6-quinone (A)
qb	2,6-quinone (B) (actually 3,7-positons)
qc	1,5-quinone (C)
qd	1,5-quinone (D) (actually 4,8-positions)
qe	1,7-quinone (E)
qf	1,7-quinone (F) (actually 2,8-positions)
qg	1,7-quinone (G) (actually 4,6-positions)
qh	1,7-quinone (H) (actually 3,5-positions)
P or Pa	: 1,4,5,8-quinone (A)
Pb	1,2,5,8-quinone (B)
Q	1,2,3,4-quinone
O or Oa	1,2,5,6-quinone (A)
Ob	1,2,7,8-quinone (B)
Oc	1,2,3,5-quinone (C)
Od	1,2,3,7-quinone (D)





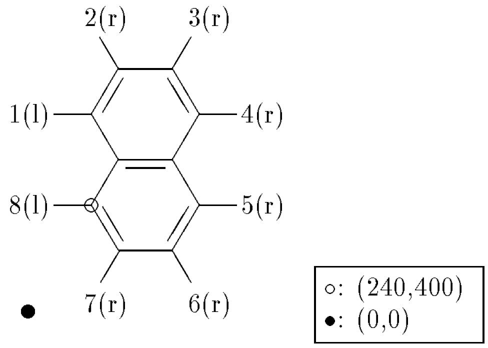


4.1.2 Horizontal Forms of Naphthalene Derivatives

The macro **`\naphdrh`** is used to draw naphthalene derivatives of horizontal type (carom.sty) as well as various naphthoquinone derivatives. The format of this command is as follows:

```
\naphdrh[OPT]{SUBSLIST}
```

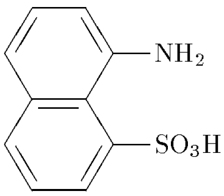
The format of the argument OPT is the same as that of **`\naphdrv`** (Tables 4.1). The format of the argument SUBSLIST is the same as collected in Tables 2.2. The locant numbering and the handedness of substitution are designed as follows:

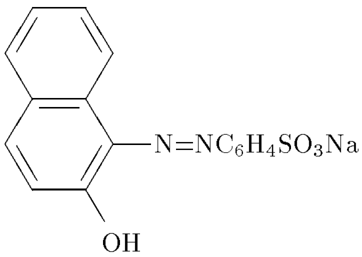


Example:

```
\naphdrh{4==NH$_{2}$;5==SO$_{3}$H}\qquad
\naphdrh{5==N=NC$_{6}$H$_{4}$SO$_{3}$Na;6==OH}
```

These commands produce:





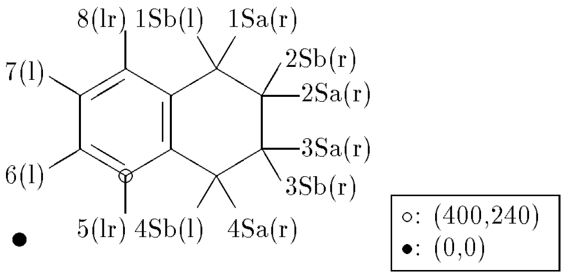
4.2 Drawing Tetraline Derivatives

4.2.1 Vertical Forms of Tetraline Derivatives

The macro **`\tetralinev`** is used to draw tetraline derivatives of vertical type (carom.sty) as well as various naphthoquinone derivatives. The format of this command is as follows:

```
\tetralinev[OPT]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument OPT is used to specify a bond pattern as shown in Table 4.2.

Table 4.2: Argument OPT for commands `\tetralinev` and `\tetralineh`

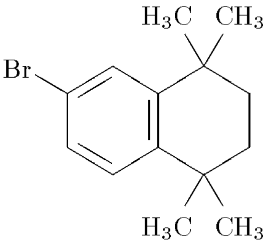
Character	Printed structure
none	tetraline
A	aromatic circle
e or ea	1,2-double bond
eb	2,3-double bond
ec	3,4-double bond

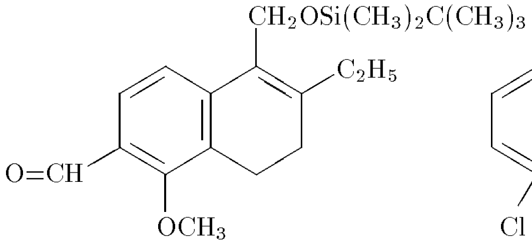
A bond modifier in the argument SUBSLIST for $n = 1$ to 4 can be one of the bond modifiers shown in Table 2.2, which allows α- or β-orientation. On the other hand a bond modifier in the argument SUBSLIST for $n = 5$ to 8 should be vacant. If there appears the overcrowding between 1- and 8-substituent or between 4- and 5-substituent, the bond modifier 5Sb or 8Sb is allowed to avoid such overcrowding.

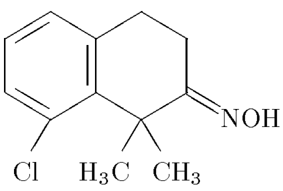
Example:

```
\tetralinev{1Sb==H$_{3}$C;1Sa==CH$_{3}$;%
4Sb==H$_{3}$C;4Sa==CH$_{3}$;7==Br}\qquad
\tetralinev[ea]{1==CH$_{2}$OSi(CH$_{3}$)$_{2}$C(CH$_{3}$)$_{3}$;
2==C$_{2}$H$_{5}$;5==OCH$_{3}$;6==O=CH}\qquad
\tetralinev{3D==NOH;4Sb==H$_{3}$C;4Sa==CH$_{3}$;5Sb==Cl}
```

These commands produce:





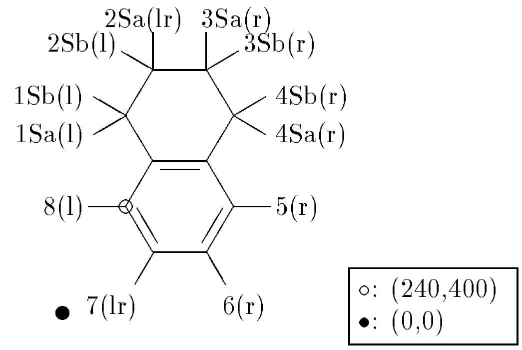


4.2.2 Horizontal Forms of Tetraline Derivatives

The `\tetralineh` is the horizontal counterpart of the command `\tetralinev`:

```
\tetralineh[OPT]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:

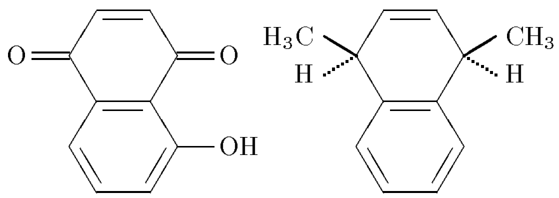


The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument OPT is used to specify a bond pattern as shown in Table 4.2. The argument SUBSLIST is the same as that of `\tetralinev`.

Example:

```
\tetralineh[eb]{1D==O;4D==O;5==OH} \qquad
\tetralineh[eb]{1SB==H$_{3}$C;1SA==H;4SB==CH$_{3}$;4SA==H}
```

These commands produce:



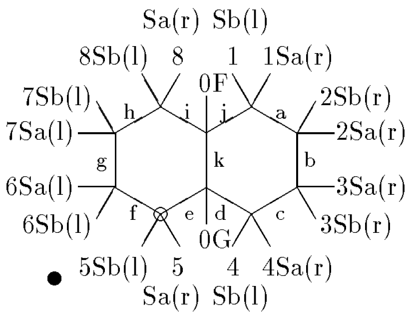
4.3 Drawing Decaline Derivatives

4.3.1 Vertical Forms of Decaline Derivatives

The macro `\decalinev` is used to draw decaline derivatives of vertical type (carom.sty). The format of this command is as follows:

```
\decalinev[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and characters for showing bonds to be doubled are represented by the following diagram:



○: (400,240)
•: (0,0)

The handedness for each oriented or double-sided position is shown with a character set in parentheses. The option argument BONDLIST is based on the assignment of characters (a–k) to respective bonds as shown in the above diagram. A bond modifier in the argument SUBSLIST for n = 1–8 can be one of bond modifiers shown in Table 2.2. The substitution at the bridgehead positions is designated as shown in Table 4.3.

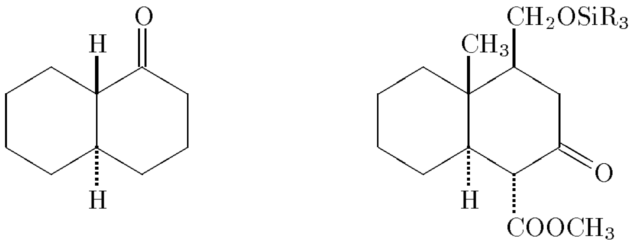
Table 4.3: SUBSLIST for bridgehead positions in `\decalinev` and `\decalineh`

Character	Printed structure
0FA	alpha single bond at 8a
0FB	beta single bond at 8a
0FU	unspecified single bond at 8a
0GA	alpha single bond at 4a
0GB	beta single bond at 4a
0GU	unspecified single bond at 4a

Example:

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

These commands produce:

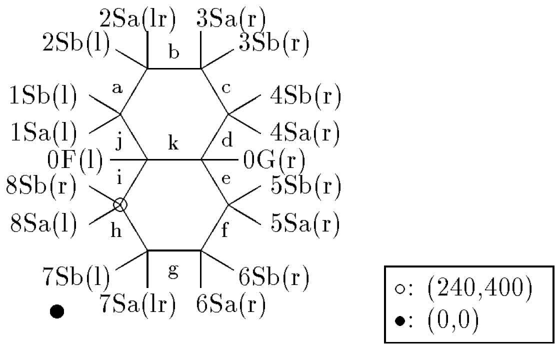


4.3.2 Horizontal Forms of Decaline Derivatives

The macro `\decalineh` (carom.sty) is the horizotal counterpart of `\decalinev`. The format and the assignment of BONDLIST and SUBSLIST of the former macro are the same as the latter (see Tables 2.2 and 4.3).

```
\decalineh[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:

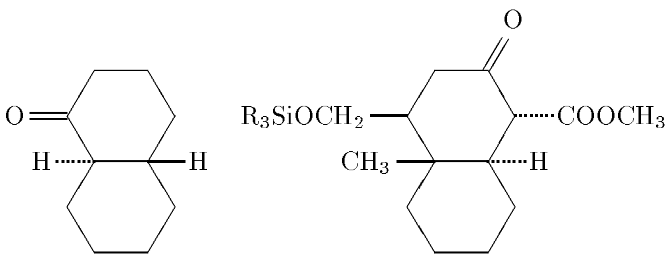


The handedness for each oriented or double-sided position is shown with a character set in parentheses.

Example:

```
\decalineh{1D==O;0FA==H;0GB==H} \qquad\qquad
\decalineh{1B==R$_{3}$SiOCH$_{2}$;3D==O;4A==COOCH$_{3}$;%
0FB==CH$_{3}$;0GA==H}
```

These commands produce:



Chapter 5

Fused Tricyclic Carbocycles and Steroids

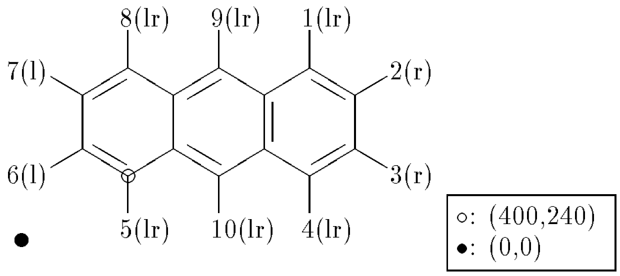
5.1 Drawing Anthracene Derivatives

5.1.1 Command for Specified Use

The macro `\anthracenev` is used to draw anthracene derivatives of vertical type (carom.sty) as well as various quinone derivatives. The format of this command is as follows:

```
\anthracenev[OPT]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:

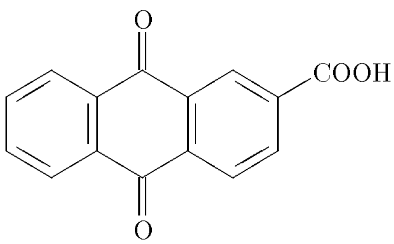


The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument OPT is used to specify a bond pattern as shown in Table 5.1. The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 10.

Example:

```
\anthracenev[pa]{9D==O;{{10}D}==O;2==COOH}\hskip1.5cm
\anthracenev[pA]{9D==O;{{10}D}==O;2==COOH}
```

These commands produce:



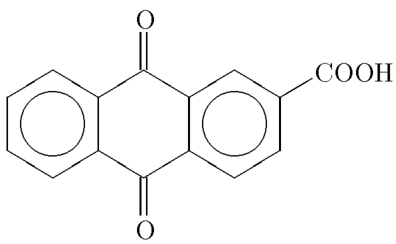


Table 5.1: Argument OPT for commands \anthracenev

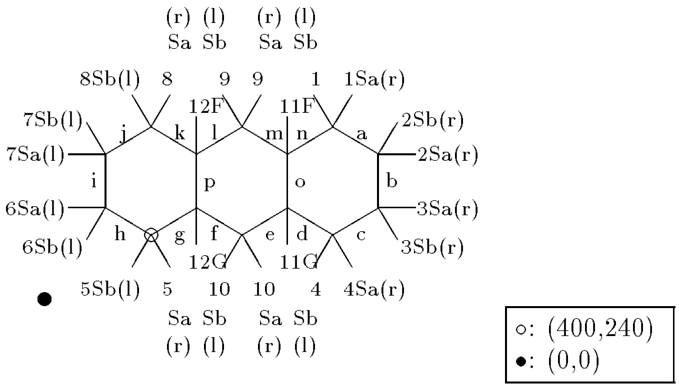
Character	Printed structure
none or r	right-handed double bonds
l	left-handed double bonds
A	aromatic circle
p or pa	9,10-anthraquinone (A)
pA	9,10-anthraquinone (circle type)
o	1,2-anthraquinone (A)
oa	1,2-anthraquinone (A')
oA	1,2-anthraquinone (circle type)
ob	2,3-antharquinone (B)
oc	1,2-anthraquinone (C)
q	1,4-anthraquinone (A)
qa	1,4-anthraquinone (A')
qA	1,4-anthraquinone (circle type)

5.1.2 Command for General Use

The macro **\hanthracenev** (carom.sty) is a more general macro than **anthracenev**, where the latter is actually a short-cut command of the former. The format of this command is as follows:

```
\hanthracenev[BONDLIST]{SUBSLIST}
```

Locant numbers (1–12) for designating substitution positions and bond descriptors (a–p) are represented by the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses. The option argument BONDLIST is based on the assignment of characters (a–p) to respective bonds as shown in the above diagram and Table 5.2. A bond modifier in the argument SUBSLIST for n = 1–10 is selected from those shown in Table 2.2. The substitution at the bridgehead positions is designated as shown in Table 5.3.

Example:

```
\hanthracenev[C]{5==\lmoiety{CH$_{3}$O};%
8==\lmoiety{CH$_{3}$O};9==CN;{{10}D}==O}\qquad
\hanthracenev[hjp]{{{11}FA}==H;{{11}GA}==H;1A==OBz;4B==OH;2D==O}
```

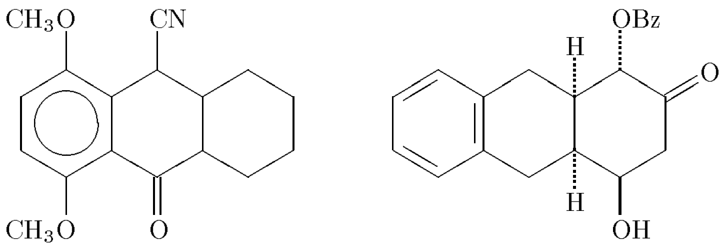
These commands produce:

Table 5.2: Argument BONDLIST for commands `\hanthracenev`

Character	Printed structure
none	perhydro-anthracene
a	1,2-double bond
b	2,3-double bond
c	3,4-double bond
d	4,4a-double bond
e	10,4a-double bond
f	10,10a-double bond
g	5,10a-double bond
h	5,6-double bond
i	6,7-double bond
j	8,7-double bond
k	8,8a-double bond
l	9,8a-double bond
m	9,9a-double bond
n	1,9a-double bond
o	4a,9a-double bond
p	10a,8a-double bond
A	right aromatic circle
B	central aromatic circle
C	left aromatic circle

Table 5.3: SUBSLIST for bridgehead positions in `\hanthracenev`

Character	Printed structure
11FA	alpha single bond at 9a
11FB	beta single bond at 9a
11FU	unspecified single bond at 9a
11GA	alpha single bond at 4a
11GB	beta single bond at 4a
11GU	unspecified single bond at 4a
12FA	alpha single bond at 8a
12FB	beta single bond at 8a
12FU	unspecified single bond at 8a
12GA	alpha single bond at 10a
12GB	beta single bond at 10a
12GU	unspecified single bond at 10a



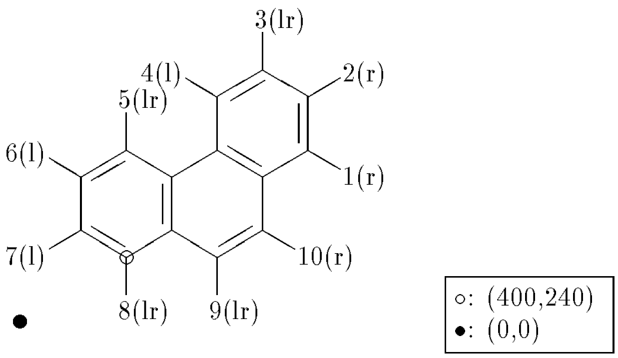
5.2 Drawing Phenanthrene Derivatives

5.2.1 Command for Specified Use

The macro `\phenanthrenev` is used to draw phenanthrene derivatives of vertical type (carom.sty) as well as various quinone derivatives. The format of this command is as follows:

```
\phenanthrenev[OPT]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument OPT is used to specify a bond pattern as shown in Table 5.4.

Table 5.4: Argument OPT for commands `\phenanthrenev`

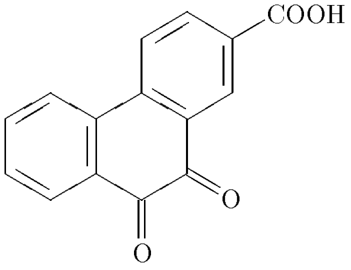
Character	Printed structure
none or r	right-handed double bonds
A	aromatic circle
p or pa	1,4-quinone (A)
pA	1,4-quinone (circle type)
o or oa	1,2-quinone (A)
oA	1,2-quinone (circle type)
ob	2,3-quinone (B)
oc	3,4-anthraquinone (C)
q or qa	9,10-quinone
qA	9,10-quinone (circle type)

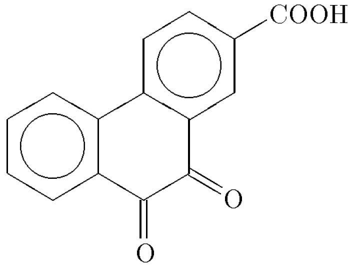
The argument SUBSLIST is employed to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is seledted to be an arabic numeral between 1 and 10.

Example:

```
\phenanthrenev[q]{9D==O;{{10}D}==O;2==COOH}\hskip1.5cm
\phenanthrenev[qA]{9D==O;{{10}D}==O;2==COOH}
```

These commands produce:



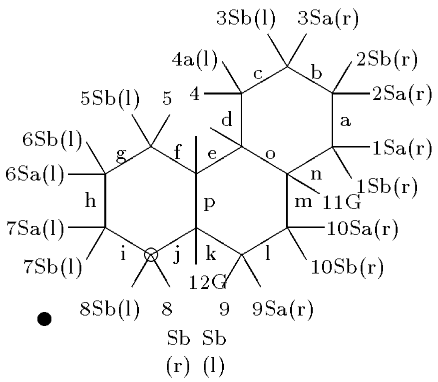


5.2.2 Command for General Use

The macro `\hphenantherev` (carom.sty) is a more general macro than `phenanthrenev`, where the latter is a short-cut command based on the former. The format of this command is as follows:

```
\hphenanthrenev[BONDLIST]{SUBSLIST}
```

Locant numbers (1–12) for designating substitution positions and bond descriptors (a–p) are represented by the following diagram:



○: (400,240)
•: (0,0)

The handedness for each oriented or double-sided position is shown with a character set in parentheses, where the designation of overcrowded positions is abbreviated.

The option argument BONDLIST is based on the assignment of characters (a–p) to respective bonds as shown in the above diagram and Table 5.5. A bond modifier in the argument SUBSLIST for n = 1–10 can be one of bond modifiers shown in Table 2.2. The substitution at the bridgehead positions is similar to that designated in Table 5.3 for `\hanthracenev`.

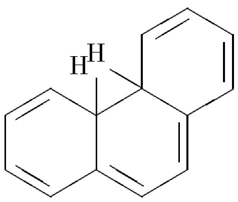
Example:

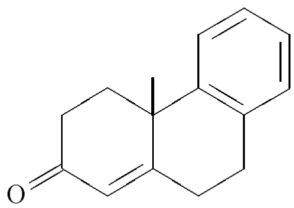
```
\hphenanthrenev[acgikm]{{{11}F}=={\kern-3em\raise1ex\hbox{H}};%
{{12}F}==\lmoiety{H~~}}\hskip1.5cm
\hphenanthrenev[acoj]{7D==O;{{12}FB}==}
```

These commands produce:

Table 5.5: Argument BONDLIST for commands `\hphenanthrenev`

Character	Printed structure
none	perhydro-phenanthrene
a	1,2-double bond
b	2,3-double bond
c	3,4-double bond
d	4,4a-double bond
e	4a,4b-double bond
f	4b,5-double bond
g	5,6-double bond
h	6,7-double bond
i	7,8-double bond
j	8,8a-double bond
k	8a,9-double bond
l	9,10-double bond
m	10,10a-double bond
n	1,10a-double bond
o	4a,10a-double bond
p	4b,8a-double bond
A	right aromatic circle
B	central aromatic circle
C	left aromatic circle



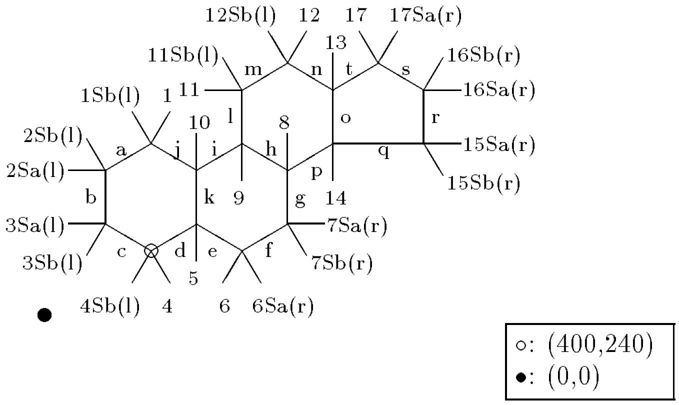


5.3 Drawing Steroid Derivatives

The macro `\steroid` (carom.sty) typsets a steroid derivative without the side chain. The format of this command is as follows:

```
\steroid[BONDLIST]{SUBSLIST}
```

Locant numbers (1–17) for designating substitution positions and bond descriptors (a–t) are represented by the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses, where the designation of overcrowded positions is abbreviated.

The option argument BONDLIST is based on the assignment of characters (a–t) to respective bonds as shown in the above diagram and Table 5.6.

Table 5.6: Argument BONDLIST for commands \steroid

Character	Printed structure	Character	Printed structure
none	steroid skeleton		
a	1,2-double bond	b	2,3-double bond
c	3,4-double bond	d	4,5-double bond
e	6,5-double bond	f	6,7-double bond
g	7,8-double bond	h	9,8-double bond
i	9,10-double bond	j	1,10-double bond
k	5,10-double bond	l	9,11-double bond
m	12,11-double bond	n	12,13-double bond
o	14,13-double bond	p	8,14-double bond
q	14,15-double bond	r	15,16-double bond
s	17,16-double bond	t	17,13-double bond
A	aromatic A ring	B	aromatic B ring
C	aromatic C ring		

A bond modifier in the argument SUBSLIST for n = 1–17 (except fused positions) is selected from the list of bond modifiers (Table 2.2). The substitution at the fused positions (n = 5,8,9,10,13 and 14) is similarly designated as for fused bicylic or tricyclic compounds (Table 5.7).

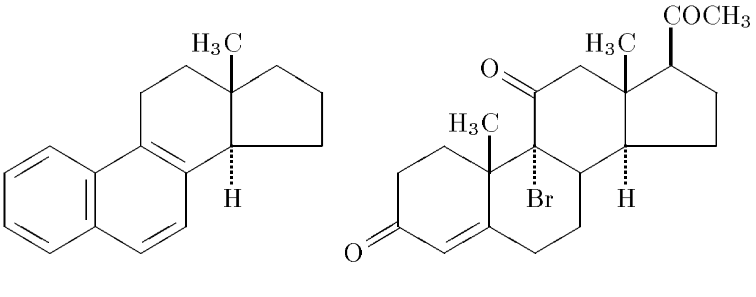
Table 5.7: SUBSLIST for fused positions in \steroid

Character	Printed structure
n or nS	exocyclic single bond at n-atom
nA	alpha single bond at n-atom (boldface)
nB	beta single bond at n-atom (dotted line)
nU	unspecified single bond at n-atom

Example:

```
\steroid[ackhf]{{{13}B}==\lmoiety{H$_{3}$C};{{14}A}==H}\hskip1cm
\steroid[d]{3D==O;9A==Br;{{11}D}==O;%
{{17}B}==COCH$_3$;{{14}A}==H;%
{{13}B}==\lmoiety{H$_3$C};{{10}B}==\lmoiety{H$_3$C}}
```

These commands produce:

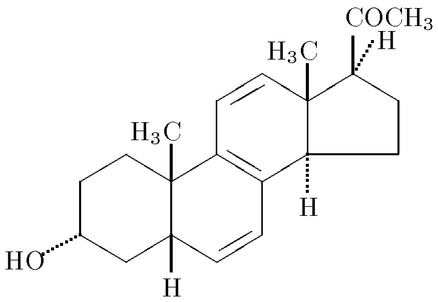


In order to avoid the overcrowding of substitution, you can use TEX primitive commands such as `\raise` and `\kern`.

Example:

```
\steroid[fhm]{3A==HO;5B==H;{{10}B}==\lmoiety{H$_{3}$C};%
{{13}B}==\lmoiety{H$_{3}$C};%
{{14}A}==H;{{17}B}==\raise.5ex\hbox{COCH$_{3}$};%
{{17}SA}=={\kern.5em\lower1.5ex\hbox{H}}}
```

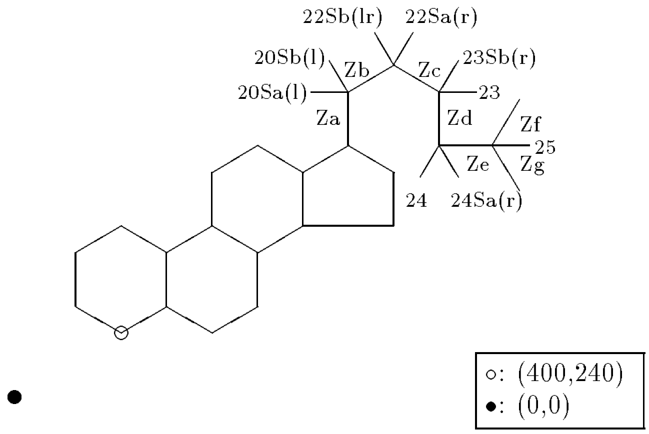
These commands produce:



The macro `\steroidchain` (carom.sty) is to draw a steroid derivative with the side chain. The format of this command is as follows:

```
\steroidchain[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and bond descriptors for the side chain are represented by the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses, where the designation of overcrowded positions is abbreviated.

The option argument BONDLIST is based on the assignment of characters (a–t) to respective bonds as shown in the above diagram and Table 5.6. The locant-numbering of chain carbons is also designated with the BONDLIST in the form of two-character indicators (Za–Zg) as collected in Table 5.8. A bond

Table 5.8: Argument BONDLIST for chain carbons (`\steroidchain`)

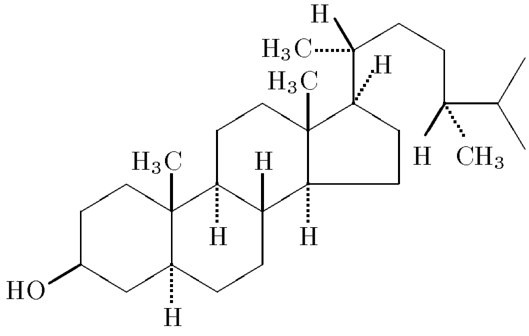
Character	Printed structure	Character	Printed structure
Z	no action		
Za	17,20-double bond	Zb	20,22-double bond
Zc	22,23-double bond	Zd	23,24-double bond
Ze	24,25-double bond	Zf	25,26-double bond
Zg	25,27-double bond		

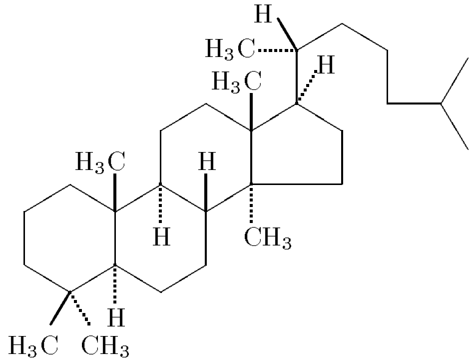
modifier in the argument SUBSLIST for n = 1–25 (except fused positions and terminal positions not to be specified, *e.g.*, 18) can be one of bond modifiers shown in Table 2.2. On the other hand, a bond modifier in the argument SUBSLIST for n = 5, 8, 9, 10, 13, 14, or 25 (fused positions *etc.*) can be selected from bond modifiers shown in Table 5.7.

For example, the `\steroidchain` macro prints (24*R*)-24-methyl-5α-cholestan-3β-ol (campestanol) and 5α-lanostane only by replacing substituents in argument SUBSLIST. Thus, the statements

```
\steroidchain{3B==HO;5A==H;{{10}B}==\lmoiety{H$_3$C};9A==H;8B==H;%
{{17}SA}==\lower1ex\hbox{ H};{{13}B}==\lmoiety{H$_3$C};{{14}A}==H;%
{{20}SA}==H$_3$C;{{20}SB}==H;{{24}SA}==CH$_3$;{{24}SB}==H}
\steroidchain{4SB==\lmoiety{H$_3$C};4SA==CH$_3$;5A==H;%
{{17}SA}==\lower1ex\hbox{ H};%
{{10}B}==\lmoiety{H$_3$C};9A==H;8B==H;{{13}B}==\lmoiety{H$_3$C};%
{{14}A}==CH$_3$;{{20}SA}==\lmoiety{H$_3$C};{{20}SB}==H}
```

typeset the following structural diagrams:

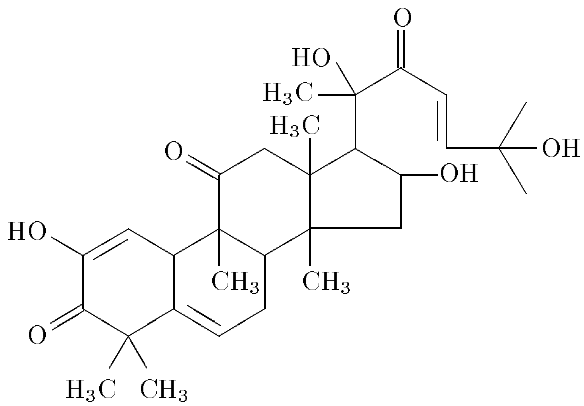




The following example of drawing cucurbitacin I illustrates the designation of double bonds in the side chain. Thus, a single macro is capable of covering a wide variety of derivatives by altering the description in arguments BONDLIST and SUBSLIST.

```
\steroidchain[ae{Zd}]{2==HO;3D==O;4Sb==\lmoiety{H$_3$C};4Sa==CH$_3$;%
9Sa==CH$_{3}$;{{11}D}==O;{{13}}==\lmoiety{H$_3$C};%
{{14}}==CH$_3$;{{20}Sa}==\lmoiety{H$_3$C};{{20}Sb}==HO;%
{{16}Sa}==OH;{{22}D}==O;{{25}}==OH}
```

produces



Chapter 6

Five- or Lower-Membered Carbocycles

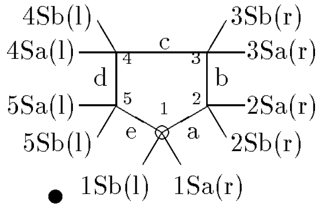
6.1 Drawing Five-Membered Carbocycles

6.1.1 Vertical Forms

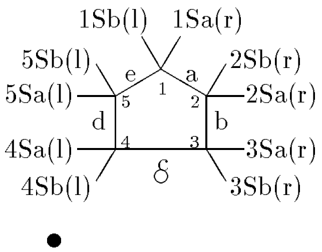
The macro `\cyclopentanev` and the corresponding inverse macro are used to draw five-membered carbocyclic compounds of vertical type (lowcycle.sty). The formats of these commands are as follows:

```
\cyclopentanev[BONDLIST]{SUBSLIST}
\cyclopentanevi[BONDLIST]{SUBSLIST}
```

The following diagrams show the numbering of the commands for designating substitution positions (1–5) and bond descriptors (a–e):



○: (400,240)
•: (0,0)



○: (400,240)
•: (0,0)

In drawing five-membered rings, only commands for general use are ready to use so that they can be employed to typeset both saturated and unsaturated derivatives. Commands for specified use have not been developed since they are not so desirable as compared with the counterparts of six-membered rings.

The optional argument BONDLIST shows bonds to be doubled as shown in Table 6.1. The default structure is a fully saturated form.

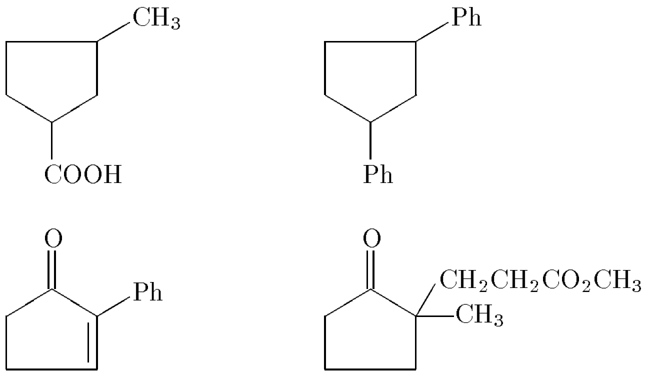
The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 5. For example, the statements,

```
\cyclopentanev{1==COOH;3==CH$_{3}$}\qquad\qquad
\cyclopentanev{1==Ph;3==Ph} \par
\cyclopentanevi[b]{1D==O;2==Ph}\qquad\qquad
\cyclopentanevi{1D==O;2Sa==CH$_{3}$;%
2Sb==CH$_{2}$CH$_{2}$CO$_{2}$CH$_{3}$}
```

produce the following structures:

Table 6.1: BONDLIST for commands \cyclopentanev and \cyclopentaneh

Character	Printed structure
none	mother nucleus
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,1-double bond
A	aromatic circle
{n+}	plus at the n-nitrogen atom (n = 1 to 5)
{0+}	plus (or minus) at the center



The command is capable of typesetting a delocalized and a localized form of cyclopentadienyl anion as follows.

```
\cyclopentanev[A{0{$-$}}]{} \qquad
\cyclopentanev[bd{1{\lower1.2ex\hbox{$-$}}}]{}
```

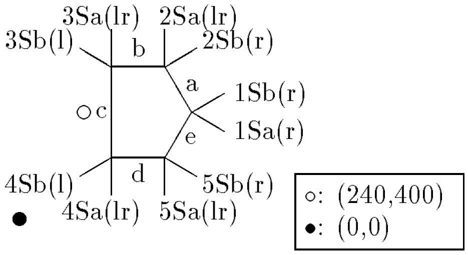
These statements produce

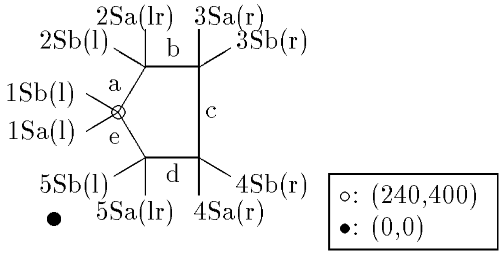
6.1.2 Horizontal Forms

The macro \cyclopentaneh and the corresponding inverse macro are used to draw five-membered carbocyclic compounds of horizontal type (lowcycle.sty). The formats of these commands are as follows:

```
\cyclopentaneh[BONDLIST]{SUBSLIST}
\cyclopentanehi[BONDLIST]{SUBSLIST}
```

The following diagrams show locant numbers for designating substitution positions as well as bond descriptors for showing double bonds:



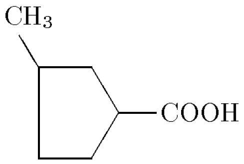


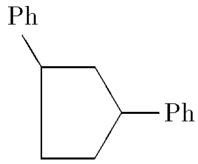
in which the same macro is used to typeset both saturated and unsaturated derivatives. For BONDLIST, see Table 6.1.

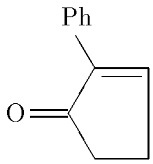
Example:

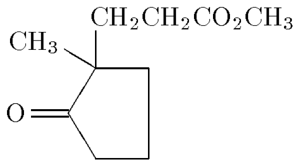
```
\cyclopentaneh{1==COOH;3==CH$_{3}$}\qquad\qquad
\cyclopentaneh{1==Ph;3==Ph} \par
\cyclopentanehi[b]{1D==O;2==Ph}\qquad\qquad
\cyclopentanehi{1D==O;2Sb==CH$_{3}$;%
2Sa==CH$_{2}$CH$_{2}$CO$_{2}$CH$_{3}$}
```

produce the following structures:







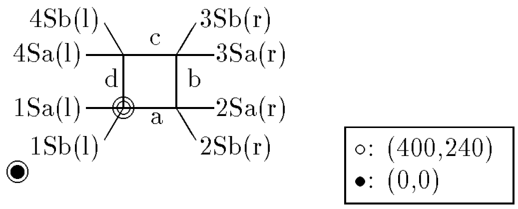


6.2 Drawing Four-Membered Carbocycles

The macro `\cyclobutane` is a command for drawing four-membered carbocycles by using the following format (lowcycle.sty).

```
\cyclobutane[BONDLIST]{SUBSLIST}
```

Locant numbers (1–4) and bond descriptors (a–d) are shown in the following diagram:



The handedness for each oriented position is shown with a character set in parentheses. The optional argument BONDLIST specifies double bonds as shown in Table 6.2.

Table 6.2: BONDLIST for commands `\cyclobutane`

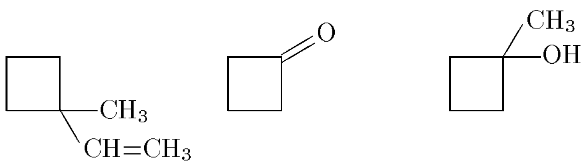
Character	Printed structure	Character	Printed structure
none	mother skeleton (fully saturated)		
a	1,2-double bond	b	2,3-double bond
c	3,4-double bond	d	4,1-double bond
{n+}	plus at the n-nitrogen atom (n = 1 to 4)		

The argument SUBSLIST is filled in to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 4.

Example:

```
\cyclobutane{2Sa==CH$_{3}$;2Sb==CH=CH$_{3}$}
\cyclobutane{3D==O}
\cyclobutane{3Sa==OH;3Sb==CH$_{3}$}
```

produce the following structures:

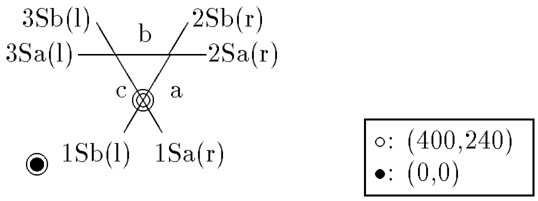


6.3 Drawing Three-Membered Heterocycles

The macro `\cyclopropane` for drawing threee-membered carbocycles has the following format (lowcyclo.sty).

```
\cyclopropane[BONDLIST]{SUBSLIST}
```

Thus, the locant numbering (1–2) and the bond description (a–c) are common as shown in the following diagram:



The handedness for each oriented position is shown with a character set in parentheses. The optional argument BONDLIST is written down to specify double bonds as shown in Table 6.3.

Table 6.3: Argument BONDLIST for commands `\cyclopropane`

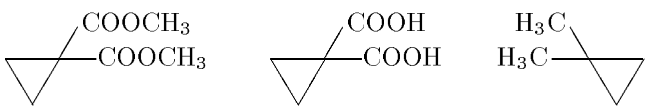
Character	Printed structure
none	saturated
a	1,2-double bond
b	2,3-double bond
c	3,1-double bond
A	aromatic circle
$\{n+\}$	plus at the n-hetero atom (n = 1 to 3)
	$n = 4$ – outer plus at 1 position
	$n = 5$ – outer plus at 2 position
	$n = 6$ – outer plus at 3 position
{0+}	plus at the center of a cyclopropane ring

The argument SUBSLIST is entered to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 3.

Example:

```
\cyclopropane{2Sa==COOCH$_{3}$;2Sb==COOCH$_{3}$}\qquad
\cyclopropane{2Sa==COOH;2Sb==COOH}\qquad\qquad
\cyclopropane{3Sa==H$_{3}$C;3Sb==H$_{3}$C}
```

produce the following structures:

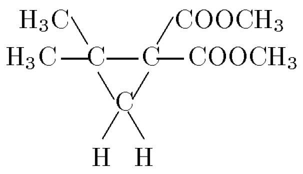


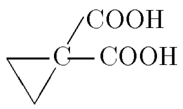
This macro is based on the macro `\threehetero` in which the ATOMLIST of the latter command is set beforehand. In order to draw a carbon atom on a cyclopropane ring, you can use the command `\threehetero` instead of `\cyclopropane`.

Example:

```
\threehetero[H]{1==C;2==C;3==C}%
 {1Sa==H;1Sb==H;2Sa==COOCH$_{3}$;2Sb==COOCH$_{3}$;%
  3Sa==H$_{3}$C;3Sb==H$_{3}$C}\qquad\qquad\qquad
\threehetero[H]{2==C}{2Sa==COOH;2Sb==COOH}
```

produce the following structures:





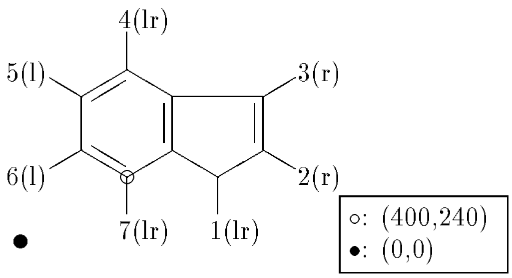
6.4 Drawing Indane Derivatives

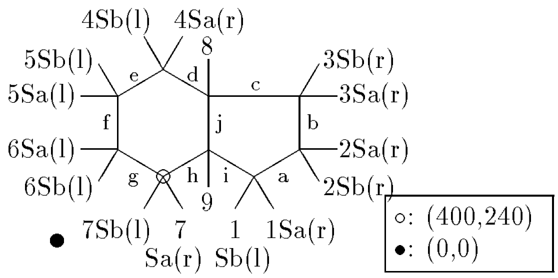
6.4.1 Vertical Forms of Indanes

Since the macros `\indanev` and `\indanevi` are included in the style file 'lowcycle.sty', they are introduced here. The format of `\indanv` is:

```
\indanev[BONDLIST]{SUBSLIST}
```

The locant numbering (1–9) and the bond description (a–j) have a common format as shown in the following diagrams:





The handedness for each oriented or double-sided position is shown with a character set in parentheses. Each character in the optional argument BONDLIST indicates a specific double bond as shown in Table 6.4. The default setting of BONDLIST produces a fully unsaturated structure, when the option BONDLIST is omitted. If you want to draw a fully saturated structure, you should write down a null option ([]) or [H].

The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 7. Substitution on 8 (3a position) or 9 (7a position) can be assigned in the same way.

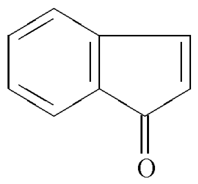
Example:

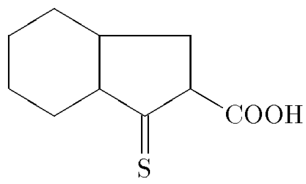
```
\indanev{1D==O} \qquad
\indanev[H]{1D==S;2==COOH}\par
\indanev[egj]{2D==O;3Sa==H;3Sb==Ph}\qquad
\indanev[A]{2D==O;3Sa==H;3Sb==Ph}
```

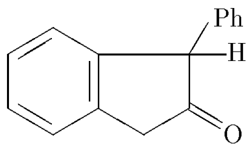
produce the following structures:

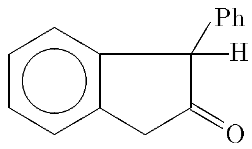
Table 6.4: Argument BONDLIST for commands `\indolev` and others

Character	Printed structure	Character	Printed structure
none or r	aromatic six-membered ring	H or []	fully saturated form
a	1,2-double bond	b	2,3-double bond
c	3,3a-double bond	d	4,3a-double bond
e	4,5-double bond	f	5,6-double bond
g	6,7-double bond	h	7,7a-double bond
i	1,7a-double bond	j	3a,4a-double bond
A	aromatic circle (six-membered ring)		
B	aromatic circle (five-membered ring)		
{n+}	plus at the n-nitrogen atom (n = 1 to 9)		





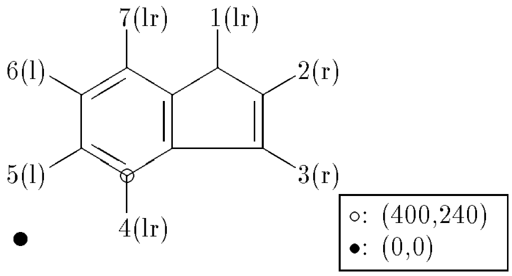


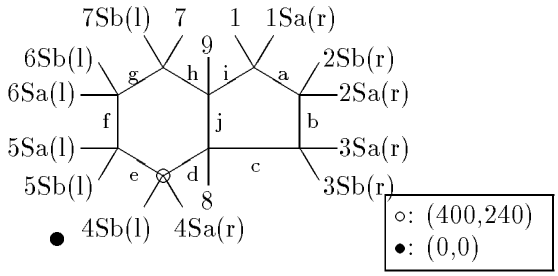


The macro `\indanevi` for drawing indane derivatives of inverse vertical type has the following format (lowcycle.sty).

```
\indanevi[BONDLIST]{SUBSLIST}
```

The locant numbering and the bond description are common with the vertical counterpart as shown in the following diagrams:



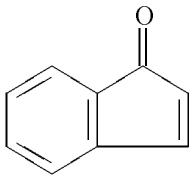


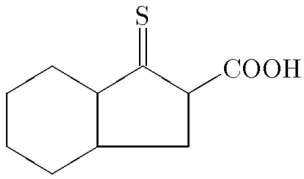
The handedness for each oriented or double-sided position is shown with a character set in parentheses; this is however omitted in the overcrowded position (between 7 and 1). The optional argument BONDLIST specifies bonds to be doubled as shown in Table 6.4.

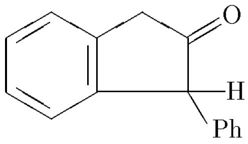
Example:

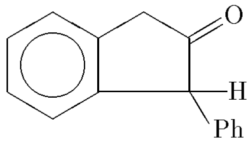
```
\indanevi{1D==O} \qquad
\indanevi[H]{1D==S;2==COOH}\par
\indanevi[egj]{2D==O;3Sa==H;3Sb==Ph}\qquad
\indanevi[A]{2D==O;3Sa==H;3Sb==Ph}
```

produce the following structures:







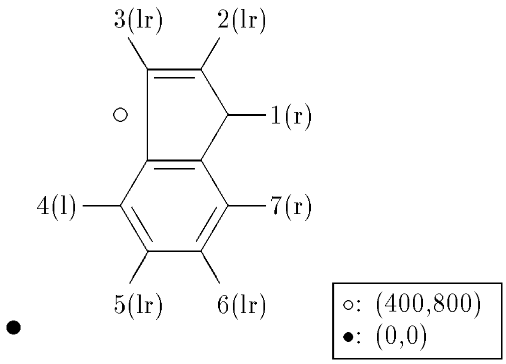


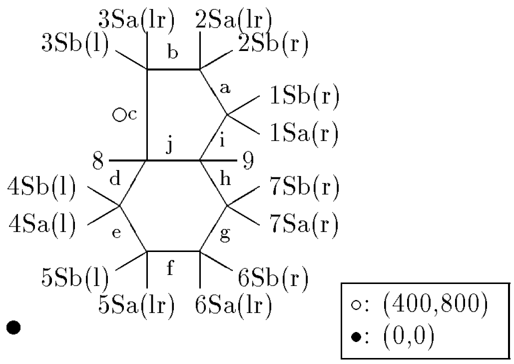
6.4.2 Horizontal Forms of Indanes

The macro `\indaneh` for drawing indane derivatives of horizontal type has the following format (lowcycle.sty).

```
\indaneh[BONDLIST]{SUBSLIST}
```

Locant numbers (1–9) for designating substitution positions and bond descriptors (a–j) are represented by the following diagram:



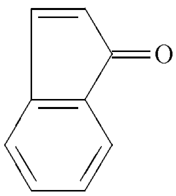


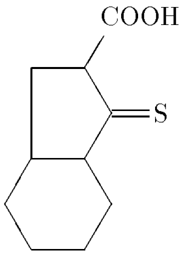
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST gives the description of double bonds as shown in Table 6.4.

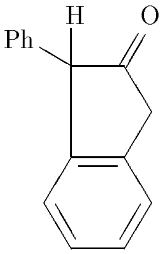
Example:

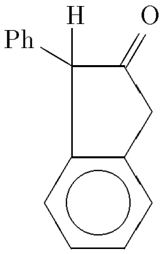
```
\indaneh{1D==O} \qquad
\indaneh[H]{1D==S;2==COOH}\par
\indaneh[egj]{2D==O;3Sa==H;3Sb==Ph}\qquad
\indaneh[A]{2D==O;3Sa==H;3Sb==Ph}
```

produce the following structures:





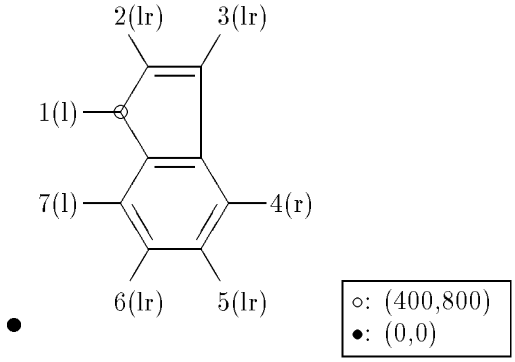


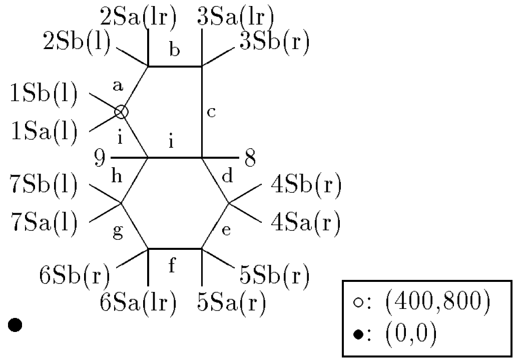


The macro `\indanehi` is the inverse counterpart of `\indaneh`, which aims at drawing indane derivatives of inverse horizontal type (lowcycle.sty).

```
\indanehi[BONDLIST]{SUBSLIST}
```

Locant numbers (1–9) for designating substitution positions and characters (a–j) for describing double bonds are shown in the following diagram:

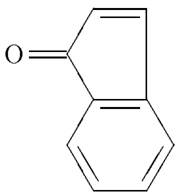


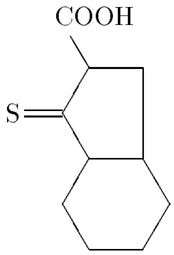


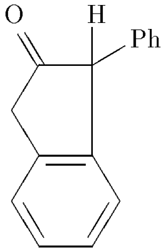
Example:

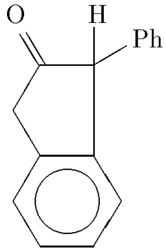
```
\indanehi{1D==O} \qquad
\indanehi[H]{1D==S;2==COOH}\par
\indanehi[egj]{2D==O;3Sa==H;3Sb==Ph}\qquad
\indanehi[A]{2D==O;3Sa==H;3Sb==Ph}
```

produce the following structures:









Chapter 7

Six-Membered Heterocycles

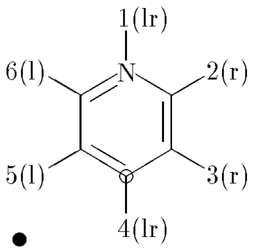
7.1 Drawing Vertical Forms of Six-Membered Heterocycles

7.1.1 Commands for Specified Use

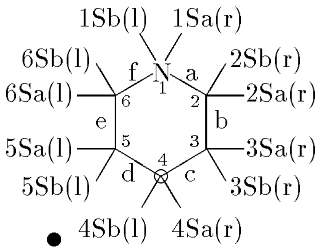
The macro `\pyridinev` and the related macros are used to draw six-membered heterocyclic compounds of vertical type (hetarom.sty). Each of these commands typesets heterocycles with the specific arrangement of heteroatoms on its skeleton. The formats of these commands are as follows:

```
\pyridinev[BONDLIST]{SUBSLIST}
\pyrazinev[BONDLIST]{SUBSLIST}
\pyrimidinev[BONDLIST]{SUBSLIST}
\pyridazinev[BONDLIST]{SUBSLIST}
\triazinev[BONDLIST]{SUBSLIST}
```

By using the command `\pyridinev` as an example, the mode of locant numbering for designating substitution positions is shown as follows along with the bond descriptors for assigning inner double bonds:



○: (400,240)
•: (0,0)



○: (400,240)
•: (0,0)

The optional argument BONDLIST specifies bonds to be doubled as shown in Table 7.1. Since a specific character is assigned to a specific bond of each heterocycle, the concrete meaning of the character is different from one heterocycle to another. However, the methodology is common in drawing all heterocycles so that the commands of XΥMTEX are easy to use.

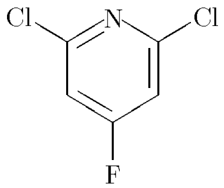
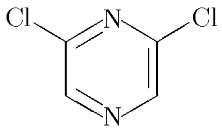
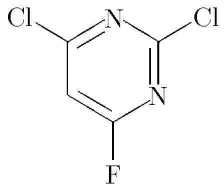
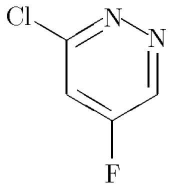
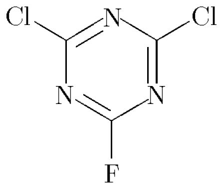
The argument SUBSLIST shows each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 6. For example, the statements,

```
\pyridinev{2==Cl;6==Cl;4==F}
\pyrazinev{2==Cl;6==Cl}
\pyrimidinev{2==Cl;6==Cl;4==F}
\pyridazinev{6==Cl;4==F}
\triazinev{2==Cl;6==Cl;4==F}
```

produce the following structures:

Table 7.1: Argument BONDLIST for commands `\pyridinev`, *etc.*

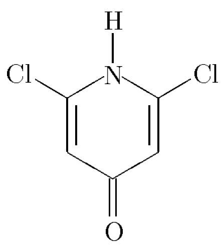
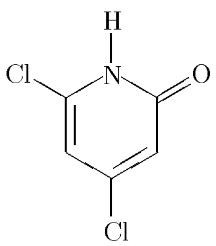
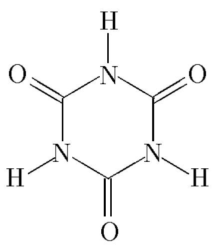
Character	Printed structure
none or r	pyridine (right-handed)
l	pyridine (left-handed)
H or [ ]	fully saturated ring
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond
A	aromatic circle
$\{n+\}$	plus at the n-nitrogen atom ($n = 1$ to 6)

It should be noted that the default setting of the BONDLIST is to depict a fully unsaturated ring (usually an aromatic ring). By setting an appropriate character string, a sigle macro is used to typeset both partially saturated and unsaturated derivatives. Moreover, a fully saturated ring can be obtained by setting a null argument or H in BONDLIST. This specification can be illustrated with the following examples.

```
\pyridinev[be]{1==H;2==Cl;6==Cl;4D==O}\qquad
\pyridinev[ce]{1==H;4==Cl;6==Cl;2D==O}\qquad
\triazinev[H]{2D==O;4D==O;6D==O;1==H;3==H;5==H}
```

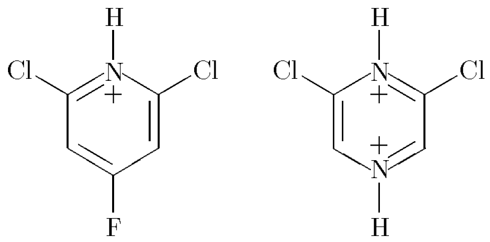
produce the following structures:

In order to depict a charge on a nitrogen, you write the statements, for example:

```
\pyridinev[r{1+}]{1==H;2==Cl;6==Cl;4==F}\qquad
\pyrazinev[l{1+}{4+}]{1==H;4==H;2==Cl;6==Cl}
```

Then you obtain the following structures:



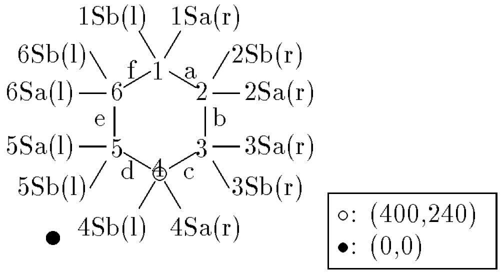
In these cases, a character 'r' or 'l' should be added to the argument BONDLIST, since the defaults are hidden by writing other characters in the BONDLIST.

7.1.2 Commands for General Use

The command **\sixheterov** is a general macro used to draw six-memered heterocyclic derivatives of vertical type (hetarom.sty). It is especially useful to draw heterocyclic compounds having other skeletal atoms than nitrogen atoms. The format of this command is as follows:

```
\sixheterov[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers for designating substitution positions and characters for bond-description are shown in the following diagram:



Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros because of the lack of spaces to print otherwise.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge specified by the character. The bond-specification is rather arbitrary in some cases but conforms to chemical conventions as faithfully as possible if such conventions are presence (Table 7.2). Since the default prints a fully unsaturated form, an option argument [H] should be written to typeset a saturated form.

The augument ATOMLIST is a list of heteroatoms, *e.g.*, 1==N for a nitrogen atom at 1-position. It should be emphasized that, in order to typeset a heteroatom at a given position, the edges incident to the heteroatom are automatically truncated to put space for printing the heteroatrom. Compare the following examples.

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

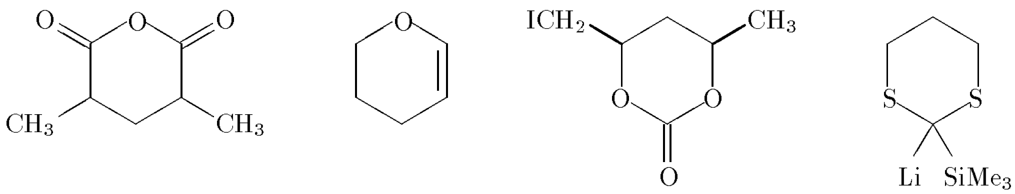
Example:

```
\sixheterov[H]{1==O}{2D==O;6D==O;3==CH$_{3}$;5==CH$_{3}$}\qquad
\sixheterov[b]{1==O}{}\qquad
\sixheterov[H]{3==O;5==O}{4D==O;6B==ICH$_{2}$;2B==CH$_{3}$}\qquad
\sixheterov[H]{3==S;5==S}{4Sa==SiMe$_{3}$;4Sb==Li}
```

Table 7.2: Argument BONDLIST for commands `\sixheterov` and `\sixheterovi`

Character	Printed structure
none or r	sixhetero (right-handed)
l	sixhetero (left-handed)
H or []	fully saturated form
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond
A	aromatic circle
{n+}	plus at the n-nitrogen atom ($n = 1$ to 6)

produce

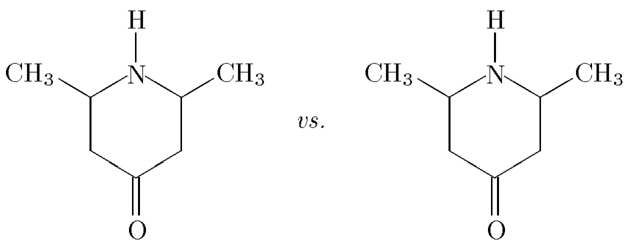


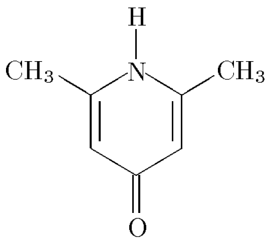
It should be noted that the same compound can be drawn in different ways. This fact is obvious because all the commands, `\pyridinev`, `\pyrazinev`, `\pyrimidinev`, `\pyridazinev`, and `\triazinev`, are based on the macro `\sixheterov`.

Example:

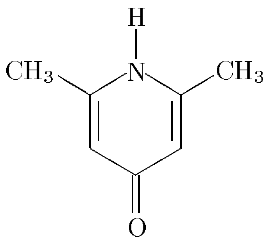
```
\pyridinev[H]{1==H;4D==O;2==CH$_{3}$;6==CH$_{3}$}\qquad
\raisebox{1.5cm}{\em vs.} \qquad
\sixheterov[H]{1==N}{1==H;4D==O;2==CH$_{3}$;6==CH$_{3}$} \par
\bigskip
\pyridinev[be]{1==H;4D==O;2==CH$_{3}$;6==CH$_{3}$}\qquad
\raisebox{1.5cm}{\em vs.} \qquad
\sixheterov[be]{1==N}{1==H;4D==O;2==CH$_{3}$;6==CH$_{3}$}
```

produce





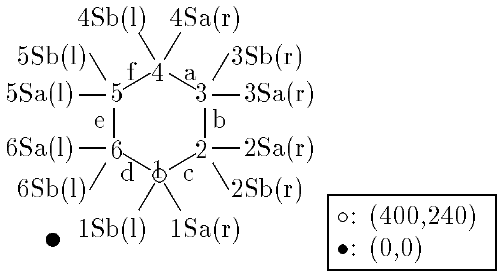
vs.



The command `\sixheterovi` is a general macro used to draw six-memered heterocyclic derivatives of inverse vertical type (hetarom.sty). The format of this command is as follows:

```
\sixheterovi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers (1–6) for designating substitution positions and bond descriptors (a–f) are shown in the following diagram:

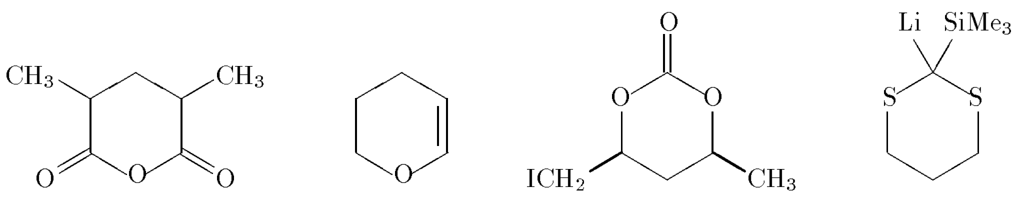


The following examples are the ones in which the `\sixheterov` commands in the above examples are replaced by `\sixheterovi`.

Example:

```
\sixheterovi[H]{1==O}{2D==O;6D==O;3==CH$_{3}$;5==CH$_{3}$}\qquad
\sixheterovi[b]{1==O}{}\qquad
\sixheterovi[H]{3==O;5==O}{4D==O;6B==ICH$_{2}$;2B==CH$_{3}$}\qquad
\sixheterovi[H]{3==S;5==S}{4Sa==SiMe$_{3}$;4Sb==Li}
```

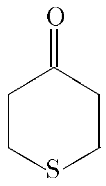
produce

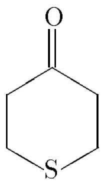


The commands `\sixheterov` and `\sixheterovi` can yield the equivalent results if the modes of numbering are altered in ATOMLIST and SUBSLIST. For example, the following two statements

```
\sixheterov[H]{4==S}{1D==O} \qquad
\sixheterovi[H]{1==S}{4D==O}
```

produce the same strucure as follows.





However, the latter is preferred to the former because the numbering of the ring atoms comforms to the chemical nomenclature. This is the reason why we have made such macros of inverse type.

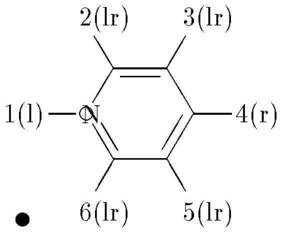
7.2 Drawing Horizontal Forms of Six-Membered Heterocycles

7.2.1 Commands for Specified Use

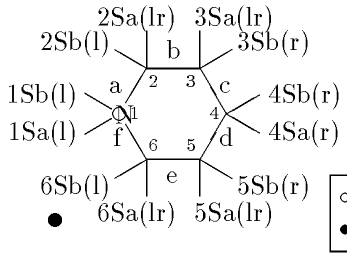
The macro `\pyridineh` and the related macros are used to draw six-membered heterocyclic compounds of horizontal type (hetaromh.sty). The formats of these commands are as follows:

```
\pyridineh[BONDLIST]{SUBSLIST}
\pyrazineh[BONDLIST]{SUBSLIST}
\pyrimidineh[BONDLIST]{SUBSLIST}
\pyridazineh[BONDLIST]{SUBSLIST}
\triazineh[BONDLIST]{SUBSLIST}
```

The following diagrams show the numbering for designating substitution positions as well as the bond specification for placing double bonds:



○: (240,400)
•: (0,0)

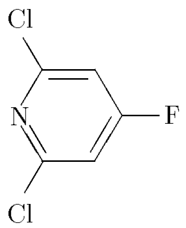


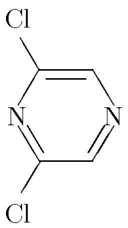
○: (240,400)
•: (0,0)

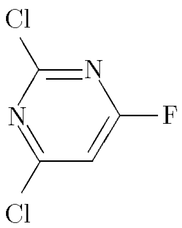
Each macro can be used to typeset both saturated and unsaturated derivatives. For example, the statements,

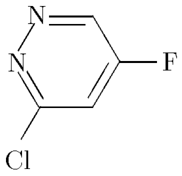
```
\pyridineh{2==Cl;6==Cl;4==F}
\pyrazineh{2==Cl;6==Cl}
\pyrimidineh{2==Cl;6==Cl;4==F}
\pyridazineh{6==Cl;4==F}
\triazineh{2==Cl;6==Cl;4==F}
```

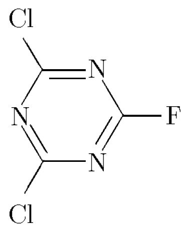
produce the following structures:







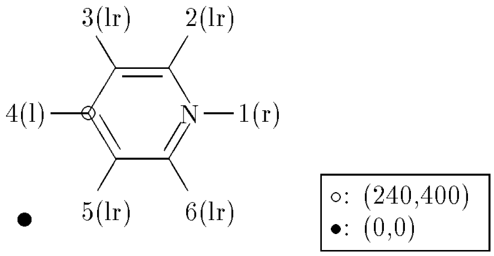


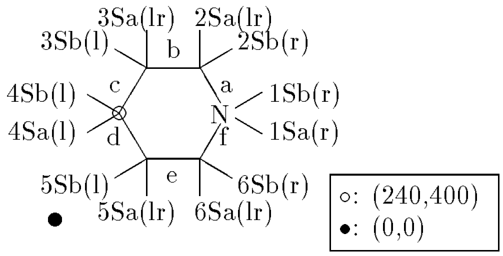


The macro `\pyridinehi` and the related macros are used to draw six-membered heterocyclic compounds of inverse horizontal type (hetarom.sty). The formats of these commands are as follows:

```
\pyridinehi[BONDLIST]{SUBSLIST}
\pyrazinehi[BONDLIST]{SUBSLIST}
\pyrimidinehi[BONDLIST]{SUBSLIST}
\pyridazinehi[BONDLIST]{SUBSLIST}
\triazinehi[BONDLIST]{SUBSLIST}
```

The numbering for designating substitution positions and the bond specification are shown in the following diagrams:

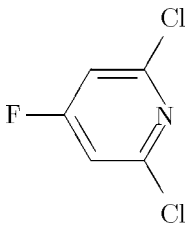


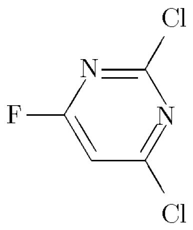


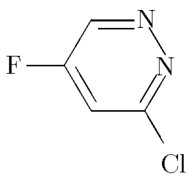
Each macro can typeset both saturated and unsaturated derivatives, where the default produces a fully unsaturated (aromatic) one. For example, the statements,

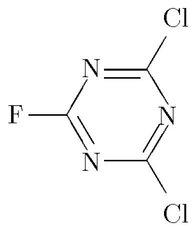
```
\pyridinehi{2==Cl;6==Cl;4==F}
\pyrimidinehi{2==Cl;6==Cl;4==F}
\pyridazinehi{6==Cl;4==F}
\triazinehi{2==Cl;6==Cl;4==F}
```

produce the following structures:







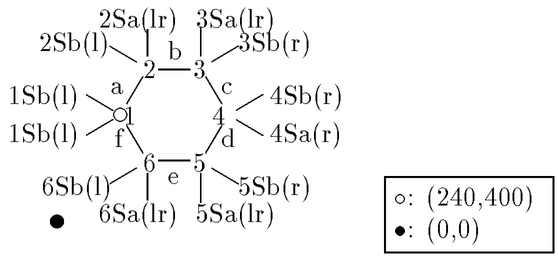


7.2.2 Commands for General Use

The macro `\sixheteroh` is a general user command for drawing six-membered heterocycles of horizontal type (hetaromh.sty). The format of this command is as follows:

```
\sixheteroh[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers for designating substitution positions as well as bond descriptors are shown in the following diagram:

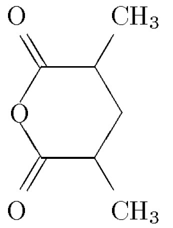


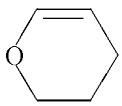
Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros. The SUBSLIST and the BONDLIST format are shown in Table 2.2 and 7.2, respectivey.

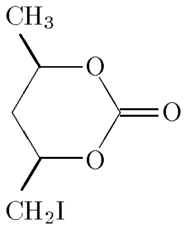
Example:

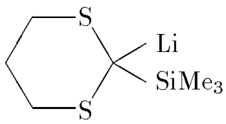
```
\sixheteroh[H]{1==O}{2D==O;6D==O;3==CH$_{3}$;5==CH$_{3}$}\qquad
\sixheteroh[b]{1==O}{}\qquad
\sixheteroh[H]{3==O;5==O}{4D==O;6B==CH$_{2}$I;2B==CH$_{3}$}\qquad
\sixheteroh[H]{3==S;5==S}{4Sa==SiMe$_{3}$;4Sb==Li}
```

produce





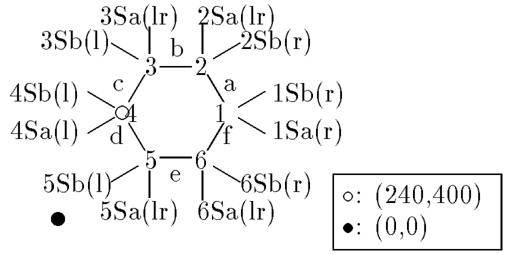




The macro **\sixheterohi** is used to draw six-membered hetrocycles of inverse horizontal type (hetaromh.sty). The format of this command is as follows:

```
\sixheterohi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The following diagram shows locant numbers (1–6) for designating substitution positions along with bond descriptors (a–f) for setting double bonds.

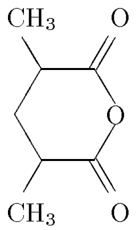


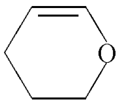
Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros. The SUBSLIST and the BONDLIST format are shown in Table 2.2 and Table 7.2, respectivey.

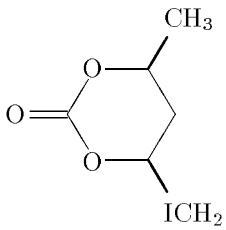
Example:

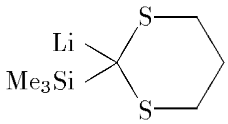
```
\sixheterohi[H]{1==O}{2D==O;6D==O;3==CH$_{3}$;5==CH$_{3}$}\qquad
\sixheterohi[b]{1==O}{}\qquad
\sixheterohi[H]{3==O;5==O}{4D==O;6B==ICH$_{2}$;2B==CH$_{3}$}\qquad
\sixheterohi[H]{3==S;5==S}{4Sa==Me$_{3}$Si;4Sb==Li}
```

produce









Chapter 8

Five- or Lower-Membered Heterocycles

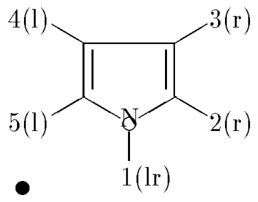
8.1 Drawing Vertical Forms of Five-Membered Heterocycles

8.1.1 Commands for Specified Use

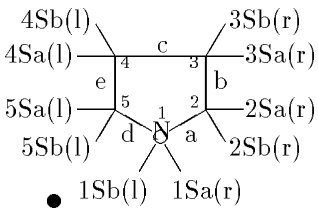
The macro `\pyrrolev` and the related macros typeset five-membered heterocyclic compounds of vertical type (hetarom.sty). The formats of these commands are as follows:

```
\pyrrolev[BONDLIST]{SUBSLIST}
\pyrazolev[BONDLIST]{SUBSLIST}
\imidazolev[BONDLIST]{SUBSLIST}
\isoxazolev[BONDLIST]{SUBSLIST}
\oxazolev[BONDLIST]{SUBSLIST}
```

The following diagrams show the numbering for designating substitution positions as well as the bond specification for writing double bonds:



○: (400,240)
•: (0,0)



○: (400,240)
•: (0,0)

Each of the macros is capable of typesetting both saturated and unsaturated derivatives. The optional argument BONDLIST specifies bond to be doubled as shown in Table 8.1. The default setting is to produce a fully unsaturated ring; on the other hand a null augument or H in BONDLIST produces a fully saturated ring.

The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 5. For example, the statements,

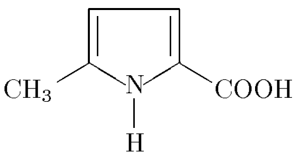
```
\pyrrolev{1==H;2==COOH;5==CH$_{3}$}\qquad\qquad\qquad
\pyrazolev{1==H;3==Ph;5==Ph}\qquad
\imidazolev{1==H;2==CH$_{3}$}
```

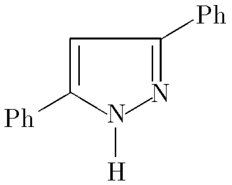
Table 8.1: Argument BONDLIST for commands `\pyrrolev`, *etc.*

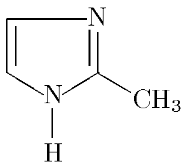
Character	Printed structure
none	mother nucleus
H or [ ]	fully saturated form
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,1-double bond
A	aromatic circle
$\{n+\}$	plus at the n-nitrogen atom (n = 1 to 5)

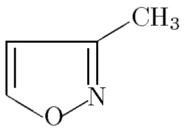
```
\isoxazolev{3==CH$_{3}$}\qquad
\oxazolev{2==CH$_{3}$}
```

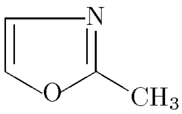
produce the following structures:







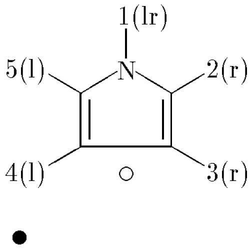




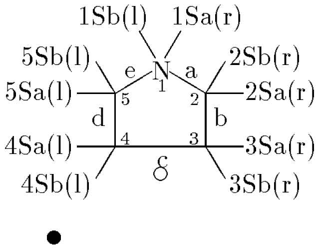
The macro `\pyrrolevi` and the related macros are used to draw five-membered heterocyclic compounds of inverse vertical type (hetarom.sty). The formats of these commands are as follows:

```
\pyrrolevi[BONDLIST]{SUBSLIST}
\pyrazolevi[BONDLIST]{SUBSLIST}
\imidazolevi[BONDLIST]{SUBSLIST}
\isoxazolevi[BONDLIST]{SUBSLIST}
\oxazolevi[BONDLIST]{SUBSLIST}
```

The locant numbering and the bond specification are shown in the following diagrams.



○: (400,240)
•: (0,0)



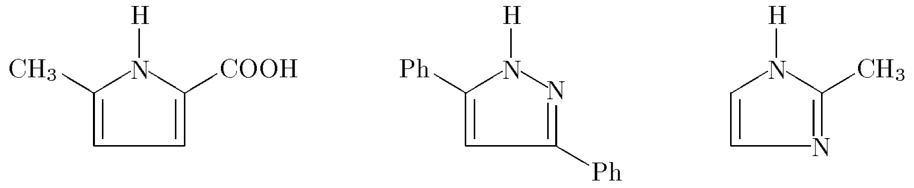
○: (400,240)
•: (0,0)

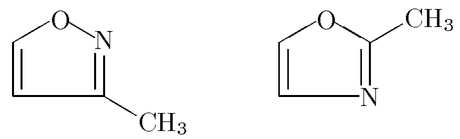
The arguments BONDLIST and SUBSLIST have the same formats as above (Tables 8.1 and 2.2).

Example:

```
\pyrrolevi{1==H;2==COOH;5==CH$_{3}$}\qquad\qquad\qquad
\pyrazolevi{1==H;3==Ph;5==Ph}\qquad
\imidazolevi{1==H;2==CH$_{3}$}\par
\isoxazolevi{3==CH$_{3}$}\qquad
\oxazolevi{2==CH$_{3}$}
```

produce the following structures:



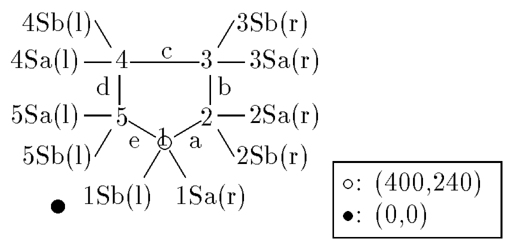


8.1.2 Commands for General Use

The command `\fiveheterov` is a general macro used to draw five-memered heterocyclic derivatives of vertical type (hetarom.sty). The format of this command is as follows:

```
\fiveheterov[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers for designating substitution positions and bond descriptors for setting double bonds are represented by the following diagram:



Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros.

The option argument BONDLIST is a character string in a pair of brackets, where each character indicates the presence of a double bond at the edge specified by the character (Table 8.2).

Since the default of BONDLIST prints a fully saturated form, the `\fiveheterov` requires no option argument [H] in contrast to `\sixheterov`.

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

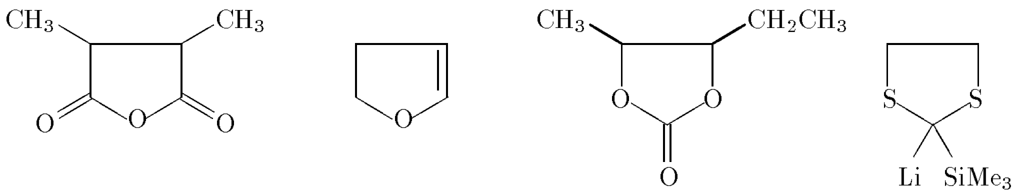
Example:

Table 8.2: Argument BONDLIST for commands `\fiveheterov` and `\fiveheterovi`

Character	Printed structure
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,1-double bond
A	aromatic circle
{n+}	plus at the n-nitrogen atom (n = 1 to 6)
{0+}	plus (or minus) at the center

```
\fiveheterov{1==O}{2D==O;5D==O;3==CH$_{3}$;4==CH$_{3}$}\qquad
\fiveheterov[b]{1==O}{}\qquad
\fiveheterov{2==O;5==O}{1D==O;3B==CH$_{2}$CH$_{3}$;4B==CH$_{3}$}\qquad
\fiveheterov{2==S;5==S}{1Sa==SiMe$_{3}$;1Sb==Li}
```

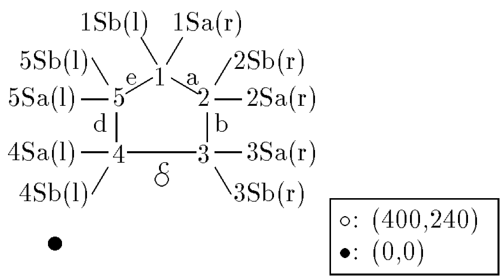
produce



The macro `\fiveheterovi` is employed to draw five-membered heterocyclic compounds of inverse vertical type (hetarom.sty). The format of this command is as follows:

```
\fiveheterovi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The following diagram shows the numbering for designating substitution positions:



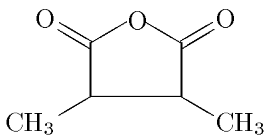
The optional argument BONDLIST specifies double bonds as shown in Table 8.2, where any combination of characters (a–d) enables us to draw both saturated and unsaturated derivatives.

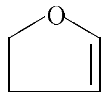
The argument SUBSLIST specifies each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 5.

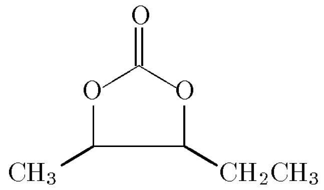
Example:

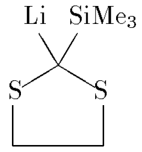
```
\fiveheterovi{1==O}{2D==O;5D==O;3==CH$_{3}$;4==CH$_{3}$}\qquad
\fiveheterovi[b]{1==O}{}\qquad
\fiveheterovi{2==O;5==O}{1D==O;3B==CH$_{2}$CH$_{3}$;4B==CH$_{3}$}\qquad
\fiveheterovi{2==S;5==S}{1Sa==SiMe$_{3}$;1Sb==Li}
```

produce









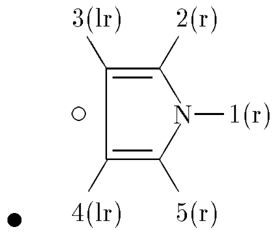
8.2 Drawing Horizontal Forms of Five-Membered Heterocycles

8.2.1 Commands for Specified Use

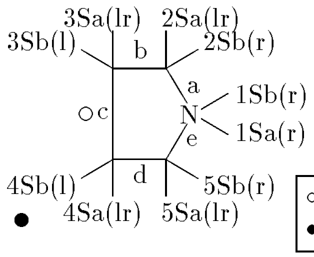
The macro `\pyrroleh` and the related macros are used to draw five-membered heterocyclic compounds of horizontal type (hetaromh.sty). The formats of these commands are as follows:

```
\pyrroleh[BONDLIST]{SUBSLIST}
\pyrazoleh[BONDLIST]{SUBSLIST}
\imidazoleh[BONDLIST]{SUBSLIST}
\isoxazoleh[BONDLIST]{SUBSLIST}
\oxazoleh[BONDLIST]{SUBSLIST}
```

The following diagrams show the numbering for designating substitution positions:



∘: (240,400)
•: (0,0)

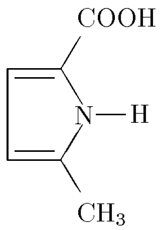


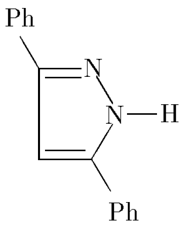
∘: (240,400)
•: (0,0)

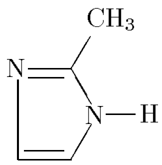
For BONDLIST, see Table 8.2. For example, the statements,

```
\pyrroleh{1==H;2==COOH;5==CH$_{3}$}\qquad\qquad\qquad
\pyrazoleh{1==H;3==Ph;5==Ph}\qquad
\imidazoleh{1==H;2==CH$_{3}$} \par
\isoxazoleh{3==CH$_{3}$}\qquad
\oxazoleh{2==CH$_{3}$}
```

produce the following structures:



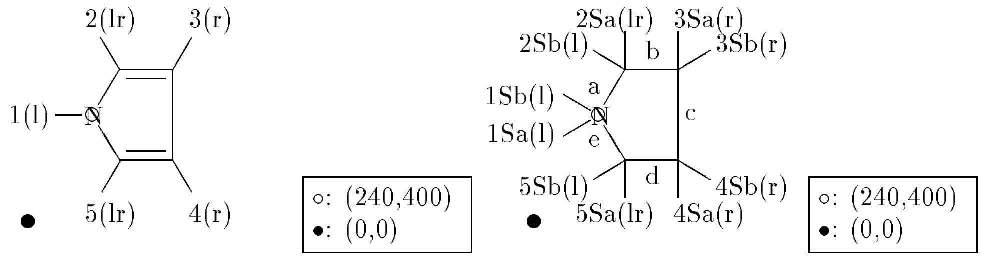




The macro `\pyrrolehi` and the related macros are used to draw five-membered heterocyclic compounds of inverse horizontal type (hetaromh.sty). The format of this command is as follows:

```
\pyrrolehi[BONDLIST]{SUBSLIST}
\pyrazolehi[BONDLIST]{SUBSLIST}
\imidazolehi[BONDLIST]{SUBSLIST}
\isoxazolehi[BONDLIST]{SUBSLIST}
\oxazolehi[BONDLIST]{SUBSLIST}
```

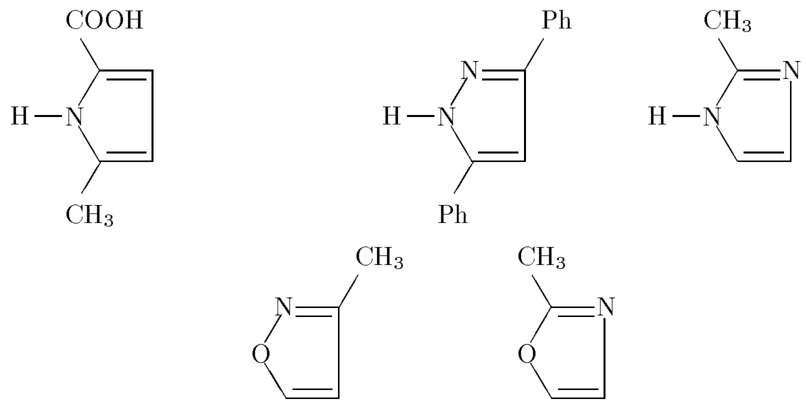
The locant numbering for designating substitution positions and the bond specification for setting double bonds are shown in the following diagram:



For example, the statements,

```
\pyrrolehi{1==H;2==COOH;5==CH$_{3}$}\qquad\qquad\qquad
\pyrazolehi{1==H;3==Ph;5==Ph}\qquad
\imidazolehi{1==H;2==CH$_{3}$}\par
\isoxazolehi{3==CH$_{3}$}\qquad
\oxazolehi{2==CH$_{3}$}
```

produce the following structures:

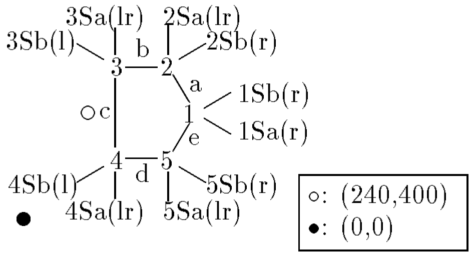


8.2.2 Commands for General Use

The command `\fiveheteroh` is a general macro used to draw five-memered heterocyclic derivatives of horizontal type (hetaromh.sty). The format of this command is as follows:

```
\fiveheteroh[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The locant numbers for designating substitution positions are represented by the following diagram:



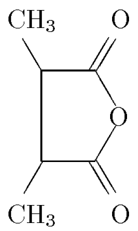
Each character set in parentheses represents the handedness of the corresponding position, which is fixed in this type of macros.

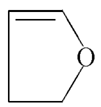
The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character (Table 8.2). The argument ATOMLIST lists a set of atoms placed on the edges assigned. The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

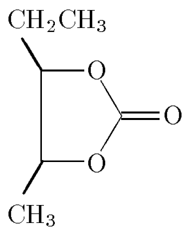
Example:

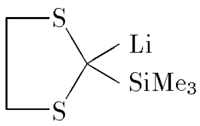
```
\fiveheteroh{1==O}{2D==O;5D==O;3==CH$_{3}$;4==CH$_{3}$}\qquad
\fiveheteroh[b]{1==O}{}\qquad
\fiveheteroh{2==O;5==O}{1D==O;3B==CH$_{2}$CH$_{3}$;4B==CH$_{3}$}\qquad
\fiveheteroh{2==S;5==S}{1Sa==SiMe$_{3}$;1Sb==Li}
```

produce





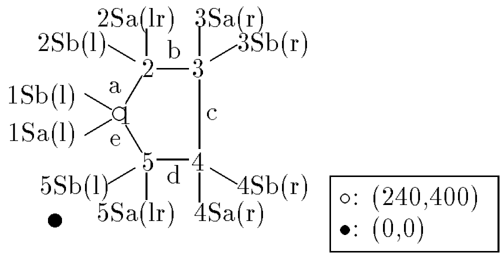




The command `\fiveheterohi` is a general macro for drawing five-memered heterocyclic derivatives of inverse horizontal type (hetaromh.sty). The format of this command is as follows:

```
\fiveheterohi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

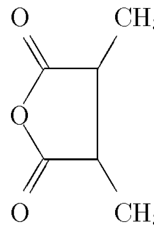
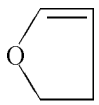
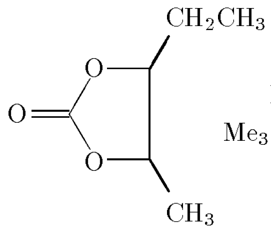
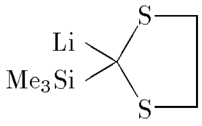
The following diagram shows the numbering for designating substitution positions as well as the bond specification for writing double bonds:



Example:

```
\fiveheterohi{1==O}{2D==O;5D==O;3==CH$_{3}$;4==CH$_{3}$}\qquad
\fiveheterohi[b]{1==O}{}\qquad
\fiveheterohi{2==O;5==O}{1D==O;3B==CH$_{2}$CH$_{3}$;4B==CH$_{3}$}\qquad
\fiveheterohi{2==S;5==S}{1Sa==Me$_{3}$Si;1Sb==Li}
```

produce the following structures:

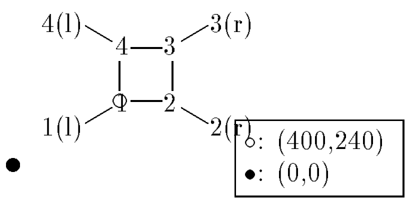





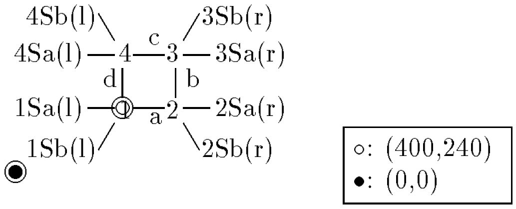
8.3 Drawing Four-Membered Heterocycles

The macro `\fourhetero` is a command for general use, which is capable of giving skeletal atoms as an ATOMLIST. This macro is designed for drawing four-membered heterocycles by using the following format (hetarom.sty).

```
\fourhetero[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The locant numbering is common in these commands as shown in the following diagram:





The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST is used for the bond specification shown in Table 8.3.

Table 8.3: Argument BONDLIST for commands `\fourhetero` and others

Character	Printed structure	Character	Printed structure
none	mother compound (fully saturated)		
a	1,2-double bond	b	2,3-double bond
c	3,4-double bond	d	4,1-double bond
$\{n+\}$	plus at the n-nitrogen atom ($n = 1$ to 4)		

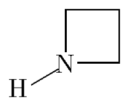
The argument ATOMLIST takes a usual format with respect to heteroatoms attached to $n = 1$ to 4, *e.g.*, 1==N for a nitrogen atom at 1-position.

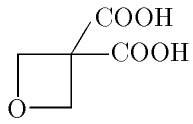
The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 4.

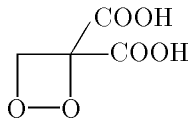
Example:

```
\fourhetero{1==N}{1==H}
\fourhetero{1==O}{3Sa==COOH;3Sb==COOH}
\fourhetero{1==O;2==O}{3Sa==COOH;3Sb==COOH}
```

produce the following structures:





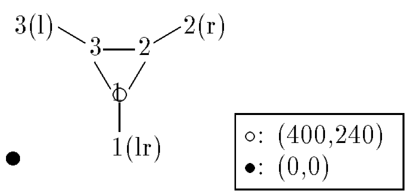


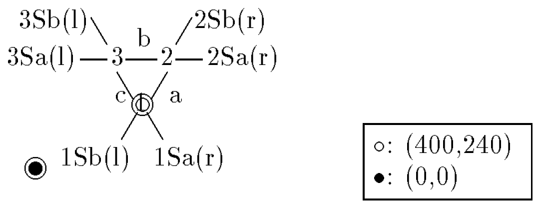
8.4 Drawing Three-Membered Heterocycles

The macro `\threehetero` for drawing threee-membered heterocycles has the following format (hetarom.sty).

```
\threehetero[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The locant numbering is common as shown in the following diagram:





The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST specifies double bonds as shown in Table 8.4.

Table 8.4: Argument BONDLIST for commands `\threehetero` and others

Character	Printed structure
none	saturated
a	1,2-double bond
b	2,3-double bond
c	3,1-double bond
A	aromatic circle
{n+}	plus at the n-hetero atom (n = 1 to 3)
	$n = 4$ – outer plus at 1 position
	$n = 5$ – outer plus at 2 position
	$n = 6$ – outer plus at 3 position
{0+}	plus at the center of a cyclopropane ring

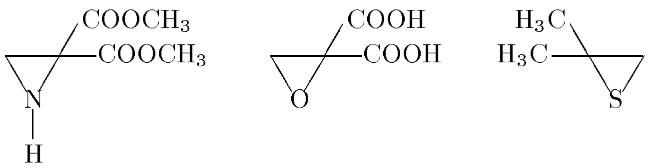
The argument ATOMLIST takes a usual format with respect to heteroatoms attached to $n = 1$ to 3, *e.g.*, 1==N for a nitrogen atom at 1-position.

The argument SUBSLIST describes each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 3.

Example:

```
\threehetero{1==N}{1==H;2Sa==COOCH$_{3}$;2Sb==COOCH$_{3}$}\qquad
\threehetero{1==O}{2Sa==COOH;2Sb==COOH}\qquad\qquad
\threehetero{1==S}{3Sa==H$_{3}$C;3Sb==H$_{3}$C}
```

produce the following structures:



Chapter 9

Heterocycles with Fused Six-Membered Rings

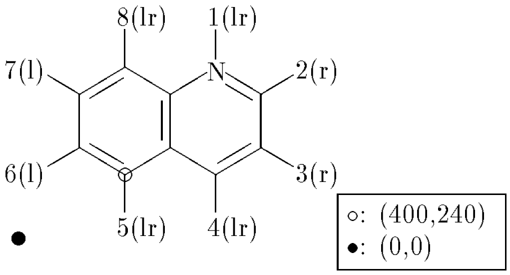
9.1 Drawing Vertical Forms

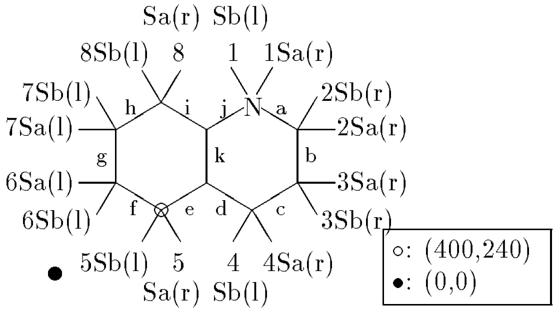
9.1.1 Commands for Specified Use

The macro `\quinolinev` is used to draw quinoline derivatives of vertical type (hetarom.sty). Macros for drawing other fused heterocycles are also defined. The formats of these commands are as follows:

```
\quinolinev[BONDLIST]{SUBSLIST}
\isoquinolinev[BONDLIST]{SUBSLIST}
\quinoxalinev[BONDLIST]{SUBSLIST}
\quinazolinev[BONDLIST]{SUBSLIST}
\cinnolinev[BONDLIST]{SUBSLIST}
\pteridinev[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions as well as bond descriptors for setting double bonds are shown in the following diagram:





The handedness for each oriented or double-sided position is shown with a character set in parentheses. Each character in the optional argument BONDLIST specifies an inner (endocyclic) double bond as shown in Table 9.1.

The argument SUBSLIST is employed to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 8. Sibstitution on 9 (4a position) or 10 (8a position) can be assigned in the same way.

Example:

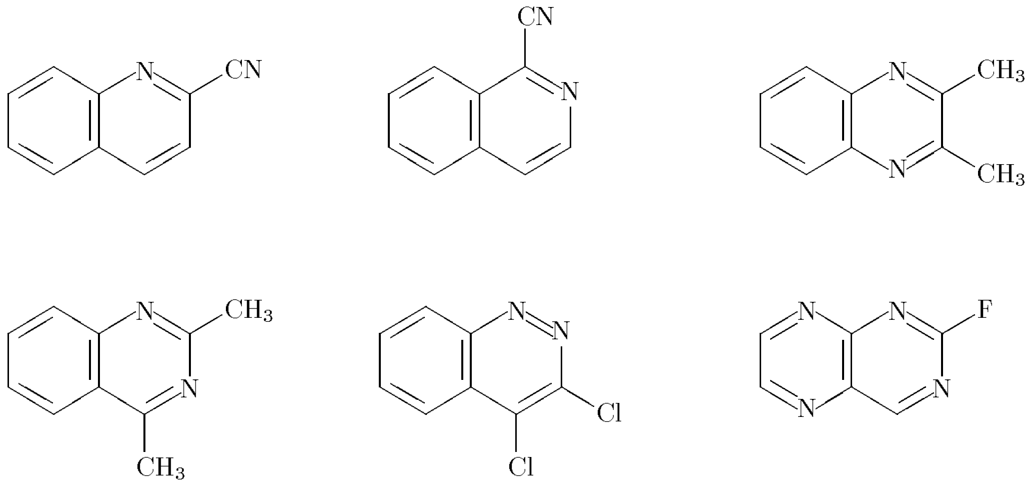
```
\quinolinev{2==CN} \qquad
```

Table 9.1: Argument BONDLIST for commands `\quinolinev` and others

Character	Printed structure	Character	Printed structure
none or r	decahetero (right-handed)	l	decahetero (left-handed)
H or [ ]	fully saturated form		
a	1,2-double bond	b	2,3-double bond
c	4,3-double bond	d	4,4a-double bond
e	4a,5-double bond	f	5,6-double bond
g	6,7-double bond	h	7,8-double bond
i	8,8a-double bond	j	1,8a-double bond
k	4a,8a-double bond		
A	aromatic circle	B	aromatic circle
{n+}	plus at the n-nitrogen atom (n = 1 to 10)		

```
\isoquinolinev{1==CN}\qquad
\quinoxalinev{2==CH$_{3}$;3==CH$_{3}$} \par
\quinazolinev{2==CH$_{3}$;4==CH$_{3}$}\qquad
\cinnolinev{4==Cl;3==Cl} \qquad
\pteridinev{2==F}
```

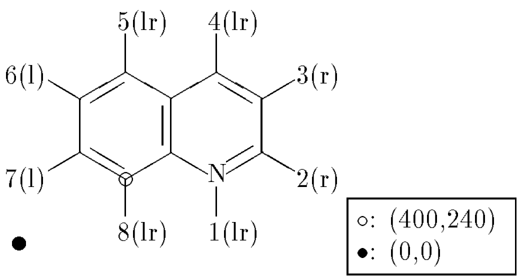
produce the following structures:

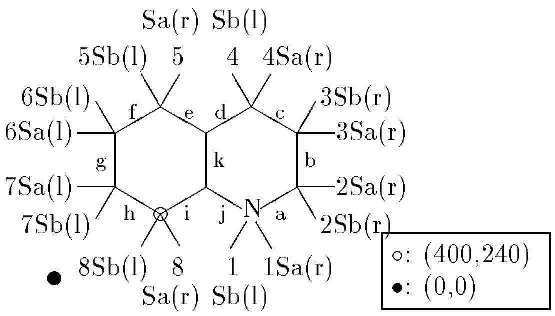


The macro `\quinolinevi` is used to draw quinoline derivatives of inverse vertical type (hetarom.sty). Macros for depicting other fused heterocycles are also defined. The formats of these commands are as follows:

```
\quinolinevi[BONDLIST]{SUBSLIST}
\isoquinolinevi[BONDLIST]{SUBSLIST}
\quinazolinevi[BONDLIST]{SUBSLIST}
\cinnolinevi[BONDLIST]{SUBSLIST}
\pteridinevi[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions along with bond descriptors are represented by the following diagram:

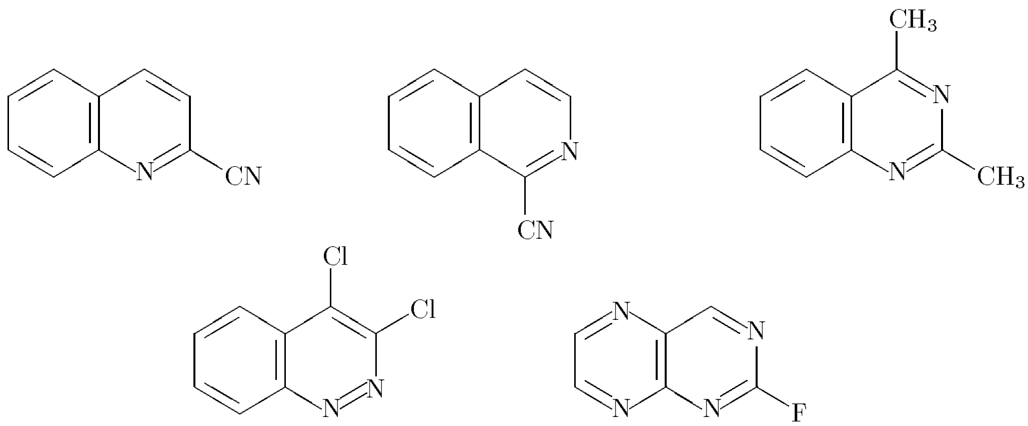




Example:

```
\quinolinevi{2==CN} \qquad
\isoquinolinevi{1==CN}\qquad
\quinazolinevi{2==CH$_{3}$;4==CH$_{3}$}\par
\cinnolinevi{4==Cl;3==Cl} \qquad
\pteridinevi{2==F}
```

produce the following structures:

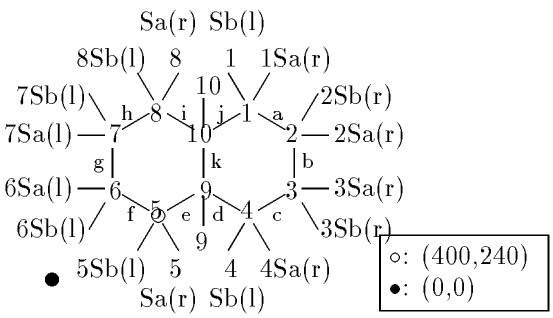


9.1.2 Commands for General Use

Such commands as `\quinolinev` (for specified use) are based on the macro `\decaheterov`, which is generally used to draw six-six-fused heterocycles of vertical type (hetarom.sty).

```
\decaheterov[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers for designating substitution positions as well as characters for setting double bonds are shown in the following diagram:



The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST is used to specify a bond pattern as shown in Table 9.1. Note that the default structure is the fully unsaturated one.

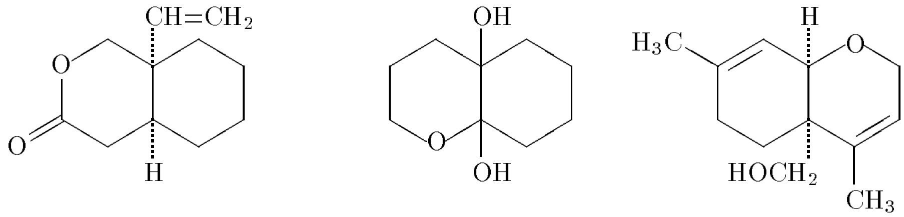
The argument ATOMLIST has a similar format for positions of $n = 1$ to 8. A hetero-atom on the 4a-position is designated to be 4a==N or 9==N; and a hetero-atom on the 8a-position is given as to be 8a==N or {{10}}==N.

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used. Note that 9 and 10 should be used for designating 4a and 8a positions.

Example:

```
\decaheterov[H]{7==O}{6D==O;9A==H;{{10}A}==CH=CH$_{2}$}
\decaheterov[H]{5==O}{9==OH;{{10}}==OH}
\decaheterov[ch]{1==O}{9A==\lmoiety{HOCH$_{2}$};{{10}A}==H;%
4==CH$_{3}$;7==H$_{3}$C}
```

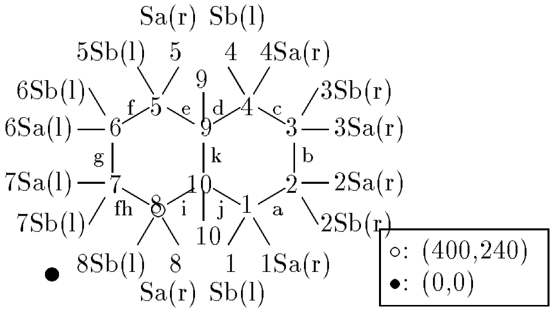
produce the following structures:



The command `\decaheterovi` is the inverse-type macro of `\decaheterov` described above (hetarom.sty).

```
\decaheterovi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers (1–10) for designating substitution positions and bond descriptors (a–f) for setting double bonds are represented by the following diagram:

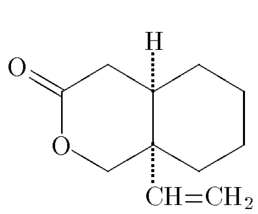


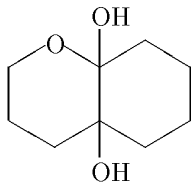
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The arguments are given in the same way as in `\decaheterov`.

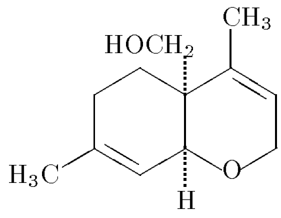
Example:

```
\decaheterovi[H]{7==O}{6D==O;9A==H;{{10}A}==CH=CH$_{2}$}
\decaheterovi[H]{5==O}{9==OH;{{10}}==OH}
\decaheterovi[ch]{1==O}{9A==\lmoiety{HOCH$_{2}$};{{10}A}==H;%
4==CH$_{3}$;7==H$_{3}$C}
```

produce the following structures:







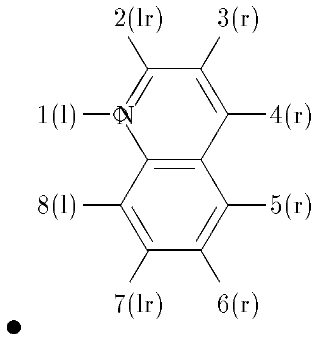
9.2 Drawing Horizontal Forms

9.2.1 Commands for Specified Use

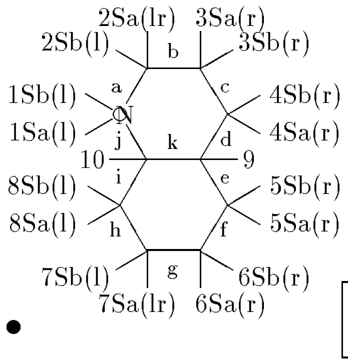
The horizontal counterparts of the commands of vertical type (`\quinolinev`, *etc*) are defined similarly in the style file, hetaromh.sty.

```
\quinolineh[BONDLIST]{SUBSLIST}
\isoquinolineh[BONDLIST]{SUBSLIST}
\quinoxalineh[BONDLIST]{SUBSLIST}
\quinazolineh[BONDLIST]{SUBSLIST}
\cinnolineh[BONDLIST]{SUBSLIST}
\pteridineh[BONDLIST]{SUBSLIST}
```

Locant numbers (1–10) for designating substitution positions and bond descriptors (a–k) are found in the following diagram:



○: (400,800)
•: (0,0)



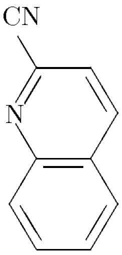
○: (400,800)
•: (0,0)

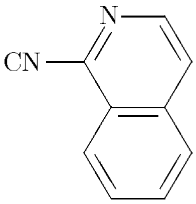
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST specifies double bonds to be typeset, as shown in Table 9.1.

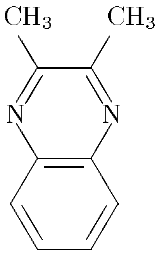
Example:

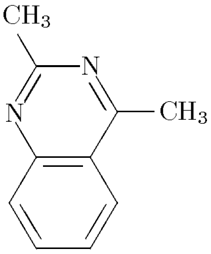
```
\quinolineh{2==CN} \qquad
\isoquinolineh{1==CN}\qquad
\quinoxalineh{2==CH$_{3}$;3==CH$_{3}$} \par
\quinazolineh{2==CH$_{3}$;4==CH$_{3}$}\qquad
\cinnolineh{4==Cl;3==Cl} \qquad
\pteridineh{2==F}
```

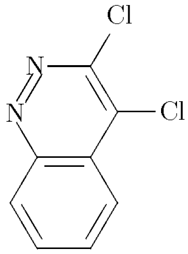
produce the following structures:

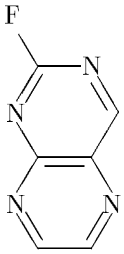








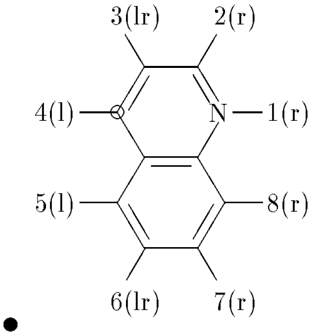




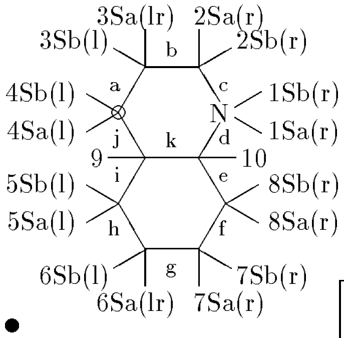
The macro **\quinolinehi** is used to draw quinoline derivatives of inverse horizontal type (hetaromh.sty). Macros for drawing other fused heterocycles are also defined in the hetaromh.sty. The formats of these commands are as follows:

```
\quinolinehi[BONDLIST]{SUBSLIST}
\isoquinolinehi[BONDLIST]{SUBSLIST}
\quinazolinehi[BONDLIST]{SUBSLIST}
\cinnolinehi[BONDLIST]{SUBSLIST}
\pteridinehi[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and characters (a–f) for designating bouble bonds are shown in the following diagram:



○: (400,800)
•: (0,0)

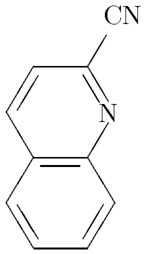


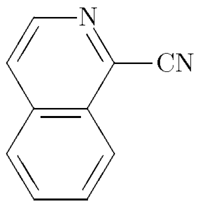
○: (400,800)
•: (0,0)

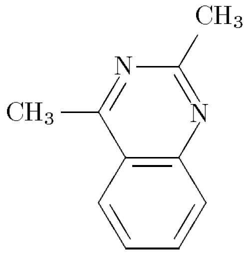
Example:

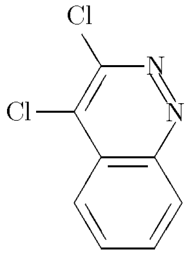
```
\quinolinehi{2==CN} \qquad
\isoquinolinehi{1==CN}\qquad
\quinazolinehi{2==CH$_{3}$;4==CH$_{3}$}\par
\cinnolinehi{4==Cl;3==Cl} \qquad
\pteridinehi{2==F}
```

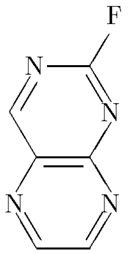
produce the following structures:









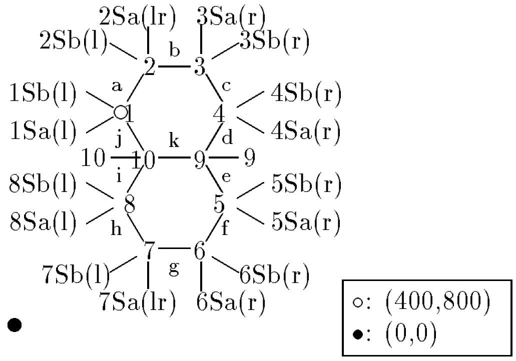


9.2.2 Commands for General Use

The macro `\decaheteroh` (carom.sty) is the horizotal counterpart of `\decaheterov`. The format and the assignment of BONDLIST and SUBSLIST of the former macro are the same as those of the latter described above (see Tables 2.2 and 9.1).

```
\decaheteroh[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers for designating substitution positions and bond descriptors for typesetting double bonds are represented by the following diagram:

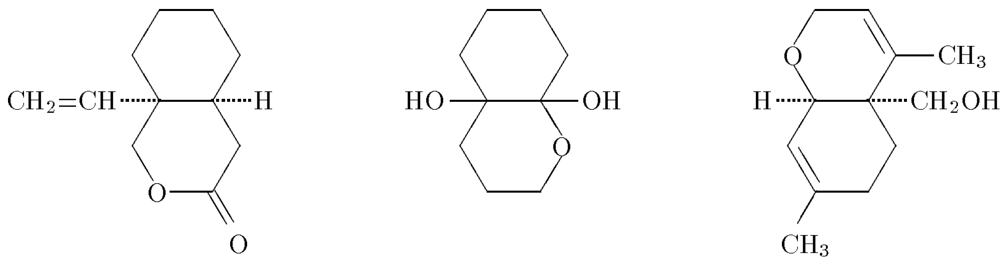


The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST contains a characher string selected from Table 9.1.

Example:

```
\decaheteroh[H]{7==O}{6D==O;9A==H;{{10}A}==CH$_{2}$=CH}
\decaheteroh[H]{5==O}{9==OH;{{10}}==HO}
\decaheteroh[ch]{1==O}{9A==CH$_{2}$OH;{{10}A}==H;%
4==CH$_{3}$;7==CH$_{3}$}
```

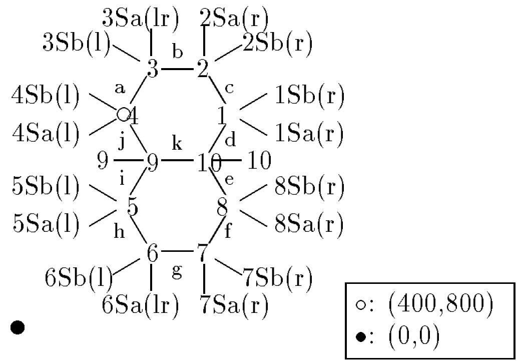
produce the following structures:



The macro `\decaheterohi` (carom.sty) is the inverse counterpart of `\decaheteroh`. The format and the assignment of BONDLIST and SUBSLIST of the former macro are the same as the latter (see Tables 2.2 and 9.1).

```
\decaheterohi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

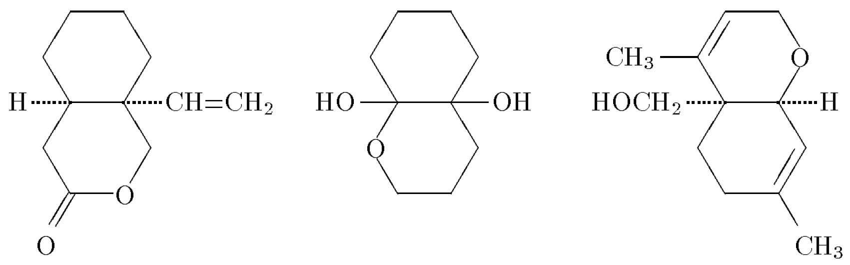
Locant numbers for designating substitution positions and bond descriptors for setting double bonds are represented by the following diagram:



Example:

```
\decaheterohi[H]{7==O}{6D==O;9A==H;{{10}A}==CH=CH$_{2}$}
\decaheterohi[H]{5==O}{9==HO;{{10}}==OH}
\decaheterohi[ch]{1==O}{9A==\lmoiety{HOCH$_{2}$};{{10}A}==H;%
4==CH$_{3}$;7==CH$_{3}$}
```

produce the following structures:



Chapter 10

Heterocycles with Fused Six- and Five-Membered Rings

10.1 Drawing Vertical Forms

10.1.1 Commands for Specified Use

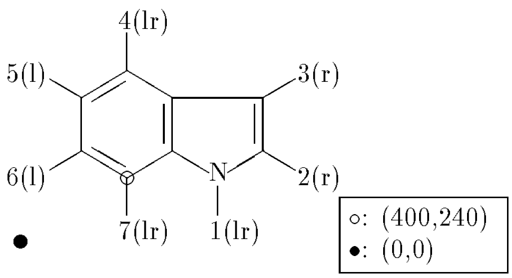
X$^\Upsilon$MT$_E$X involves macros for drawing representative fused N-heterocycles that consist of a six- and a five-membered ring. These have the following formats (hetarom.sty).

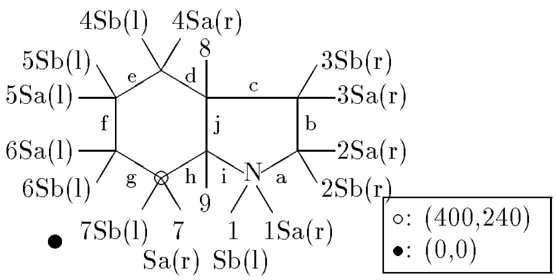
```
\indolev[BONDLIST]{SUBSLIST}
\isoindolev[BONDLIST]{SUBSLIST}
\purinev[BONDLIST]{SUBSLIST}
```

Macros for drawing fused N,O-heterocycles are also available (hetarom.sty). They are the same formats of arguments.

```
\benzofuranev[BONDLIST]{SUBSLIST}
\isobenzofuranev[BONDLIST]{SUBSLIST}
\benzoxazolev[BONDLIST]{SUBSLIST}
```

The locant numbering is common in these commands as shown in the following diagram:





The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST specifies edges with a double bond (Table 10.1).

The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 2.2, in which n is an arabic numeral between 1 and 7. Sibstitution on 8 (3a position) or 9 (7a position) can be assigned in the same way.

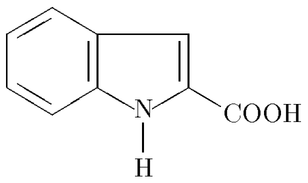
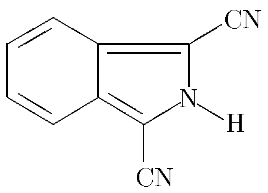
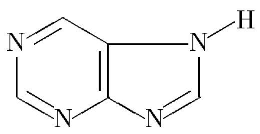
Example:

Table 10.1: Argument BONDLIST for commands `\indolev` and others

Character	Printed structure	Character	Printed structure
none or r	aromatic six-membered ring	H or []	fully saturated form
a	1,2-double bond	b	2,3-double bond
c	3,3a-double bond	d	4,3a-double bond
e	4,5-double bond	f	5,6-double bond
g	6,7-double bond	h	7,7a-double bond
i	1,7a-double bond	j	3a,4a-double bond
A	aromatic circle (six-membered ring)		
B	aromatic circle (five-membered ring)		
$\{n+\}$	plus at the n-nitrogen atom (n = 1 to 9)		

```
\indolev{1==H;2==COOH}\qquad
\isoindolev{2==H;1==CN;3==CN}\qquad
\purinev{3==H}
```

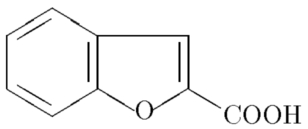
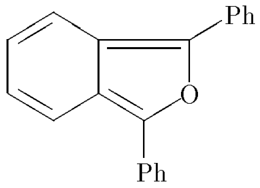
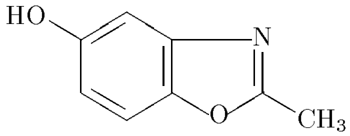
produce the following structures:

Example:

```
\benzofuranev{2==COOH}\qquad
\isobenzofuranev{1==Ph;3==Ph}\qquad
\benzoxazolev{2==CH$_{3}$;5==HO}
```

produce the following structures:

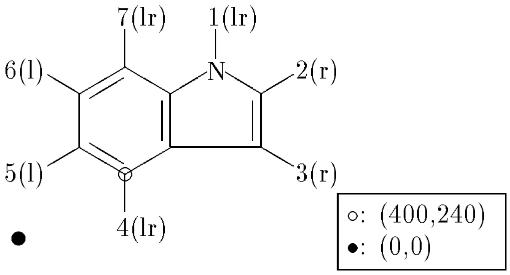
Macros for drawing fused N-heterocycles of inverse vertical type have the following formats (hetarom.sty).

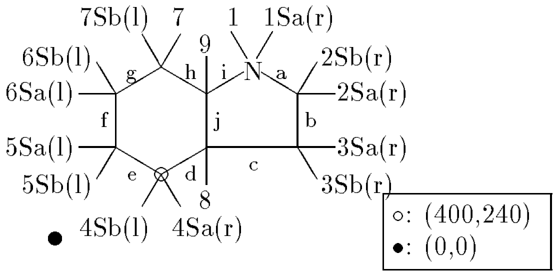
```
\indolevi[BONDLIST]{SUBSLIST}
\isoindolevi[BONDLIST]{SUBSLIST}
\purinevi[BONDLIST]{SUBSLIST}
```

Macros for drawing fused N,O-heterocycles of inverse vertical type have the following formats. They are also contained in the style file 'hetarom.sty'.

```
\benzofuranevi[BONDLIST]{SUBSLIST}
\isobenzofuranevi[BONDLIST]{SUBSLIST}
\benzoxazolevi[BONDLIST]{SUBSLIST}
```

They are the counterparts of the commands without suffix 'i' described above. The locant numbering is common in these commands as shown in the following diagram:



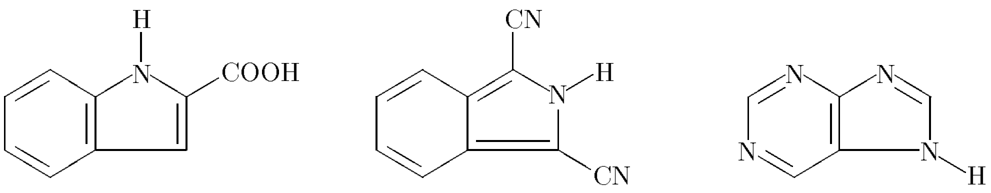


The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST is used in a usual way (Table 10.1).

Example:

```
\indolevi{1==H;2==COOH}\qquad
\isoindolevi{2==H;1==CN;3==CN}\qquad
\purinevi{3==H}
```

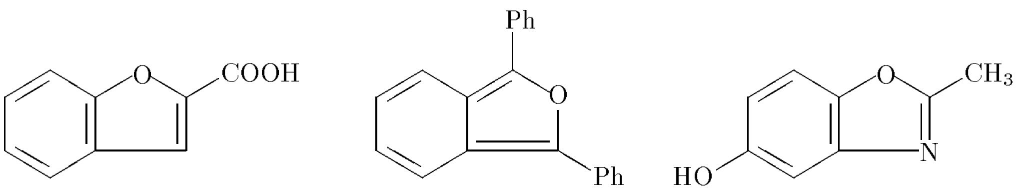
produce the following structures:



Example:

```
\benzofuranevi{2==COOH}\qquad
\isobenzofuranevi{1==Ph;3==Ph}\qquad
\benzoxazolevi{2==CH$_{3}$;5==HO}
```

produce the following structures:

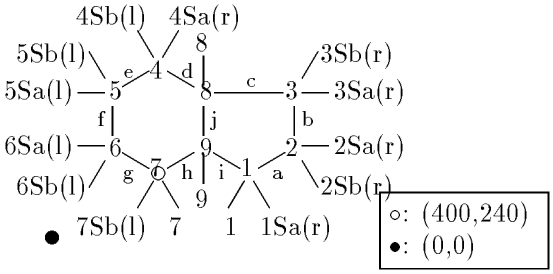


10.1.2 Commands for General Use

Macros for specified use such as `\indolev` are short-cut commands based on a general command `\nonaheterov`. Such a general command enables us to draw a further variety of heterocyclic compounds. It has the following format, the definition of which is contained also in hetarom.sty.

```
\nonaheterov[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbers (1–9) and bond descriptors (a–j) are defined as shown in the following diagram:



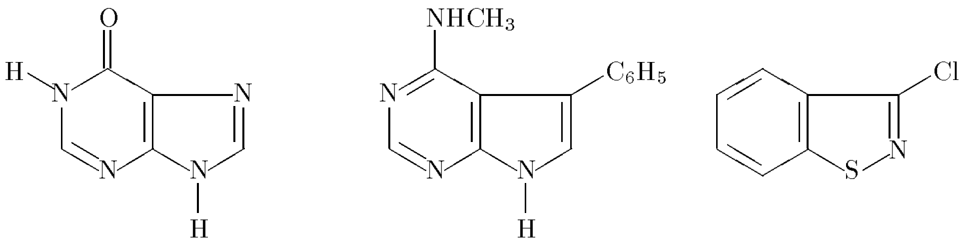
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST is used to specify double bonds as shown in Table 10.1.

The argument ATOMLIST takes a usual format with respect to heteroatoms attached to $n = 1$ to 7, *e.g.*, 1==N for a nitrogen atom at 1-position. Hetero atoms at 3a- and 7a-positions are represented as to be 3a==N (or 8==N) for a nitrogen at 3a-position, 7a==N (or 9==N) for at a nitrogen at 7a-position, and so on. The augument SUBSLIST takes a usual format except that the locant numbers 3a and 7a are replaced by 8 and 9.

Example:

```
\nonaheterov[bjg]{1==N;3==N;5==N;7==N}{1==H;5==H;4D==O}
\nonaheterov[bjge]{1==N;5==N;7==N}%
 {1==H;3==C$_{6}$H$_{5}$;4==NHCH$_{3}$}
\nonaheterov[bjge]{1==S;2==N}{3==Cl}
```

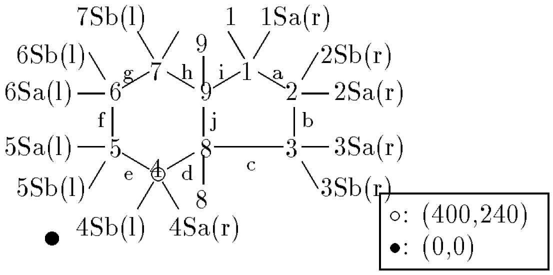
produce the following structures:



The inverse conterpart `\nonaheterovi` has the following format:

```
\nonaheterovi[BONDLIST]{ATOMLIST}{SUBSLIST}
```

Locant numbering is usually defined as shown in the following diagram:

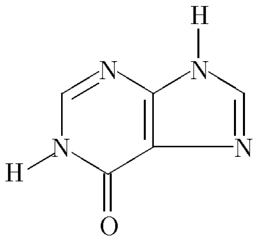


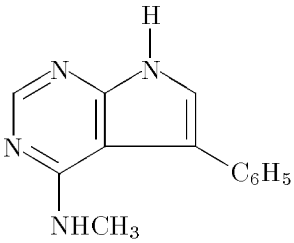
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The same format of the optional argument BONDLIST is used as shown in Table 10.1.

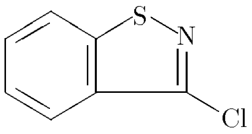
Example:

```
\nonaheterovi[bjg]{1==N;3==N;5==N;7==N}{1==H;5==H;4D==O}
\nonaheterovi[bjge]{1==N;5==N;7==N}%
 {1==H;3==C$_{6}$H$_{5}$;4==NHCH$_{3}$}
\nonaheterovi[bjge]{1==S;2==N}{3==Cl}
```

produce the following structures:







10.2 Drawing Horizontal Forms

10.2.1 Commands for Specified Use

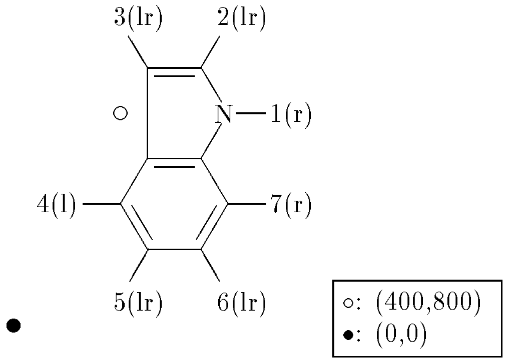
Macros for drawing N-heterocycles of horizontal type have the following formats (hetaromh.sty).

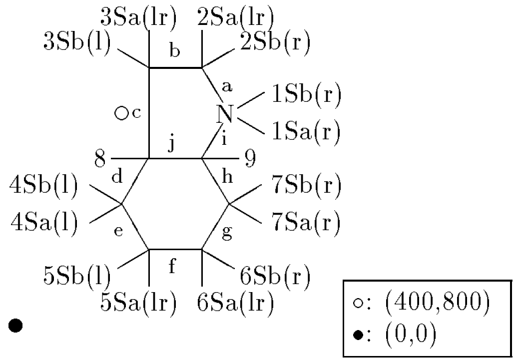
```
\indoleh[BONDLIST]{SUBSLIST}
\isoindoleh[BONDLIST]{SUBSLIST}
\purineh[BONDLIST]{SUBSLIST}
```

Macros for drawing N,O-heterocycles are available by setting the option style file 'hetaromh.sty'. They have the following formats.

```
\benzofuraneh[BONDLIST]{SUBSLIST}
\isobenzofuraneh[BONDLIST]{SUBSLIST}
\benzoxazoleh[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:



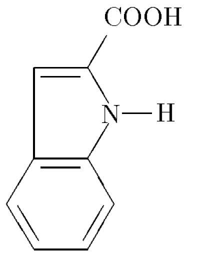


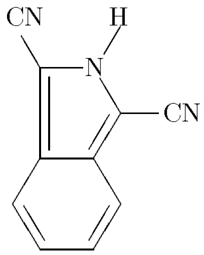
The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST specifies double bonds by using chracters selected from Table 9.1.

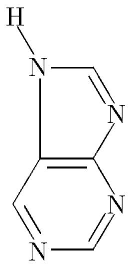
Example:

```
\indoleh{1==H;2==COOH}\qquad
\isoindoleh{2==H;1==CN;3==CN}\qquad
\purineh{3==H}
```

produce the following structures:



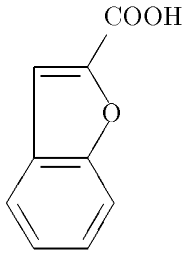


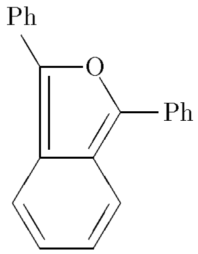


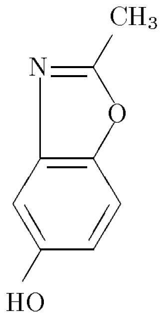
Example:

```
\benzofuraneh{2==COOH}\qquad
\isobenzofuraneh{1==Ph;3==Ph}\qquad
\benzoxazoleh{2==CH$_{3}$;5==HO}
```

produce the following structures:



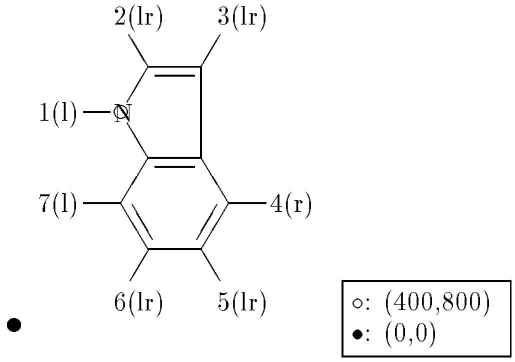


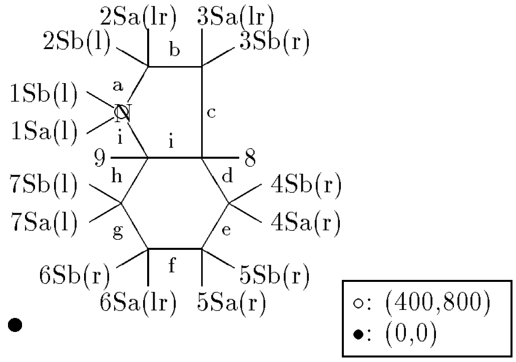


The macro **\indolehi** is used to draw inodele derivatives of inverse horizontal type (hetaromh.sty). Macros for drawing other fused heterocycles are also defined in the hetaromh.sty. The format of these commands is as follows:

```
\indolehi[BONDLIST]{SUBSLIST}
\isoindolehi[BONDLIST]{SUBSLIST}
\purinehi[BONDLIST]{SUBSLIST}
\benzofuranehi[BONDLIST]{SUBSLIST}
\isobenzofuranehi[BONDLIST]{SUBSLIST}
\benzoxazolehi[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and characters for describing bonds to be doubled are shown in the following diagram:

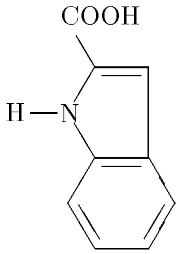


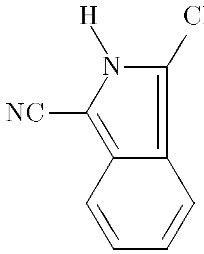


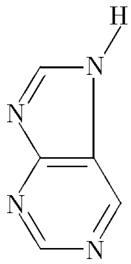
Example:

```
\indolehi{1==H;2==COOH}\qquad
\isoindolehi{2==H;1==NC;3==CN}\qquad
\purinehi{3==H}
```

produce the following structures:



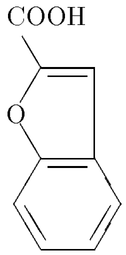


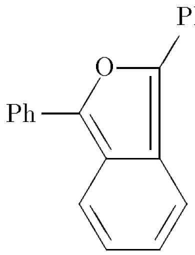


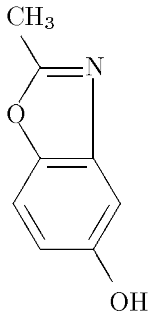
Example:

```
\benzofuranehi{2==COOH}\qquad
\isobenzofuranehi{1==Ph;3==Ph}\qquad
\benzoxazolehi{2==CH$_{3}$;5==OH}
```

produce the following structures:





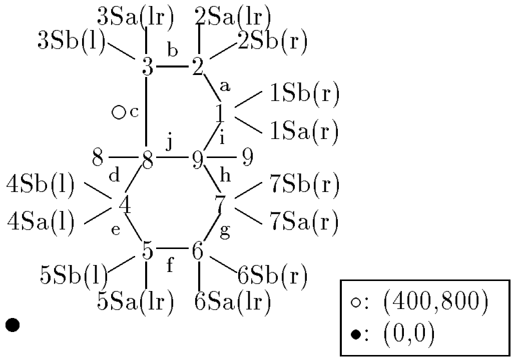


10.2.2 Commands for General Use

Macros for specified use such as `\indoleh` are based on a general command `\nonaheteroh`. This command enable us to draw a further variety of heterocyclic compounds. This macro has the following format which is contained also in hetaromh.sty.

```
\nonaheteroh[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The locant numbering is common in these commands as shown in the following diagram:



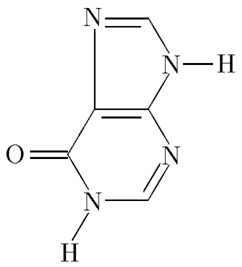
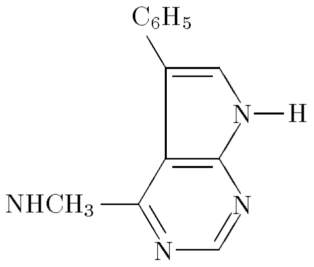
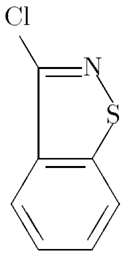
The handedness for each oriented or double-sided position is shown with a character set in parentheses. Characters listed in Table 10.1 are also used to specify double bonds by setting them into the optional argument BONDLIST.

The argument ATOMLIST takes a usual format with respect to heteroatoms attached to $n = 1$ to 7, *e.g.*, 1==N for a nitrogen atom at 1-position. Hetero-atoms at 3a- and 7b-positions are represented as to be 3a==N (or 8==N) for a nitrogen at 3a-position, 7a==N (or 9==N) for at a nitrogen at 7a-position, and so on. The augument SUBSLIST takes a usual format except that the locant numbers 3a and 7a are replaced by 8 and 9.

Example:

```
\nonaheteroh[bjg]{1==N;3==N;5==N;7==N}{1==H;5==H;4D==O}
\nonaheteroh[bjge]{1==N;5==N;7==N}%
 {1==H;3==C$_{6}$H$_{5}$;4==NHCH$_{3}$}
\nonaheteroh[bjge]{1==S;2==N}{3==Cl}
```

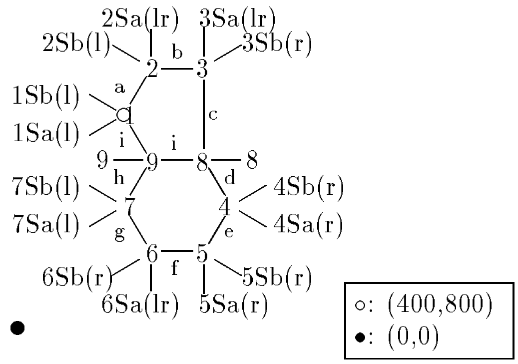
produce the following structures:

The inverse conterpart `\nonaheterohi` are also available by setting 'hetaromh.sty'. Its format is:

`\nonaheterohi[BONDLIST]{ATOMLIST}{SUBSLIST}`

Its locant numbering is common with the normal counterpart as shown in the following diagram:

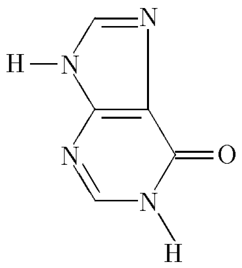
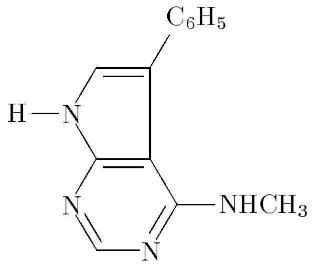
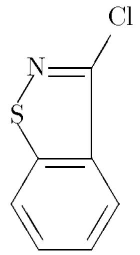


The handedness for each oriented or double-sided position is shown with a character set in parentheses. The optional argument BONDLIST uses characters listed in Table 10.1 so as to specify double bonds.

Example:

```
\nonaheterohi[bjg]{1==N;3==N;5==N;7==N}{1==H;5==H;4D==O}
\nonaheterohi[bjge]{1==N;5==N;7==N}%
 {1==H;3==C$_{6}$H$_{5}$;4==NHCH$_{3}$}
\nonaheterohi[bjge]{1==S;2==N}{3==Cl}
```

produce the following structures:

Chapter 11

Building Blocks

11.1 Six-Membered Blocks

The macro `\sixunitv` provides a six-membered fragment that can be fused to another ring structure, producing a new ring system.

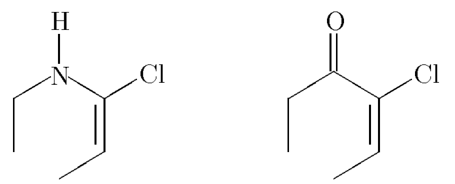
```
\sixunitv[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

The modes of numbering for positions and for edges are the same as those of `\sixheterov`. Hence, the arguments BONDLIST, ATOMLIST, and SUBSLIST are written in the same way. The argument OMIT indicates bonds to be deleted, where characters are selected from the table prepared for the BONDLIST of `\sixheterov`. It should be noted that the assignment of a null argument to ATOMLIST produces a carbocyclic building block.

Example:

```
\sixunitv[b]{1==N}{1==H;2==Cl}{d} \qquad
\sixunitv[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:



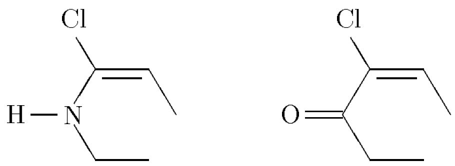
The macro `\sixunith` is the horizontal counterpart of `\sixunitv`. It produces a six-membered fragment of horizontal type,

```
\sixunith[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

Example:

```
\sixunith[b]{1==N}{1==H;2==Cl}{d} \qquad
\sixunith[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:



11.2 Five-Membered Blocks

The macro `\fiveunitv` produces a five-membered fragment that can be fused to another ring structure to produce a new ring system.

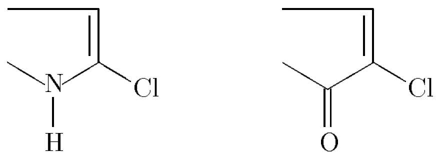
```
\fiveunitv[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

The numbering of positions and the designation of edges are the same as those of `\fiveheterov`. Hence, the arguments BONDLIST, ATOMLIST, and SUBSLIST are written in the same way. The argument OMIT indicates bonds to be deleted. It is a list of the same format as the BONDLIST of `\fiveheterov`.

Example:

```
\fiveunitv[b]{1==N}{1==H;2==Cl}{d} \qquad
\fiveunitv[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:



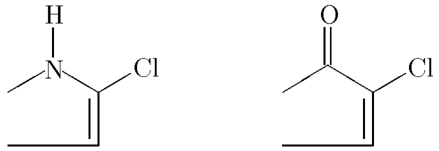
The macro `\fiveunitvi` produces a five-membered fragment of inverse type that can be fused to another ring structure to produce a new ring system.

```
\fiveunitvi[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

Example:

```
\fiveunitvi[b]{1==N}{1==H;2==Cl}{d} \qquad
\fiveunitvi[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:



The macro `\fiveunith` is a five-membered fragment of horizontal type that can be fused to another ring structure to produce a new ring system.

```
\fiveunith[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

Example:

```
\fiveunith[b]{1==N}{1==H;2==Cl}{d} \qquad
\fiveunith[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:

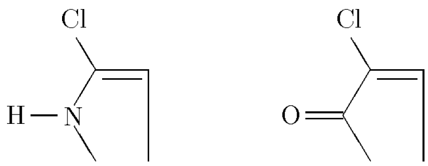
The macro `\fiveunithi` is the inverse counterpart of `\fiveunith`. It produces a five-membered fragment of another horizontal type so that it can be fused to another ring structure to produce a new ring system.

```
\fiveunithi[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

Example:

```
\fiveunithi[b]{1==N}{1==H;2==Cl}{d} \qquad
\fiveunithi[b]{}{1D==O;2==Cl}{d}
```

produce the following structures:



11.3 Setting Locant Numbers

The `\bdloocant` prints six characters on the edges of a six-membered ring of vertical type (locant.sty).

```
\bdloocant{#1}{#2}{#3}{#4}{#5}{#6}
```

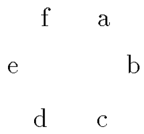
On the other hand, the `\bdloocnth` prints six characters on the edges of a six-membered ring of horizontal type.

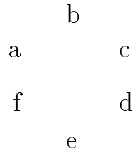
```
\bdloocnth{#1}{#2}{#3}{#4}{#5}{#6}
```

Example:

```
\bdloocant{a}{b}{c}{d}{e}{f} \qquad
\bdloocnth{a}{b}{c}{d}{e}{f}
```

produce the following structures:





The `\sxloocant` prints six characters on the vertices of a six-membered ring of vertical type.

```
\sxloocant{#1}{#2}{#3}{#4}{#5}{#6}
```

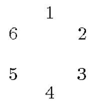
On the other hand, the `\sxloocnth` prints six characters on the vertices of a six-membered ring of horizontal type.

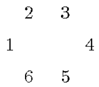
```
\sxloocnth{#1}{#2}{#3}{#4}{#5}{#6}
```

Example:

```
\sxloocant{1}{2}{3}{4}{5}{6} \qquad
\sxloocnth{1}{2}{3}{4}{5}{6}
```

produce the following structures:



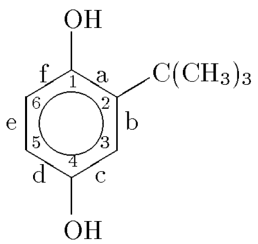


These commands can be used by combining with a structure-drawing macro in a picture environment to show the locant numbering of the structure.

Example:

```
\begin{picture}(1000,1000)(0,0)
\put(0,0){\sxloocant{1}{2}{3}{4}{5}{6}}
\put(0,0){\bdloocant{a}{b}{c}{d}{e}{f}}
\put(0,0){\bzdrv[c]{1==OH;2==C(CH$_{3}$)$_{3}$;4==OH}}
\end{picture}
```

produces the following structure:



Chapter 12

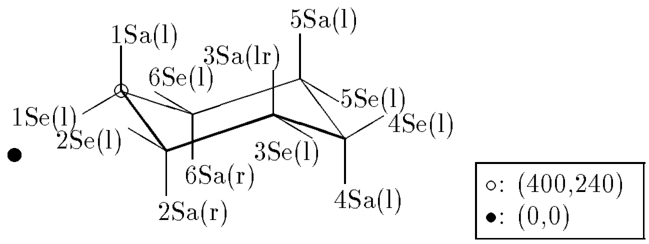
Further Cyclic Compounds

12.1 Drawing Chair Form of Cylohexane

The macro `\chair` is used to draw cyclohexane derivatives of chair-form (ccycle.sty). The format of this command is as follows:

`\chair[BONDLIST]{SUBSLIST}`

Locant numbers for designating substitution positions are represented by the following diagram:



Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character. The bond-correspondence is rather arbitrary in some cases but conforms to chemical conventions as faithfully as possible if such conventions are presence (Table 12.1).

Table 12.1: Argument BONDLIST for commands `\chair`

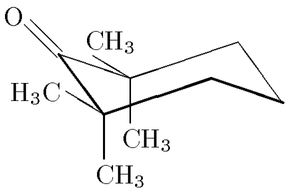
Character	Printed structure
none	cyclohexane
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond

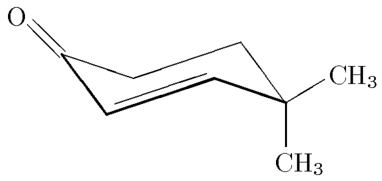
The argument SUBSLIST for this macro takes a general format, except that modifiers are selected from ‘Sa’ for an axial substitutent, ‘Se’ for an equatorial substitutent, and ‘D’ for a substitutent through an double bond.

Example:

```
\chair{1D==O;2Se==H$_{3}$C;2Sa==CH$_{3}$;%
6Se==CH$_{3}$;6Sa==CH$_{3}$} \qquad\qquad
\chair[b]{1D==O;4Se==CH$_{3}$;4Sa==CH$_{3}$}
```

produce the following diagrams:



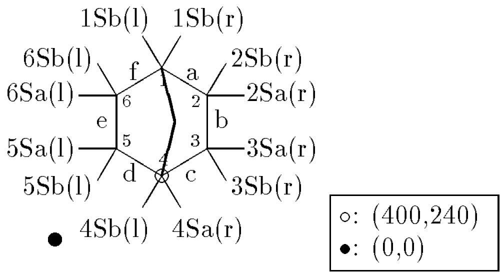


12.2 Drawing Bicyclo[2.2.1]heptane

The macro `\bicychepv` is used to draw bicyclo[2.2.1]heptane derivatives of vertical type in a flat fashion. The format of this command is as follows:

```
\bicychepv[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and bond descriptors for assigning double bonds are shown in the following diagram:



Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character (Table 12.2).

Table 12.2: Argument BONDLIST for commands `\bicychepv` and `\bicycheph`

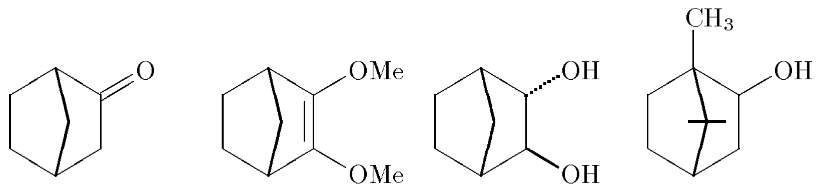
Character	Printed structure
none	cyclohexane
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond
A	aromatic circle
7	7,7-dimethyl

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

Example:

```
\bicychepv{2D==O}
\bicychepv[b]{2==OMe;3==OMe}
\bicychepv{3B==OH;2A==OH}
\bicychepv[7]{1==CH$_{3}$;2==OH}
```

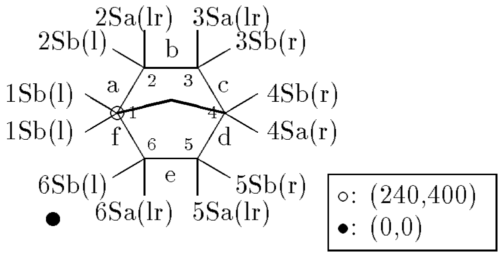
produce the following diagrams:



The macro `\bicycheph` is used to draw bicyclo[2.2.1]heptane derivatives of vertical type in a flat fashion. The format of this command is as follows:

```
\bicycheph[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions along with bond desciptors are found in the following diagram:

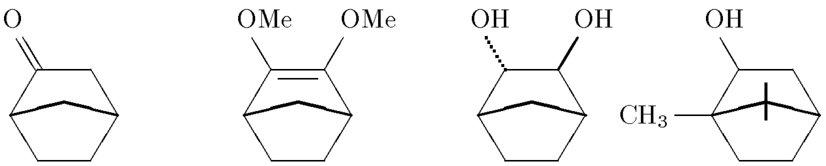


Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros. For the SUBSLIST and the BONDLIST, see Table 2.2 and 12.2. .

Example:

```
\bicycheph{2D==O}
\bicycheph[b]{2==OMe;3==OMe}
\bicycheph{3B==OH;2A==OH}
\bicycheph[7]{1==CH$_{3}$;2==OH}
```

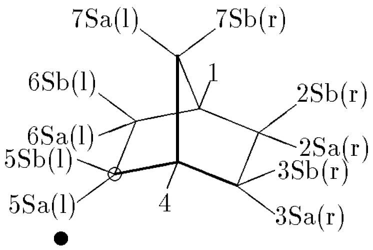
produce the following diagrams:



For the purpose of depicting the stereochemisty of bicyclo[2.2.1]heptane derivatives, you can use the command `\bornane` instead of the commands `\bicychepv` and `\bicycheph`. The format of this command is as follows:

```
\bornane[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions are represented by the following diagram:



○: (200,240)
●: (0,0)

Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character (Table 12.3). The SUBSLIST format is shown in Table 2.2.

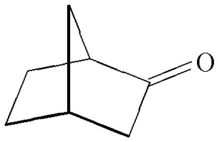
Table 12.3: Argument BONDLIST for commands `\bornane`

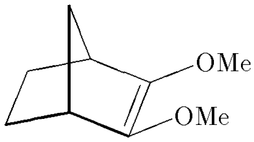
Character	Printed structure
none	cyclohexane
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond
g	1,7-double bond
h	4,7-double bond

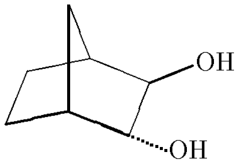
Example:

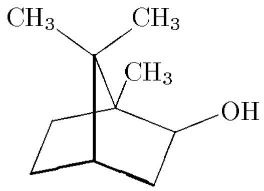
```
\bornane{2D==O}
\bornane[b]{2==OMe;3==OMe}\par
\bornane{3B==OH;2A==OH}
\bornane{7Sa==CH$_{3}$;7Sb==CH$_{3}$;1==CH$_{3}$;2==OH}
```

produce the following diagrams:







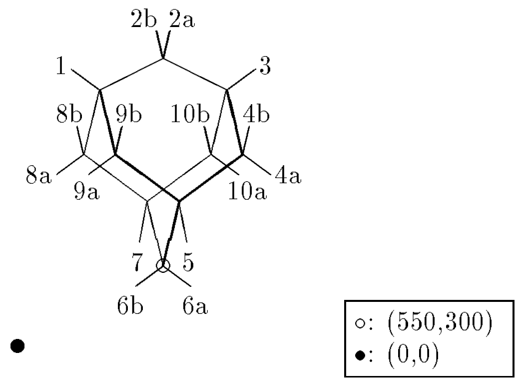


12.3 Drawing Adamantane Derivatives

The macro `\adamantane` prints adamantane derivatives by means of the following format:

```
\adamantane[BONDLIST]{SUBSLIST}
```

where BONDLIST is not effective in the present specification.



The argument SUBSLIST is slightly different from general conventions, as shown in Table 12.4.

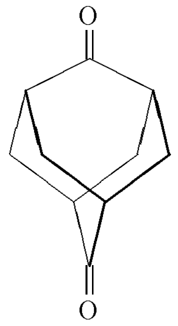
Example:

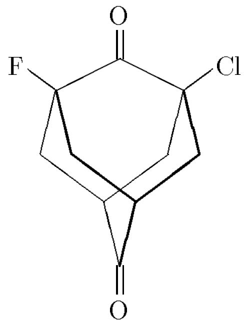
```
\adamantane{2D==O;6D==O}
\adamantane{2D==O;6D==O;1==F;3==Cl}
```

produce the following diagrams:

Table 12.4: Argument SUBSLIST for command `\adamantane`

Character	Printed structure
for $n = 1, 3, 5$, and 7 (bridgeheads)	
n or na	exocyclic single bond at n-atom
for $n = 2, 4, 6, 8, 9$, and 10 (bridges)	
na	exocyclic single bond at n-atom (axial)
nb	exocyclic single bond at n-atom (equatorial)
nD	exocyclic double bond at n-atom (2 and 6)



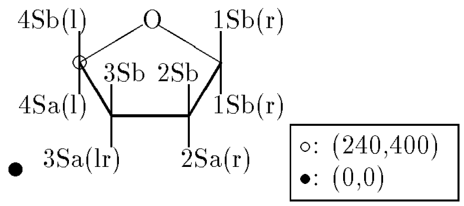


12.4 Drawing Furanoses and Pyranoses

For drawing furanoses, the command `furanose` is used. The format of this command is as follows:

```
\furanose[BONDLIST]{SUBSLIST}
```

Locant numbers for designating substitution positions and bond descriptors are represented by the following diagram:



Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros.

The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the edge corresponding to the character (Table 12.5).

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

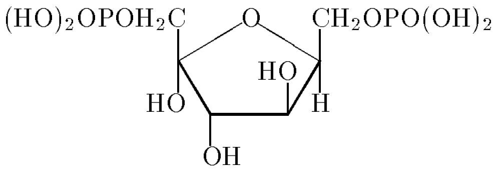
Example:

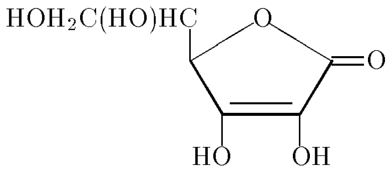
```
\furanose{1Sa==H;1Sb==CH$_{2}$OPO(OH)$_{2}$;2Sb==\lmoiety{HO};3Sa==OH;%
4Sb==(HO)$_{2}$OPOH$_{2}$C;4Sa==HO}\hskip5cm
\furanose[b]{1D==O;2Sa==OH;3Sa==\lmoiety{HO};4Sb==HOH$_{2}$C(HO)HC}
```

Table 12.5: Argument BONDLIST for commands `\bicychepv` and `\bicycheph`

Character	Printed structure
none	mother skeleton
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,1-double bond

produce the following diagrams:

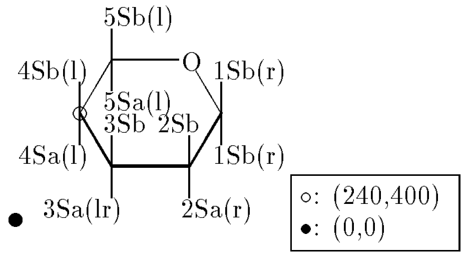




For drawing furanoses, the command `pyranose` is used. The format of this command is as follows:

`\pyranose[BONDLIST]{SUBSLIST}`

Locant numbers for designating substitution positions are represented by the following diagram:



Each character set in parentheses represents the handedness of the corresponding postion, which is fixed in this type of macros.

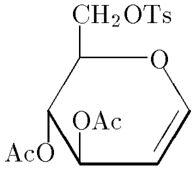
The option argument BONDLIST is an character string in a pair of brackets, where each character indicates the presence of a double bond at the corresponding edge (Table 12.6).

The argument SUBSLIST for this macro takes a general format, in which the modifiers listed in Table 2.2 are used.

Example:

```
\pyranose[a]{3Sb==OAc;4Sa==AcO;5Sb==CH$_{2}$OTs}
\pyranose[b]{2D==O;5Sb==CH$_{2}$OTs}
```

produce the following diagrams:



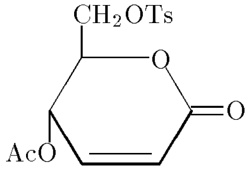


Table 12.6: Argument BONDLIST for commands `\bicychepv` and `\bicycheph`

Character	Printed structure
none	mother skeleton
a	1,2-double bond
b	2,3-double bond
c	4,3-double bond
d	4,5-double bond
e	5,6-double bond
f	6,1-double bond

Chapter 13

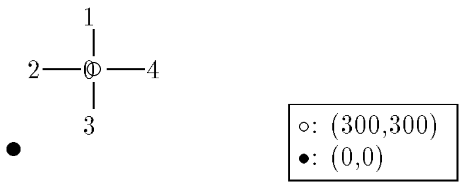
Aliphatic Compounds

13.1 Drawing Tetrahedral Units

The macro `\tetrahedral` is used to draw a tetrahedral unit (aliphat.sty). The format of this command is as follows:

```
\tetrahedral[AUXLIST]{SUBSLIST}
```

The following diagram shows the numbering for designating substitution positions:



in which the same macro is used to typeset both saturated and unsaturated derivatives.

The optional argument AUXLIST is used to specify a charge on the central atom: *i.e.*, {0+} represents a + charge (or another one charararacter) on the center.

The argument SUBSLIST is used to specify each substituent with a locant number and a bond modifier shown in Table 13.1, in which n is an arabic numeral between 1 and 4.

Table 13.1: SUBSLIST for `\tetrahedral`

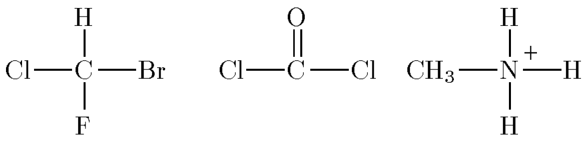
Character	Structures printed
nT	triple bond at n-atom
nD	double bond at n-atom
n or nS	single bond at n-atom
nA	alpha single bond at n-atom
nB	beta single bond at n-atom

The central carbon atom is asigned by writing 0==C. The structural formula of an ammonium ion can also be obtained with this command.

Example:

```
\tetrahedral{0==C;1==H;2==Cl;3==F;4==Br}\qquad
\tetrahedral{0==C;1D==O;2==Cl;4==Cl}\qquad
\tetrahedral[{}{0+}]{0==N;1==H;2==CH$_{3}$;3==H;4==H}
```

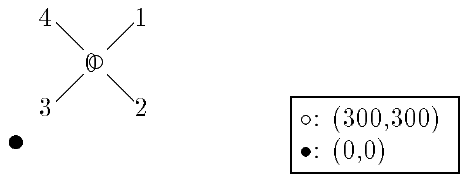
produce the following structures:



The macro `\square` is used to draw a tetrahedral unit of another type (aliphat.sty). The format of this command is as follows:

```
\square[AUXLIST]{SUBSLIST}
```

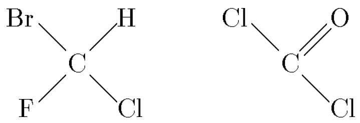
The following diagram shows the numbering for designating substitution positions:



Example:

```
\square{0==C;1==H;2==Cl;3==F;4==Br}\qquad
\square{0==C;1D==O;2==Cl;4==Cl}
```

produce the following structures:



13.2 Drawing Trigonal Units

The macro `\rtrigonal` and `\ltrigonal` are used to draw right-handed and left-handed trigonal units (aliphat.sty). The formats of these commands are as follows:

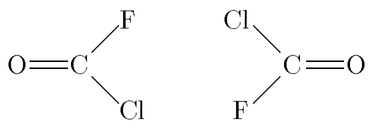
```
\rtrigonal[AUXLIST]{SUBSLIST}
\ltrigonal[AUXLIST]{SUBSLIST}
```

The bond angles of 2–0–3 are 90° in the trigonal units printed with these commands. The arguments AUXLIST and SUBSLIST are the same as those of `\tetrahedral`.

Example:

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

produce the following structures:



The macros `\utrigonal` and `\Utrigonal` are used to draw upward trigonal units with angles 90° and 120° (aliphat.sty). The formats of these commands are as follows:

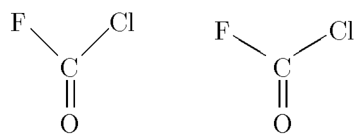
```
\utrigonal[AUXLIST]{SUBSLIST}
\Utrigonal[AUXLIST]{SUBSLIST}
```

The arguments AUXLIST and SUBSLIST are the same as those of `\tetrahedral`.

Example:

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

produce the following structures:



On the other hand, the macros `\dtrigonal` and `\Dtrigonal` are used to draw downward trigonal units with angles 90° and 120° (aliphat.sty). The formats of these commands are as follows:

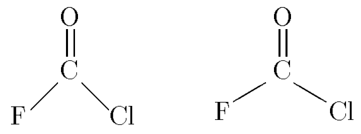
```
\dtrigonal[AUXLIST]{SUBSLIST}
\Dtrigonal[AUXLIST]{SUBSLIST}
```

The arguments AUXLIST and SUBSLIST are the same as those of `\tetrahedral`.

Example:

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

produce the following structures:

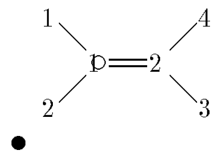


13.3 Drawing Ethylene Derivatives

The macro `\ethylene` is used to draw ethylene derivatives with angles 90° (aliphat.sty). The format of this command is as follows:

```
\ethylene[BONDLIST]{ATOMLIST}{SUBSLIST}
```

The following diagram shows the numbering for designating substitution positions:



○: (300,300)
●: (0,0)

Table 13.2: BONDLIST for `\ethylene`

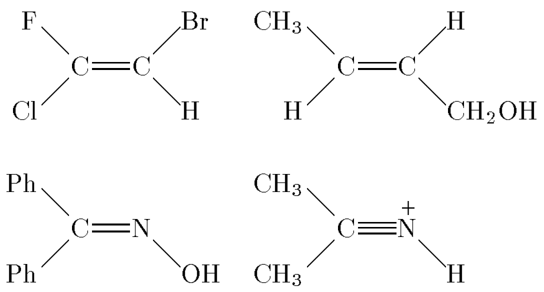
Character	Structures printed
{n+}	+ charge (or another one chararacter) on n-atom
d	inner double bond (between centers 1 and 2)
t	inner triple bond (between centers 1 and 2)

The argument ATOMLIST is used for giving central atoms. The argument SUBSLIST is the same as that of `\tetrahedral`.

Example:

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

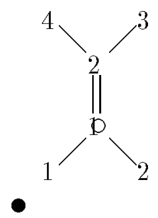
produce the following structures:



The macro `\ethylenev`, which is the vertical counterpart of `\ethylene`, is used to draw ethylene derivatives with angles 90° (aliphat.sty). The format of this command is as follows:

`\ethylenev[BONDLIST]{ATOMLIST}{SUBSLIST}`

The following diagram shows the numbering for designating substitution positions:

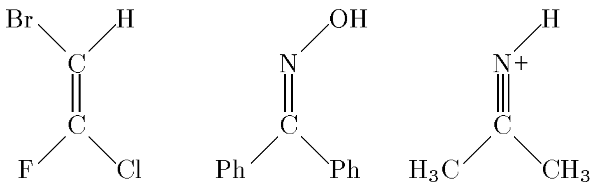


○: (300,300)
●: (0,0)

Example:

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

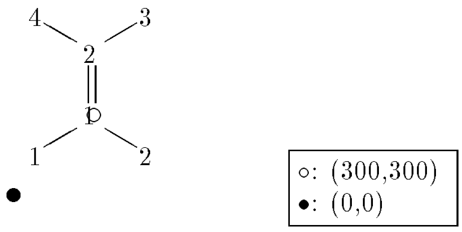
produce the following structures:



The macro `\Ethylenev` is used to draw ethylene derivatives with angles 120° (aliphat.sty). It is the vertical counterpart of `\ethylene`. The format of the command is as follows:

```
\Ethylenev[BONDLIST]{ATOMLIST}{SUBSLIST}
```

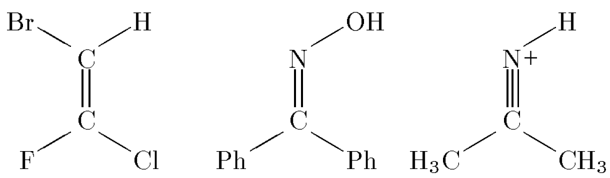
The following diagram shows the numbering for designating substitution positions:



Example:

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

produce the following structures:



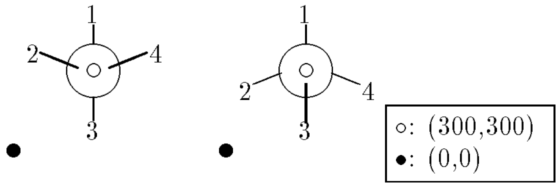
13.4 Drawing Configurations

The macros `tetrastereo` and `dtetrastereo` typset fragments which show actural configuration of a tetrahedral carbon in different modes of projections. The formats of these commands are as follows:

```
\tetrastereo[AUXLIST]{SUBSLIST}
\dtetrastereo[AUXLIST]{SUBSLIST}
```

The arguments AUXLIST and SUBSLIST are the same as those of `\tetrahedral`.

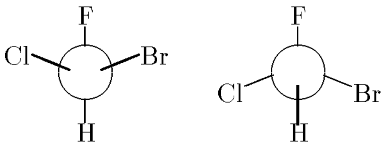
The following diagram shows the numbering for designating substitution positions:



Example:

```
\tetrastereo{1==F;2==Cl;3==H;4==Br}\qquad
\dtetrastereo{1==F;2==Cl;3==H;4==Br}
```

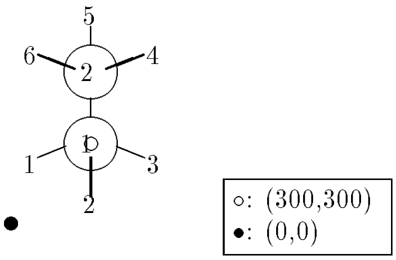
produce the following structures:



The configuration of ethane is typeset by the macro `\ethanestereo`. The format of the command is as follows:

```
\ethanestereo[AUXLIST]{ATOMLIST}{SUBSLIST}
```

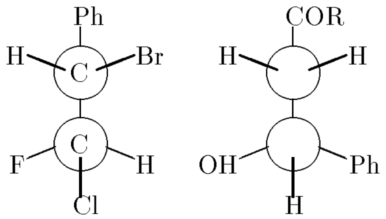
The argument ATOMLIST is used for giving central atoms. The arguments AUXLIST and SUBSLIST are the same as those of `\tetrahedral`.



Example:

```
\ethanestereo{1==C;2==C}{1==F;2==Cl;3==H;4==Br;6==H;5==Ph}\qquad
\ethanestereo{}{1==OH;2==H;3==Ph;4==H;5==COR;6==H}
```

produce the following structures:



Further examples of typesetting the configurations of ethane derivatives have been described in an article concerning sterochemistry [4].

Chapter 14

Combining structures

14.1 General Remarks

14.1.1 Coordinates of the Picture Environment

The macros described in the other chapters of this manual can be combined to construct a more complicated structural formula. This treatment is based on the fact that two or more picture environments of LaTeX can be nested, recognizing each inner picture environment as a LaTeX picture box.

A picture environment of LaTeX is set up with the following statement:

```
\begin{picture}(Lx,Ly)(Sx,Sy),
⋮
\end{picture}
```

This command produces an $L_x \times L_y$ area for drawing a structural formula, where the origin (0, 0) can be shifted by giving differences (S_x, S_y).

The `\put(`P_x, P_y`)` command places an inner picture box (*e.g.*, a fragment created by a macro of the present paper) so that the reference point of the inner picture is located on the (P_x, P_y) point of the outer picture environment.

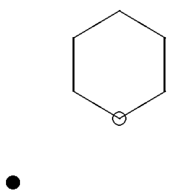
14.1.2 Reference Points and Inner Origins

A macro of XΥMTEX is based on an inner picture environment, which has an original point for drawing a structure and a set of sifted values. Suppose the definition of the macro contains an inner picture environment represented by

`\begin{picture}(`ℓ_x, ℓ_y`)(`s_x, s_y`).`

The point (s_x, s_y) of the inner environment becomes the (0,0) point of the structure generated by the macro. This point is called the reference point of the macro in the present manual. On the other hand, the origin of the inner environment becames the $(-s_x, -s_y)$ point of the generated structure. It is called the inner origin of the macro.

For example, the command `\cyclohexanev` generates a skeleton,



in which the symbol ∘ represents the inner origin and the symbol • represents a reference point. The macro `\cyclohexanev` is defined on the basis of an inner picture environment:

`\begin{picture}(800, 800)(-400, -240).`

As a result, the inner origin is referred to as the (400, 200) point of the resulting macro; and the inner $(-400, -240)$ point is regarded as the new origin (0, 0), which is the reference point of the macro.

Each macro is characterized by the referece point and the inner origin, which are shown in a framed box beside the specification of the macro. The reference point and the inner origin of each macro are revealed by stating `\origpttrue` in the preamble of a manuscript. Then, they are printed with the symbols ∘ and •; and the values of them appear on the display. For example, the above cyclohexane structure is typeset by the following statement:

```
{\origpttrue
\begin{center}
\cyclohexanev{}
\end{center}}
```

or by an equivalent statement:

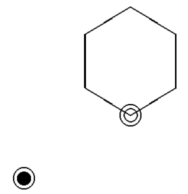
```
\begin{xymspec}
\cyclohexanev{}
\end{xymspec}
```

14.1.3 Setting Coordinates

The command `\put` typesets an object, which may be a character string, a structure generated with a macro, or others. When a macro is written as an argument of the command `\put` in an outer picture environment, a structure due to the macro is typeset so that the reference point of the macro is placed on the point designated by the `\put` command. For example,

```
{\origpttrue
\begin{picture}(1000,700)(0,0)
\put(0,0){\cyclohexanev{}}
\put(0,0){\circle{80}}
\put(400,240){\circle{80}}
\end{picture}
}
```

produces

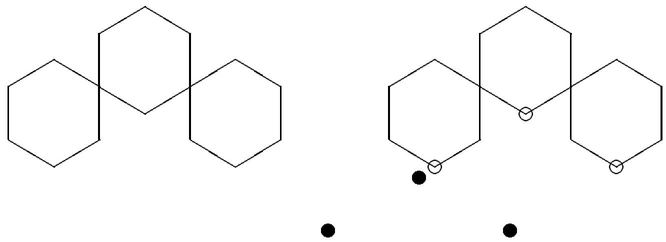


The reference point with • is encircled by an outer circle representing the origin of the outer picture environment. The inner origin represented with an open circle is encircled by an outer circle centered at the $(400, 240)$ point of the outer environment, resulting in a double circle.

Since we adopt a bond length equal to 200 and a bond slope of (5, 3) or (3, 5), such values as 200, 171, and 103 (and any combinations of these values) appear frequently in typsetting combined structures. Note that 171 is approximately equal to $200 \times (5/\sqrt{34})$ and 103 is aproximately equal to $200 \times (3/\sqrt{34})$. For example, a spiro compound can be typeset by the statement:

```
\begin{picture}(1200,900)(0,0)
\put(0,0){\cyclohexanev{}}
\put(342,200){\cyclohexanev{}}
\put(684,0){\cyclohexanev{}}
\end{picture}
```

The resulting structures are



The right-hand structure is to show the reference points and the inner origins of the fragements used. In this case, the shifted values $(-400, -240)$ of each fragment are equal to those of another fragment, since each fragment is generated by the same macro. Hence, the argument coordinates of the `\put` can be calculated without considering such shifted values. Thus, the value 342 is equal to 171×2, and 684 is equal to 171×4.

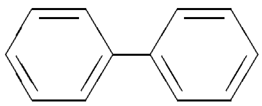
14.2 Combination of Macros Through a Bond

Since each of the macros described in the other chapters of the present manual is based on a picture environment, one of the simplest ways of combining structures is to place individual structures into an outer picture environment. Such combination of macros increases the variety of structural diagrams.

In order to illustrate the method of calculating coordinates, we take the drawing of biphenyl as the first example:

```
\begin{picture}(1200,600)(0,0)
\put(0,0){\bzdrh{4==}}
\put(546,0){\bzdrh{}}
\end{picture}
```

This statement produces the following structure:



The first argument of each `\put` command represents the coordinates of the point on which the structure is printed.

The inner origin of the macro `\bzdrh` is the leftmost position of the benzene ring. The structure typeset by the command `\put(0,0){\bzdrh{4==}}` has a rightmost terminal point at $(546, 0)$ with respect to the inner picture environment.[1] The value 546 is calculated by $406 + 140$, where 406 is the length of the horizontal hexagon ($= 103 + 200 + 103$) and 140 is the bond length produced by the argument `{4==}`.

The command `\put(546,0){\bzdrh{}}` prints another benzene ring so that the inner origin of this benzene is placed on the terminal position of the former benzene ring. Note again that the argument

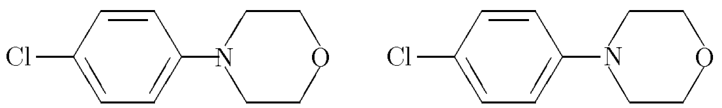
[1] The absolute cooridnates with respect to the outer picture environment is $(546 + 400, 0 + 240)$ in this case.

coordinates of `\put` can be calculated without considering such shifted values, $(400, 240)$, since each of the fragments is generated by the same macro.

Let us draw 1-chloro-4-morphorinobenzene by means of two different ways.

```
\begin{picture}(1200,600)(0,0)
\put(0,0){\bzdrh{1==Cl;4==}}
\put(546,0){\sixheteroh[H]{1==N;4==O}{}}
\end{picture}
\qquad
\begin{picture}(1200,600)(0,0)
\put(0,0){\bzdrh{1==Cl;4==N}}
\put(566,0){\sixheteroh[H]{1=={ };4==O}{}}
\end{picture}
```

These statements produce essentially the same structure:

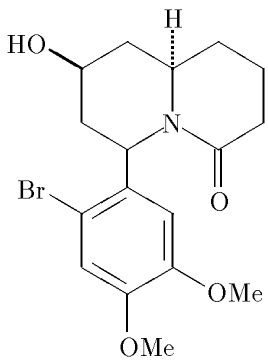


It should be noted that `{4==}` in SUBSLIST produces a bond without a substituent at the 4-position of the benzene ring, while `1=={␣}` in ATOMLIST creates a vacancy to accomodate the nitrogen atom.

The following example illustrates a more complicated structure with a vertical bond linking two fragment structures. Thus, the statement

```
\begin{picture}(1200,1500)(-200,-600)
\put(0,0){\decaheterov[H]{4a==N}{4D==O;7B==HO;{{10}A}==H}}
\put(0,-546){\bzdrv{1==;3==OMe;4==OMe;6==Br}}
\end{picture}
```

prints the following diagram:

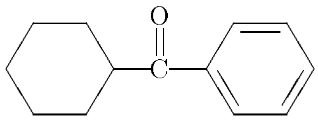


The first argument of each `\put` command represents the coordinates of the point on which the structure is printed. The value -546 is calculated by 140 (bond length) + 406 (the height of the hexagon $= 103 + 200 + 103$), because the inner origin of the structure printed by `\decaheterov` is position 5 (the left carbon atom adjacent to the nitrogen atom) and that of the latter structure is position 4 (the bottom carbon attached by the methoxy group).

The following example illustrates a combined structure in which two cyclic substructures are linked through an aliphatic unit

```
\begin{picture}(800,1000)(0,0)
\put(0,0){\cyclohexaneh[H]{4==}}
\put(754,0){\bzdrh{1==}}
\put(520,100){\tetrahedral{0==C;1D==O}}
\end{picture}
```

This statement produces



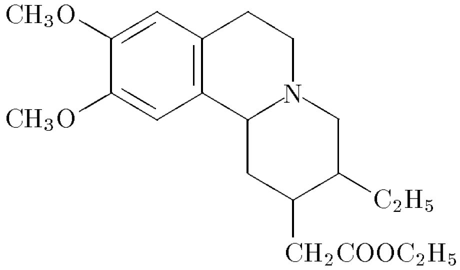
The calculation of the values for `\tetrahedral` is slightly complicated, since its inner origin is different from those of the other commands. The right terminal position due to the `\cyclohexaneh` is the point $(546, 0)$, the x-coordinate of which is equal to the length of a benzene ring (406) plus a bond length (140). The left terminal position due to the `\bzdrh` is the point $(614, 0)$, because $754 - 140 = 614$. Then, the aliphatic unit (`\tetrahedral`) should be placed at the average position of x-coordinate $(546 + 614)/2 = 580$. Since the inner origin of the the `\cyclohexaneh` is $(400, 240)$ and that of the `\tetrahedral` is $(300, 300)$, the x-coordinate is calculated to be $580-(300-240) = 520$ while the y-coordinate is calculated to be $400 - 300 = 100$.

14.3 Using Building Blocks

Macros `\sixunitv` and `\fiveunitv` are designed for building a new fused ring system:

```
\sixunitv[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
\fiveunitv[BONDLIST]{ATOMLIST}{SUBSLIST}{OMIT}
```

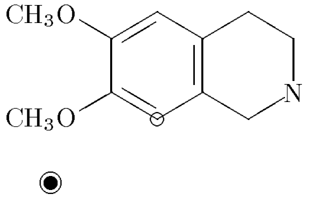
where argument OMIT (a–f for `\sixunitv` and a–e for `\fiveunitv`) is a list of characters, each of which represents one bond to be omitted. The other arguments have the same formats as described in the preceding sections. These macros produce five- and six-membered fragments respectively, in which the bond assigned by argument OMIT is deleted to be a fused vacant bond. They include the mechanism of the hetroatom truncation in order to be applied to typesetting both carbocycles and heterocycles. For example, a tricyclic system



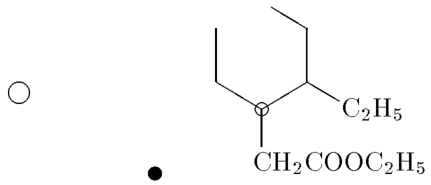
is typeset with the statement:

```
\begin{picture}(1200,1500)(-200,-600)
\put(0,0){\decaheterov[fhk]{3==N}{6==CH$_3$O;7==CH$_3$O}}
\put(513,-303){\sixunitv[H]{1=={ }}%
  {3==C$_2$H$_5$;4==CH$_2$COOC$_2$H$_5$}{f}}
\end{picture}
```

In order to examine the details of the combination, let us typeset the structure with the first command:



and separately the structure with the secdond command:



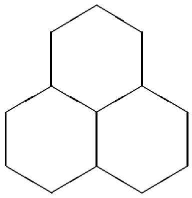
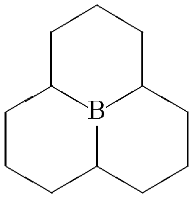
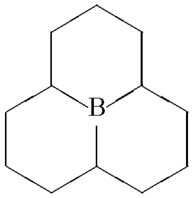
It should be noted that argument ATOMLIST in the `\sixunitv` macro contains the assignment "`1=={␣}`" which assures the vacant bridgehead position. This vacancy is occupied by the bridgehead nitrogen printed by the `\decaheterov` macro.

The following examples illustrate combinations of `decaheterov` and `\sixunitv` to produce a borane and the related carbocycle.

```
\begin{picture}(1200,1000)(0,0)
\put(0,0){\decaheterov[H]{}{}}
\put(171,303){\sixunitv[H]{4=={ }}{}{cd}}
\end{picture}
\qquad
\begin{picture}(1200,1000)(0,0)
\put(0,0){\decaheterov[H]{8a==B}{}}
\put(171,303){\sixunitv[H]{4=={ }}{}{cd}}
\end{picture}
```

```
\qquad
\begin{picture}(1200,1000)(0,0)
\put(0,0){\sixunitv[H]{2=={ }}{}{a}}
\put(342,0){\sixunitv[H]{}{}{ef}}
\put(171,303){\sixheterovi[H]{1==N}{}}
\end{picture}
```

These statements produce the following structures.

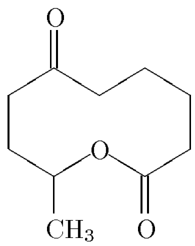
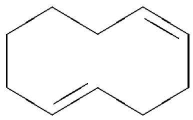




The second and third examples above show alternative ways to depict the carborane. Note that the argument `{2=={␣}}` in the third example is necessary to print the desired structures.

The following two exmaples involve a combination of two `\sixunitv` commands.

```
\begin{picture}(1200,800)(0,0)
\put(0,0){\sixunitv[H]{3==O}{1D==O;4==CH$_{3}$}{b}}
\put(342,0){\sixunitv[H]{5=={ }}{4D==O}{e}}
\end{picture}
\qquad
\begin{picture}(1200,800)(0,0)
\put(0,0){\sixunitv[c]{}{}{b}}
\put(342,0){\sixunitv[a]{}{}{e}}
\end{picture}
```

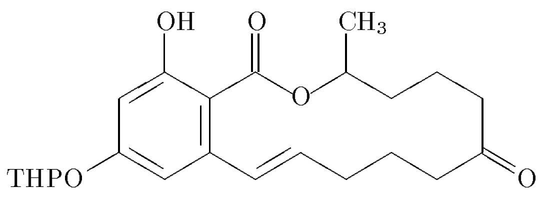
These statements provide

The following exmaple involves a combination of three `\sixunitv` commands and one `\bzdrv` command.

```
\begin{picture}(1600,800)(0,0)
\put(0,0){\bzdrv[r]{1==OH;5==THPO}}
\put(342,0){\sixunitv[c]{2==O}{1D==O}{be}}
\put(684,0){\sixunitv[H]{6=={ }}{1==CH$_{3}$}{be}}
\put(1026,0){\sixunitv[H]{}{3D==O}{e}}
\end{picture}
```

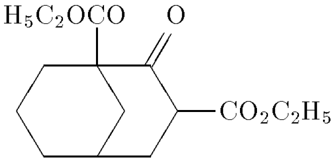
This statement provides

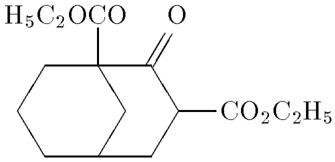


A bicyclo[3.3.1]nonane is typeset by this technique.

```
\begin{picture}(1600,800)(0,0)
\put(0,0){\cyclohexaneh[H]{3Sa==\lmoiety{H$_{5}$C$_{2}$OCO\kern2em}}}
\put(200,0){\sixunith[H]{}{3D==O;4==CO$_{2}$C$_{2}$H$_{5}$}{af}}
\end{picture}
\qquad
\begin{picture}(1600,800)(0,0)
\put(0,0){\cyclohexaneh[H]{3Sa==\lmoiety{H$_{5}$C$_{2}$OCO\kern2em}}}
\put(200,0){\fiveunith[H]{}{2D==O;1==CO$_{2}$C$_{2}$H$_{5}$}{c}}
\end{picture}
```

These statements provide equivalent results as follows.

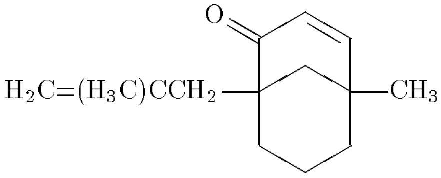




A vertical form of bicyclo[3.3.1]nonane is also typeset by this technique.

```
\begin{picture}(800,1000)(0,0)
\put(0,0){\cyclohexanev[H]{6Sa==\lmoiety{H$_{2}$C=(H$_{3}$C)CCH$_{2}$};
2Sa==CH$_{3}$}}
\put(0,200){\sixunitv[a]{}{6D==O}{cd}}
\end{picture}
```

This statement provides

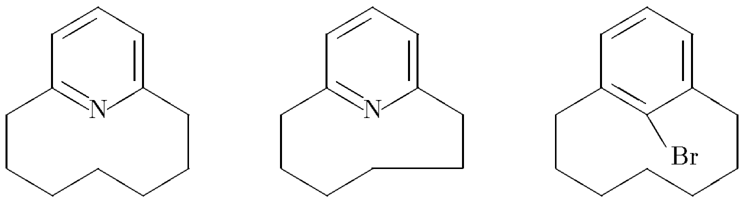


[7](2,6)- and [6](2,6)Pyridinophanes are other examples typeset by this technique. In a similar way, 13-Bromo-(2,6)metacyclophane can be printed easily.

```
\begin{picture}(1200,1000)(0,0)
\put(0,0){\sixunitv[H]{2=={ }}{}{ab}}
```

```
\put(342,0){\sixunitv[H]{6=={ }}{}{ef}}
\put(171,303){\pyridinevi{}}
\end{picture}
\qquad
\begin{picture}(1200,1000)(0,0)
\put(0,0){\sixunitv[H]{2=={ }}{}{ab}}
\put(342,0){\fiveunitvi[H]{5=={ }}{}{de}}
\put(171,303){\pyridinevi{}}
\end{picture}
\qquad
\begin{picture}(1200,1000)(0,0)
\put(0,0){\sixunitv[H]{2=={ }}{}{ab}}
\put(342,0){\sixunitv[H]{6=={ }}{}{ef}}
\put(171,303){\bzdrv{4Sa==\kern.5em\raise1ex\hbox{Br}}}
\end{picture}
```

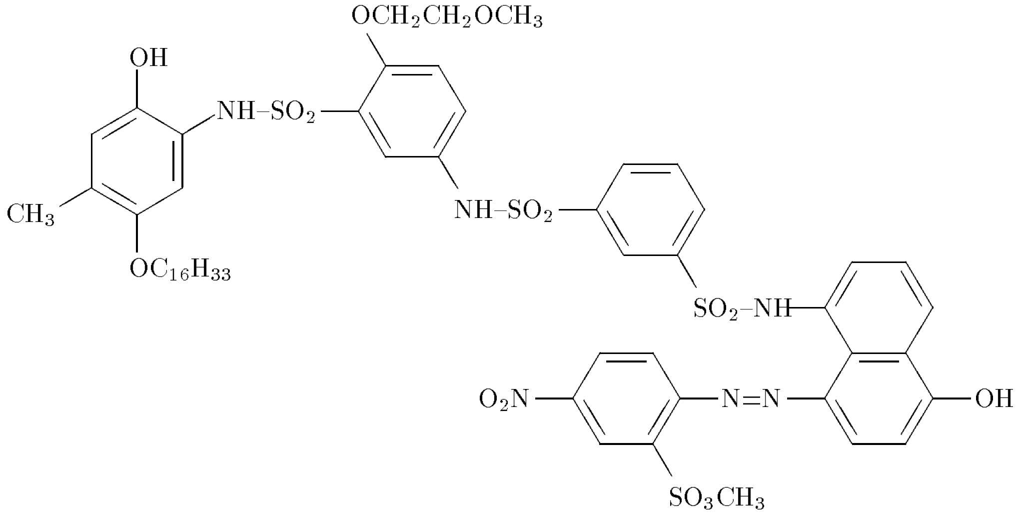
These statements provide



We have reported an article on dye releasers for instant color photography, in which a variety of structural formulas have been typeset by means of original utilities of the LaTeX picture environment [4]. The present XΥMTeX provides us with a more versatile tool of drawing such complex molecules. Thus, the formula of a cyan dye releaser for instant color photography is typeset by the statement:

```
\begin{picture}(4000,2000)(0,-1000)
\put(0,0){\bzdrv{1==OH;2==NH--SO$_{2}$;4==OC$_{16}$H$_{33}$;5==CH$_{3}$}}
\put(993,230){\bzdrh{1==;2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
5==NH--SO$_{2}$}}
\put(1890,-140){\bzdrh{1==;5==SO$_{2}$--NH}}
\put(2750,-850){\naphdrh{1==;5==OH;8==}}
\put(1800,-850){\bzdrh{1==O$_{2}$N;5==SO$_{3}$CH$_{3}$;4==N=N}}
\end{picture}
%}
```

These commands produce the following structure:



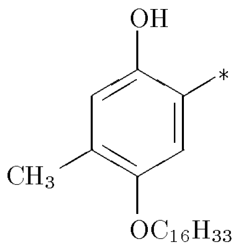
Chapter 15

Large Substituents

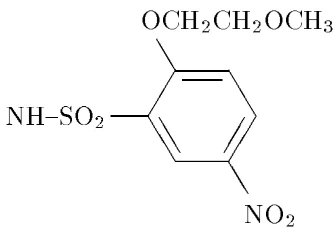
15.1 Basic Ideas

In all of the preceding chapters, any substituents described in SUBSLIST are rather simple ones, which at most vary from an atom of one- or two-character to a group of several characters. How about such a complex substituent as produced by a macro?

Let us consider the substitution of



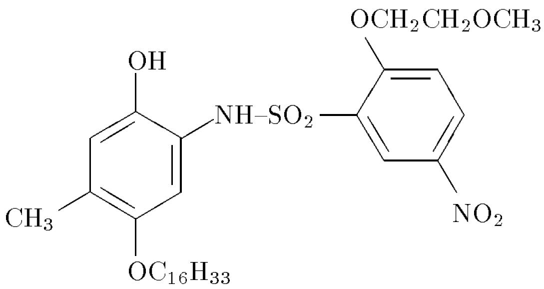
at the 2-position (*)with the substituent represented by



This task can be accomplished in the light of the technique introduced in the preceding chapter. Thus, the statement

```
\begin{picture}(2000,1000)(0,0)
\put(0,0){\bzdrv{1==OH;2==;4==OC$_{16}$H$_{33}$;5==CH$_{3}$}}
\put(993,230){\bzdrh{1==NH--SO$_{2}$;%
2==OCH$_{2}$CH$_{2}$OCH$_{3}$;5==NO$_{2}$}}
\end{picture}
```

provides



This methodology implies that both of the parts are regarded as fragments to be combined together.

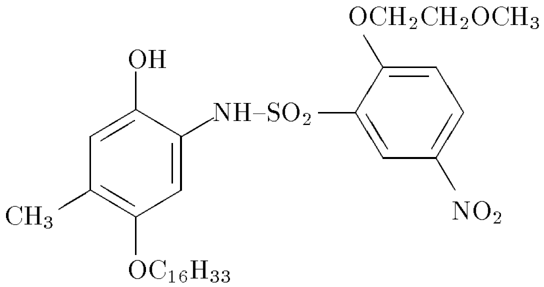
On the other hand, another useful technique is available, if you use the TEX command `\setbox` and the related commands. In the light of this technique, either one is regarded as a substituent of the other. First, a structure regarded as a substituent is constructed in a `\hbox` and stored in `\box4` by means of the command `\setbox` as follows:

```
\setbox4=\hbox{%
 \begin{picture}(0,0)(-285,370)%
%  \put(-285,370){\circle{50}}%change reference point
  \put(0,0){\bzdrh{1==NH--SO$_{2}$;2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
   5==NO$_{2}$}}%
 \end{picture}}%
```

The inner picture environment has the width of 0pt and the height of 0pt, where the reference point is shifted into the $(-285, 370)$ point which is the rightmost point of the NH–SO$_2$ group. This reference point is regared as the $(0, 0)$ point of the substituent stored in `\box4`. Then, the substituent `\box4` is written in SUBSLIST of the command `\bzdrv`, *i.e.*,

```
\bzdrv{1==OH;2==\box4;4==OC$_{16}$H$_{33}$;5==CH$_{3}$}
```

This statement produces



It should be noted that the token `2==\box4` creates such a complex fragment that is impossible to be directly assigned to an argument list. This technique is also useful to avoid the overcrowding of substituents, since the reference point of the substituent can be changed appropriately.

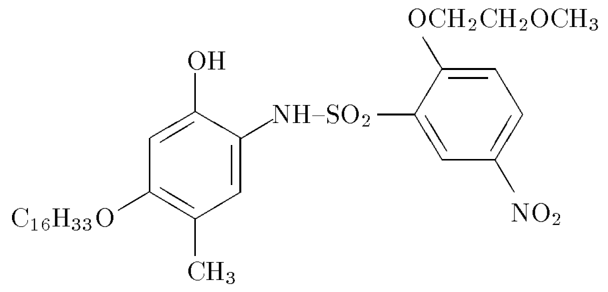
When you multiple times use the stored substituent, you can use the command `\copy` instead of `\box`:

```
\bzdrv{1==OH;2==\copy4;4==OC$_{16}$H$_{33}$;5==CH$_{3}$}
```

Then, you are able to use the stored substituent in another context.

```
\setbox5=\hbox{%
\bzdrv{1==OH;2==\box4;5==C$_{16}$H$_{33}$O;4==CH$_{3}$}}%
\mbox{\box5}
```

This statement provides another derivative having the same substituents.



15.2 Nested Substituents

The lastest sample reveals that a structure constructed by the present techique can be further nested to be a substituent of another macro. The following example illustrates multiple nesting for drawing the same dye releaser as depicted in the preceding chapter.

First, the formula of 2-methanesulfonyl-4-nitro-phenyl-1-azo group (A) is constructed in the box `\box4` by means of following statement:

```
\setbox4=\hbox{%
 \begin{picture}(0,0)(996,370)%
%  \put(996,370){\circle{50}}%
  \put(0,0){\bzdrh{1==O$_{2}$N;5==SO$_{3}$CH$_{3}$;4==N=N}}%
 \end{picture}}%
```

Note that the value (996,370) shifts the reference point into the rightmost terminal of the azo group, which is a linking point in the next step. The formula (A) strored in `\box4` is placed at the 8-position of a naphalene ring. The resulting formula (B) is, in turn, stored into `\box5`.

```
\setbox5=\hbox{%
 \begin{picture}(0,0)(-250,712)%
%  \put(-250,712){\circle{50}}%
  \put(0,0){\naphdrh{1==SO$_{2}$NH;5==OH;8==\box4}}%
 \end{picture}%
 }%
```

The value $(-250, 712)$ shifts the reference point into the leftmost terminal of the sulfonamido group at the 1-position of the naphthalene ring. The formula B an a sulfamoyl group are placed at the meta position of a benzen ring to produce formula C.

```
\setbox4=\hbox{%
 \begin{picture}(0,0)(-285,370)%
%  \put(-285,370){\circle{50}}%
  \put(0,0){\bzdrh{1==NH--SO$_{2}$;5==\box5}}%
 \end{picture}%
}%
```

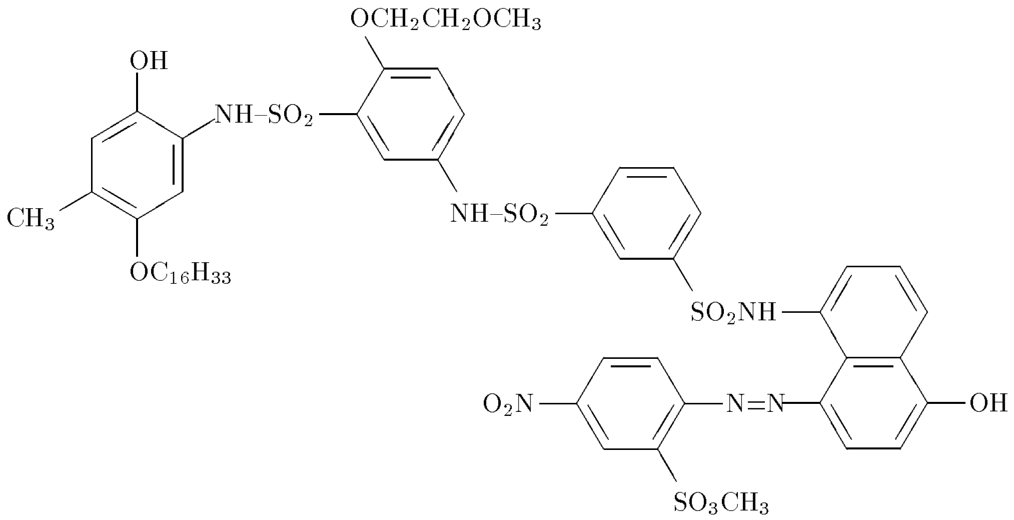
The resulting formula C is further placed on another benzene ring to generate the formula (D) of a complex substituent.

```
\setbox5=\hbox{%
 \begin{picture}(0,0)(-285,370)%
%  \put(-285,370){\circle{50}}%
  \put(0,0){\bzdrh{1==NH--SO$_{2}$;2==OCH$_{2}$CH$_{2}$OCH$_{3}$;%
   5==\box4}}%
 \end{picture}%
}%
```

Finally, the substituent D is placed at the ortho position to a hydroxyl group on a benzene ring.

```
\setbox4=\hbox{%
\bzdrv{1==OH;2==\box5;4==OC$_{16}$H$_{33}$;5==CH$_{3}$}}%
\mbox{\box4}
```

The formula stored in `\box4` is printed by means of the command `\box4`, giving the following structure.



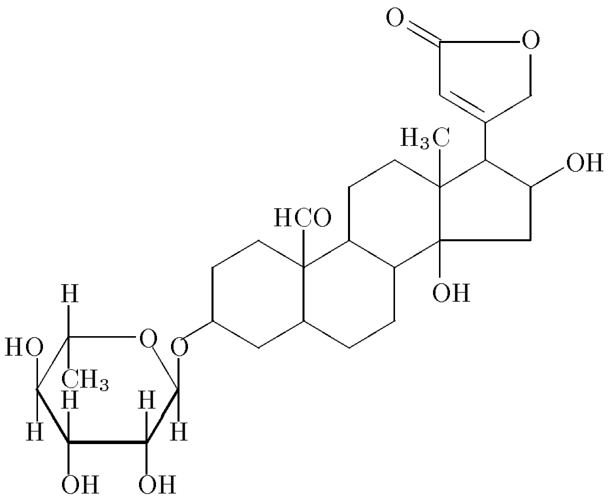
One of the merits of the present methodology is that we can use relative coordinates in each step of combining two structures. Hence, the calculation of coordinates is simpler than that based on the method of the preceding chapter.

The structural formula of adonitoxin can be written in a similar way, where two complex substituents stored in `\box0` and `\box1` are placed on a steroid skeleton.

```
\setbox0=\hbox{%
 \begin{picture}(0,0)(369,257)%
%  \put(369,257){\circle{50}}%
  \put(0,0){\fiveheterov[e]{3==O}{4D==O}}
 \end{picture}}%
\setbox1=\hbox{%
 \begin{picture}(0,0)(772,530)%
%  \put(772,530){\circle{50}}%
  \put(0,0){\pyranose{1Sb==O;1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;%
  4Sb==HO;4Sa==H;5Sb==H;5Sa==CH$_{3}$}}%
 \end{picture}}%
\setbox2=\hbox{%
   \steroid{{{10}}==\lmoiety{HCO\kern-.7em};{{14}}==OH;%
   {{13}}==\lmoiety{H$_{3}$C};%
   {{16}}==OH;{{17}}==\box0;3==\box1}}%
\medskip
\begin{center}
%\fbox{
\begin{picture}(2500,1800)(-600,-300)
\put(0,0){\mbox{\box2}}
\end{picture}
```

```
%}
\end{center}
```

These commands produce



Bibliography

[1] Knuth D., *The TEXbook*, Addison-Wesley, Reading (1984).

[2] Ito T., *Kagaku to Kogyo*, **46**, 66 (1993). This article described that the Chemical Society of Japan changed the publishing process of its journal (*Bull. Chem. Soc. Jpn.*) on January 1993 into the one that is based on the combination of TEX and SGML (Standard Generalized Mark-up Language).

[3] Lamport L., LATEX *A document Preparation System*, Addison-Wesley, Reading (1986).

[4] Haas R. T. & O'Kane K. C., *Comput. Chem.*, **11**, 251 (1987).

[5] Ramek, M., in Clark, M. (ed), TEX: Applications, Uses, Methods, Ellis Horwood, London (1990), p. 277.

[6] Fujita S., "Typesetting structural formulas with the text formatter TEX/LATEX", *Comput. Chem.*, in press.

[7] Fujita S., *Kagakusha-Seikagakusha no tame no* LATEX *(*LATEX *for Chemists and Biochemists)*, Tokyo Kagaku Dozin, Tokyo (1993).

[8] Podar S., "Enhancements to the picture environment of LATEX", Manual for Version 1.2 dated July 14, 1986.

[9] Fujita S., "Promolecules with subsymmetry of $\mathbf{D}_{\infty h}$. Combinatorial enumeration and stereochemical properties", *J. Chem. Inf. Comput. Sci.*, **32**, 354–363 (1992).

[10] Fujita S., Koyama K., & Ono S., "Dye releasers for instant color photography", *Rev. Heteroatom Chem.*, **7**, 229–267 (1992).

Appendix A

List of Commands

A.1 aliphat.sty

The style file 'aliphat.sty' contains the following commands

```
%
%  <Macros for tetravalent atoms>
%
%     \tetrahedral                       \@tetrahedral
%     \square                            \@square
%
%  <Macros for trivalent atoms>
%
%     \rtrigonal                         \@rtrigonal
%     \ltrigonal                         \@ltrigonal
%     \utrigonal                         \@utrigonal
%     \Utrigonal                         \@Utrigonal
%     \dtrigonal                         \@dtrigonal
%     \Dtrigonal                         \@Dtrigonal
%
%  <Macros for two-carbon compounds>
%
%     \ethylene                          \@ethylene
%     \ethylenev                         \@ethylenev
%     \Ethylenev                         \@Ethylenev
%
%  <Macros for stereo-projection>
%
%     \tetrastereo                       \@tetrastereo
%     \dtetrastereo                      \@dtetrastereo
%     \ethanestereo                      \@ethanestereo
%
```

A.2 carom.sty

The style file 'carom.sty' contains the following commands.

```
%
```

```
%   <VERTICAL TYPE>
%
%     \cyclohexanev               \@cyclohexanev
%     \bzdrv                      \@bzdrv
%     \decalinev                  \@decalinev
%     \naphdrv                    \@naphdrv
%     \tetralinev                 \@tetralinev
%     \hanthracenev               \@hanthracenev
%     \anthracenev                \@anthracenev
%     \hphenanthrenev             \@hphenanthrenev
%     \phenanthrenev              \@phenanthrenev
%     \steroid                    \@steroid
%     \steroidchain               \@steroidchain
%
%   <HORIZONTAL TYPE>
%
%     \cyclohexaneh               \@cyclohexaneh
%     \bzdrh                      \@bzdrh
%     \decalineh                  \@decalineh
%     \naphdrh                    \@naphdrh
%     \tetralineh                 \@tetralineh
%
```

A.3 lowcycle.sty

The style file 'lowcycle.sty' contains the following commands.

```
%
%     \cyclopentanev                      \@cyclopentanev
%     \cyclopentanevi                     \@cyclopentanevi
%     \cyclopentaneh                      \@cyclopentaneh
%     \cyclopentanehi                     \@cyclopentanehi
%     \indanev                            \@indanev
%     \indanevi                           \@indanevi
%     \indaneh                            \@indaneh
%     \indanehi                           \@indanehi
%     \cyclobutane                        \@cyclobutane
%     \cyclopropane                       \@cyclopropane
%
%
```

A.4 ccycle.sty

The style file 'ccycle.sty' contains the following commands.

```
%
%  <Basic Macros>
%
%     \chair                      \@chair
%     \bicychepv                  \@bicychepv
%     \bicycheph                  \@bicycheph
```

```
%     \bornane                    \@bornane
%     \adamantane                 \@damantane
%
```

A.5 hetarom.sty

The style file 'hetarom.sty' contains the following commands.

```
%
%  <Six-Membered Heterocycles>

%    Basic Macros
%
%     \sixheterov                \@sixheterov
%     \sixheterovi               \@sixheterovi
%
%    Application Macros
%
%     \pyridinev                 \@pyridinev
%     \pyridinevi                \@pyridinevi
%     \pyrazinev                 \@pyrazinev
%     \pyrimidinev               \@pyrimidinev
%     \pyrimidinevi              \@pyrimidinevi
%     \pyridazinev               \@pyridazinev
%     \pyridazinevi              \@pyridazinevi
%     \triazinev                 \@triazinev
%     \triazinevi                \@triazinevi
%
%  <Five-Membered Heterocycles>
%    Basic Macros
%
%     \fiveheterov               \@fiveheterov
%     \fiveheterovi              \@fiveheterovi
%
%    Application Macros
%
%     \pyrrolev                  \@pyrrolev
%     \pyrazolev                 \@pyrazolev
%     \imidazolev                \@imidazolev
%     \isoxazolev                \@isoxazolev
%     \oxazolev                  \@oxazolev
%     \pyrrolevi                 \@pyrrolevi
%     \pyrazolevi                \@pyrazolevi
%     \imidazolevi               \@imidazolevi
%     \isoxazolevi               \@isoxazolevi
%     \oxazolevi                 \@oxazolevi
%
%  <Six-Six-Fused Heterocycles>
%    Basic Macros
%
%     \decaheterov               \@decaheterov
%     \decaheterovi              \@decaheterovi
```

```
%
%   Application Macros
%
%    \quinolinev              \@quinolinev
%    \quinolinevi             \@quinolinevi
%    \isoquinolinev           \@isoquinolinev
%    \isoquinolinevi          \@isoquinolinevi
%    \quinoxalinev            \@quinoxalinev
%    \quinazolinev            \@quinazolinev
%    \quinazolinevi           \@quinazolinevi
%    \cinnolinev              \@cinnolinev
%    \cinnolinevi             \@cinnolinevi
%    \pteridinev              \@pteridinev
%    \pteridinevi             \@pteridinevi
%
%  <Six-Five-Fused Heterocycles>
%   Basic Macros
%
%    \nonaheterov             \@nonaheterov
%    \nonaheterovi            \@nonaheterovi
%
%   Application Macros
%
%    \purinev                 \@purinev
%    \purinevi                \@purinevi
%    \indolev                 \@indolev
%    \indolevi                \@indolevi
%    \indolizinev             \@indolizinev
%    \indolizinevi            \@indolizinevi
%    \isoindolev              \@isoindolev
%    \isoindolevi             \@isoindolevi
%    \benzofuranev            \@benzofuranev
%    \benzofuranevi           \@benzofuranevi
%    \isobenzofuranev         \@isobenzofuranev
%    \isobenzofuranevi        \@isobenzofuranevi
%    \benzoxazolev            \@benzoxazolev
%    \benzoxazolevi           \@benzoxazolevi
%
%  <Four-Membered Heterocycles>
%
%    \fourhetero              \@fourhetero
%
%  <Four-Membered Heterocycles>
%
%    \threehetero             \@threehetero
%
%  <Building Units>
%
%    \sixunitv                \@sixunitv
%    \fiveunitv               \@fiveunitv
%    \fiveunitvi              \@fiveunitvi
%
```

A.6 hetaromh.sty

The style file 'hetaromh.sty' contains the following commands.

```
%
%  <Six-membered heterocycles (horizontal)>
%
%    Basic Macros
%
%     \sixheteroh                 \@sixheteroh
%     \sixheterohi                \@sixheterohi
%
%    Application Macros
%
%     \pyridineh                  \@pyridineh
%     \pyridinehi                 \@pyridinehi
%     \pyrazineh                  \@pyrazineh
%     \pyrimidineh                \@pyrimidineh
%     \pyrimidinehi               \@pyrimidinehi
%     \pyridazineh                \@pyridazineh
%     \pyridazinehi               \@pyridazinehi
%     \triazineh                  \@triazineh
%     \triazinehi                 \@triazinehi
%
%  <Five-membered heterocycles (horizontal)>
%
%    Basic Macros
%
%     \fiveheteroh                \@fiveheteroh
%     \fiveheterohi               \@fiveheterohi
%
%    Application Macros
%
%     \pyrroleh                   \@pyrroleh
%     \pyrazoleh                  \@pyrazoleh
%     \imidazoleh                 \@imidazoleh
%     \isoxazoleh                 \@isoxazoleh
%     \oxazoleh                   \@oxazoleh
%     \pyrrolehi                  \@pyrrolehi
%     \pyrazolehi                 \@pyrazolehi
%     \imidazolehi                \@imidazolehi
%     \isoxazolehi                \@isoxazolehi
%     \oxazolehi                  \@oxazolehi
%
%  <Six-Six fused heterocycles (horizontal)>
%
%    Basic Macros
%
%     \decaheteroh                \@decaheteroh
%     \decaheterohi               \@decaheterohi
%
%    Application Macros
%
```

```
%     \quinolineh                \@quinolineh
%     \quinolinehi               \@quinolinehi
%     \isoquinolineh             \@isoquinolineh
%     \isoquinolinehi            \@isoquinolinehi
%     \quinoxalineh              \@quinoxalineh
%     \quinazolineh              \@quinazolineh
%     \quinazolinehi             \@quinazolinehi
%     \cinnolineh                \@cinnolineh
%     \cinnolinehi               \@cinnolinehi
%     \pteridineh                \@pteridineh
%     \pteridinehi               \@pteridinehi
%
%  <Six-Five fused heterocycles (horizontal)>
%
%    Basic Macros
%
%     \nonaheteroh               \@nonaheteroh
%     \nonaheterohi              \@nonaheterohi
%
%    Application Macros
%
%     \purineh                   \@purineh
%     \purinehi                  \@purinehi
%     \indoleh                   \@indoleh
%     \indolehi                  \@indolehi
%     \indolizineh               \@indolizineh
%     \indolizinehi              \@indolizinehi
%     \isoindoleh                \@isoindoleh
%     \isoindolehi               \@isoindolehi
%     \benzofuraneh              \@benzofuraneh
%     \benzofuranehi             \@benzofuranehi
%     \isobenzofuraneh           \@isobenzofuraneh
%     \isobenzofuranehi          \@isobenzofuranehi
%     \benzoxazoleh              \@benzoxazoleh
%     \benzoxazolehi             \@benzoxazolehi
%
%   <Building units>
%
%     \sixunith                  \@sixunith
%     \fiveunith                 \@fiveunith
%     \fiveunithi                \@fiveunithi
%
```

A.7 hcycle.sty

The style file 'hcycle.sty' contains the following commands.

```
%
% <Pyranose and Furanose>
%
%     \pyranose                 \@pyranose
%     \furanose                 \@furanose
```

```
%
```

A.8 chemstr.sty

The style file 'chemstr.sty' contains the following commands.

```
%
%  <Convention>
%
%     \rmoiety
%     \lmoiety
%     \putlatom
%     \putratom
%     \putlratom
%     \Putlratom

%   <Setting of atoms and bonds>
%
%     \setsixringv      (on a vertical six-membered ring)
%     \setdecaringv     (on a decaline (six-six) ring)
%     \setfusedbond     (at fused bond positions)
%     \setatombond      (at an appropiate position)
%     \setsixringh       (on a horizontal six-membered ring)
%
```

A.9 locant.sty

The style file 'locant.sty' contains the following commands.

```
%
%     \sxlocant      \sxloocant
%     \bdlocant      \bdloocant
%     \sxlocnth      \sxloocnth
%     \bdlocnth      \bdloocnth
%
```