The XeTeX System for Publishing Interdisciplinary Chemistry/Mathematics Books

Shinsaku Fujita

Shonan Institute of Chemoinformatics and Mathematical Chemistry

2013/10/26

TUG 2013 (Tokyo)

My Interests and Targets

- **Main Targets** — Interdisciplinary Approach
  http://xymtex.com/fujitas/fujitae.html
  1. Synthetic Organic Chemistry — Development of Organic Compounds for Photography
  2. Chemoinformatics — Database for Organic Reactions Based on the Concept of Imaginary Transition Structures
  3. Mathematical Stereochemistry — The USCI Approach, the Proligand Method, and the Stereoisogram Approach
- **Subsidiary Targets** — Development of Writing Tools
  1. XyMTEX — Development of Packages for Drawing Chemical Structural formulas
     http://xymtex.com/fujitas3/xymtex/index.html
  2. LATEX Packages for Japanese Typesetting
     http://xymtex.com/fujitas/rd/texlatex.html
  3. Essay for Time-Space Trips in Kyoto by Following Old Jintan's Street Markers 「仁丹の町名看板をよすがに京めぐり」
     http://xymtex.com/kyomeguri/index.html

Activities Aiming at Main Targets

Recent Account Reports on Main Targets:

- Shinsaku Fujita,
  "Numbers of Alkanes and Monosubstituted Alkanes. A Long-Standing Interdisciplinary Problem Over 130 Years"
  Bull. Chem. Soc. Jpn, **83**, 1–18 (2010).
  http://www.jstage.jst.go.jp/article/bcsj/83/1/83_20090008/_pdf
- Shinsaku Fujita,
  "Extended Pseudoasymmetry and Geometric Prochirality Clarifying the Scope of the Concepts of Holantimers and Stereoisograms",
  Tetrahedron: Asymmetry, **23**, 623–634 (2012).

Caricature"The Heavens of Fujita"

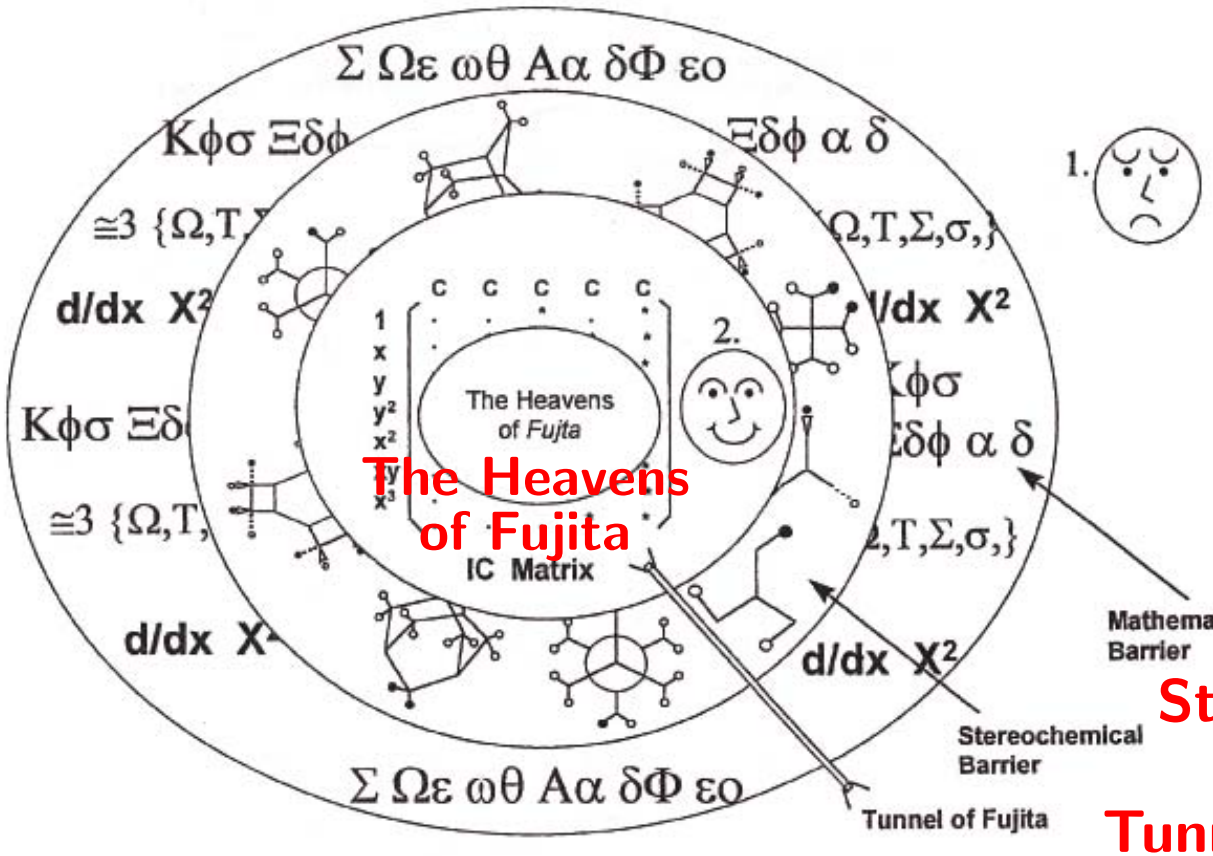


FIG35 Pictorial illustration of a paradox:An organic chemist (who is not interested in mathematics) is trying to make his way through the "heavens of Fujita".Such heavens can only be reached by mathematics! C.f. comments a-c in Section 3.1

The Heavens of Fujita

Mathematical Barrier

Stereochemical Barrier

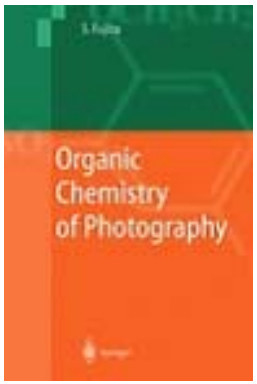
Tunnel of Fujita

Figure 35 of Sherif El-Basil,
"Combinatorial Organic Chemistry: An Educational Approach",
Nova Science (2000).

Monographs on Main Targets

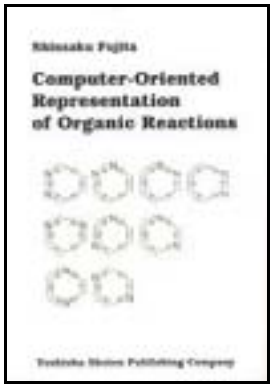
— Invitation to "the Heavens of Fujita"

Synthetic Organic Chemistry



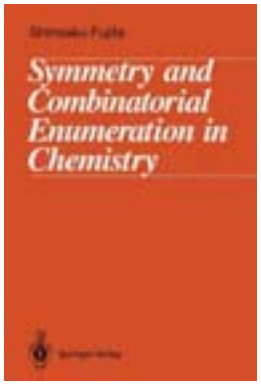
2004

Chemoinformatics



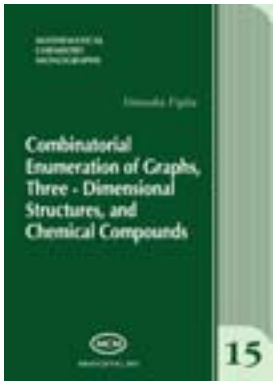
2001

Mathematical Stereochemistry



1991

2007



2013

Activities Aiming at Subsidiary Targets

- My Private Laboratory:
  Shonan Institute of Chemoinformatics and Mathematical Chemistry
  http://xymtex.com/
- Recent Report on XyMTeX:
  Shinsaku Fujita,
  "Articles, Books, and Internet Documents with Structural Formulas Drawn by XyMTeX — Writing, Submission, Publication, and Internet Communication in Chemistry",
  Asian J. TeX, **3**, 89–108 (2009).
  http://ajt.ktug.kr/2009/0302fujita.pdf

Books on TEX/LATEX in Japanese

1993

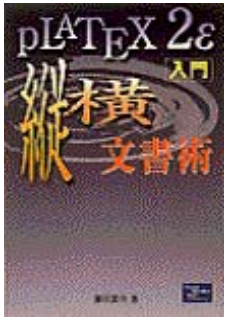
1995

1996

1996

1997

1998



2000

2000

2003

2009

2009

2010

2010

TEX/LATEX with XƎMTEX has supported the main targets. How?

Short personal history of XyMTEX with LATEX

1989 Start of writing articles with Japanese MicroTEX (Ascii Co.) on PC-9800 (NEC).

1991 LATEX-typesetting and publication of "Symmetry and Combinatorial Enumeration in Chemistry" from Springer-Verlag (Heidelberg-Berlin).

1993 LATEX-typesetting and publication of "LATEX for Chemists and Biochemists" (in Japanese) from Tokyo Kagaku Dojin (Tokyo).

1993* First release of XyMTEX (Version 1.00) for typesetting chemical structural formulas.

1997* XyMTEX/LATEX-typesetting and publication of "XyMTEX—Typesetting Chemical Structural Formulas" from Addison-Wesley Japan (Tokyo).

1999* Release of XyMTEX Version 2.00 for supporting the XyM notation as a linear notation of structural formulas.

2001 LATEX-typesetting and publication of "Computer-Oriented Representation of Organic Reactions" from Yoshioka-Shoten (Kyoto).

2002* Release of XyMTEX Version 4.00 for supporting PostScript language.

2004 XyMTEX/LATEX-typesetting and publication of "Organic Chemistry of Photography" from Springer-Verlag (Heidelberg-Berlin).

2007 XyMTEX/LATEX-typesetting and publication of "Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers" from University of Kragujevac (Kragujevac).

2009* Release of XyMTEX Version 4.04 for supporting complicated formulas such as steroids.

2010* Release of XyMTEX Version 5.00 for supporting the PDF mode

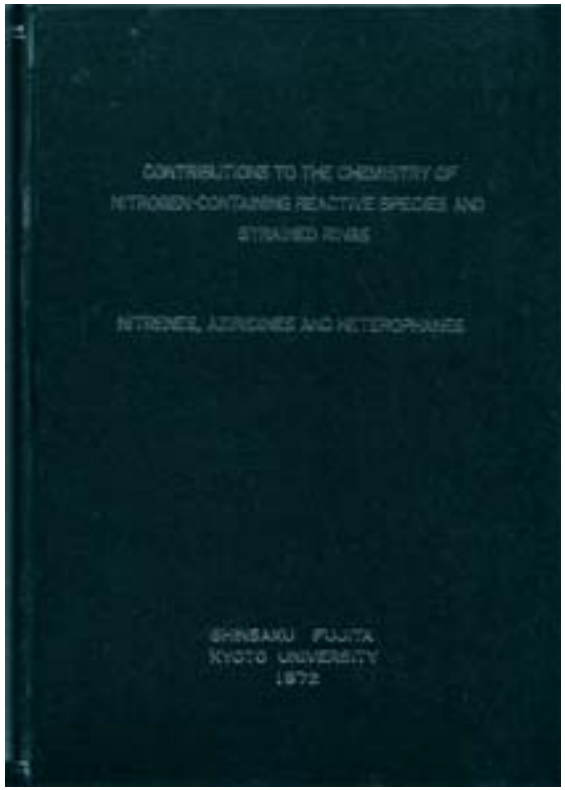
2013* Release of XyMTEX Version 5.01 for supporting a comprehensive on-line manual

2013 XyMTEX/LATEX-typesetting and publication of "Combinatorial Enumeration of Graphs, Three-Dimensional Structures, and Chemical Compounds" from University of Kragujevac (Kragujevac).

Before TEX/LATEX

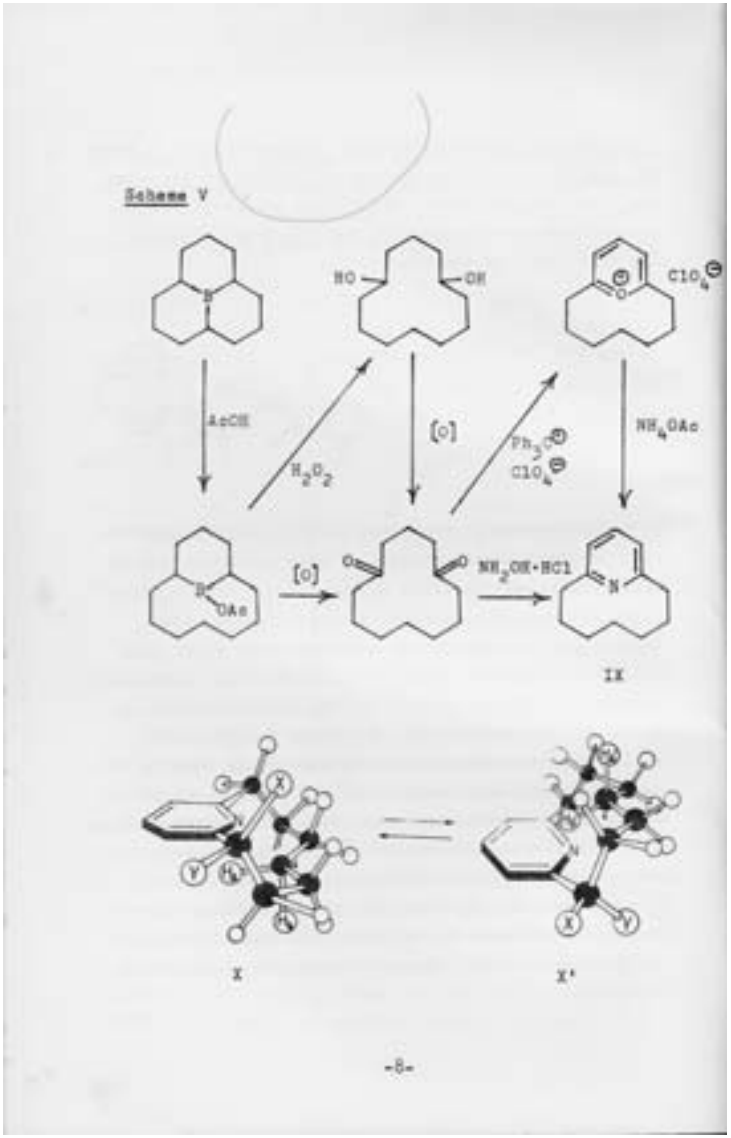
Manual Typewriter for Writing a Camera-Ready Manuscript

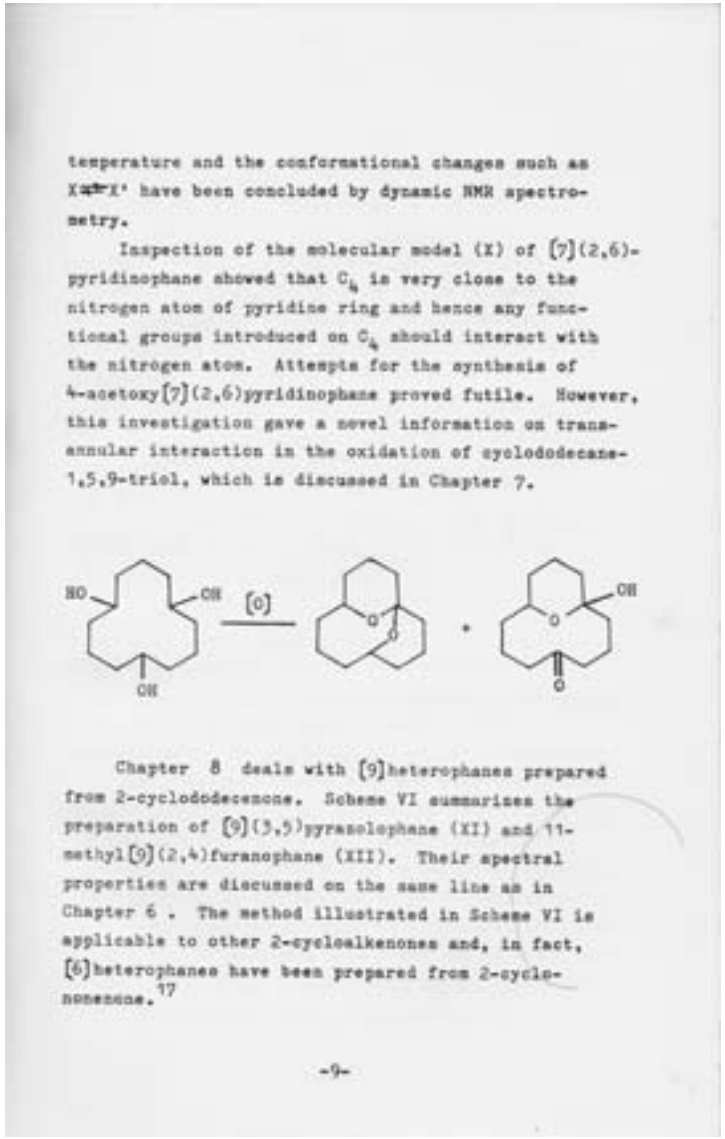
Book Written with Manual Typewriter



(Thesis)
Shinsaku Fujita,
"Contributions to the Chemistry of Nitrogen-Containing Reactive Species and Strained Rings—Nitrene, Aziridines and Heterophanes", (1972) 137pp.

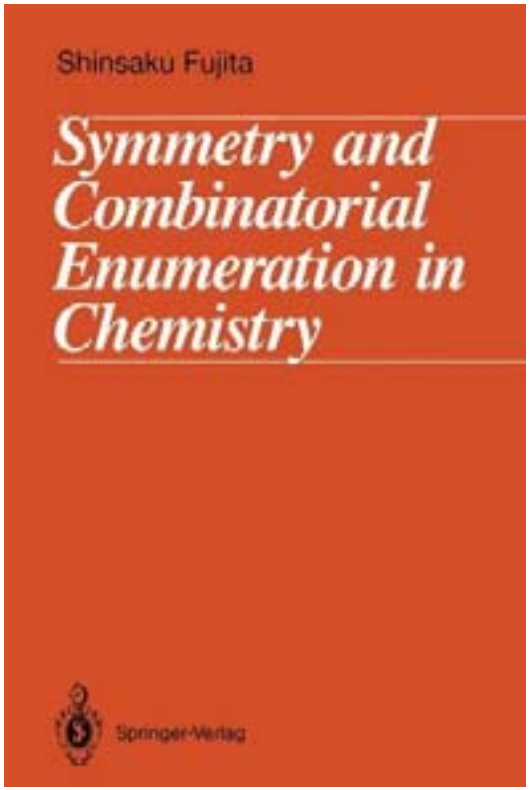
Book Written with Manual Typewriter





TEX/LATEX (without XMTEX)

Book Written with LaTeX



Shinsaku Fujita,
"Symmetry and Combinatorial Enumeration in Chemistry", Springer-Verlag (1991) 368pp.

(Book Reviews)
C. A. Mead, *J. Am. Chem. Soc.*, **1992**, *114*, 4018–4019.
S. J. Cyvin, *Structural Chemistry*, **1994**, *5*, 145.
C. A. Mead, D. J. Klein, *Theor Chim Acta* **1992**, *82*, 339-340.

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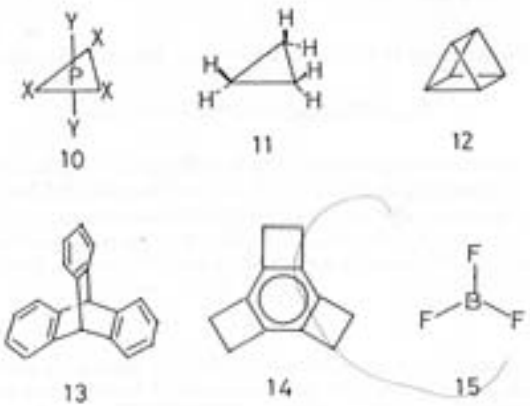
Delivery form:	A camera-ready manuscript.

Book Written with LaTeX

70 CHAPTER 6. SYSTEMATIC CLASSIFICATION OF MOLECULAR SYMMETRIES

Table 6.3: SCR Notations of D_{3h}-molecules

molecule	SCR notation
10	$D_{3h}[/C_{2v}(X_2);\ /C_{2v}(Y_2);/D_{3h}(P)]$
11	$D_{3h}[/C_s(H_6);\ /C_{3v}(C_3)]$
12	$D_{3h}[/C_s(C_6H_6)]$
13	$D_{3h}[/C_s(3C_6,2H_6);\ /C_{2v}(C_2\ ,H_2)]$
14	$D_{3h}[/C_1(H_{12});\ /C_s'(2C_6)]$
15	$D_{3h}[/C_{2v}(F_2);\ /D_{3h}(B)]$



10 11 12

13 14 15

6.2. SCR NOTATION 71

$$\begin{pmatrix}
1/24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1/8 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1/4 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1/6 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1/4 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1/12 & -1/4 & 0 & 0 & 0 & 1/6 & 0 & 0 & 0 & 0 & 0 \\
1/4 & -1/4 & -1/2 & 0 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 \\
1/2 & 0 & -1 & -1/2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1/2 & 0 & 0 & -1/2 & -1/2 & -1/2 & 0 & 1 & 0 & 0 \\
1/6 & 0 & 0 & -1/2 & 0 & -1/6 & 0 & 0 & 0 & 1/2 & 0 \\
-1/2 & 0 & 1 & 1/2 & 0 & 1/2 & 0 & -1 & -1 & -1/2 & 1
\end{pmatrix}$$

$$= (0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0\,1),$$

wherein the second 11×11 matrix is the inverse matrix. The resulting vector indicates

$$\mathbf{P}_{\mathbf{T}_d} = \mathbf{T}_d(/\mathbf{C}_{3v}) + \mathbf{T}_d(/\mathbf{T}_d), \tag{6.5}$$

became a set of CRs is SCR = { $\mathbf{T}_d(/\mathbf{C}_1)$, $\mathbf{T}_d(/\mathbf{C}_2)$, $\mathbf{T}_d(/\mathbf{C}_s)$, $\mathbf{T}_d(/\mathbf{C}_3)$, $\mathbf{T}_d(/\mathbf{S}_4)$, $\mathbf{T}_d(/\mathbf{D}_2)$, $\mathbf{T}_d(/\mathbf{C}_{2v})$, $\mathbf{T}_d(/\mathbf{C}_{3v})$, $\mathbf{T}_d(/\mathbf{D}_{2d})$, $\mathbf{T}_d(/\mathbf{T})$, $\mathbf{T}_d(/\mathbf{T}_d)$} in this case. We can easily assign these CRs to the sets of equivalent atoms, i.e., $\mathbf{T}_d(/\mathbf{C}_{3v})$ to the Δ_1 orbit (H_4) and $\mathbf{T}_d(/\mathbf{T}_d)$ to the Δ_2 orbit (C). This result is summarized by the SCR notation, $\mathbf{T}_d[/\mathbf{C}_{3v}(H_4);\ /\mathbf{T}_d(C)]$.

Table 6.4 collects SCR notations for several $\mathbf{T}_d$-molecules. The compound (**17**) is named tetrahedrane after its geometrical form. The compound (**18**) is called adamantane because of its diamond structure (Greek: adamas). The geometrical relationship between **17** and **18** will be discussed in Chapter 17. The compound (**19**) is derived by substituting nitrogen atoms for four methines of cubane. The substitution reduces the original $\mathbf{O}_h$ symmetry of cubane into $\mathbf{T}_d$.

The original version[3] of the SCR notation consists of type I and II notations. The type II notation is based on the subduction of coset representations, characterizing the symmetry of a molecule as well as that of a parent skeleton. The type I notation is an abbreviation of the type I notation, where information about the skeleton is omitted. The present version essentially succeeds to the type I notation, whereas the distinction between molecules and skeletons are not taken into consideration.

In Chapter 7, we will show that any point of a $\mathbf{G}(/\mathbf{G}_i)$ orbit belongs to the local symmetry $\mathbf{G}_i$. The $\mathbf{G}(/\mathbf{G}_i)$ determines the permutational properties as well as the local symmetry of the orbit. The symbol $(\mathbf{G}(/\mathbf{G}_i))$ is convenient to indicate such inherent nature of the orbit.

Development of XeTeX

Short personal history of XƎMTEX with LATEX

1989 Start of writing articles with Japanese MicroTEX (Ascii Co.) on PC-9800 (NEC).

1991 LATEX-typesetting and publication of "Symmetry and Combinatorial Enumeration in Chemistry" from Springer-Verlag (Heidelberg-Berlin).

1993 LATEX-typesetting and publication of "LATEX for Chemists and Biochemists" (in Japanese) from Tokyo Kagaku Dojin (Tokyo).

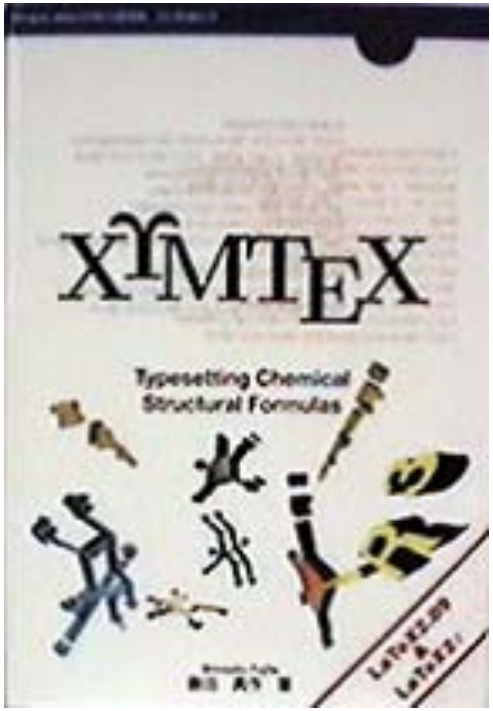
1993* First release of XƎMTEX (Version 1.00) for typesetting chemical structural formulas.

1997* XƎMTEX/LATEX-typesetting and publication of "XƎMTEX—Typesetting Chemical Structural Formulas" from Addison-Wesley Japan (Tokyo).

1999* Release of XƎMTEX Version 2.00 for supporting the XƎM notation as a linear notation of structural formulas.

2001 LATEX-typesetting and publication of "Computer-Oriented Representation of Organic Reactions" from Yoshioka-Shoten (Kyoto).

XeTeX Book



Shinsaku Fujita,
"XeTeX—Typesetting Chemical Structural Formulas",
Addison-Wesley Japan (1997) 352pp.

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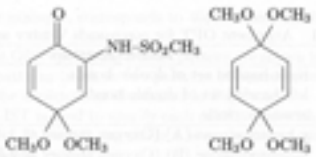
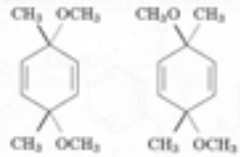
Structural Formulas:	Drawn by XeTeX.
Delivery form:	dvi file (converted by pTeXsT).
	CD-ROM submission.



Stereoisomers can be depicted distinctly by using bond modifiers for \bndrvz. Thus, the code

```
\bndrv[pa]{1SB=-CH$_{3}$;1SA=-OCH$_{3}$;4SB=-CH$_{3}$;4SA=-OCH$_{3}$}
\bndrv[pa]{1SB=-CH$_{3}$H0;1SA=-CH$_{3}$;4SB=-CH$_{3}$;4SA=-OCH$_{3}$}
```

typesets the following structures:

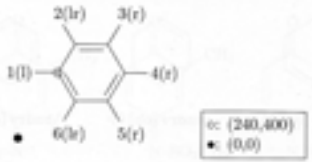


3·1·2 Horizontal Forms of Benzene Derivatives

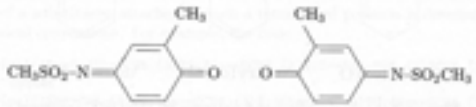
You can use the macro \bndrh to draw benzene derivatives of horizontal type (caron.sty). The format of this command is as follows:

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

The formats of the arguments are the same as those of \bndrv (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:

```
\bndrh[pa]{4O=O;1O=-CH$_{3}$SO$_{2}$H$\sim$5;3=-CH$_{3}$} \qquad
\bndrh[pa]{1O=O;4O=-SO$_{2}$HCH$_{3}$;2=-CH$_{3}$}
```

It should be noted the the commands \bndrv and \bndrh are based respectively on the commands \cyclohexanev and \cyclohexanh 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 (see Figures 3·1 and 3·2).

3·2 Drawing Cyclohexane Derivatives

3·2·1 Vertical Forms of Cyclohexane Derivatives

The macro \cyclohexanev (caron.sty) is used to draw cyclohexane derivatives of vertical type. 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 a 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). Several examples for drawing endocyclic double bonds are listed in Figure 3·2. Note that Figure 3·2 provides alternative ways for designating endocyclic double bonds. Compare this with the results collected in Figure 3·1.

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:

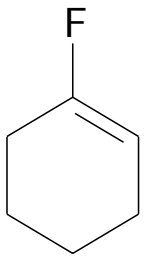
```
\cyclohexanev{2O=O;1Sb=NH$_{3}$H$^{-}$C;1Sa=-CH$_{3}$H;%
3Sb=-CH$_{3}$H;3Sa=-CH$_{3}$H} \qquad\qquad
\cyclohexanev[b]{1O=O;5Sb=-CH$_{3}$H;5Sa=-CH$_{3}$H}
```

The first example illustrates a 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:

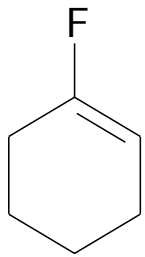
XMNotation as a New Linear Notation

S. Fujita, N. Tanaka, *J. Chem. Inf. Comput. Sci.*, **39**, 903–914 (1999).

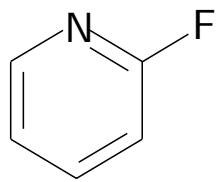
1. mother skeleton
2. skeletal bond list (option)
3. bond list (option)
4. atom list (option)
5. substitution list
6. omit list (option)



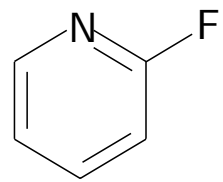

```
\sixheterov
[a]{}{1==F}
```




```
\cyclohexanev
[a]{1==F}
```

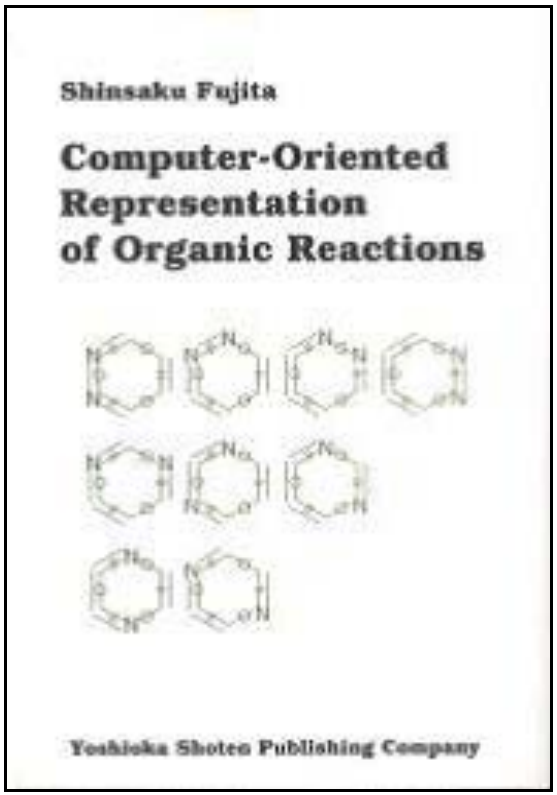



```
\sixheterov
[ace]{1==N}{2==F}
```




```
\pyridinev
[ace]{2==F}
```

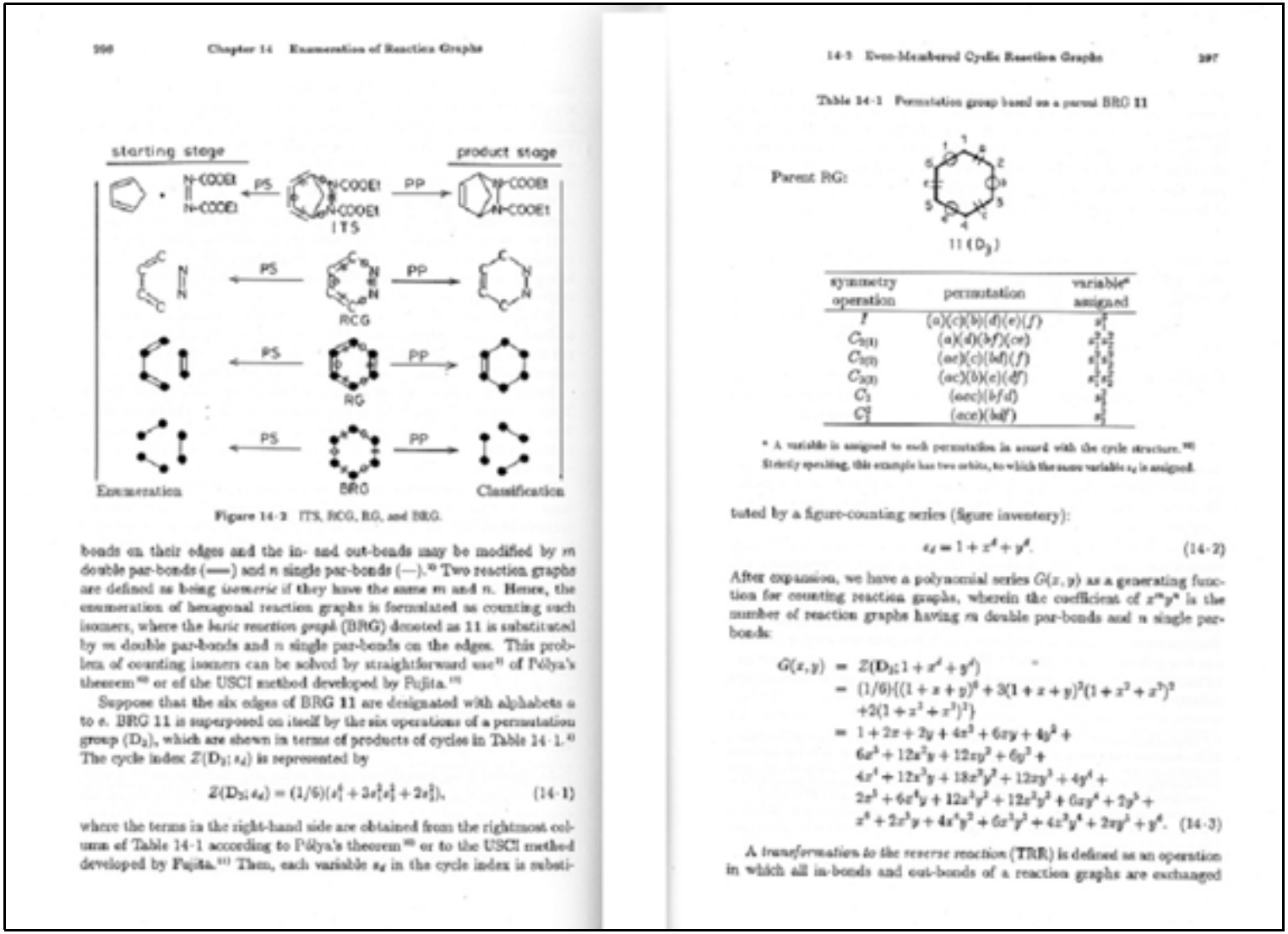
Book Written with LaTeX



Shinsaku Fujita,
"Computer-Oriented Representation of Organic Reactions",
Yoshioka-Shoten (2001) 371pp.

Text:	Typeset by LaTeX 2_ε.
Structural Formulas:	Manual drawing with rotring pens. Paste up.
Delivery form:	A camera-ready manuscript.

Book Written with LaTeX



200 Chapter 14 Enumeration of Reaction Graphs

Figure 14-3 ITS, RCG, RG, and BRG.

bonds on their edges and the in- and out-bonds may be modified by m double par-bonds (═) and n single par-bonds (—).[9] Two reaction graphs are defined as being *isomeric* if they have the same m and n. Hence, the enumeration of hexagonal reaction graphs is formulated as counting such isomers, where the *basic reaction graph* (BRG) denoted as 11 is substituted by m double par-bonds and n single par-bonds on the edges. This problem of counting isomers can be solved by straightforward use[11] of Pólya's theorem[10] or of the USCI method developed by Fujita.[11]

Suppose that the six edges of BRG 11 are designated with alphabets a to e. BRG 11 is superposed on itself by the six operations of a permutation group (D_3), which are shown in terms of products of cycles in Table 14-1.[12] The cycle index $Z(D_3; e_d)$ is represented by

$$Z(D_3; e_d) = (1/6)(s_1^6 + 3s_2^3 s_1^0 + 2s_3^2). \qquad (14\text{-}1)$$

where the terms in the right-hand side are obtained from the rightmost column of Table 14-1 according to Pólya's theorem[10] or to the USCI method developed by Fujita.[11] Then, each variable s_d in the cycle index is substi-

14-3 Even-Membered Cyclic Reaction Graphs 207

Table 14-1 Permutation group based on a parent BRG 11

Parent RG:

11 (D_3)

symmetry operation	permutation	variable* assigned
I	$(a)(c)(b)(d)(e)(f)$	s_1^6
$C_{2(1)}$	$(a)(d)(bf)(ce)$	$s_1^2 s_2^2$
$C_{2(2)}$	$(ac)(c)(bd)(f)$	$s_1^2 s_2^2$
$C_{2(3)}$	$(ac)(b)(e)(df)$	$s_1^2 s_2^2$
C_3	$(ace)(bfd)$	s_3^2
C_3^2	$(ace)(bdf)$	s_3^2

* A variable is assigned to each permutation in accord with the cycle structure.[10] Strictly speaking, this example has two orbits, to which the same variable s_d is assigned.

tuted by a figure-counting series (figure inventory):

$$e_d = 1 + x^d + y^d. \qquad (14\text{-}2)$$

After expansion, we have a polynomial series $G(x, y)$ as a generating function for counting reaction graphs, wherein the coefficient of $x^m y^n$ is the number of reaction graphs having m double par-bonds and n single par-bonds:

$$\begin{aligned} G(x,y) &= Z(D_3; 1 + x^d + y^d) \\ &= (1/6)\{(1 + x + y)^6 + 3(1 + x + y)^2(1 + x^2 + x^2)^2 \\ &\quad +2(1 + x^3 + x^3)^2\} \\ &= 1 + 2x + 2y + 4x^2 + 6xy + 4y^2 + \\ &\quad 6x^3 + 12x^2y + 12xy^2 + 6y^3 + \\ &\quad 4x^4 + 12x^3y + 18x^2y^2 + 12xy^3 + 4y^4 + \\ &\quad 2x^5 + 6x^4y + 12x^3y^2 + 12x^2y^3 + 6xy^4 + 2y^5 + \\ &\quad x^6 + 2x^5y + 4x^4y^2 + 6x^3y^3 + 4x^2y^4 + 2xy^5 + y^6. \end{aligned} \qquad (14\text{-}3)$$

A *transformation to the reverse reaction* (TRR) is defined as an operation in which all in-bonds and out-bonds of a reaction graphs are exchanged

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Short personal history of XeTeX with LaTeX

2002* Release of XeTeX Version 4.00 for supporting PostScript language.

2004 XeTeX/LaTeX-typesetting and publication of "Organic Chemistry of Photography" from Springer-Verlag (Heidelberg-Berlin).

2007 XeTeX/LaTeX-typesetting and publication of "Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers" from University of Kragujevac (Kragujevac).

XyMTeX-PostScript (XyMTeX Version 4.00) of Printing Quality

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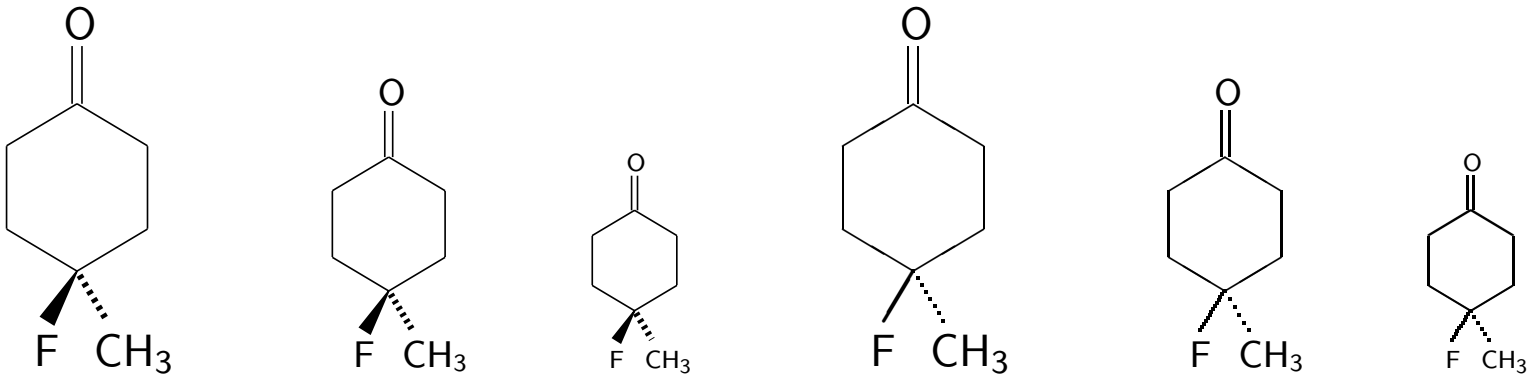


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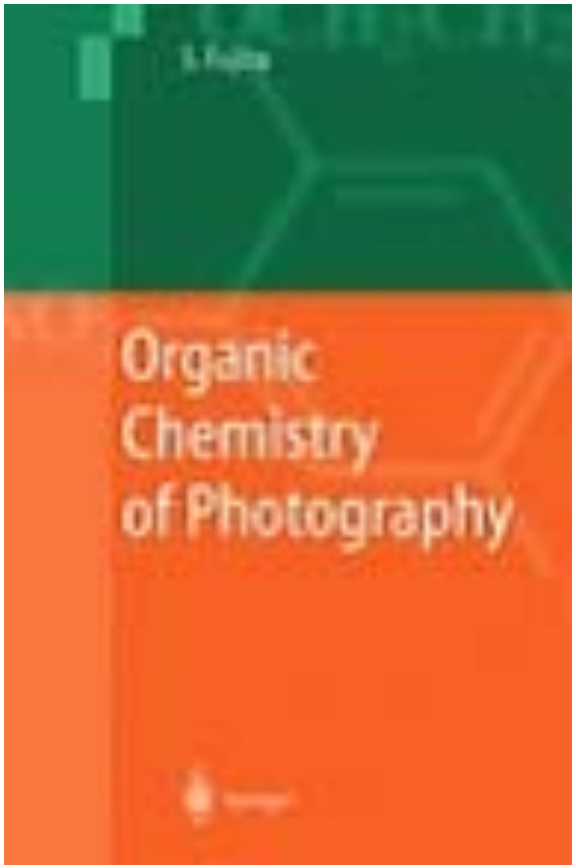

Shinsaku Fujita,
"Organic Chemistry of Photography",
Springer-Verlag (2004) 587pp.

(Book Review)
M. W. Tausch, *Angew. Chem. Int. Ed.* **2005**, *44*, 2629.

Readers will be especially impressed by the structural formulas in the text, created by software that the author has developed himself; as well as showing the molecular structure very clearly, they also give complete information about functional groups, substituents, counterions, etc.

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In particular, the presence of a 2-methoxyethoxy group has been found to enhance the dye-releasing efficiency. This enhancement has been presumed to stem from an intramolecular chelating effect, as shown in Fig. 19.15 [9,10]. The 1,2-attack of a hydroxide ion to the sulfonimido group of **44** gives an adduct (**45**), where the 2-methoxyethoxy group chelates the hydrogen atom of the hydroxy group in terms of hydrogen bonding. This chelation results in the formation of an eight-membered ring of the intermediate (**45**), as designated by ⑧. The releasing of the sulfonamide (**39**) requires a further intermediate (**46**), which contains a six-membered ring designated by ⑥. The six-membered ring is presumed to be more plausible than the eight-membered ring.

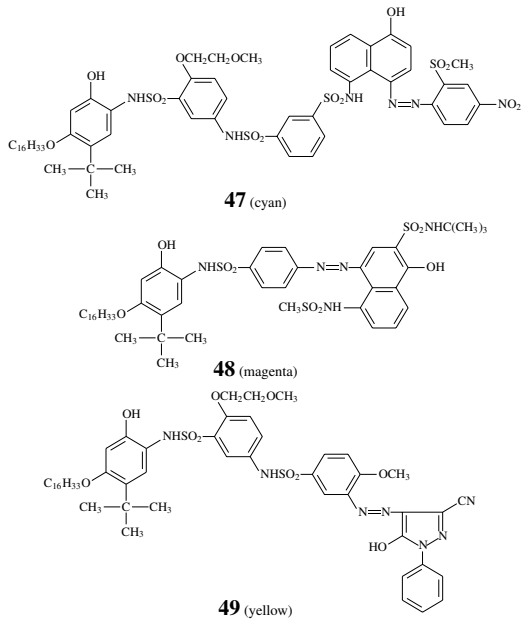

Figure 19.16. An improved set of cyan, magenta, and yellow *o*-sulfonamidophenol dye releasers for color reproduction in instant color photography [22].

The design of *o*-sulfonamidophenol moieties by using the model compounds described above has arrived at an improved set of dye releasers, as shown in Fig. 19.16 [22]. The specification of this patent contains experimental comparisons between dye releasers having a *t*-butyl group and the ones having a methyl group by using practical photographic films. Moreover, the effect of 2-alkoxyethoxy groups has been also incorporated in the dye releasers shown in Fig. 19.16 [23]. This type of *o*-sulfonamidophenol dye releasers has been used in the FI-10 film for the FOTORAMA system marketed by Fuji Photo Film in 1981 [1].

Syntheses

As collected in Table 19.2, various benzoxazole intermediates (**34a**–**34g**) for preparing 2-amino-4-alkyl-5-alkoxyphenols have been easily obtained in high yields. In particular, **34c** serves as a starting material for preparing the dye releasers listed in Fig. 19.16 [16,22].

Another versatile method for preparing 2-amino-4-alkyl-5-alkoxyphenols is the Friedel-Crafts alkylation of 2-acetamido-5-alkoxyphenol, as shown in Fig. 19.17 [24]. Thus, the key step is the conversion of **51** into **52**, where isobutene is used as a carbon source and Amberlite 15 (a synthetic ion-exchange resin from Rohm & Haas Co.) is used as a catalyst.

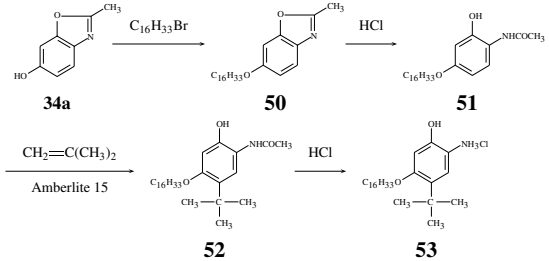

Figure 19.17. Synthesis of 2-amino-4-*t*-butyl-5-hexadecyloxyphenol by a Friedel-Crafts alkylation [24]. Homologs having other *t*-butyl groups have also been reported. This is a key for preparing *o*-sulfonamidophenol dye releasers.

Since the presence of a 2-alkoxyethoxy group has been found to enhance the dye-releasing efficiency in the model experiments described above [9,10] as well as in practical usage [22,23], 2-(2-alkoxyethoxy)benzenesulfonic acids having a nitrogen function have become important as key intermediates for preparing dye releasers of high efficiency. The introduction of such a 2-alkoxyethoxy group at the ortho position of a sulfonyl function is illustrated in Fig. 19.18 [25]. The first method described in one of the patents [23] has used sodium 2-methoxyethylate ($Na^+ \ ^-OCH_2CH_2OCH_3$) prepared by adding sodium hydride

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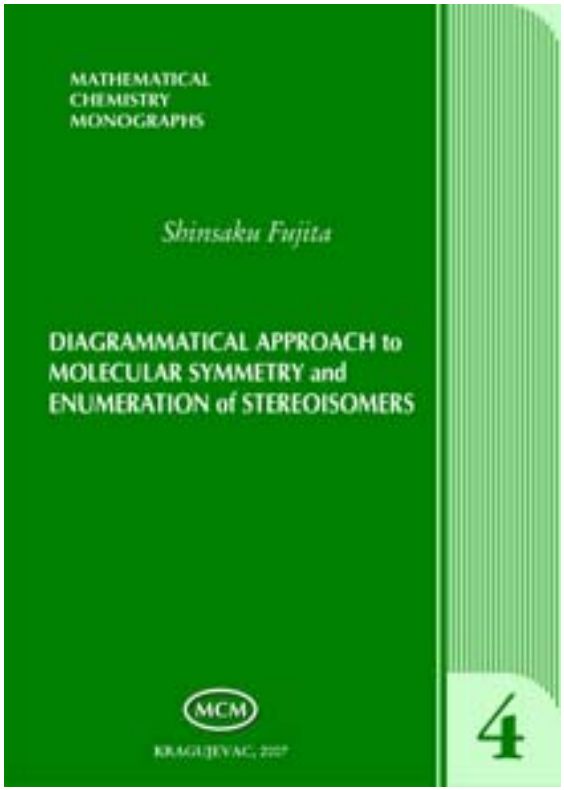

Shinsaku Fujita,
"Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers", University of Kragujevac (2007) 206pp.

(Book Review)
N. Trinajsti, *Croatica Chemica Acta* **2009**, *81*, A27–A28.

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Table 7.4. Subduction Table Based on LCRs for $\mathbf{D}_{2d}$ [2]

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}'_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{S}_4$	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{D}_2$	$\downarrow\mathbf{D}_{2d}$
$\mathbf{D}_{2d}(/\mathbf{C}_1)$	$8\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_1)$	$4\mathbf{C}'_2(/\mathbf{C}_1)$	$4\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{S}_4(/\mathbf{C}_1)$	$2\mathbf{C}_{2v}(/\mathbf{C}_1)$	$2\mathbf{D}_2(/\mathbf{C}_1)$	$\mathbf{D}_{2d}(/\mathbf{C}_1)$
$\mathbf{D}_{2d}(/\mathbf{C}_2)$*	$4\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_2)$	$2\mathbf{C}'_2(/\mathbf{C}_1)$	$2\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{S}_4(/\mathbf{C}_2)$	$2\mathbf{C}_{2v}(/\mathbf{C}_2)$	$2\mathbf{D}_2(/\mathbf{C}_2)$	$\mathbf{D}_{2d}(/\mathbf{C}_2)$
$\mathbf{D}_{2d}(/\mathbf{C}'_2)$	$4\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$	$\mathbf{C}'_2(/\mathbf{C}_1)$ $+2\mathbf{C}'_2(/\mathbf{C}'_2)$	$2\mathbf{C}_s(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$	$\mathbf{D}_2(/\mathbf{C}'_2)$ $+\mathbf{D}_2(/\mathbf{C}''_2)$	$\mathbf{D}_{2d}(/\mathbf{C}'_2)$
$\mathbf{D}_{2d}(/\mathbf{C}_s)$	$4\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}'_2(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{S}_4(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_s)$ $+\mathbf{C}_{2v}(/\mathbf{C}'_s)$	$\mathbf{D}_2(/\mathbf{C}_1)$	$\mathbf{D}_{2d}(/\mathbf{C}_s)$
$\mathbf{D}_{2d}(/\mathbf{S}_4)$*	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}'_2(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{S}_4(/\mathbf{S}_4)$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{D}_2(/\mathbf{C}_2)$	$\mathbf{D}_{2d}(/\mathbf{S}_4)$
$\mathbf{D}_{2d}(/\mathbf{C}_{2v})$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}'_2(/\mathbf{C}_1)$	$2\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{S}_4(/\mathbf{C}_2)$	$2\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{D}_2(/\mathbf{C}_2)$	$\mathbf{D}_{2d}(/\mathbf{C}_{2v})$
$\mathbf{D}_{2d}(/\mathbf{D}_2)$*	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$2\mathbf{C}'_2(/\mathbf{C}'_2)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_2)$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$2\mathbf{D}_2(/\mathbf{D}_2)$	$\mathbf{D}_{2d}(/\mathbf{D}_2)$
$\mathbf{D}_{2d}(/\mathbf{D}_{2d})$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}'_2(/\mathbf{C}'_2)$	$\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{S}_4(/\mathbf{S}_4)$	$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{D}_2(/\mathbf{D}_2)$	$\mathbf{D}_{2d}(/\mathbf{D}_{2d})$

* Forbidden CR. See Chapter 7 of Fujita's book [2].

$\mathcal{A}^{\dagger}$, the two permutation diagrams corresponding to $\mathbf{C}_s = \{I, \sigma_{d(1)}\}$ are selected so as to give Fig. 7.10 (for I and $\sigma_{d(1)}$), which corresponds to Fig. 7.9. By careful comparison between the first box of the top row and the counterpart of the bottom row in Fig. 7.9, we could find that the eight vertices of **1** are divided into four orbits (i.e., $\{1,2\}$, $\{3,8\}$, $\{4,7\}$, and $\{5,6\}$).[l] In contrast, this division can be found more easily by Fig. 7.10, because one of such orbits (i.e., $\{1,2\}$) is marked with solid circles.[m] Hence, the fixation of the first box of the top row during the action of $\mathbf{C}_s = \{I, \sigma_{d(1)}\}$ is more clearly demonstrated so as to give the first box of the bottom row in Fig. 7.10.

Thus, by comparing the two diagrams of Fig. 7.10, one can find easily that the $\{\mathcal{A}^{\dagger}_1\}$ and the $\{\mathcal{A}^{\dagger}_3\}$ are respectively immobile (fixed or stabilized), while the $\mathcal{A}^{\dagger}_2$ and the $\mathcal{A}^{\dagger}_4$ are interchanged into each other.[n] As a result, the symmetry restriction from $\mathbf{D}_{2d}$ to $\mathbf{C}_s$ divides the four-membered orbit of assemblies ($\mathcal{A}^{\dagger}$) into two one-membered orbits ($\{\mathcal{A}^{\dagger}_1\}$ and $\{\mathcal{A}^{\dagger}_3\}$) and a two-membered orbit($\{\mathcal{A}^{\dagger}_2, \mathcal{A}^{\dagger}_4\}$).

Because the resulting one-membered orbit $\{\mathcal{A}^{\dagger}_1\}$ (or $\{\mathcal{A}^{\dagger}_3\}$) is fixed by $\mathbf{C}_s$, the orbit is concluded to be governed by the LCR $\mathbf{C}_s(/\mathbf{C}_s)$. Because the two-membered orbit of assemblies $\{\mathcal{A}^{\dagger}_2, \mathcal{A}^{\dagger}_4\}$ is fixed by $\mathbf{C}_1$ and the two assemblies $\mathcal{A}^{\dagger}_2$ and $\mathcal{A}^{\dagger}_4$ are permuted by the action of the $\sigma_{d(1)}$-operation, the orbit is concluded to be governed by the LCR $\mathbf{C}_s(/\mathbf{C}_1)$. Thereby, the subduction represented by Fig. 7.10 is summarized into eq. 7.46. This procedure shows that Fig. 7.10 is capable of deriving results equivalent to those derived by Fig. 7.9. Thus, the same subduction table as Table 7.4 can be alternatively obtained. Then,

[l] Strictly speaking, this division of the eight vertices is controlled by the subduction of the RRR $(\mathbf{C}_1 \backslash \mathbf{D}_{2d} \downarrow \underline{\mathbf{C}_s}$ (cf. eq. 6.58 in Chapter 6), where the underlined $\mathbf{C}_s$ is the local symmetry of the LCR $\mathbf{D}_{2d}(/\underline{\mathbf{C}_s})$, which governs the orbit of assemblies $\mathcal{A}^{\dagger} = \{\mathcal{A}^{\dagger}_1, \mathcal{A}^{\dagger}_2, \mathcal{A}^{\dagger}_3, \mathcal{A}^{\dagger}_4\}$. In general, the symmetrical behavior of a **K**-molecule derived from a regular body of **G** is described by the LCR $\mathbf{G}(/\underline{\mathbf{K}})$, while the division of $|\mathbf{G}|$ vertices in the regular body of **G** is controlled by the subduction $(\mathbf{C}_1 \backslash \mathbf{G} \downarrow \underline{\mathbf{K}}$. Note that the underlined **K**'s are selected to be common. This feature is the basis of the concept of mandalas, as described in the next chapter.

[m] Although the formulation using $\mathcal{A}^{\dagger}$ is more understandable than the formulation using $\mathcal{A}^{*}$, the latter is adopted as a primary formulation because its generality is superior to the former. For example, one can select $\{3,8\}$, $\{1,2\}/\{3,8\}$, or $\{1,2\}/\{4,7\}$ as vertices to be marked with solid circles. The formulation using $\mathcal{A}^{*}$ connotes these alternatives as well as the special case shown in Fig. 7.10 (i.e., the selection of $\{1,2\}$).

[n] Do not confuse an orbit of vertices with an orbit of assemblies. The discussion described here is concerned with the subduction of the orbit of assemblies, i.e., $\mathcal{A}^{\dagger} = \{\mathcal{A}^{\dagger}_1, \mathcal{A}^{\dagger}_2, \mathcal{A}^{\dagger}_3, \mathcal{A}^{\dagger}_4\}$, which is governed by the LCR $\mathbf{D}_{2d}(/\mathbf{C}_s)$.

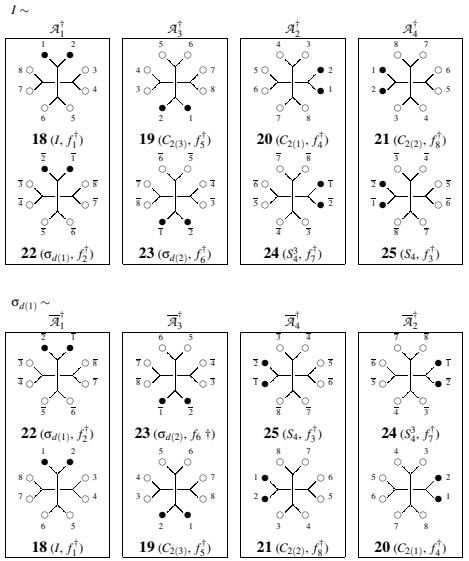

Figure 7.10. The action of I and $\sigma_{d(1)}$ on the $\mathbf{C}_s$-molecule (the four $\mathbf{C}_s$-assemblies) listed in Fig. 7.8. The alignment shown in this diagram corresponds to an ordered set, $\mathcal{A}^{\dagger}_o = \{\mathcal{A}^{\dagger}_1, \mathcal{A}^{\dagger}_3, \mathcal{A}^{\dagger}_4, \mathcal{A}^{\dagger}_2\}$.

the other tables for the LCRs (the USCI-CF table, the USCI table and the mark table) are obtained similarly, where they are equivalent to those for the RCRs described in Chapter 6 (Tables 6.8, 6.9, and 6.10).

Exercise 7.13. Derive eqs. 7.42–7.49 and Table 7.4 diagrammatically by following the procedure given above for Fig. 7.10. Compare the derivation with the one described for obtaining eqs. 6.61–6.68 in Chapter 6.

7.4 Mandalas as Nested Regular Bodies

The discussions described in Section 7.2 have essentially followed Chapters 13 and 15 of Fujita's book [2], although a more diagrammatical approach has been adopted by following partly the treatment reported recently [4,5]. Because the discussions have required

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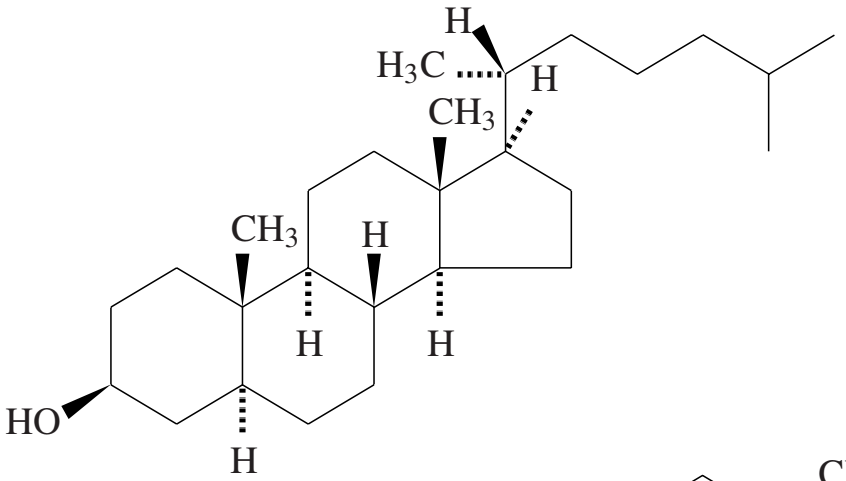
2010* Release of XeTeX Version 5.00 for supporting the PDF mode

2013* Release of XeTeX Version 5.01 for supporting a comprehensive on-line manual

2013 XeTeX/LaTeX-typesetting and publication of "Combinatorial Enumeration of Graphs, Three-Dimensional Structures, and Chemical Compounds" from University of Kragujevac (Kragujevac).

— Commands for Complicated Structures

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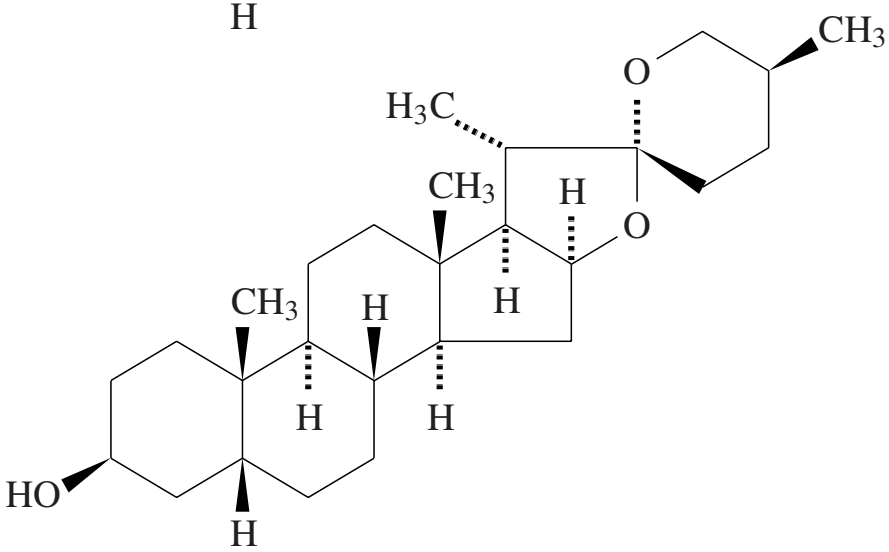


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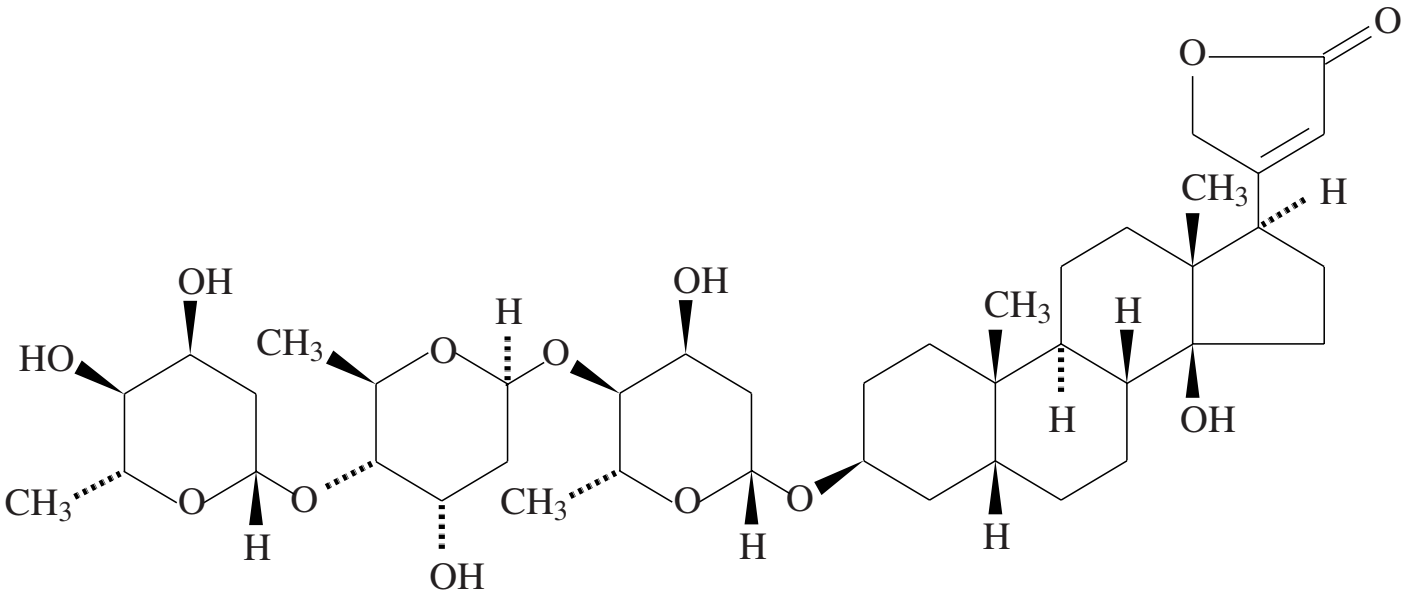
— Commands for Complicated Structures

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6A==CH$_{3}$;5B==HO}}%
}}}};%
5B==H;8B==H;9A==H;%
{10}B==CH$_{3}$;{13}B==CH$_{3}$;%
{14}B==OH;{17}GA==H;%
{{17}}==¥fiveheterov[a]{4==O}%
{1==(yl);3D==O}}
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XyMTeX Vesion 4.04 + PSTricks $\Longrightarrow$ XyMTeX Version 5.00 (PS Mode)
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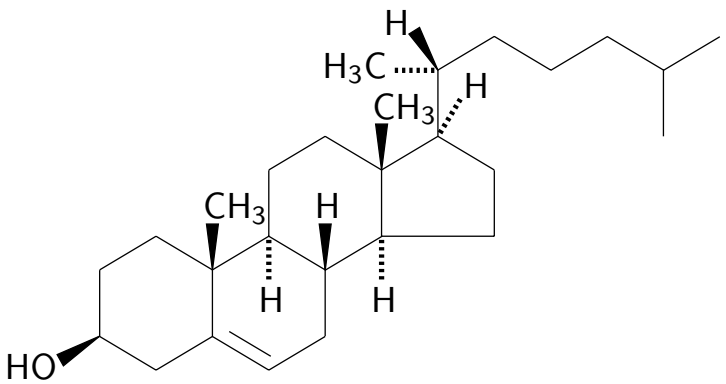


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%¥usepackage{xymtexps}%PostScript mode
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PostScript Mode vs. PDF Mode

- PostScript Mode:

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- PDF Mode:

$$\text{tex} \xrightarrow{\LaTeX} \text{dvi} \xrightarrow{\text{dvipdfmx}} \text{pdf}$$

- PDF Mode (pdftex option):

$$\text{tex} \xrightarrow{\text{pdflatex}} \text{pdf}$$

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¥end{document}
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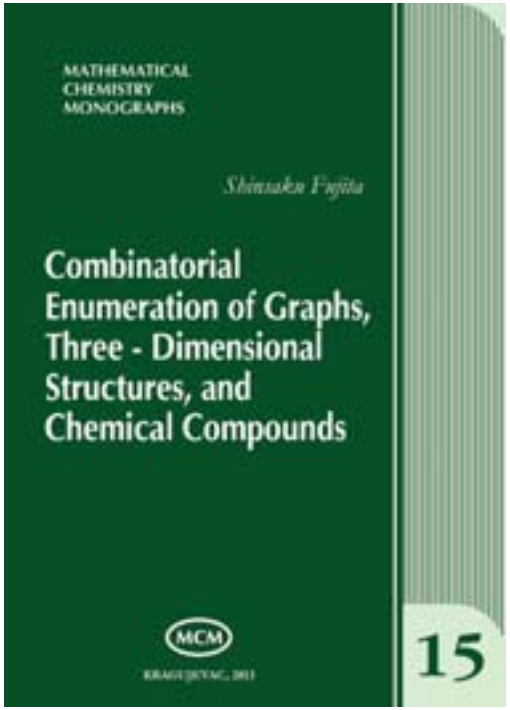

Shinsaku Fujita,
"Combinatorial Enumeration of Graphs, Three-Dimensional Structures, and Chemical Compounds",
University of Kragujevac (2013) 576pp.

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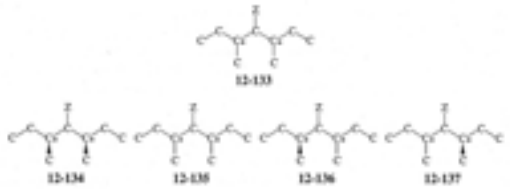


Figure 12.20. Pólya's treatment for a planted tree of carbon content 9 with 2 asymmetric carbon centers (**12-133**), which produces four steric isomers **12-134**–**12-137**. Each asymmetric carbon center is designated by an asterisk (*). A hydrogen atom on each asymmetric carbon center is omitted. The symbol Z is a root or OH. Two asymmetric carbon centers in **12-133** indicate the presence of 2^2 (= 4) steric isomers (**12-134**–**12-137**). Note that the principal node of **12-134** (or **12-135**) is symmetric (non-asymmetric) in terms of Pólya's treatment, which is incapable of detecting pseudoasymmetry.

which is a key concept to recognize the two exceptions (**12-121** (= **12-85**) and **12-122** (= **12-86**)) to be achiral, as illustrated in Fig. 12.17. In other word, Pólya's treatment is incapable of recognizing the achiralities of **12-134** and **12-135** because of the lack of reflection operations.

On the other hand, the data of the (n = 9)-row in Table 12.3, which have been evaluated by Fujita's treatment [31], show that there are 41 achiral planted 3D-trees (σ_9 = 41) and there are 255 enantiomeric pairs of chiral planted 3D-trees (C_9 = 255). The former value 41 is consistent with the presence of 41 achiral planted 3D-trees listed in Figs. 12.15–12.18 with no exceptions. The value 255 corresponds to 510 steric isomers, which is consistent with the value 512 − 2 = 510 due to Pólya's treatment, because the presence of **12-134** and **12-135** corresponds to 41 (Fujita) − 39 (Pólya) = 2 and the presence of **12-136** and **12-137** corresponds to 512 (Pólya) − 510 (Fujita) = 2. The total number of steric isomers is calculated to be 39 + 512 (Pólya) = 41 + 510 (Fujita) = 551, whether we obey Pólya's treatment or Fujita's one (cf. β_9 = 551 in Table 12.1).

The above discussions in addition to the discussions on "Asymmetry vs. Chirality" on page 429 are summarized as follows:

> "Steric isomers" due to Pólya's treatment are conceptually different from "steric isomers" due to Fujita's treatment in their connotations concerning asymmetry vs. chirality. In particular, the achirality linked to pseudoasymmetry is ignored in Pólya's treatment, while it is properly considered in Fujita's treatment. Although they give the same isomer number per carbon content, the latter "steric isomers" due to Fujita's treatment are adopted in this book because of stereochemical consistency.

12.4.2 Number of Asymmetric and Pseudoasymmetric Centers in Fujita's Enumeration

The discussions on the graph **12-133** in Fig. 12.20 have revealed that Pólya's treatment of the corresponding steric isomers **12-134**–**12-137** lacks the concept of *pseudoasymmetric*

centers. Because Pólya's treatment is based on permutation groups (i.e., the symmetric group $S^{(3)}$ and the alternating group $A^{(3)}$), it does not take account of reflection operations, so that it is incapable of recognizing the principal nodes of **12-134** and **12-135** to be pseudoasymmetric centers. This subsection is devoted to a rationalization of pseudoasymmetric centers in terms of Fujita's enumeration of 3D structures.

Fujita's Enumeration of Planted 3D-Trees with Given Numbers of Asymmetric and Pseudoasymmetric Centers

Fujita has developed the stereoisogram approach [43,45,47], where permutation groups and point groups are integrated into *RS*-stereoisomeric groups. Stereoisograms have been proposed as diagrammatical expressions of such *RS*-stereoisomeric groups. Fujita has shown that the stereoisogram approach is effective to the enumeration of achiral and chiral monosubstituted alkanes (planted 3D-trees) having given numbers of asymmetric and pseudoasymmetric centers [33].[8]

Suppose that a monosubstituted alkane (planted 3D-tree) of carbon content n has ℓ asymmetric centers and m pseudoasymmetric centers and that it is characterized by a monomial $x^n y^\ell z^m$, where x, y, and z are used to represent respective dummy variables. In a parallel way to the generating functions $a(x)$ (Eq. 12.53), $c(x^2)$ (Eq. 12.46), and $b(x)$ (Eq. 12.40), the corresponding generating functions $a(x, y, z)$, $c(x^2, y^2, z^2)$, and $b(x, y, z)$ for counting alkyl ligands of carbon content n, which have ℓ asymmetric centers and m pseudoasymmetric centers, can be generated:

$$a(x,y,z) = \sum_{n=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\alpha_{n\ell m}z^m\right)y^\ell\right)x^n \tag{12.79}$$

$$c(x^2,y^2,z^2) = \sum_{n=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\gamma_{n\ell m}z^{2m}\right)y^{2\ell}\right)x^{2n} \tag{12.80}$$

$$b(x,y,z) = \sum_{n=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\beta_{n\ell m}z^m\right)y^\ell\right)x^n. \tag{12.81}$$

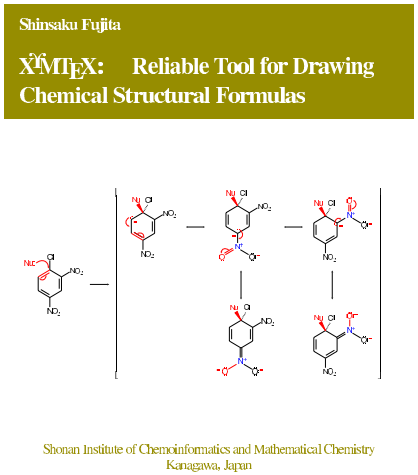
where we place $\alpha_{000} = 1$, $\gamma_{000} = 1$, and $\beta_{000} = 1$ for trivial cases of hydrogens. The series represented by Eqs. 12.79–12.81 have been already noted in Fujita's articles [33,40]. Although detailed descriptions on the derivation of these generating functions are omitted in this book, the coefficients, $\alpha_{n\ell m}$, $\gamma_{n\ell m}$, and $\beta_{n\ell m}$, can be evaluated on the basis of the stereoisogram approach [48].

The coefficient $\alpha_{n\ell m}$ itself represents the number of achiral monosubstituted alkanes (achiral planted 3D-trees) of carbon content n, where each of them has ℓ asymmetric centers and m pseudoasymmetric centers. The coefficient $\beta_{n\ell m}$ itself represents the number of monosubstituted alkanes (as steric isomers) of carbon content n with ℓ asymmetric centers and m pseudoasymmetric centers. On the other hand, the number $C_{n\ell m}$ of enantiomeric pairs of chiral monosubstituted alkanes (chiral planted 3D-trees) of carbon content n, where each of them has ℓ asymmetric centers and m pseudoasymmetric centers, is obtained as the

[8] To accomplish the itemization due to the numbers of asymmetric and pseudoasymmetric centers etc., the definitions of *RS*-stereogenic centers, asymmetric centers, and pseudoasymmetric centers have been discussed in detail [33]. This method has been further applied to the enumeration of achiral and chiral alkanes (3D-trees) with considering numbers of asymmetric and pseudoasymmetric centers [40].

XMTEX Version 5.01

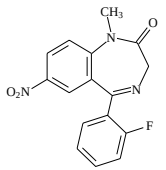
On-Line Manual of XyMTeX



Shinsaku Fujita,
"XyMTeX, A Reliable Tool for Drawing Chemical Structural Formulas",
Shonan Institute of Chemoinformatics and Mathematical Chemistry (2013) 760pp. + XX
Available from
http://xymtex.com/ and CTAN

Text:	Typeset by LaTeX 2_ε.
Structural Formulas:	Drawn by XyMTeX.
Delivery form:	PDF file (generated by the PostScript mode).
	PDF file (generated by the PDF mode).
	On-line Manual.

On-Line Manual of XyMTEX (p. 543)

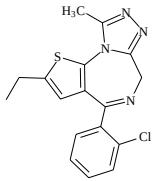


31-16

Example 31.18. The structure **31-17** of etizolam (Depas®) is drawn by the code:

```
\begin{XyMcompd}(1100,1350)(-450,-600){cpd:etizolam}{}
\FiveCycle(0,0){19}[be]{4==S;%
5s==\rotatebox{10}{\trimethylene{}{3==(yl)}};%
2s==\SevenCycle(-125,157){-6}[a]{%
2==\rotatebox{-19}{N};%
5s==\FiveCycle(0,0){-25}[bd]{%
3==\rotatebox{-13}{N};4==\rotatebox{-13}{N};%
5s==\exosinglebond{72};%
5==\put(-180,50){\rotatebox{-13}{\llap{H$_{3}$}C}}%
}[a];%
5==\rotatebox{-19}{N};%
1s==\exosinglebond{154};%
1s==\put(-70,-140){\rotatebox{-26}{\benzenev{1==(yl);2==\rotatebox{13}{Cl}}}}%
}[f]}
\end{XyMcompd}
```

where several rotation angles are determined by trial and error. This code generates the following diagram:

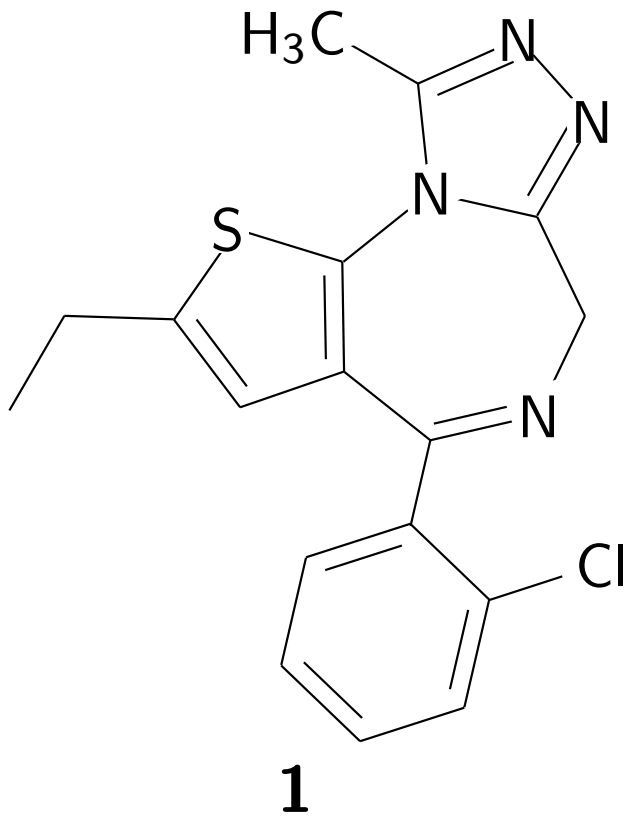


31-17

Example 31.19. The structural formula of carbamazepin, which has been shown in Section 30.2.2 (**30-7**) is alternatively drawn by the new commands defined in this chapter. Thus, the code:

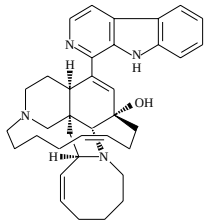
```
\begin{XyMcompd}(1050,750)(-450,0){cpd:carbamazepinZ}{}
\SevenCycle(0,0){0}[a]{%
5s==\exosinglebond{0};%
5s==\put(0,160){\trimethylenei[a]{1==O;3==NH$_{2}$}{2==(yl);2==\null}};
5==N;%
3s==\rotatebox{13}{\sixfusev[ace]{}{}{e}};%
7s==\rotatebox{-13}{\sixfusev[bdf]{}{}{B}}
\end{XyMcompd}
```

generates an equivalent structural formula **31-18** of carbamazepin as follows:



1

On-Line Manual of XyMTeX (p. 556)

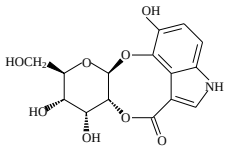


31-34

□

Example 31.36. The structure **31-35** of (−)-ovatolide, a tetracyclic indol alkaloid bearing an eight-membered ether-lactone [12], is drawn as follows:

```
\begin{XyMcompd}(1600,1100)(-950,-200){cpd:ovatolide}{}
\wedgehashedwedge
\EightCycle(-100,-242){0}{%
1==O;6==O;%
8s==\sixheterov{1==O}{3==(yl);4A==OH;5A==HO;6B==HOCH$_{2}$};%
8s==\HashWedgeAsSubst(0,0)(1,-1){100};%
7s==\WedgeAsSubst(0,0)(1,1){100};%
2s==\exodoublebond{-160};%
2==\put(80,-180){O};%
4s==\rotatebox{45}{\sixheterov[ace]{%
4s==\PutBondLine(0,0)(0,-140){0.4pt}}{5==(yl);%
1==\rotatebox{-45}{\raisebox{3pt}{OH}}%
}};%
3s==\FiveCycle(0,0){-18}[a]{3==NH}[cde]%
}[dfgh]
\end{XyMcompd}
```

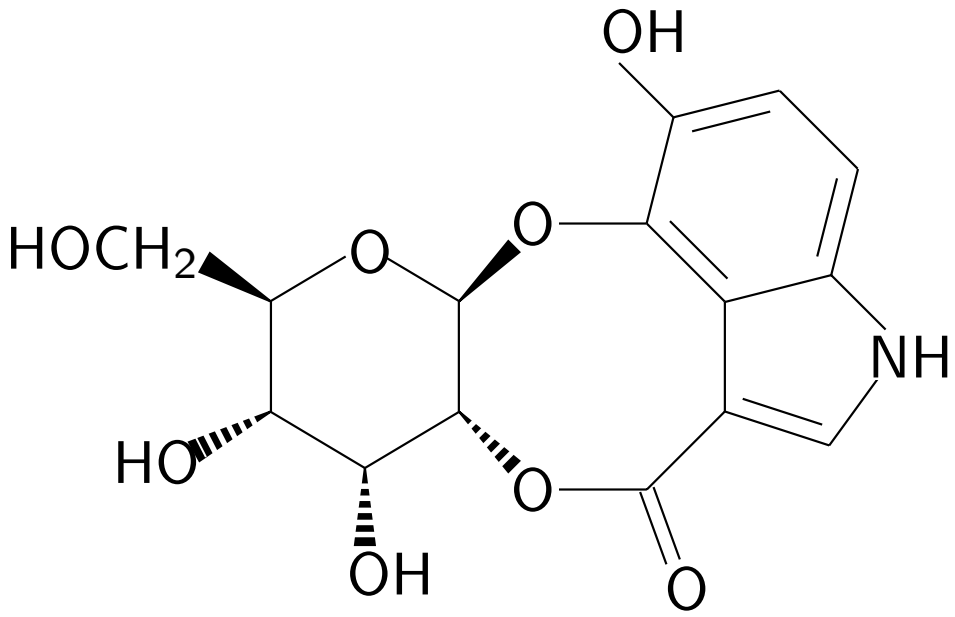


31-35

□

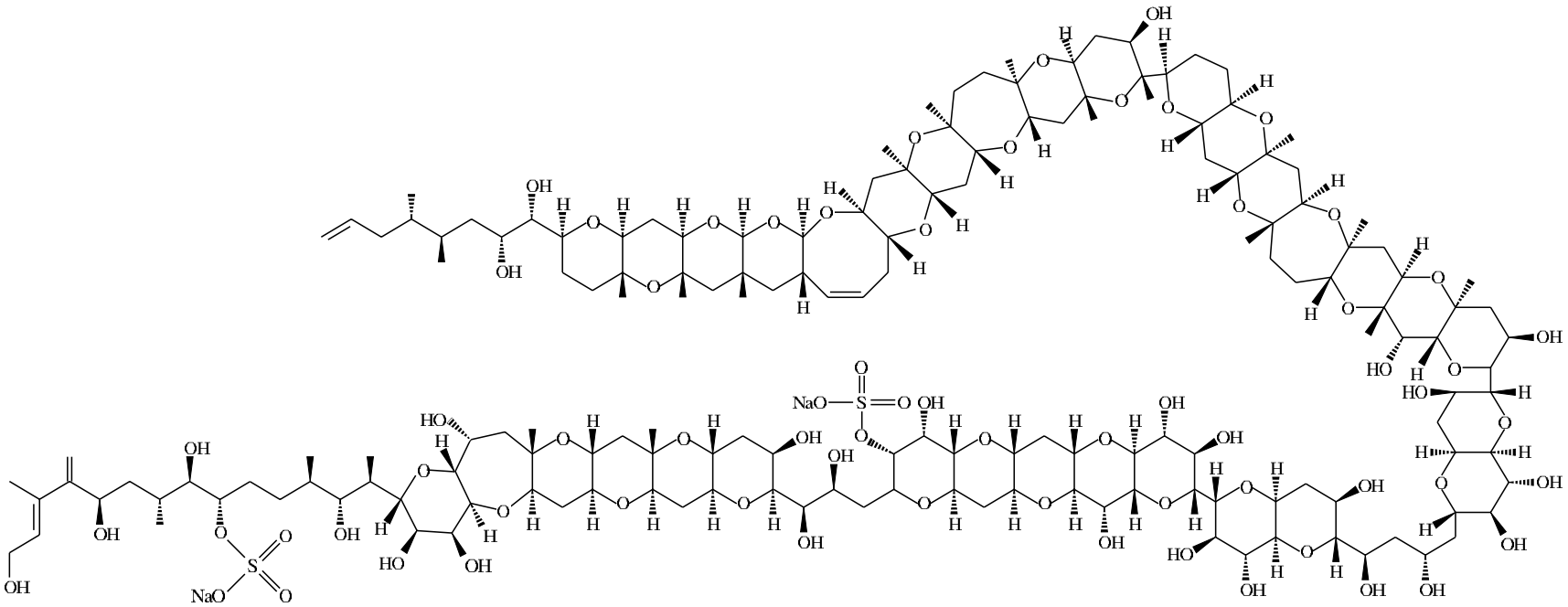
31.5 Multiple Ring Fusion

Now that we have defined commands for drawing seven- and eight-membered rings, we are ready to draw several complicated compounds of natural source.



2

On-Line Manual of XeTeX (p. 562)

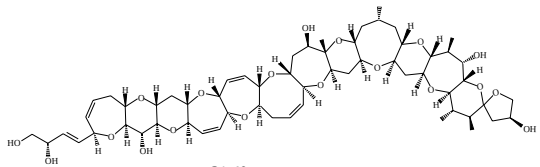


31-39 (Maitotoxin)

Figure 31.3. Structure of maitotoxin

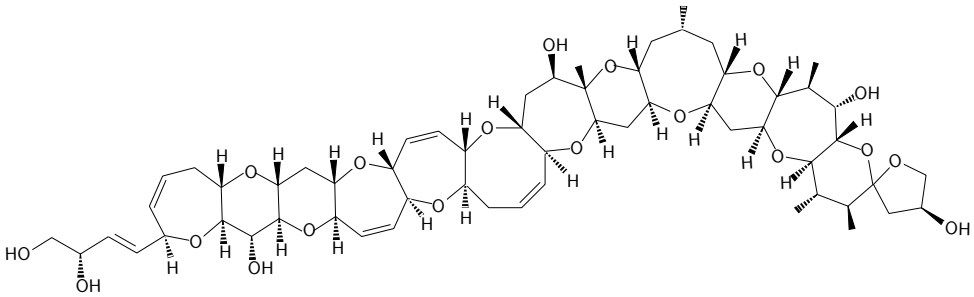
On-Line Manual of XyMTeX (p. 563)


```
4==O;%
2s==\WedgeAsSubstX(0,0)(110,-110);2==\put(160,-160){\rotatebox{-11}{OH}}
}%end M-ring
}{6==(yl);1GB==\rotatebox{-8}{H};6FA==\rotatebox{-8}{H};4B==\null;5A==\null
}[f]}%end L-ring
}%end K-ring
}{1==(yl);1FA==\rotatebox{-3}{H};2GB==\rotatebox{-3}{H};%
5GA==\rotatebox{-3}{H};4FB==\rotatebox{-3}{H}%
}[ad]}%end J-ring
}[h]%end I-ring
}{5FA==\rotatebox{-18}{H};6GB==\null;3GA==\rotatebox{-18}{H};%
2FB==\rotatebox{-18}{H}}{e}}%end H-ring
}[g];%end G-ring
%%%%%%%%%%%%%%
% left part %
%%%%%%%%%%%%%%
8s==\SevenCycle(325,157){-12}[e]{%E-ring
2==O;%
1s==\SevenCycle(325,157){26}[a]{%D-ring
5==\rotatebox{12}{O};%
3s==\HashWedgeAsSubstX(6,-12)(60,-120)[6];3==\put(80,-180){\rotatebox{12}{H}};%
4s==\WedgeAsSubstX(0,0)(-40,120)[6];4==\put(-40,200){\rotatebox{12}{H}};%
7s==\rotatebox{-12}{%BC-ring
\decaheterov{4==\rotatebox{-2}{O};8==\rotatebox{-2}{O};%
6s==\SevenCycle(325,157){-13}[f]{%A-ring
2==O;%
1s==\HashWedgeAsSubstX(6,-12)(60,-120)[7];1==\put(80,-180){\rotatebox{-1}{H}};%
1s==\rotatebox{12}{\pentamethylenei[c]{}{5==(yl);1W==HO;2A==OH}}%
}%end A-ring
}{3==(yl);2FB==\rotatebox{-2}{H};3GA==\rotatebox{-2}{H};9A==\rotatebox{-2}{H};%
{10}B==\rotatebox{-2}{H};6FA==\rotatebox{-2}{H};7GB==\rotatebox{-2}{H};%
5A==\rotatebox{-2}{OH}%
}[bg]}%endBC-ring
}[c]%end D-ring
}[c]%end E-ring
}%end F-ring
\end{XyMcompd}
}
\\
\compd\label{cpd:ciguatoxin} (Ciguatoxin 1B)
\\
\end{tabular}
```



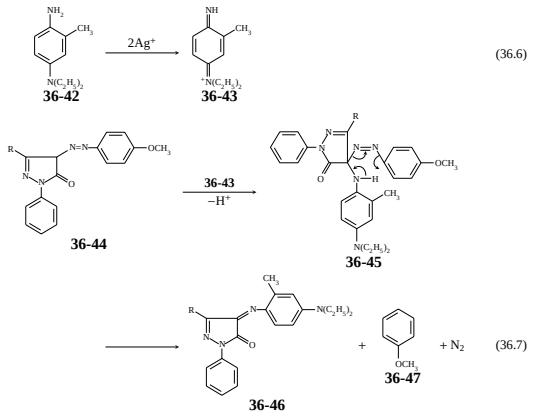
31-40 (Ciguatoxin 1B)

In the above code, each step of nested fusions is shown by a pair of comments such as `%F-ring` and `%end F-ring`. The eight-membered F-ring is selected as a skeleton, where the right part and the left part are drawn



3 (Ciguatoxin 1B)

On-Line Manual of XeTeX (p. 647)



Anisole (**36-47**) is detected as a byproduct. The resulting azomethine dye (**36-46**) is a magenta-colored dye for color photography. □

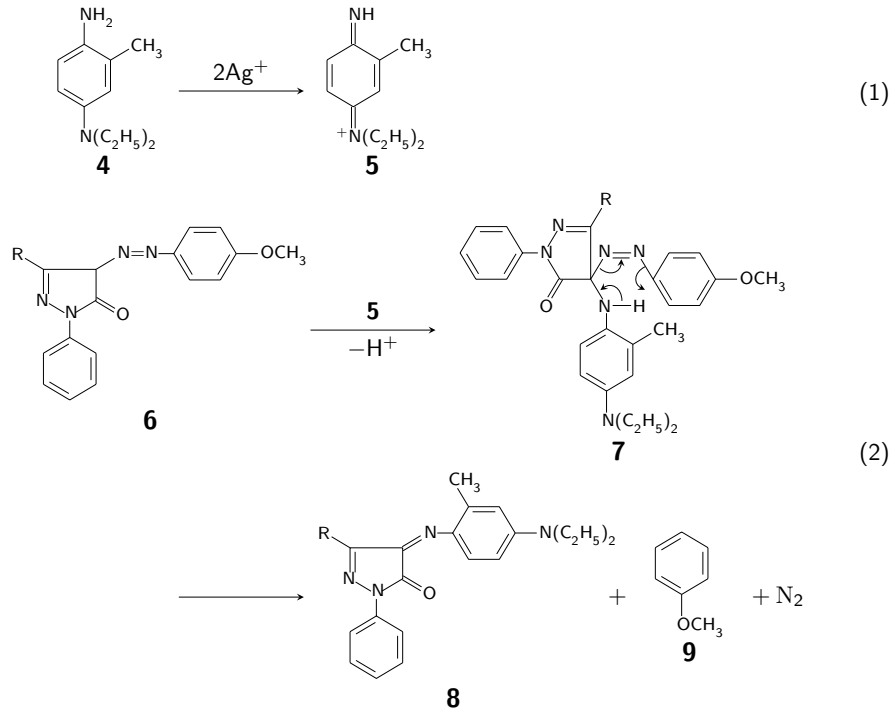
36.5 Structural Formulas in Display Chem Environments

36.5.1 Reaction Schemes in the ChemEquation-like Environments

If the molecular formula CH_3OH written above the reaction arrow in Eq. 36.1 is desired to be drawn in the display line, it is convenient to use the `ChemEquation` environment.

Example 36.17. As found in this example, the code `CH_{3}OH` can be directly declared in place of `\mbox{CH$_{3}$OH}` or `\mathrm{CH}_{3}\mathrm{OH}`, which would be required in the `equation` environment.

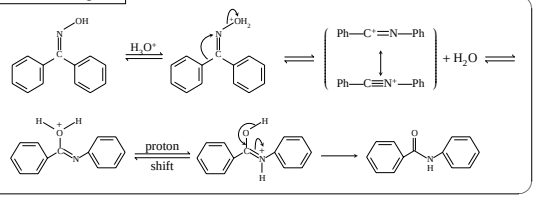
```
\begin{ChemEquation}
\resetamsmathlabel %reset \label from amsmath to LaTeX
\begin{XyMcompd}(400,750)(220,200){cpd:BPHOH2}{}
\bzdrv{1==OH}
\end{XyMcompd}
+ CH_{3}OH
\reactrarrow[10\unitlength]{-20\unitlength}{500\unitlength}
{HCl}{\ChemForm{-H_{2}O}}
\begin{XyMcompd}(400,750)(220,200){cpd:PHOME2}{}
\bzdrv{1==\ChemForm{OCH_{3}}}
\end{XyMcompd}
\label{eq:EQ2}
\end{ChemEquation}
```



On-Line Manual of XeTeX (p. 657)


```
1==\electronshiftArrowl(-40,100)(-200,200)(-80,400)(60,320);%
1==\electronshiftArrowr(60,50)(60,200)(100,200)(150,80)}%
{2==H;2W==\bzdrh{1==(yl)};1W==\bzdrh{4==(yl)};%
1==\Utrigonal{0==O;2==H;1==(yl)}}
\end{XyMcompd}
\mskip6mu \reactrarrow{0pt}{1cm}{}{} \mskip6mu
\begin{XyMcompd}(1100,500)(-400,0){}{}
\dimethylenei{2==\downnobond{N}{H}}{2W==\bzdrh{1==(yl)};1W==\bzdrh{4==(yl)};1D==O}
\end{XyMcompd}
\end{ChemEqnarray*}
\end{tboxscreen}
```

Beckmann Rearrangement



□

Note that the commands \sbond, \dbond, and \tbond are supported by the chemist packages to draw single (—), double (=), and triple bonds (≡). For the curved arrows, see Section 33.4.

36.7.3 Frames with Shadows

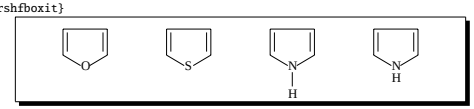
The rshfboxit Environment

The rshfboxit (right-shadow-frame-box-it) environment provides a framed box with right and bottom shadows, where the width of the box can be specified by its argument ⟨boxwidth⟩.

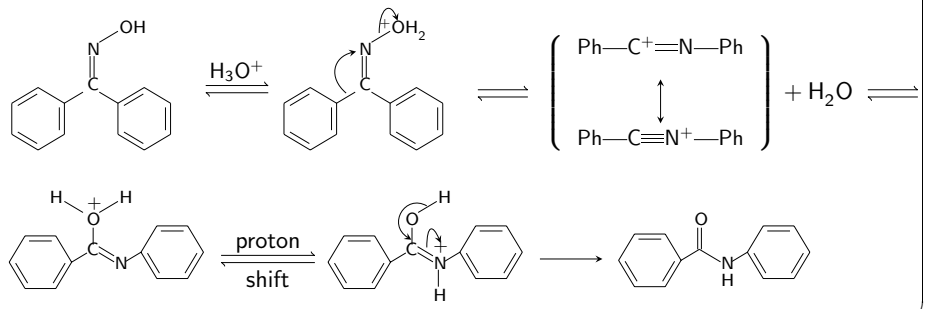
```
\begin{rshfboxit}{⟨boxwidth⟩}
(text)
\end{rshfboxit}
```

Example 36.31. The following example shows a list of commands for drawing five-membered heterocycles, which is surrounded by such a framed box.

```
\begin{rshfboxit}{12cm}
\centering
\begin{XyMcompd}(2700,550)(250,50){}{}
\furanv{} \thiophenev{} \pyrrolev{1==H}
\fiveheterov[bd]{1==\downnobond{N}{H}}{}
\end{XyMcompd}
\end{rshfboxit}
```



Beckmann Rearrangement



On-Line Manual of XyMTeX (p. 661)

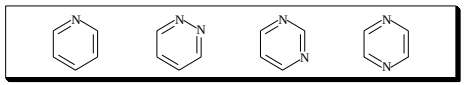
The grshfboxit Environment

A grshfboxit (gradient-right-shadow-frame-box-it) environment provides a framed box with right and bottom gradient shadows, where the width of the box can be specified by its argument ⟨boxwidth⟩.

```
\begin{grshfboxit}{⟨boxwidth⟩}
(text)
\end{grshfboxit}
```

Example 36.37. The following example shows a list of commands for drawing six-membered heterocycles, which is surrounded by such a framed box.

```
\begin{grshfboxit}{12cm}
\centering
\begin{XyMcompd}(2700,450)(250,250){}{}
\pyridinev{} \pyridazinev{} \pyrimidinev{} \pyrazinev{}
\end{XyMcompd}
\end{grshfboxit}
```



□

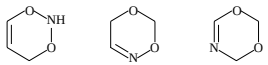
The grshfboxit environment may contain a sentence along with structural formulas.

Example 36.38. For example, you write such a statement such as

```
\begin{center}
\blue
\begin{grshfboxit}{0.7\textwidth}
\centering\black
{\red 2H,4H-1,3,2-, 2H,6H-1,3,4- and 2H,4H-1,3,5-dioxazine} \\
\sixheterov[e]{1==O;2==NH;3==O}{}
\sixheterov[d]{1==O;3==O;4==N}{}
\sixheterov[e]{1==O;3==O;5==N}{}
\end{grshfboxit}
\end{center}
```

Then, you obtain the following result:

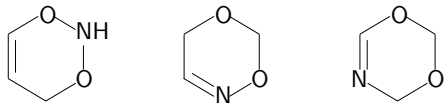
2H,4H-1,3,2-, 2H,6H-1,3,4- and 2H,4H-1,3,5-dioxazine



where the frame is colored in blue, the name is colored in red, and the structural formulas are printed out in black. □

The grshfboxit environment is based on the grshfr@meboxit environment of the chemist package. Hence, we can use the latter inner environment to change parameters.

2H,4H-1,3,2-, 2H,6H-1,3,4- and 2H,4H-1,3,5-dioxazine



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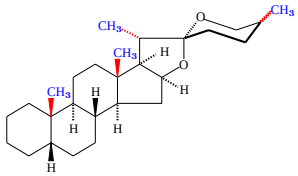


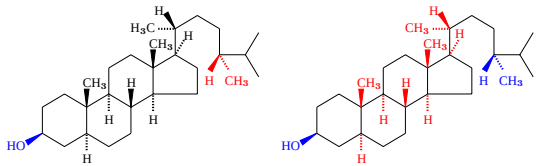
It should be emphasized that wedged bonds, dashed bold bonds, and wavy bonds for stereochemistry are colored by the same technique of bond coloring due to the `\addbscolor` command. □

Commands of high level have a fixed set of substituents, which are not changed by the systematic method described here. For the purpose of coloring the fixed set, you should use the corresponding commands of low level.

Example 38.25. For example, the high-level command `\cholestanealpha` is compared with the low-level command `\steroidchain` as follows:

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

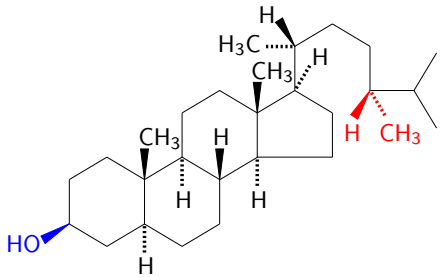
high-level macro: low-level macro



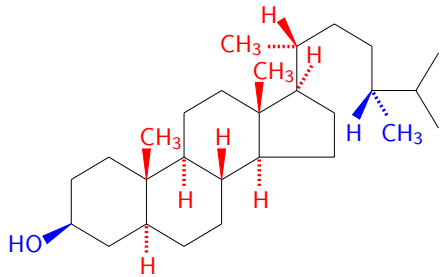
Note that the black bonds in the left structure (or the red bonds in the right structure) indicate the fixed set of substituents for the `\cholestanealpha` command of high level. □

Example 38.26. The fused structure **38-1** of morphine (or heroin) is drawn by the scheme 6 ← 6 ← 6 according to the addition technique. A furan ring and a piperidine ring are added by respective sets of low-level commands such as `\PutBondLine` and `\WedgeAsSubstX`. Hetero atoms (O and N) in morphine **38-1a**

high-level macro:



low-level macro:



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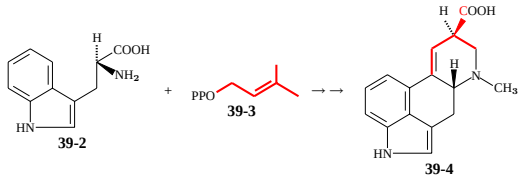
Example 39.6. Lysergic acid **39-4** is a precursor for wide range of ergoline alkaloids. Its dimethylamide (lysergic acid dimethylamide: LSD) is a semisynthetic psychedelic drug of the ergoline family. The red colored moiety of **39-4** stems from DMAPP (dimethylallyl pyrophosphate, **39-3**), which is attached to tryptophan (**39-2**) during the biosynthesis of lysergic acid (**39-4**).

```
\begin{center}
\begin{XyMcompd}(1050,800)(200,0){cpd:tryptophan}{}
\decaheterov[fhk%
{d\fivefusevi[b]{4==HN}{}{A}[e]}%
]{}{2FA==H;2==COOH;2GB==NH$_{2}$}[aj]
\end{XyMcompd}
\quad + \quad
\begin{XyMcompd}(700,300)(-50,150){cpd:DMAPP}{}
\def\thinLineWidth{1.6pt}
\redx{\tetramethylenei[b]{}{1W==\blackx{PPO};3==\null}}
\end{XyMcompd}
\quad $\rightarrow$ \quad
\begin{XyMcompd}(1100,1200)(250,0){cpd:lysergicacid}{}
\decaheterov[fhk%
{a\sixfusev[e%
{a{\replaceSKbond[1.6pt](0,0)(5,-3){171}{\red}}}%
{a{\replaceSKbond[1.6pt](0,0)(-5,-3){171}{\red}}}%
{e{\replaceSKbond[1.6pt](0,0)(0,1){200}{\red}}}%
]{3==N}{3==CH$_{3}$;1Sd==H;1Su==\addbscolor{\red}{C\blackx{OOH}}}{D}}
{d\fivefusevi[b]{4==HN}{}{A}[e]}%
]{}{2FB==H}
\end{XyMcompd}
\end{center}
```



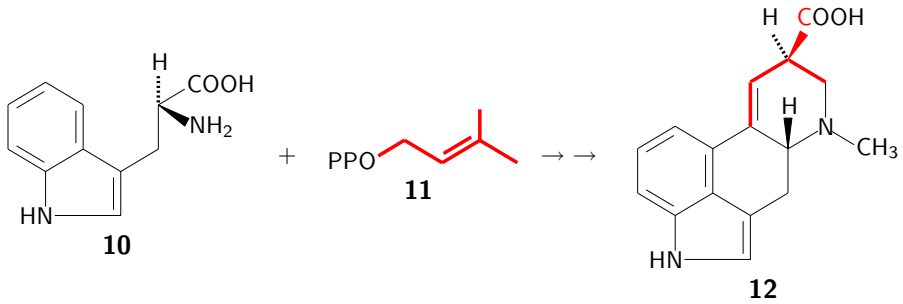
The bold bonds of **39-3** are generated by declaring `\def\thinLineWidth{1.6pt}`. The whole structure generated by `\tetramethylenei` is surrounded by `\redx` so as to be colored in red, except that the character string "PPO" remains to be black by declaring `1W==\blackx{PPO}`. The red skeletal bonds of **39-4** are generated by the command `\replaceSKbond`. □

39.2 Coloring Double Bonds

39.2.1 A Systematic Way

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

```
\adddbcolor{⟨commandsuffix⟩}{⟨skelbcolor⟩}
```



On-Line Manual of XyMTeX (p. 719)

Example 39.11. For example, Fig. 39.1 shows a reaction (a Diels-Alder reaction) and its ITS as well as related diagrams for representing the reaction in various levels of information, i.e, an imaginary transition structure (ITS), a reaction-center graph (RCG), a reaction graph (RG), and a basic reaction graph (BRG). This figure is a modification of [1, Fig. 14.2]. The process denoted by PS is a projection to a starting stage, by which the ITS produces the corresponding starting stage. The process denoted by PP is a projection to a product stage, by which the ITS produces the corresponding product stage.

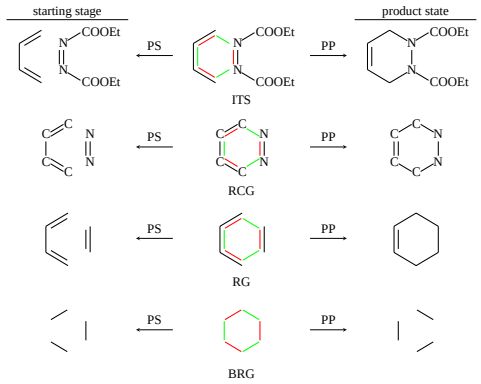
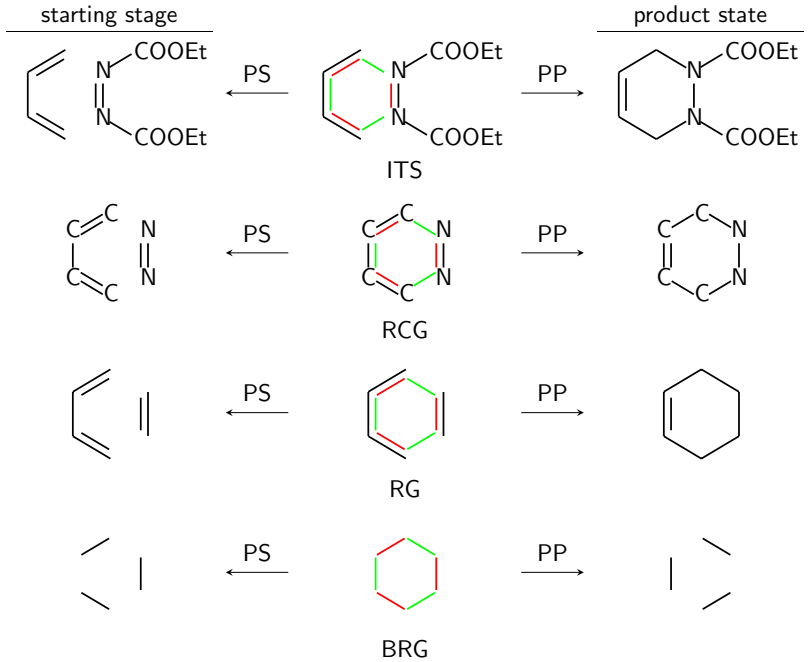


Figure 39.1. An imaginary transition structure (ITS), a reaction-center graph (RCG), a reaction graph (RG), and a basic reaction graph (BRG) for the ITS approach. This figure is a modification of [1, Fig. 14.2].

The scheme contained in Fig. 39.1 is depicted by the following code:

```
\begin{center}
\def\thinLineWidth{0.8pt}
\begin{tabular}{ccccc}
starting stage &&&& product state \\
\cline{1-1}\cline{5-5}
\noalign{\vskip3pt}
\begin{XyMcompd}(700,500)(250,200){}{}
\sixheterov[bdf]{2==N;3==N}{2==COOEt;3==COOEt}[ac]
\end{XyMcompd}
& \reactlarrow{0pt}{1cm}{PS}{\strut} &
\begin{XyMcompd}(700,500)(250,200){}{}
\sixheterov[%
{a{\adddbcolor{v}{\green}}}{b{\adddbcolor{v}{\red}}}%
{c{\adddbcolor{v}{\green}}}{d{\adddbcolor{v}{\red}}}%
{e{\adddbcolor{v}{\green}}}{f{\adddbcolor{v}{\red}}}%
]{2==N;3==N}{2==COOEt;3==COOEt}[ac]
\end{XyMcompd}
& \reactrarrow{0pt}{1cm}{PP}{\strut} &
\begin{XyMcompd}(700,500)(250,200){}{}
\sixheterov[e]{2==N;3==N}{2==COOEt;3==COOEt}
```



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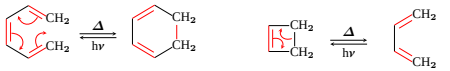
```
\noalign{\vskip10pt}
\compd\label{cpd:fourdine} \\
1,3-butadiene \\
\end{tabular}
\\
$\Delta H^{\circ} = \mathrm{-9.7~kcal\cdot mol^{-1}}$
\end{center}
\end{minipage}
\end{center}
```

Electrocyclic Reactions



40-1 *cis*-1,3,5-hexatriene

40-2 1,3-cyclo hexadiene

$\Delta H^\circ = -14.5$ kcal · mol^{-1}

40-3 cyclobutene

40-4 1,3-butadiene

$\Delta H^\circ = -9.7$ kcal · mol^{-1}

□

40.1.3 Vitamin B_2 and Related Compounds

Riboflavin (Vitamin B_2) has a benzene-fused 1,3,5,8-tetrazanaphthalene nucleus, which is attached by one ribose unit (colored in red). Flavin mononucleotide (FMN) and flavin adenine dinucleotide (FAD) are derived from riboflavin by introducing phosphate or pyrophosphate linkage.

Example 40.3. The total scheme of derivations is drawn by using the LaTeX quote environment:

```
\begin{quote}
\changeunitlength{0.08pt}
\def\thinLineWidth{0.8pt}
\let\substfont=\sffamily
\begin{tabular}{c}
\begin{XyMcompd}(1500,1450)(50,-550){}{}
\decaheterov[ej%
{b{\sixfusev[ace]{}{2==CH$_{3}$;3==CH$_{3}${E}}}%
]{1==N;4==N;5==N;7==HN}{6D==O;8D==O;%
4==\addbscolor{\red}{\sixheterov{}{1==(yl);4A==OH;5A==HO;6A==HO;3==OH}[ab]}}
\end{XyMcompd} \\
\compd\label{cpd:riboflavin} \\
riboflavin (Vitamin B$_{2}$) \\
\end{tabular}
\reactrarrow{0pt}{1cm}{}{}
\begin{tabular}{c}
\begin{XyMcompd}(1500,1450)(50,-550){}{}
\decaheterov[ej%
{b{\sixfusev[ace]{}{2==CH$_{3}$;3==CH$_{3}${E}}}%
]{1==N;4==N;5==N;7==HN}{6D==O;8D==O;%
4==\addbscolor{\red}{\sixheterov{}{1==(yl);4A==OH;5A==HO;6A==HO;%
3==\bluex{\ryl(3==O){4==%
\tetrahedral{2==(yl);0==P;1D==O;4==OH;3==O$^{-}$Na$^{+}$}}}%
}[ab]}}
\end{XyMcompd} \\
\compd\label{cpd:flavinFMN} \\
flavin mononucleotide (FMN) \\
\end{tabular}
\\[10pt]
```

Electrocyclic Reactions

13 *cis*-1,3,5-hexatriene

14 1,3-cyclo hexadiene

$\Delta H^\circ = -14.5$ kcal · mol^{-1}

15 cyclobutene

16 1,3-butadiene

$\Delta H^\circ = -9.7$ kcal · mol^{-1}

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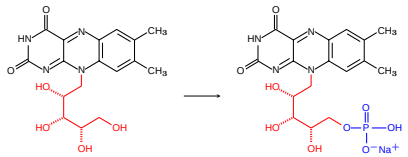
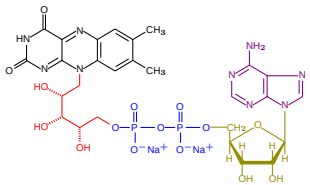
```
\mbox{}\hfill
\rule[12pt]{0.4pt}{3cm}\reactrarrow{10pt}{1cm}{}{}
\hskip1cm
\begin{tabular}{c}
\begin{XyMcompd}(2850,1750)(50,-850){}{}
\decaheterov[ej%
{b{\sixfusev[ace]{}{2==CH$_{3}$;3==CH$_{3}${E}}}%
]{1==N;4==N;5==N;7==HN}{6D==O;8D==O;%
4==\addbscolor{\red}{\sixheterov{}{1==(yl);4A==OH;5A==HO;6A==HO;%
3==\bluex{\ryl(3==O){4==\tetrahedral{2==(yl);0==P;1D==O;3==O$^{-}$Na$^{+}$;%
4==\ryl(4==O){4==\tetrahedral{2==(yl);0==P;1D==O;3==O$^{-}$Na$^{+}$;%
4==\ryl(4==O\olivex{\sbond C\rlap{H\raisebox{1pt}{$_{2}$}}}){%
8==\addbscolor{\olive}{\fivesugarh{%
1s==\violetx{\put(0,300){%
\nonaheterov[begj]{1==N;3==N;5==N;7==N}{1==(yl);4==NH$_{2}$}}};%
1s==\PutBondLine(0,00)(0,300){0.8pt};%
5==O;%
1s==\WedgeAsSubst(0,0)(-3,-5){120};4s==\WedgeAsSubst(0,0)(3,-5){120};%
3s==\PutBondLine(-17,0)(307,0){2.8pt}%
}{4==(yl);1Sa==H;2Sb==H;2Sa==OH;3Sb==H;3Sa==OH;4Sa==H}
}}}}}}}[ab]}}
\end{XyMcompd} \\
\compd\label{cpd:flavinade} \\
flavin adenine dinucleotide (FAD) \\
\end{tabular}
\end{quote}
```



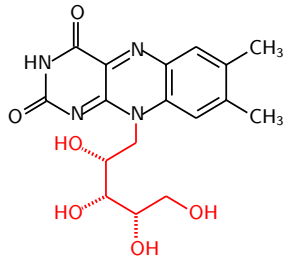
40-5
riboflavin (Vitamin B_2)

40-6
flavin mononucleotide (FMN)

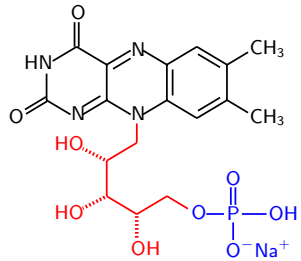


40-7
flavin adenine dinucleotide (FAD)

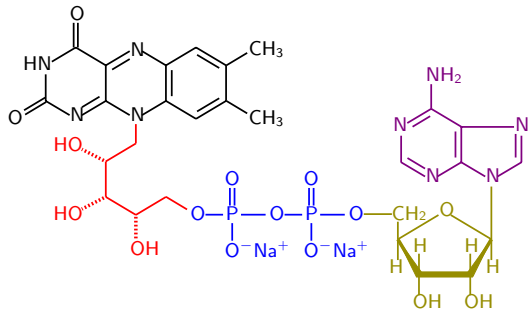
The structure **40-5** of riboflavin (Vitamin B_2) is drawn as such a benzene-fused 1,3,5,8-tetrazanaphthalene nucleus, where `\sixfusev` is declared in the ⟨atomlist⟩ of `\decaheterov` according to the addition tech-



17
riboflavin (Vitamin B_2)



18
flavin mononucleotide (FMN)



19
flavin adenine dinucleotide (FAD)

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```
}{6A==\null}{D}[bc]}}
]{}{1GA==H}{D}}}
]{}{2FB==\null;3GA==H}{D}%
}}]{}{}{C}[def]}}]{}{}{D}[ab]}}]{}{5A==HO}
\end{XyMcompd}
}
```

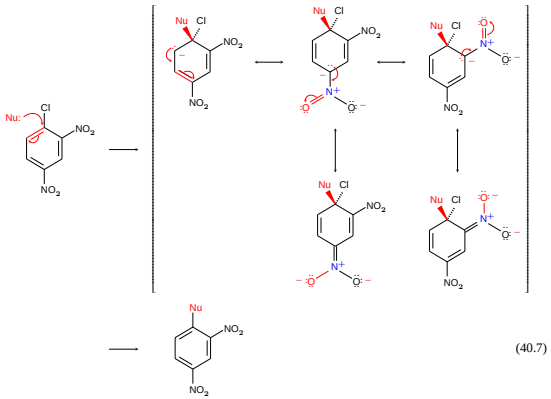
By using these macros, Fig. 40.1 is drawn by the following code:

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

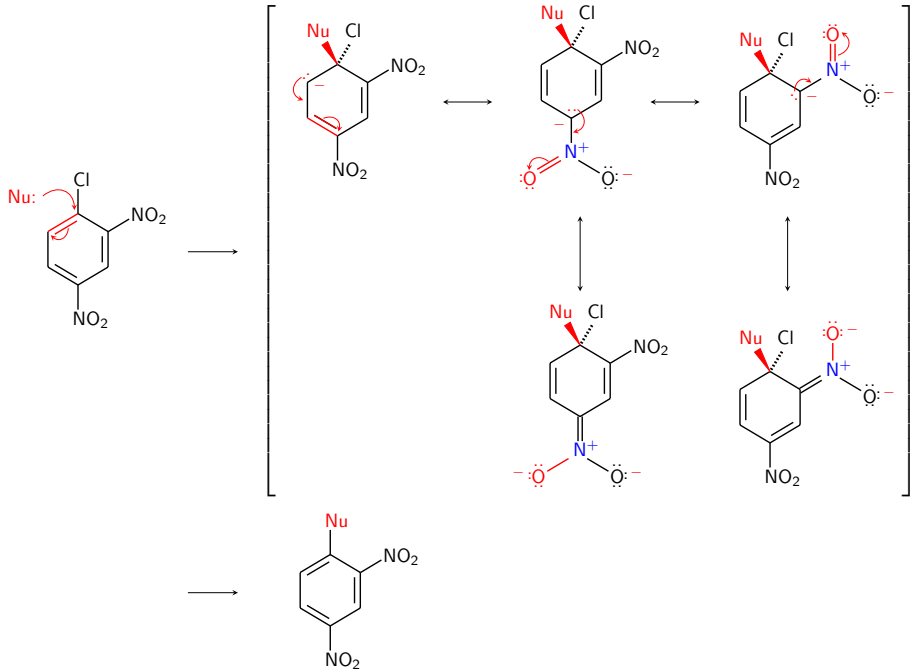
□

40.3.2 Nucleophilic Reactions

Example 40.13. A nucleophilic substitution of 1-chloro-2,4-dinitrobenzene is represented by Eq. 40.7, where curved arrows for representing electron shifts are colored in red.



(40.7)



(3)

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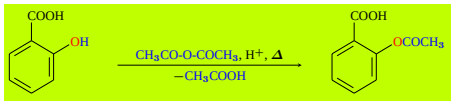
```
\reactrarrow{-10pt}{5cm}{\bluex{CH$_{3}$CO-O-COCH$_{3}$}, H$^{+}$, $\Delta$}%
{$-$\bluex{CH$_{3}$COOH}}
\qquad
\begin{XyMcompd}(750,650)(280,250){}{}
\benzenev{1==COOH;2==\redx{O}\bluex{COCH$_{3}$}}
\end{XyMcompd}}
\end{center}
```

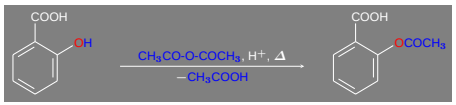
generates a colored box involving a reaction scheme:



□

Example 40.15. The default color of the ⟨text⟩ of `\colorbox` is black, unless other colors are specified, as found in the preceding output. The color of ⟨text⟩ can be changed freely. If the background color is selected to be dark, even `\white` can be declared to print ⟨text⟩. The following output is a typical example:

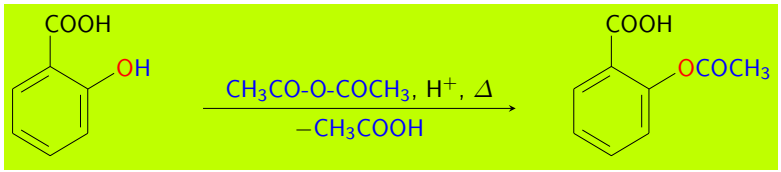
```
\begin{center}
\colorbox{gray}{\white%
\def\thinLineWidth{0.8pt}
\let\substfont=\sffamily
\sffamily
\begin{XyMcompd}(500,650)(280,250){}{}
\benzenev{1==COOH;2==\redx{O}\bluex{H}}
\end{XyMcompd}
\qquad
\reactrarrow{-10pt}{5cm}{\bluex{CH$_{3}$CO-O-COCH$_{3}$}, H$^{+}$, $\Delta$}%
{$-$\bluex{CH$_{3}$COOH}}
\qquad
\begin{XyMcompd}(750,650)(280,250){}{}
\benzenev{1==COOH;2==\redx{O}\bluex{COCH$_{3}$}}
\end{XyMcompd}}
\end{center}
```

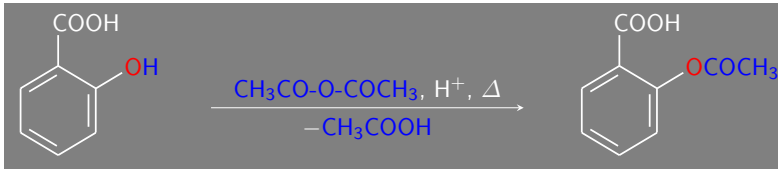


□

Example 40.16. A reaction scheme in the `ChemEquation` environment is surrounded by the `minipage` environment, the width of which is selected to be equal to the text width of your document. The `\colorbox` puts a space around the text of ⟨text⟩, where the space is adopted to be equal to `\fboxsep` (default value 3pt) of the LaTeX-command `\fbox`. Hence, you should declare `\fboxsep=0pt` to avoid the overfull warning.

```
\noindent
{\fboxsep=0pt
\colorbox{pink}{%
\begin{minipage}{\textwidth}
\begin{ChemEquation}
\begin{XyMcompd}(500,650)(280,250){}{}
\benzenev{1==COOH;2==\redx{O}\bluex{H}}
```





Summary

1. The XƎMTEX version 5.01 has recently been released.
2. A comprehensive on-line manual is now available.
3. The XƎMTEX system combined with the TEX/LATEX system has supported publication of interdisciplinary books linking chemistry and mathematics.