XΥMTEX (Version 4.05) for Typesetting Chemical Structural Formulas: A. Lewis Structures Drawn by the **lewisstruc** Package.

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Chapter 1

Introduction

1.1 History

The history of the XΥMTEX system is summarized in Table 1.1:

Table 1.1: Versions of XΥMTEX

version	package files and comments
1.00 (1993)	(for LaTeX2.09) See Ref. [1, 2]. aliphat.sty, carom.sty, lowcycle.sty, hetarom.sty, hetaromh.sty, hcycle.sty, chemstr.sty, locant.sty, xymtex.sty
1.01 (1996)	(for LaTeX 2_ε) See Ref. [3]. ccycle.sty, polymers.sty, chemist.sty
1.02 (1998)	(not released) Nested substitution by 'yl'-function.
2.00 (1998)	Enhanced version based on the XΥM Notation. See Ref. [4, 5]. fusering.sty, methylen.sty
2.01 (2001)	(not released) Size reduction, sizeredc.sty (version 1.00)
3.00 (2002)	Size reduction (sizeredc.sty, version 1.01), and reconstruction of the command system. See Ref. [6]
4.00 (2002)	(not released) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00)
4.01 (2004)	PostScript printing and length-variable central atoms [7]
4.02 (2004)	PostScript printing and wedges bonds for stereochemistry [8]
4.03 (2005)	PostScript printing and wavy bonds for stereochemistry [8]
4.04 (2009)	Macros for drawing steroids (steroid.sty, ver 1.00) [9]
4.05 (2009)	(The present version) New macros for drawing Lewis structures of the lewissturc package (lewisstruc.sty, version 1.00), revised and improved macros added to the chemist package (ver 4.05) [and the chmst-ps package (ver 1.02)], and the first release of the chemtimes package (ver 1.00)

Among the new matters of the XΥMTEX system (version 4.05) summarized in Table 1.1, this manual is concerned with macros for drawing Lewis structures of the lewissturc package (lewisstruc.sty, version 1.00).

1.2   Use of the **lewisstruc** Package

Because the lewisstruc package is part of the X͞yͪMͪTEX system, it is automatically loaded when the X͞yͪMͪTEX system is loaded by declaring ¥usepackage{xymtexps} (PostScript-compatible mode) or ¥usepackage {xymtex} (TEX/LATEX mode) in the preamble of a document to be typeset. The following template shows a typical description for loading the X͞yͪMͪTEX system including the lewisstruc package.

```
%Test405A.tex
¥documentclass{article}
¥usepackage{xymtexps}%loading the XyMTeX system (involving lewisstruc.sty)
¥usepackage{chemist,chmst-ps}%loading of the chemist package (not requisite)
¥begin{document}
(text)
¥end{document}
```

The tex file named Test405A.tex (stored in the c:¥fujita directory for example) is processed by LATEX 2$_\varepsilon$, where the following command is input in a command line (e.g., in the command-prompt window of Windows XP).

```
c>¥fujita latex Test405A
```

The resulting DVI file (Test405A.dvi) is then converted into a PostScript file by using dvips(k):

```
c>¥fujita dvipsk -D2400 -Pdl Test405A
```

Thereby, you are able to obtain Test405.ps as a PostScript file, which can be browsed by means of GSview/GhostScript.

Alternatively, the PostScript file (Test405.ps) is further converted into a PDF file by using Adobe Distiller. The resulting PDF file (Test405.pdf) can be browsed by Adobe Reader.

Note: This document uses the ¥ symbol to show each control sequence according to Japanese encoding. For example, the above template is transformed into the one with non-Japanese encoding, as follows:

```
%Test405A.tex
\documentclass{article}
\usepackage{xymtexps}%loading the XyMTeX system (involving lewisstruc.sty)
\usepackage{chemist,chmst-ps}%loading of the chemist package (not requisite)
\begin{document}
(text)
\end{document}
```

1.3   Recent Books Citing the X͞yͪMͪTEX System

Recent books on LATEX 2$_\varepsilon$ have referred to the X͞yͪMͪTEX system, e.g., pages 520–540 of [10] and pages 551–598 of Vol. II of [11].

Chapter 2

Lone Pairs and Radicals

2.1 Basic Commands for Drawing Lone Pairs

The command ¥overpair supported by the lewisstruc package (included in the X$^{I\!M}$MT$_{E}$X system) draws a lone pair over an atom specified by its argument, while the command ¥underpair draws a lone pair under an atom specified by its argument. They can be nested freely, as follows:

```
single usage: ¥overpair{O} ¥underpair{N} ¥qquad
nested usage: ¥underpair{¥overpair{O}} ¥overpair{¥underpair{N}}
```

single usage: Ö Ṇ   nested usage: Ö̤ Ṇ̈

The ¥LewisSbond command draws a lone pair in the form of a semicolon. The Lewis structures of hydrogen fluoride and water are typeset as follows:

```
HF ¥qquad H¥LewisSbond¥overpair{¥underpair{F}}¥LewisSbond{} ¥qquad
H¥sbond¥overpair{¥underpair{F}}¥LewisSbond{} ¥¥[5pt]
¥chemform{H_{2}O} ¥qquad
H¥LewisSbond¥overpair{¥underpair{O}}¥LewisSbond{}H ¥qquad
H¥sbond¥overpair{¥underpair{O}}¥sbond{}H
```

HF   H:F̈:   H——F̈:

H$_2$O   H:Ö:H   H——Ö——H

The command ¥lonepairA is capable of drawing at most four lone pairs, the positions of which are specified by its optional argument. The numbering of the four lone pairs is shown as follows:

$$4 \; :\ddot{\underset{3}{\overset{1}{O}}}: \; 2$$

where a set of numbers for drawing lone pairs (e.g., 124 etc. in an ascending order) is given as an optional argument. A list of such modes of numbering is summarized in the following example:

```
¥lonepairA{O} ¥qquad
¥lonepairA[1234]{O} ¥qquad ¥lonepairA[123]{O} ¥qquad
¥lonepairA[124]{O} ¥qquad ¥lonepairA[134]{O} ¥qquad
¥lonepairA[234]{O} ¥¥[5pt]
¥lonepairA[12]{O} ¥qquad ¥lonepairA[13]{O} ¥qquad
¥lonepairA[14]{O} ¥qquad ¥lonepairA[23]{O} ¥qquad
¥lonepairA[24]{O} ¥qquad ¥lonepairA[34]{O} ¥¥[5pt]
¥lonepairA[1]{O} ¥qquad¥lonepairA[2]{O} ¥qquad
¥lonepairA[3]{O} ¥qquad ¥lonepairA[4]{O} ¥qquad
¥lonepairA[5]{O}
```

:Ö: :Ö: Ö: :Ö: :Ö   :Ọ:

Ö: Ọ   :Ö   Ọ: :O: :Ọ

Ö   O: Ọ   :O   :Ö:

An element represented by two alphabets (e.g., Ne) can be attached by four lone pairs by using the ¥lonepairA command. Thus, the command ¥lonepairA[1234]{Ne} outputs :N̈e: properly.

By using the command ¥lonepairA, the Lewis structures of hydrogen fluoride and water are alternatively typeset as follows:

```
HF ¥qquad H¥LewisSbond¥lonepairA[123]{F}
¥qquad H¥sbond¥lonepairA[123]{F} ¥¥[5pt]
¥chemform{H_{2}O} ¥qquad
H¥LewisSbond¥lonepairA[13]{O}¥LewisSbond{}H ¥qquad
H¥sbond¥lonepairA[13]{O}¥sbond{}H
```

HF   H:F̈:   H——F̈:

H$_2$O   H:Ö:H   H——Ö——H
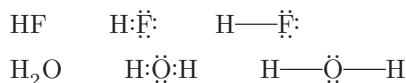
An atom with lone pairs (drawn by ¥lonepairA) can be incorporated in a structural formula due to the X$^{\Upsilon}_{\!M}$MTEX system. The following example shows benzene derivatives with hydroxyl substituents, which contain lone pairs by means of ¥lonepairA.

```
¥bzdrv[l]{1==¥lonepairA[14]{O}H;4==¥lonepairA[34]{O}H}
¥bzdrv[r]{1==¥lmoiety{H¥lonepairA[12]{O}};4==¥lmoiety{H¥lonepairA[23]{O}}}
¥bzdrv[A]{2==¥lonepairA[13]{O}H}
¥bzdrv{2==¥lonepairA[13]{O}¥LewisSbond{}H}
```
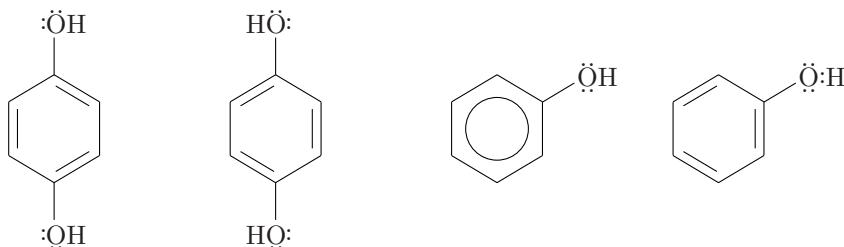
Although lone pairs of heterocyclic compounds are usually abbreviated in organic chemistry, they participate in nucleophilic reactions as neceophiles. To show such participation explicitly, lone pairs are drawn by ¥lonepairA as follows:

```
¥furanv{}
¥fiveheterov[bd]{1==¥lonepairA[13]{O}}{}
¥pyridinev{}
¥sixheterov[ace]{1==¥lonepairA[1]{N}}{}
```
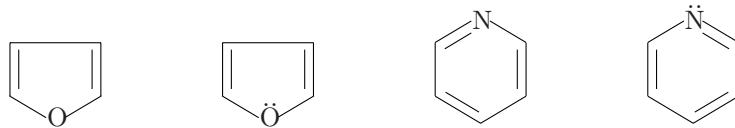
The command ¥lonepairB is capable of drawing at most four lone pairs in an alternative mode, where the positions of selected lone pairs are specified by its optional argument. The numbering of the four lone pairs is shown as follows:

$$\begin{matrix} 4 & & 1 \\ & :\ddot{O}: & \\ 3 & & 2 \end{matrix}$$

where a set of numbers for drawing lone pairs (e.g., 124 etc.) is given as an optional argument. A list of such modes of numbering is summarized in the following example:

```
¥lonepairB{O} ¥qquad
¥lonepairB[1234]{O} ¥qquad ¥lonepairB[123]{O} ¥qquad
¥lonepairB[124]{O} ¥qquad ¥lonepairB[134]{O} ¥qquad
¥lonepairB[234]{O} ¥¥[5pt]
¥lonepairB[12]{O} ¥qquad ¥lonepairB[13]{O} ¥qquad
¥lonepairB[14]{O} ¥qquad ¥lonepairB[23]{O} ¥qquad
¥lonepairB[24]{O} ¥qquad ¥lonepairB[34]{O} ¥¥[5pt]
¥lonepairB[1]{O} ¥qquad¥lonepairB[2]{O} ¥qquad
¥lonepairB[3]{O} ¥qquad ¥lonepairB[4]{O} ¥qquad
¥lonepairB[5]{O}
```

:Ö: :Ö: .Ö: ˙Ö: :Ö˙   :Ö.

Ö: .Ö˙   ˙Ö˙   .Ö.   ˙Ö.   :Ö

Ö˙   Ö.   .Ö   ˙Ö   :Ö:
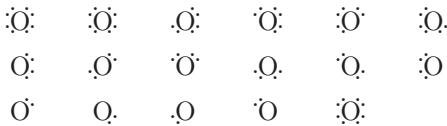
An atom with lone pairs (drawn by ¥lonepairB) can also be incorporated in a structural formula due to the XΥMTEX system. The following example shows formaldehyde derivatives with a carbonyl oxygen, which contains lone pairs by means of ¥lonepairB.

```
¥Ltrigonal{0==C;1D==¥lonepairB[12]{O};2==H;3==H} ¥qquad
¥Rtrigonal{0==C;1D==¥lonepairB[34]{O};2==H;3==H} ¥qquad
¥Utrigonal{0==C;1D==¥lonepairB[23]{O};2==H;3==H} ¥qquad
¥Dtrigonal{0==C;1D==¥lonepairB[14]{O};2==H;3==H}
```
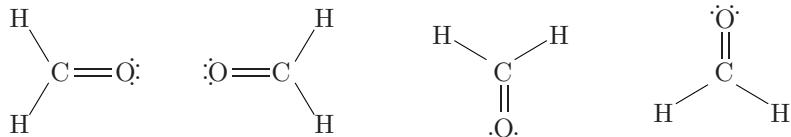

2.2   Basic Commands for Drawing Radicals

In analogy to the command ¥lonepairA, the command ¥chemradicalA is capable of drawing at most four electrons (dots), the positions of which are specified by its optional argument. The numbering of the four electrons is shown as follows:

$$4 \cdot \overset{1}{\underset{3}{\dot{O}}} \cdot 2$$

where a set of numbers for drawing unpaired electrons (e.g., 124 etc. in an ascending order) is given as an optional argument. A list of such modes of numbering is summarized in the following example:

```
¥chemradicalA{O} ¥qquad ¥chemradicalA[1234]{O} ¥qquad
¥chemradicalA[123]{O} ¥qquad ¥chemradicalA[124]{O} ¥qquad
¥chemradicalA[134]{O} ¥qquad ¥chemradicalA[234]{O} ¥¥[5pt]
```

```
¥chemradicalA[12]{O} ¥qquad ¥chemradicalA[13]{O} ¥qquad
¥chemradicalA[14]{O} ¥qquad ¥chemradicalA[23]{O} ¥qquad
¥chemradicalA[24]{O} ¥qquad ¥chemradicalA[34]{O} ¥¥[5pt]
¥chemradicalA[1]{O} ¥qquad ¥chemradicalA[2]{O} ¥qquad
¥chemradicalA[3]{O} ¥qquad ¥chemradicalA[4]{O} ¥qquad
¥chemradicalA[5]{O} ¥qquad
```

·Ö·   ·Ȯ·   Ȯ·   ·Ö·   ·Ö   ·Ö·

Ȯ·   Ö   ·Ȯ   Ö·   ·Ö·   ·Ö

Ö   Ö·   Ö   ·Ö   ·Ȯ·
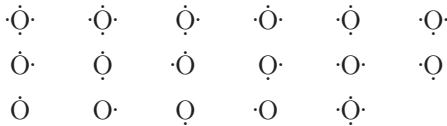
A Lewis structure of acetylene is drawn by using the ¥chemradicalA command.

```
¥begin{ChemEquation}
¥chemradicalA[2]{H} ¥quad ¥chemradicalA[1234]{C} ¥quad
¥chemradicalA[1234]{C} ¥quad ¥chemradicalA[4]{H} ¥quad
¥rightarrow ¥quad
H¥sbond¥chemradicalA[13]{C}¥sbond¥chemradicalA[13]{C}¥sbond{}H
¥quad = ¥quad H¥sbond{}C¥tbond{}C¥sbond{}H
¥end{ChemEquation}
```

$$\text{H· ·Ċ· ·Ċ· ·H} \quad \rightarrow \quad \text{H——Ċ——Ċ——H} \quad = \quad \text{H——C≡C——H} \qquad (2.1)$$
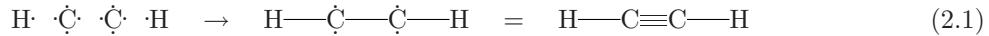
Note the ChemEquation environment is supported by the chemist package.

In analogy to the command ¥lonepairB, the command ¥chemradicalB is capable of drawing at most four electrons (dots), the positions of which are specified by its optional argument. The numbering of the four electrons is shown as follows:

$$\overset{4 \quad \cdot \quad 1}{\underset{3 \quad \cdot \quad 2}{:\!O\!:}}$$

where a set of numbers for drawing electrons (e.g., 124 etc. in an ascending order) is given as an optional argument. A list of such modes of numbering is summarized in the following example:

```
¥chemradicalB{O} ¥qquad ¥chemradicalB[1234]{O} ¥qquad
¥chemradicalB[123]{O} ¥qquad ¥chemradicalB[124]{O} ¥qquad
¥chemradicalB[134]{O} ¥qquad ¥chemradicalB[234]{O} ¥¥[5pt]
¥chemradicalB[12]{O} ¥qquad ¥chemradicalB[13]{O} ¥qquad
¥chemradicalB[14]{O} ¥qquad ¥chemradicalB[23]{O} ¥qquad
¥chemradicalB[24]{O} ¥qquad ¥chemradicalB[34]{O} ¥¥[5pt]
¥chemradicalB[1]{O} ¥qquad ¥chemradicalB[2]{O} ¥qquad
¥chemradicalB[3]{O} ¥qquad ¥chemradicalB[4]{O} ¥qquad
¥chemradicalB[5]{O} ¥qquad
```

:O: :O: .O: :O.   :O   O:

O: .O: .O.   .O   .O   O

O.   O.   .O   O.   .O:
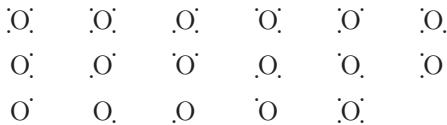
A Lewis structure of ethylene is drawn by using the ¥chemradicalB command, where the first structure is drawn by using the picture environment of the native LATEX 2ε.

```
¥begin{ChemEquation}
¥raisebox{-18pt}{¥unitlength=0.1pt
¥begin{picture}(425,380)(-103,-171)
¥put(-103,171){¥chemradicalB[2]{H}}
¥put(-103,-171){¥chemradicalB[1]{H}}
```

```
¥put(0,0){¥chemradicalB{C}}
¥put(200,0){¥chemradicalB{C}}
¥put(303,171){¥chemradicalB[3]{H}}
¥put(303,-171){¥chemradicalB[4]{H}}
¥end{picture}} ¥qquad
¥rightarrow
¥raisebox{-28pt}{%
¥Ltrigonal{0==¥chemradicalB[2]{C};2==H;3==H;%
1==¥Rtrigonal{0==¥chemradicalB[3]{C};1==(yl);2==H;3==H}}}
¥qquad¥qquad = ¥qquad
¥raisebox{-28pt}{¥ethylene{}{1==H;2==H;3==H;4==H}}
¥end{ChemEquation}
```

$$\begin{array}{ccccc} \overset{\cdot}{H} \quad \overset{\cdot}{H} & & H \qquad H & & H \qquad H \\ \overset{\cdot\cdot}{\underset{\cdot\cdot}{C}} \ \ \overset{\cdot\cdot}{\underset{\cdot\cdot}{C}} & \rightarrow & \diagdown C — \overset{\cdot}{C} \diagup & = & \diagdown C = C \diagup \\ \overset{\cdot}{H} \quad \overset{\cdot}{H} & & H \qquad H & & H \qquad H \end{array} \qquad (2.2)$$

2.3   Lewis Structures

2.3.1   Atoms with an Atom through a Lone Pair

The command ¥overpairover{A}{B} is used to draw an atom (A) attached upward by another atom (B) through a lone pair, while the command ¥underpairunder{A}{B} is used to draw an atom (A) attached downward by another atom (B) through a lone pair. These commands can be nested freely.

```
--- ¥overpairover{A}{B} ¥qquad ¥underpairunder{A}{B} ¥qquad
¥underpairunder{¥overpairover{A}{B}}{X} ¥qquad
¥overpairover{¥underpairunder{A}{B}}{X} ---
```

$$— \overset{B}{\underset{}{\ddot{A}}} \qquad \overset{}{\underset{\ddot{B}}{A}} \qquad \overset{B}{\underset{X}{\ddot{A}}} \qquad \overset{X}{\underset{B}{\ddot{A}}} —$$
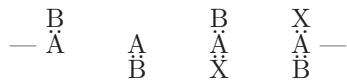
Such nested usage of these commands allows us to draw Lewis structures of methane and ammonia, as follows:

```
H¥LewisSbond¥underpairunder{¥overpairover{C}{H}}{H}¥LewisSbond{}H ¥qquad
H¥LewisSbond¥overpairover{¥underpair{N}}{H}¥LewisSbond{}H
```

$$\begin{array}{cc} \overset{H}{\underset{\ddot{H}}{H \! : \! \ddot{C} \! : \! H}} & \overset{H}{H \! : \! \ddot{N} \! : \! H} \end{array}$$

The command ¥leftlonepairover{A}{B} is used to draw an atom (A) attached by another atom (B) through a lone pair in the northwest direction, while the command ¥rightlonepairover{A}{B} is used to draw an atom (A) attached by another atom (B) through a lone pair in the northeast direction. These commands can be nested freely.

```
--- ¥leftlonepairover{A}{B} ¥qquad
¥rightlonepairover{A}{B} ¥qquad
¥rightlonepairover{¥leftlonepairover{A}{B}}{X} ¥qquad
¥leftlonepairover{¥rightlonepairover{A}{B}}{X} ---
```

$$— \overset{B\cdot}{\underset{}{A}} \qquad \overset{\cdot B}{\underset{}{A\cdot}} \qquad \overset{B\cdot \ X}{\underset{}{\cdot A \cdot}} \qquad \overset{X\cdot \ B}{\underset{}{\cdot A \cdot}} —$$
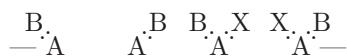
Downward counterparts of these commands are also supported by the lewisstruc package. Thus, the command ¥leftlonepairunder{A}{B} is used to draw an atom (A) attached by another atom (B) through a lone pair in the southwest direction, while the command ¥rightlonepairunder{A}{B} is used to draw an atom (A) attached by another atom (B) through a lone pair in the southeast direction. These commands can be nested freely.

```
--- ¥leftlonepairunder{A}{B} ¥qquad
¥rightlonepairunder{A}{B} ¥qquad
¥rightlonepairunder{¥leftlonepairunder{A}{B}}{X} ¥qquad
¥leftlonepairunder{¥rightlonepairunder{A}{B}}{X} ---
```

—.A   A.   .A.   .A.—
   B   B   B X   X   B

These upward-type and downward-type commands can be nested freely, as exemplified by the following outputs:

```
--- ¥rightlonepairunder{¥leftlonepairover{A}{B}}{X} ¥qquad
¥leftlonepairover{¥leftlonepairunder{A}{B}}{X} ¥qquad
¥rightlonepairover{¥rightlonepairunder{¥leftlonepairover{A}{B}}{X}}{Y} ¥qquad
¥leftlonepairunder{¥rightlonepairover{%
¥rightlonepairunder{¥leftlonepairover{A}{B}}{X}}{Y}}{Z} ---
```

   B.   X.   B. Y   B. Y
—.A.   .A   .A.   .A.—
    X   B   X   Z   X
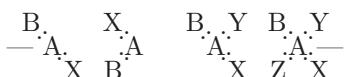
2.3.2   Tetrahedral Lewis Structures

The command ¥LewistetrahedralA is capable of drawing at most four atoms through lone pairs, where the positions of selected atoms with lone pairs are specified by its optional argument. The numbering of the four atoms with lone pairs is shown as follows:

$$4\!:\!\overset{\displaystyle 1}{\underset{\displaystyle 3}{\ddot{C}}}\!:\!2$$

Following examples show the applicability of the command ¥LewistetrahedralA.

```
¥LewistetrahedralA{0==C;1==A;2==B;3==X;4==Y} ¥qquad¥qquad
¥LewistetrahedralA{0==C;1==A;2==B;3==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;1==A;2==B;4==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;1==A;3==Y;4==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;2==B;3==Y;4==X} ¥¥[15pt]
¥LewistetrahedralA{0==C;1==A;2==B} ¥qquad¥qquad
¥LewistetrahedralA{0==C;1==A;3==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;1==A;4==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;2==B;3==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;2==B;4==X} ¥qquad¥qquad
¥LewistetrahedralA{0==C;3==Y;4==X} ¥¥[15pt]
¥LewistetrahedralA{0==C;1==A} ¥qquad¥qquad
¥LewistetrahedralA{0==C;2==B} ¥qquad¥qquad
¥LewistetrahedralA{0==C;3==B} ¥qquad¥qquad
¥LewistetrahedralA{0==C;4==B}
```

$$
\begin{array}{cccccc}
& A & & A & & A \\
Y\colon\!\ddot{C}\colon\!B & & \ddot{C}\colon\!B & & X\colon\!\ddot{C}\colon\!B & & X\colon\!\ddot{C} & & X\colon\!\ddot{C}\colon\!B \\
X & & X & & & & Y & & Y
\end{array}
$$

A·Ċ·H etc. — (top rows of Lewis structures)

A
Ċ:B

A
Ċ
X

X:Ċ

Ċ:B
X

X:C:B

X:Ċ
Y

A
Ċ

C:B

C
B

B:C

A Lewis structure of methane is drawn by using the **¥Lewistetrahedral A** command. The first structure is drawn by using the array environment of the native LaTeX 2ε, where **¥chemradicalA** commands are used to draw component radical structures.

```
¥begin{ChemEquation}
¥begin{array}{ccc}
& ¥chemradicalA[3]{H} & ¥¥[5pt]
¥chemradicalA[2]{H} & ¥chemradicalA[1234]{C} & ¥chemradicalA[4]{H} ¥¥[5pt]
& ¥chemradicalA[1]{H} & ¥¥
¥end{array}
¥quad ¥rightarrow ¥quad
¥LewistetrahedralA{0==C;1==H;2==H;3==H;4==H}
¥quad = ¥quad
¥raisebox{-28pt}{¥tetrahedral{0==C;1==H;2==H;3==H;4==H}}
¥end{ChemEquation}
```

$$
\begin{array}{ccc}
& \dot{H} & \\
H\cdot\ \ \cdot\dot{C}\cdot\ \ \cdot H & & \\
& \dot{H} &
\end{array}
\quad\rightarrow\quad
\begin{array}{c}
H \\
H\colon\!\ddot{C}\colon\!H \\
H
\end{array}
\quad=\quad
\begin{array}{c}
H \\
| \\
H\!-\!\!-\!C\!-\!\!-\!H \\
| \\
H
\end{array}
\tag{2.3}
$$
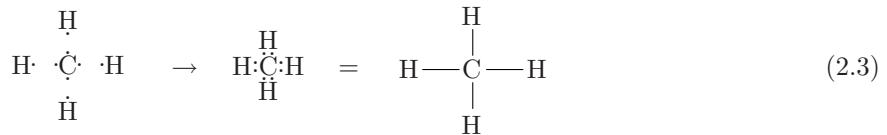
A Lewis structure of ammonia is also drawn by using the **¥Lewistetrahedral A** command. The first structure is drawn by using the array environment of the native LaTeX 2ε, where **¥chemradicalA** commands are used to draw component radical structures. When inner math modes may cause troubles, the use of the **¥mbox** command is sometimes useful as follows:

```
¥begin{ChemEquation}
¥raisebox{8pt}{%
$¥begin{array}{ccc}
& ¥chemradicalA[3]{H} & ¥¥[5pt]
¥chemradicalA[2]{H} & ¥chemradicalA[124]{¥underpair{N}} & ¥chemradicalA[4]{H} ¥¥
¥end{array}$}
¥quad ¥rightarrow ¥quad
¥mbox{¥LewistetrahedralA{0==¥underpair{N};1==H;2==H;4==H}}
¥quad = ¥quad
¥raisebox{-28pt}{¥tetrahedral{0==¥underpair{N};1==H;2==H;4==H}}
¥end{ChemEquation}
```

$$
\begin{array}{c}
\dot{H} \\
H\cdot\ \ \cdot\ddot{N}\cdot\ \ \cdot H
\end{array}
\quad\rightarrow\quad
\begin{array}{c}
H \\
H\colon\!\ddot{N}\colon\!H
\end{array}
\quad=\quad
\begin{array}{c}
H \\
| \\
H\!-\!\!-\!\ddot{N}\!-\!\!-\!H
\end{array}
\tag{2.4}
$$
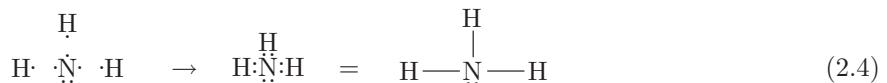
The command **¥LewistetrahedralB** is capable of drawing at most four atoms through lone pairs in an alternative mode, where the positions of selected atoms with lone pairs are specified by its optional argument. The numbering of the four atoms with lone pairs is shown as follows:

$$\overset{4\ \ 1}{\underset{3\ \ 2}{\cdot\dot{C}\cdot}}$$

The following examples show the applicability of the command ¥LewistetrahedralB.

```
¥LewistetrahedralB{0==C;1==A;2==B;3==X;4==Y} ¥qquad¥qquad
¥LewistetrahedralB{0==C;1==A;2==B;3==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;1==A;2==B;4==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;1==A;3==Y;4==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;2==B;3==Y;4==X} ¥¥[15pt]
¥LewistetrahedralB{0==C;1==A;2==B} ¥qquad¥qquad
¥LewistetrahedralB{0==C;1==A;3==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;1==A;4==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;2==B;3==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;2==B;4==X} ¥qquad¥qquad
¥LewistetrahedralB{0==C;3==Y;4==X} ¥¥[15pt]
¥LewistetrahedralB{0==C;1==A} ¥qquad¥qquad
¥LewistetrahedralB{0==C;2==B} ¥qquad¥qquad
¥LewistetrahedralB{0==C;3==B} ¥qquad¥qquad
¥LewistetrahedralB{0==C;4==B}
```

In some cases, ¥LewistetrahedralB is incapable of accepting a substituent derived from such a command as ¥lonepairB. To avoid troubles of this type, a rather dirty technique using ¥setbox may be effective, as shown in the following example.

```
¥begingroup
¥fboxrule=0pt¥fboxsep=1pt
¥setbox0=¥hbox{¥lonepairB[234]{¥fbox{¥kern0.6pt F}}}
¥setbox1=¥hbox{¥lonepairB[134]{¥fbox{¥kern0.6pt F}}}
¥setbox2=¥hbox{¥lonepairA[123]{¥kern0.6pt F¥kern0.6pt}}
¥setbox3=¥hbox{¥LewistetrahedralA{0==B;2==¥box2}}
¥LewistetrahedralB{0==¥box3;3==¥raise1pt¥box0¥kern-1pt;4==¥lower2pt¥box1¥kern-1pt}
¥endgroup
```

The following examples show the difference between ¥LewistetrahedralA and ¥lonepairA as well as the difference between ¥LewistetrahedralB and ¥lonepairB.

```
¥LewistetrahedralA{0==C;1=={};2=={};3=={};4=={}}␣¥quad
¥LewistetrahedralA{0==C;1=={␣};2=={␣};3=={␣};4=={␣}}␣¥quad
¥lonepairA[1234]{C}␣¥¥[10pt]
¥LewistetrahedralB{0==C;1=={};2=={};3=={};4=={}}␣¥quad
¥LewistetrahedralB{0==C;1=={␣};2=={␣};3=={␣};4=={␣}}␣¥quad
¥lonepairB[1234]{C}
```

C   :Ċ: :Ċ:

C   :Ċ: :Ċ:
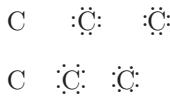
### 2.3.3 Nested Tetrahedral Lewis Structures

Because the command ¥Lewistetrahedral A is incapable of drawing nested structures, another approach should be taken to to avoid such drawback. For this purpose, the lewisstruc package of the XⓎMTEX system supports the command ¥LewisTetrahedralA, which has been defined in an alternative methodology based on the ¥tetrahedral command of the aliphat package of the XⓎMTEX system. This means that the argument of ¥LewisTetrahedralA is capable of accommodating a so-called (yl)-function which is widely adopted in the XⓎMTEX system. In addition, the argument of ¥LewisTetrahedralA supports an additional function, which gives us a tool of drawing two pairs of electrons for representing a double bond (D), three pairs of electrons for representing a triple bond (T), and a straight line for representing a single bond.

```
¥LewisTetrahedralA{0==C;1==A;2==B;3==X;4==Y}
¥LewisTetrahedralA{0==C;1==A;2N==B;3==X;4N==Y}
¥LewisTetrahedralA{0==C;1D==A;2D==B;3D==X;4D==Y}
¥LewisTetrahedralA{0==C;1T==A;2T==B;3T==X;4T==Y}
```

$$
\begin{array}{cccc}
\text{A} & \text{A} & \text{A} & \text{A} \\
\text{B:C:Y} & \text{B——C——Y} & \text{B::C::Y} & \text{B:::C:::Y} \\
\text{X} & \text{X} & \text{X} & \text{X}
\end{array}
$$
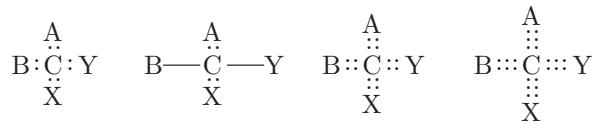
By declaring 2==(yl) in an inner ¥LewisTetrahedralA, a substituent is produced so as to be attached to the 4-position of an outer ¥LewisTetrahedralA. Thereby, the two tetrahedral Lewis structures are linked to each other as follows:

```
¥LewisTetrahedralA{0==C;1==A;2==B;3==X;%
4==¥LewisTetrahedralA{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralA{0==C;1==A;2==B;3==X;%
4D==¥LewisTetrahedralA{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralA{0==C;1==A;2==B;3==X;%
4T==¥LewisTetrahedralA{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralA{0==C;1==A;2==B;3==X;%
4N==¥LewisTetrahedralA{2==(yl);0==C;1==A;3==X;4==Y}}
```

$$
\begin{array}{cccc}
\text{A A} & \text{A A} & \text{A A} & \text{A A} \\
\text{B:C:C:Y} & \text{B:C::C:Y} & \text{B:C:::C:Y} & \text{B:C——C:Y} \\
\text{X X} & \text{X X} & \text{X X} & \text{X X}
\end{array}
$$

By declaring 4==(yl) in an inner ¥LewisTetrahedralA, another substituent is produced so as to be attached to the 2-position of an outer ¥LewisTetrahedralA. Thereby, the two tetrahedral Lewis structures are linked to each other as follows:

```
¥LewisTetrahedralA{0==C;1==A;4==B;3==X;%
2==¥LewisTetrahedralA{4==(yl);0==C;1==A;3==X;2==Y}}
¥LewisTetrahedralA{0==C;1==A;4==B;3==X;%
2D==¥LewisTetrahedralA{4==(yl);0==C;1==A;3==X;2==Y}}
```

```
\LewisTetrahedralA{0==C;1==A;4==B;3==X;%
2T==\LewisTetrahedralA{4==(yl);0==C;1==A;3==X;2==Y}}
\LewisTetrahedralA{0==C;1==A;4==B;3==X;%
2N==\LewisTetrahedralA{4==(yl);0==C;1==A;3==X;2==Y}}
```

$$\begin{array}{cccc}
\overset{\cdot\cdot}{A}\ \overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A}\ \overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A}\ \overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A}\qquad\ \overset{\cdot\cdot}{A} \\
Y\!:\!\overset{}{\underset{}{C}}\!:\!\overset{}{\underset{}{C}}\!:\!B & Y\!:\!\overset{}{\underset{}{C}}\!:\!\!:\!\overset{}{\underset{}{C}}\!:\!B & Y\!:\!\overset{}{\underset{}{C}}\!:\!\!:\!\!:\!\overset{}{\underset{}{C}}\!:\!B & Y\!:\!\overset{}{\underset{}{C}}\!\!-\!\!-\!\!\overset{}{\underset{}{C}}\!:\!B \\
\underset{\cdot\cdot}{X}\ \underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X}\ \underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X}\ \underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X}\ \underset{\cdot\cdot}{X}
\end{array}$$

Lewis structures of vertical linkage can be drawn in a similar way.

```
\LewisTetrahedralA{0==C;2==A;4==B;3==X;%
1==\LewisTetrahedralA{3==(yl);0==C;1==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;3==X;%
1D==\LewisTetrahedralA{3==(yl);0==C;1==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;3==X;%
1T==\LewisTetrahedralA{3==(yl);0==C;1==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;3==X;%
1N==\LewisTetrahedralA{3==(yl);0==C;1==A;4==X;2==Y}}
```

$$\begin{array}{cccc}
\overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A} & \overset{\cdot\cdot}{A} \\
Y\!:\!C\!:\!X & Y\!:\!C\!:\!X & Y\!:\!C\!:\!X & Y\!:\!C\!:\!X \\
A\!:\!C\!:\!B & A\!:\!C\!:\!B & A\!:\!C\!:\!B & A\!:\!C\!:\!B \\
\underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X} & \underset{\cdot\cdot}{X}
\end{array}$$

Another set of Lewis structures of vertical linkage can be drawn in a similar way.

```
\LewisTetrahedralA{0==C;2==A;4==B;1==X;%
3==\LewisTetrahedralA{1==(yl);0==C;3==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;1==X;%
3D==\LewisTetrahedralA{1==(yl);0==C;3==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;1==X;%
3T==\LewisTetrahedralA{1==(yl);0==C;3==A;4==X;2==Y}}
\LewisTetrahedralA{0==C;2==A;4==B;1==X;%
3N==\LewisTetrahedralA{1==(yl);0==C;3==A;4==X;2==Y}}
```

$$\begin{array}{cccc}
\overset{\cdot\cdot}{X} & \overset{\cdot\cdot}{X} & \overset{\cdot\cdot}{X} & \overset{\cdot\cdot}{X} \\
A\!:\!C\!:\!B & A\!:\!C\!:\!B & A\!:\!C\!:\!B & A\!:\!C\!:\!B \\
Y\!:\!C\!:\!X & Y\!:\!C\!:\!X & Y\!:\!C\!:\!X & Y\!:\!C\!:\!X \\
\underset{\cdot\cdot}{A} & \underset{\cdot\cdot}{A} & \underset{\cdot\cdot}{A} & \underset{\cdot\cdot}{A}
\end{array}$$

Because the command \Lewistetrahedral B is incapable of drawing nested structures, another approach should be taken to to avoid such drawback. For this purpose, the lewisstruc package of the X^MT_EX system supports the command \LewisTetrahedralB, which has been defined in an alternative methodology based on the \squareplanar command (renamed from \square) of the aliphat package of the X^MT_EX system. This means that the argument of \LewisTetrahedralB is capable of accommodating a so-called (yl)-function which is widely adopted in the X^MT_EX system. In addition, the argument of \LewisTetrahedralB supports an additional function, which gives us a tool of drawing two pairs of electrons for representing a double bond (D), three pairs of electrons for representing a triple bond (T), and a straight line for representing a single bond.

```
¥LewisTetrahedralB{0==C;1==A;2==B;3==X;4==Y}
¥LewisTetrahedralB{0==C;1==A;2N==B;3==X;4N==Y}
¥LewisTetrahedralB{0==C;1D==A;2D==B;3D==X;4D==Y}
¥LewisTetrahedralB{0==C;1T==A;2T==B;3T==X;4T==Y}
```
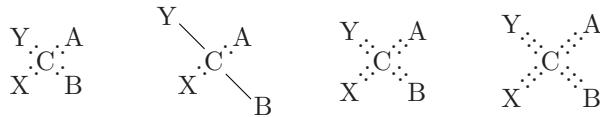
By declaring `2==(yl)` in an inner `¥LewisTetrahedralB`, a substituent is produced so as to be attached to the 4-position of an outer `¥LewisTetrahedralB`. Thereby, the two tetrahedral Lewis structures are linked to each other as follows:

```
¥LewisTetrahedralB{0==C;1==A;2==B;3==X;%
4==¥LewisTetrahedralB{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralB{0==C;1==A;2==B;3==X;%
4D==¥LewisTetrahedralB{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralB{0==C;1==A;2==B;3==X;%
4T==¥LewisTetrahedralB{2==(yl);0==C;1==A;3==X;4==Y}}
¥LewisTetrahedralB{0==C;1==A;2==B;3==X;%
4N==¥LewisTetrahedralB{2==(yl);0==C;1==A;3==X;4==Y}}
```
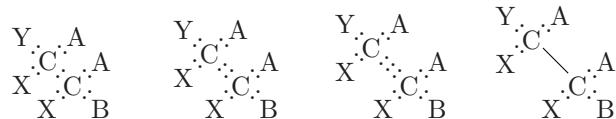
By declaring `4==(yl)` in an inner `¥LewisTetrahedralB`, another substituent is produced so as to be attached to the 2-position of an outer `¥LewisTetrahedralB`. Thereby, the two tetrahedral Lewis structures are linked to each other as follows:

```
¥LewisTetrahedralB{0==C;1==A;4==B;3==X;%
2==¥LewisTetrahedralB{4==(yl);0==C;1==A;3==X;2==Y}}
¥LewisTetrahedralB{0==C;1==A;4==B;3==X;%
2D==¥LewisTetrahedralB{4==(yl);0==C;1==A;3==X;2==Y}}
¥LewisTetrahedralB{0==C;1==A;4==B;3==X;%
2T==¥LewisTetrahedralB{4==(yl);0==C;1==A;3==X;2==Y}}
¥LewisTetrahedralB{0==C;1==A;4==B;3==X;%
2N==¥LewisTetrahedralB{4==(yl);0==C;1==A;3==X;2==Y}}
```
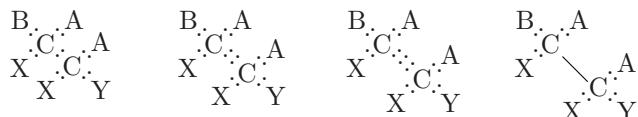
Lewis structures of northeast linkage can be drawn in a similar way.

```
¥LewisTetrahedralB{0==C;2==A;4==B;3==X;%
1==¥LewisTetrahedralB{3==(yl);0==C;1==A;4==X;2==Y}}
¥LewisTetrahedralB{0==C;2==A;4==B;3==X;%
1D==¥LewisTetrahedralB{3==(yl);0==C;1==A;4==X;2==Y}}
```

```
¥LewisTetrahedralB{0==C;2==A;4==B;3==X;%
1T==¥LewisTetrahedralB{3==(yl);0==C;1==A;4==X;2==Y}}
¥LewisTetrahedralB{0==C;2==A;4==B;3==X;%
1N==¥LewisTetrahedralB{3==(yl);0==C;1==A;4==X;2==Y}}
```
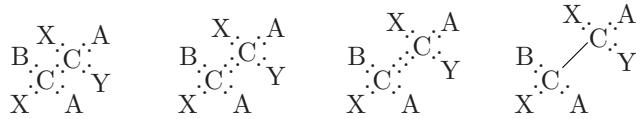

Another set of Lewis structures of southwest linkage can be drawn in a similar way.

```
¥LewisTetrahedralB{0==C;2==A;4==B;1==X;%
3==¥LewisTetrahedralB{1==(yl);0==C;3==A;4==X;2==Y}}
¥LewisTetrahedralB{0==C;2==A;4==B;1==X;%
3D==¥LewisTetrahedralB{1==(yl);0==C;3==A;4==X;2==Y}}
¥LewisTetrahedralB{0==C;2==A;4==B;1==X;%
3T==¥LewisTetrahedralB{1==(yl);0==C;3==A;4==X;2==Y}}
¥LewisTetrahedralB{0==C;2==A;4==B;1==X;%
3N==¥LewisTetrahedralB{1==(yl);0==C;3==A;4==X;2==Y}}
```
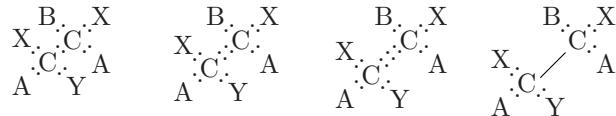

A rather dirty technique is necessary to draw a Lewis structure of boron trifluoride.

```
¥begingroup
¥fboxrule=0pt¥fboxsep=1pt
¥LewisTetrahedralB{%
0==B¥LewisSbond¥raisebox{-1.3pt}{¥lonepairA[123]{¥fbox{¥kern0.6pt F}}};%
3==¥raisebox{1.6pt}{¥lonepairB[234]{¥fbox{¥kern0.6pt F}}}¥kern-2pt;%
4==¥raisebox{-1.9pt}{¥lonepairB[134]{¥fbox{¥kern0.6pt F}}}¥kern-2pt}
%%
¥LewisTetrahedralB{%
0==B¥sbond¥raisebox{-1.3pt}{¥lonepairA[123]{¥fbox{¥kern0.6pt F}}};%
3N==¥raisebox{1.6pt}{¥lonepairB[234]{¥fbox{¥kern0.6pt F}}}¥kern-2pt;%
4N==¥raisebox{-1.9pt}{¥lonepairB[134]{¥fbox{¥kern0.6pt F}}}¥kern-2pt}
¥endgroup
```
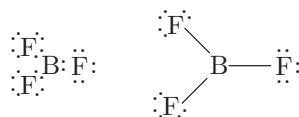

2.4   Additional Examples for Compounds with Lone Pairs

1-Isothiocyanato-(4S)-(methylsulfonyl)butane (an anti-cancer agent contained in broccoli) has the following structure:

```
¥begin{XyMcompd}(1300,450)(100,100){}{}
¥dtetrahedralS{0==S;1D==¥lonepairA[24]{O};4B==CH$_{3}$;3A==¥lonepairB[1]{¥null};%
2==¥tetramethylene{}{1==(yl);4W==¥lonepairA[3]{N}¥dbond C¥dbond¥lonepairA[13]{S}}}
¥end{XyMcompd}
¥qquad
¥begin{XyMcompd}(1400,450)(100,100){}{}
¥dtetrahedralS{0==S;1D==¥lonepairA[24]{O};4B==CH$_{3}$;3A==¥lonepairB[1]{¥null};%
0==¥phantom{S}%
¥raisebox{-0.4em}{%
¥pentamethylenei{}{1==(yl);5W==¥lonepairA[3]{N}¥dbond C¥dbond¥lonepairA[13]{S}}}}
¥end{XyMcompd}
```
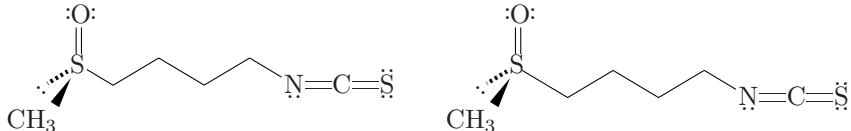

The latter structure has a more plausible length of an S—C bond. An alternative code can typeset the same compound:

```
¥begin{XyMcompd}(1400,450)(100,100){}{}
¥dtetrahedralS{0==%
¥pentamethylenei{1==S}{1==(yl);5W==¥lonepairA[3]{N}¥dbond C¥dbond¥lonepairA[13]{S}};%
1D==¥lonepairA[24]{O};4B==CH$_{3}$;3A==¥lonepairB[1]{¥null}}
¥end{XyMcompd}
```
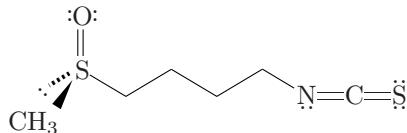

The S=O bond of a sulfoxide can be regarded as being delocalized to give S^{+}——O^{-}. For example, the sulfoxide part of sparsomycin is drawn by means of the following code:

```
¥begin{XyMcompd}(2100,800)(100,200){}{}
¥sixheterov[a]{4==¥downnobond{N}{H};6==¥llap{H}{N};
2s==¥nonamethylene[b]{5==¥downnobond{N}{H};8==¥downnobond{S}{$^{+}$};%
9s==¥trimethylene{2==S}{1==(yl)}}
{1==(yl);4D==O;6SA==H;6==¥dimethylenei{1==¥upnobond{O}{H}}{2==(yl)};%
8SB==¥llap{$^{-¥:}$}¥lonepairA[124]{O};8SA==¥kern4pt¥nelonepair}}%
{1==CH$_{3}$;3D==O;5D==O}
¥end{XyMcompd}
```
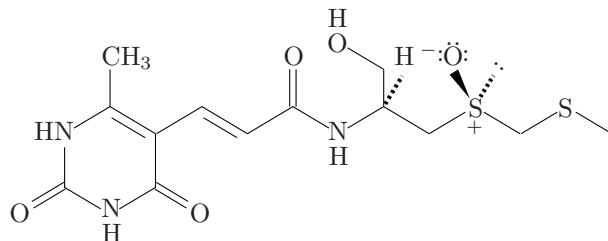

It should be noted that the organochemical convention allows us to omit lone pairs if unnecessary. Thus, the nitrogen atoms and the oxygen atoms (except the oxygen of the sulfoxide moiety) in the above structural formula of sparsomycin have no information on lone pairs. As a further example, the formula of 1-isothiocyanato-(4S)-(methylsulfonyl)butane is allowed to be represented by an abbreviated form, where the lone pairs except that of the sulfur atom (necessary to show the (4S)-configuration) are omitted as follows.

```
¥begin{XyMcompd}(1400,450)(100,100){}{}
¥dtetrahedralS{0==%
¥pentamethylenei{1==S}{1==(yl);5W==N¥dbond C¥dbond S};%
1D==O;4B==CH$_{3}$;3A==¥lonepairB[1]{¥null}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(1400,450)(100,100){}{}
¥dtetrahedralS{0==%
¥pentamethylenei{1==S¥rlap{$^{+}$}}{1==(yl);5W==N¥dbond C¥dbond S};%
1==O$^{-}$;4B==CH$_{3}$;3A==¥lonepairB[1]{¥null}}
¥end{XyMcompd}
```
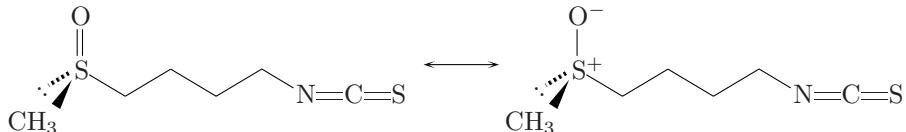

The right canonical formula shows that unnecessary lone pairs can be omitted even for canonical formulas with formal charges (cf. Section 3.1 on page 21).

Chapter 3

Chemical Schemes with Lewis Structures

3.1 Resonance Forms

For an approximation of quantum-chemical calculation, organic chemistry uses a resonance form in which two or more representative structural formulas (canonical formulas) are linked with double-headed arrows. For example, nitromethane is represented by the following resonance form, where two structural formulas with formal charges are linked by a double-headed arrow so as to show the neutral nature of the nitromethane molecule.

```
¥begin{XyMcompd}(450,450)(0,100){}{}
¥Rtrigonal{0==N$^{¥:+}$;1==H$_{3}$C;3D==O;2==O$^{-}$}
¥end{XyMcompd}
¥reactlrarrow{0pt}{3cm}{arrow for}{a resonance form}
¥begin{XyMcompd}(450,450)(0,100){}{}¥quad
¥Rtrigonal{0==N$^{¥:+}$;1==H$_{3}$C;2D==O;3==O$^{-}$}
¥end{XyMcompd}
```
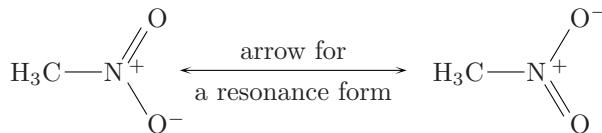
The above resonance form is an abbreviated representation of the following resonance form with full information of lone pairs, where two Lewis structures are linked with a double-headed arrow.

```
¥begin{XyMcompd}(450,450)(0,100){}{}
¥Rtrigonal{0==N$^{¥:+}$;1==H$_{3}$C;3D==¥lonepairA[12]{O};2==¥lonepairA[234]{O}$_{¥:-}$}
¥end{XyMcompd}
¥reactlrarrow{0pt}{3cm}{arrow for}{a resonance form}
¥begin{XyMcompd}(450,450)(0,100){}{}¥quad
¥Rtrigonal{0==N$^{¥:+}$;1==H$_{3}$C;2D==¥lonepairA[23]{O};3==¥lonepairA[124]{O}$^{¥:-}$}
¥end{XyMcompd}
```

21
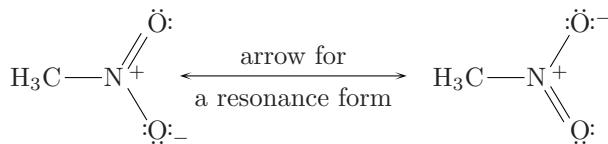
Note that lone pairs around each central nitrogen are replaced by usual bonds (—— and ==) and a polarized bond (N$^+$——O$^-$).

A bent arrow (curved arrow) is used to explain the relationship between the two Lewis structures, where the start of the arrow is located at a lone pair to be shifted and the arrowhead is located at a bond to be formed in one case; or, in the other case, the start of the arrow is located at a bond to be deleted and the arrowhead is located at a lone pair to be formed. The following example is to show such an explanation.

```
¥begin{center}
¥begin{XyMcompd}(450,450)(0,100){}{}
¥Rtrigonal{0==N$^{¥:+}$;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(90,150)(70,250)(150,250);%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(110,-70)(50,-130)(140,-160);%
1==H$_{3}$C;3D==¥lonepairA[12]{O};2==¥lonepairA[234]{O}$_{¥:-}$}
¥end{XyMcompd}
¥reactlrarrow{0pt}{3cm}{arrow for}{a resonance form}
¥begin{XyMcompd}(450,450)(0,100){}{}¥quad
¥Rtrigonal{0==N$^{¥:+}$;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(120,140)(70,240)(130,250);%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(100,-70)(50,-130)(140,-170);%
1==H$_{3}$C;2D==¥lonepairA[23]{O};3==¥lonepairA[124]{O}$^{¥:-}$}
¥end{XyMcompd}
¥end{center}
```

where each red bent arrow is drawn by the ¥pscurve command supported by the PSTricks package [12], which is loaded automatically when ¥usepackage{xymtexps} is declared to load the XⅰMTEX system of POSTSCRIPT-compatible mode. The resulting output is shown as follows:
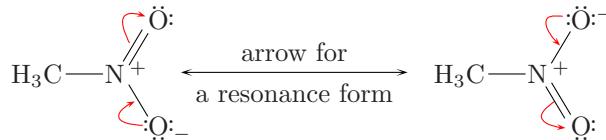
Another resonance form can be drawn as follows, where a three-membered canonical formula is involved. Note that the three atoms of the resulting three-membered ring (the right-hand formula) are located at the same positions of the left-handed open-chain formula.

```
¥begin{center}
¥begin{XyMcompd}(450,450)(0,100){}{}
¥Rtrigonal{0==N$^{¥:+}$;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{<-}%
(30,80)(30,160)(90,150);%
2==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(100,30)(150,100)(150,170)(80,250);%
1==H$_{3}$C;3D==¥lonepairA[12]{O};2==¥lonepairA[234]{O}$_{¥:-}$}
¥end{XyMcompd} ¥qquad
¥reactlrarrow{0pt}{3cm}{arrow for}{a resonance form}
¥begin{XyMcompd}(450,450)(0,100){}{}¥quad
¥Rtrigonal{0==¥lonepairA[1]{N};%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(30,100)(20,160)(100,150);%
2==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{<-}%
```

```
(100,30)(150,100)(150,170)(70,250);%
1==H$_{3}$C;2==¥lonepairA[23]{O};3==¥lonepairA[12]{O};%
2==¥psline[unit=¥unitlength,linewidth=0.4pt](40,90)(40,380)}
¥end{XyMcompd}
¥end{center}
```

where in the vertical bond in the right-hand formula is drawn by using ¥psline supported by the PSTricsks package.
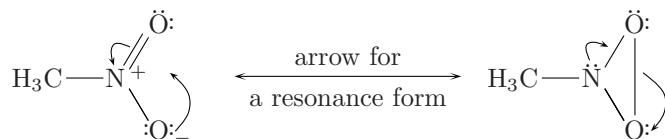
In standard viewpoints of organic chemistry, such a three-membered canonical formula is recognized not to exhibit so large contribution to a resonance form.

If such a three-membered ring has N—O and O—O bonds of ordinary bond lengths for three-membered rings, the same electron shift as above should be regarded as an equilibrium so that the two Lewis structures are not canonical formulas for constructing a resonance form:

```
¥begin{center}
¥begin{XyMcompd}(450,450)(0,100){}{}
¥Rtrigonal{O==N$^{¥:+}$;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{<-}%
(30,80)(30,160)(90,150);%
2==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(100,30)(150,100)(150,170)(80,250);%
1==H$_{3}$C;3D==¥lonepairA[12]{O};2==¥lonepairA[234]{O}$_{¥:-}$}
¥end{XyMcompd} ¥qquad
¥reactlarrow{0pt}{3cm}{%
¥reactrarrow{0pt}{1.5cm}{}{}¥¥[-8pt]}{¥strut}¥qquad
¥begin{XyMcompd}(450,300)(50,200){}{}
¥threeheterohi{1==¥lonepairA[1]{N};2==¥lonepairA[23]{O};3==¥lonepairA[12]{O}}%
{1==H$_{3}$C}
¥end{XyMcompd}
¥end{center}
```
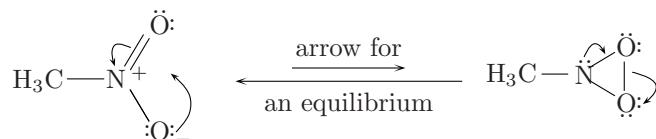
p-Methoxybenzaldehyde exhibits delocalization through the benzene ring, where the electron-donating methoxy interacts the electron-withdrawing carbonyl group according to the following resonance form:

```
¥begin{XyMcompd}(1100,350)(-100,250){}{}
¥bzdrh{1==CH$_{3}$$¥lonepairA[13]{O};%
4==¥rtrigonal{1==(yl);0==C;2==H;3D==¥lonepairA[13]{O}}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{1cm}{}{} ¥quad
¥begin{XyMcompd}(1150,350)(-150,250){}{}
¥bzdrh[pa]{1D==CH$_{3}$$¥lonepairA[3]{O}$^{+}$;%
4D==¥rtrigonal{1==(yl);0==C;2==H;3==¥lonepairA[123]{O}¥rlap{$^{¥:-}$}}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{1cm}{}{} ¥quad etc.
```
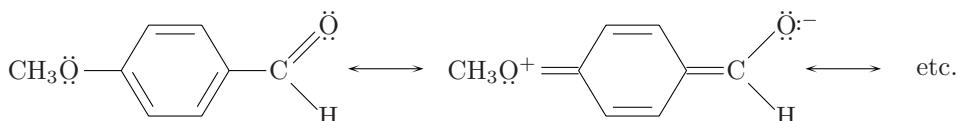
3.2   Radical Fissions

A radical fission of a C—H bond of methane is represented in two ways, i.e., a scheme due to Lewis structures and a scheme due to usual structural formulas.

```
¥begin{ChemEquation}
¥begin{XyMcompd}(250,400)(150,100){}{}
¥dtetrahedralS{0==C;1==H;2==H;3A==H;4B==H}
¥end{XyMcompd}
¥qquad = ¥qquad
¥left¥{%
¥begin{array}{ccc}
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥put(0,0){¥blue ¥circle{30}}
¥put(0,0){¥LewistetrahedralA{0==C;1==H;2==H;3==H;4==H}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(185,70)(200,150)(240,80)
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(170,0)(200,-80)(220,-50)(190,0)
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{energy}{$¥Delta ¥mathit{H}^{¥circ}=439~kJ/mol$}
&
¥setbox0=¥hbox{¥chemradicalA[2]{C}}
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥LewistetrahedralA{0==¥box0;1==H;3==H;4==H}
¥end{XyMcompd}
+ ¥quad ¥chemradicalA[4]{H} ¥¥
¥noalign{¥vskip8pt}
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==C;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(40,70)(80,150)(120,50);%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(140,50)(170,150)(220,70);%
1==H;2==H;3==H;4==H}
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{energy}{$¥Delta ¥mathit{H}^{¥circ}=439~kJ/mol$}
&
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==¥chemradicalA[2]{C};1==H;2==H;3==H}
¥end{XyMcompd}
+ ¥quad ¥chemradicalA[4]{H} ¥¥
¥end{array}¥right.
¥end{ChemEquation}
```

Because the XyMcompd environment is based on the picture environment of LATEX 2$_\varepsilon$, commands of LATEX 2$_\varepsilon$ such as ¥put and ¥circle can be used in addition to commands of X͞Y͞MTEX. Thus, the command ¥put(0,0){¥blue ¥circle{30}} outputs a blue circle at the original point. Moreover, commands of PSTricks package (e.g., ¥pscurve) can be declared directly in the XyMcompd environment.

$$
\begin{array}{ccc}
& & \text{energy} \\
\mathrm{H}:\overset{\mathrm{H}}{\underset{\mathrm{H}}{\mathrm{C}}}:\mathrm{H} & \xrightarrow{\hspace{1.5cm}} & \mathrm{H}:\overset{\mathrm{H}}{\underset{\mathrm{H}}{\mathrm{C}}}\cdot \quad + \quad \cdot\mathrm{H} \\
& \Delta H^\circ = 439 \text{ kJ/mol} &
\end{array}
$$
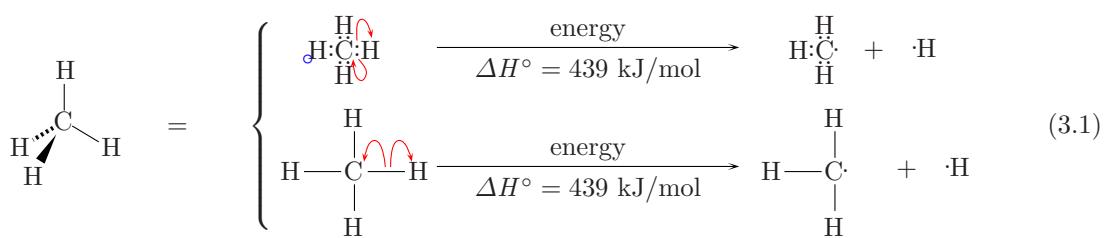
It should be noted that each bent arrow in a radical fission represents the shift of a single electron, while each bent arrow in a resonance form represents the shift of a lone pair (two electrons). Bent arrows of the former type are usually represented as harpoons (e.g., $\rightharpoonup$), which are not supported by the PSTricks package. This will be an open target to be developed.

3.3 Carbocations

A carbocation can be dissociated from methane by extracting a hydride ion. Two expressions of such dissociation are shown as follows:

```
¥begin{ChemEquation}
¥left¥{%
¥begin{array}{ccc}
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥put(0,0){¥LewistetrahedralA{0==C;1==H;2==H;3==H;4==H}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(185,70)(200,150)(240,80)
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{}{}
&
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥LewistetrahedralA{0==C¥rlap{$^{+}$};1==H;3==H;4==H}
¥end{XyMcompd}
+ ¥quad ¥lonepairA[4]{H}^{-} ¥¥
¥noalign{¥vskip8pt}
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==C;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(140,50)(170,150)(220,70);%
1==H;2==H;3==H;4==H}
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{}{}
&
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==C¥rlap{$^{+}$};1==H;2==H;3==H}
¥end{XyMcompd}
+ ¥quad ¥lonepairA[4]{H}^{-} ¥¥
¥end{array}¥right.
¥end{ChemEquation}
```

$$
\left\{
\begin{array}{l}
\text{(reaction scheme)}
\end{array}
\right. \tag{3.2}
$$
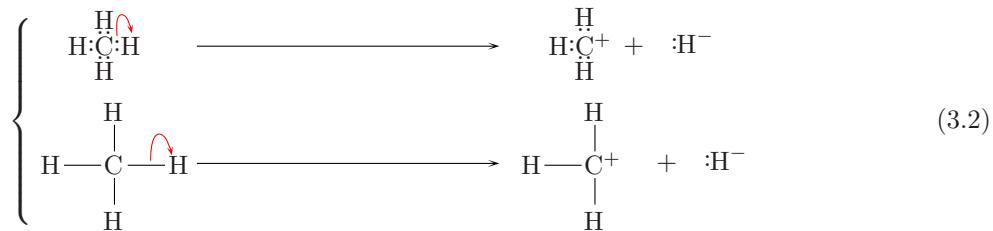
The addition of hydrogen chloride to 2,3-dimethylbut-2-ene produces 2-chloro-2,3-dimethylbutane, where the first protonation produces a carbocation, which is converted to the final product by chlorination.

```
¥begin{center}
¥begin{XyMcompd}(800,700)(50,100){}{}
¥put(600,700){H¥sbond¥lonepairA[123]{Cl}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=green]{->}%
(400,330)(400,600)(600,730)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=green]{->}%
(750,720)(800,600)(850,700)%
¥put(0,0){¥Ethyleneh{}{1==CH$_{3}$;2==CH$_{3}$;3==CH$_{3}$;4==CH$_{3}$}}
¥end{XyMcompd}
¥reactlarrow{-15pt}{3cm}{%
¥reactrarrow{0pt}{1.5cm}{}{}¥¥[-8pt]}{protonation}¥qquad
¥begin{XyMcompd}(850,700)(50,100){}{}
¥put(750,700){¥lonepairA[1234]{Cl}$^{¥:-}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(500,330)(500,600)(700,730)%
¥put(0,0){%
¥Ltrigonal{0==C$^{+}$;1==¥tetrahedral{2==(yl);0==C;1==H;4==CH$_{3}$;3==CH$_{3}$};%
2==CH$_{3}$;3==CH$_{3}$}}
¥end{XyMcompd} ¥¥
¥reactrarrow{0pt}{3cm}{¥strut}{{}¥¥[-18pt]%
¥reactlarrow{0pt}{1.5cm}{}{chlorination}}¥qquad
¥begin{XyMcompd}(900,500)(-50,100){}{}
¥tetrahedral{0==C;4==¥tetrahedral{2==(yl);0==C;1==H;4==CH$_{3}$;3==CH$_{3}$};%
1==¥lonepairA[124]{Cl};2==CH$_{3}$;3==CH$_{3}$}
¥end{XyMcompd}
¥end{center}
```
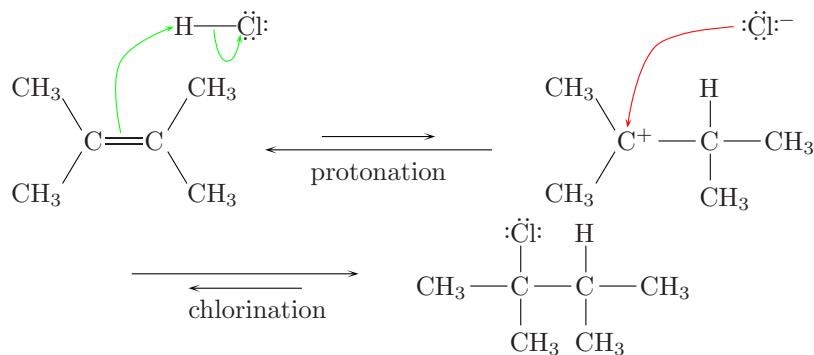
3.4   Nucleophilic Substitutions of Order Two

An acid-catalyzed bromination (bromine substitution) of ethanol runs through an S_N2 mechanism, which causes the stereochemical inversion of the central carbon, although the case of ethanol exhibits no effect of such an inversion.

```
¥begin{XyMcompd}(900,450)(100,100){}{}
¥put(0,0){¥ltetrahedralS{0==C;2==H$_{3}$C;3A==H;4B==H;1==¥lonepairA[13]{O}H}}
¥put(650,275){+}
¥put(750,275){H¥sbond ¥lonepairA[123]{Br}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(500,370)(575,450)(675,450)(750,370)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(900,350)(950,450)(1000,380)%
¥end{XyMcompd}
¥qquad
¥reactrarrow{0pt}{3cm}{¥strut}{{}¥¥[-18pt]%
¥reactlarrow{0pt}{1.5cm}{}{}}¥qquad
¥begin{XyMcompd}(900,450)(100,100){}{}
¥put(0,0){¥ltetrahedralS{0==C;2==H$_{3}$C;3A==H;4B==H;%
1==¥llap{¥raisebox{2pt}{$^{¥:+}$}}¥lonepairA[3]{O}H$_{2}$}}
¥put(780,275){+}
¥put(950,275){¥lonepairA[1234]{Br}$^{¥:-}$}
¥end{XyMcompd}
¥¥
¥begin{XyMcompd}(900,450)(100,100){}{}
¥put(400,0){¥ltetrahedralS{0==C;2==H$_{3}$C;3A==H;4B==H;%
1==¥llap{¥raisebox{2pt}{$^{¥:+}$}}¥lonepairA[3]{O}H$_{2}$}}
%¥put(800,275){+}
¥put(100,200){¥lonepairA[1234]{Br}$^{¥:-}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(200,300)(350,400)(500,400)(650,320)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(775,310)(820,450)(900,350)%
¥end{XyMcompd}
¥qquad
¥reactrarrow{0pt}{3cm}{S$_{¥mathrm{N}}$2}{{}¥¥[-18pt]%
¥reactlarrow{0pt}{1.5cm}{}{}}¥qquad
¥begin{XyMcompd}(900,450)(100,100){}{}
¥put(0,0){¥rtetrahedralS{0==C;2==CH$_{3}$$;3A==H;4B==H;%
1==¥lonepairA[134]{Br}}}
¥put(700,275){+}
¥put(870,275){H$_{2}$$¥lonepairA[13]{O}}
¥end{XyMcompd}
```
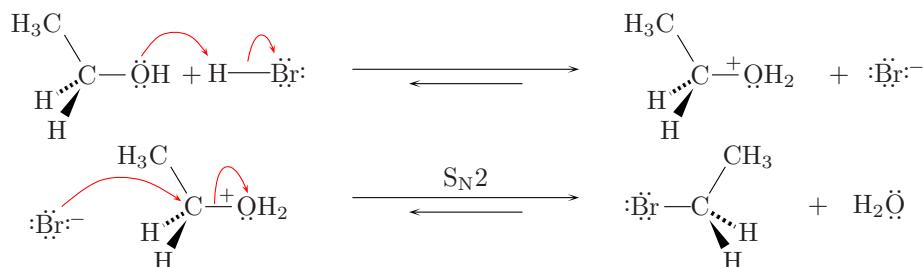

3.5   Carboanions

A carboanion can be dissociated from methane by extracting a proton. Two expressions of such dissociation are shown as follows:

```
¥begin{ChemEquation}
¥left¥{%
```

```
¥begin{array}{ccc}
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥put(0,0){¥LewistetrahedralA{0==C;1==H;2==H;3==H;4==H}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(170,0)(200,-80)(220,-50)(190,0)
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{}{}
&
¥setbox0=¥hbox{¥lonepairA[2]{C}¥rlap{$^{¥:-}$}}
¥begin{XyMcompd}(100,200)(100,-50){}{}
¥LewistetrahedralA{0==¥box0;1==H;3==H;4==H}
¥end{XyMcompd}
+ H^{+} ¥¥
¥noalign{¥vskip8pt}
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==C;%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(40,70)(80,150)(120,50);%
1==H;2==H;3==H;4==H}
¥end{XyMcompd}
&
¥reactrarrow{0pt}{4cm}{}{}
&
¥begin{XyMcompd}(350,450)(100,100){}{}
¥tetrahedral{0==¥lonepairA[2]{C}$^{¥:-}$;1==H;2==H;3==H}
¥end{XyMcompd}
+ ¥quad H^{+} ¥¥
¥end{array}¥right.
¥end{ChemEquation}
```


$$(3.3)$$
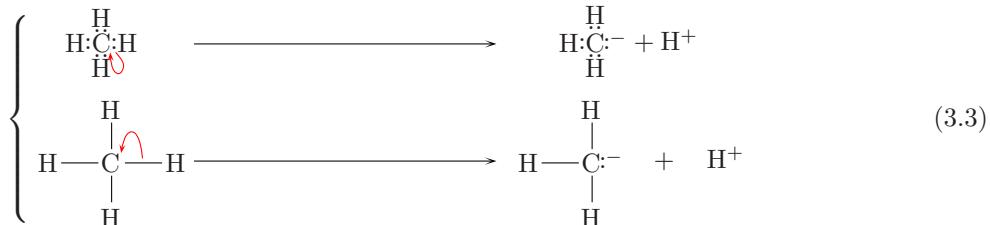
3.6 Aromatic Nucleophilic Substitutions

Aromatic nucleophilic substitutions have been already discussed in Chapter 4 of the online manual of XΥMT$_E$X version 4.01 (xymtx401.pdf). The present section provides further examples in which lone pairs are drawn explicitly. A methoxide anion attacks 1-chloro-2,4-dinitrobenzene at the carbon atom attached by chlorine so as to give a Meisenheimer complex, in which the resulting negative charge is delocalized through the benzene ring by the nitro groups.

```
¥begin{ChemEqnarray}
¥lefteqn{%
¥begin{XyMcompd}(850,900)(-50,0){}{}
¥put(0,0){¥bzdrv{4==¥lonepairA[234]{Cl};3==NO$_{2}$;1==NO$_{2}$}}
¥put(-100,0){CH$_{3}$$¥lonepairA[123]{O}$^{¥:-}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(120,100)(180,200)(380,230)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
```

```
(240,350)(300,450)(335,335)%
¥end{XyMcompd} ¥reactrarrow{0pt}{2cm}{¥strut}{CH$_{3}$OH}}&& ¥nonumber ¥¥
&&
¥left[%
¥begin{XyMcompd}(650,900)(150,0){}{}
¥put(0,0){¥bzdrv[od]{4Sb==CH$_{3}$$¥lonepairA[23]{O};%
4Sa==¥lonepairA[234]{Cl};3==NO$_{2}$;1==NO$_{2}$}}
¥put(150,320){$_{¥:-}$¥lonepairB[1]{~}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(650,900)(150,0){}{}
¥put(0,0){¥bzdrv[pa]{4Sb==CH$_{3}$$¥lonepairA[23]{O};%
4Sa==¥lonepairA[234]{Cl};3==NO$_{2}$;1==NO$_{2}$}}
¥put(305,620){$^{¥:-}$¥lonepairA[3]{~}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(650,900)(150,0){}{}
¥put(0,0){¥bzdrv[oc]{4Sb==CH$_{3}$$¥lonepairA[23]{O};%
4Sa==¥lonepairA[234]{Cl};3==NO$_{2}$;1==NO$_{2}$}}
¥put(538,320){¥lonepairB[4]{~}$^{¥:-}$}
¥end{XyMcompd}¥quad¥right] =
¥begin{XyMcompd}(650,900)(150,0){}{}
¥put(0,0){¥bzdrv[Z]{4Sb==CH$_{3}$$¥lonepairA[23]{O};%
4Sa==¥lonepairA[234]{Cl};3==NO$_{2}$;1==NO$_{2}$}}
¥put(400,450){¥makebox(0,0){¥scriptsize $-$}}
¥psline[unit=¥unitlength,linewidth=0.4pt,linestyle=dashed,dash=2pt 1pt]{-}%
(250,350)(250,530)(400,620)(550,530)(550,350)%
¥end{XyMcompd}
¥end{ChemEqnarray}
```


$$\tag{3.4}$$

The Chichibabin reaction is a 2-amination of pyridine by means of potassium amide to produce 2-aminopyridine.

```
¥begin{center}
¥begin{XyMcompd}(950,500)(150,150){}{}
¥put(0,0){¥sixheterovi[ace]{1==¥lonepairA[3]{N}}{}}
¥put(700,300){$^{¥:-}$¥lonepairA[13]{N}H$_{2}$}
```

```
¥put(1050,300){K$^{+}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(590,350)(700,450)(810,390)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(410,300)(450,450)(480,380)%
¥end{XyMcompd}
¥reactrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(950,500)(150,150){}{}
¥put(0,0){¥sixheterovi[ce]{1==¥llap{$_{-}$}¥lonepairA[13]{N}}{%
2Sa==¥lonepairA[1]{N}H$_{2}$;2Sb==H}}
¥put(950,100){K$^{+}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(410,200)(450,120)(510,290)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(610,260)(650,100)(790,100)(850,120)%
¥end{XyMcompd}
¥reactrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(1000,500)(150,150){}{}
¥put(0,0){¥sixheterovi[ace]{1==¥lonepairA[3]{N}}{%
2==¥lonepairA[1]{N}H$_{2}$}}
¥put(950,100){K$^{+}$$~$^{-¥:}$¥lonepairA[4]{H}}
¥end{XyMcompd} ¥¥ ¥vskip15pt
¥reactrarrow{0pt}{1cm}{}{}
¥begin{XyMcompd}(1050,500)(150,150){}{}
¥put(0,0){¥sixheterovi[ace]{1==¥lonepairA[3]{N}}{%
2==¥llap{$_{-}$}¥lonepairA[13]{N}H}}
¥put(900,100){K$^{+}$ + H$_{2}$}
¥end{XyMcompd}
¥reactrarrow{0pt}{1cm}{H$_{2}$¥lonepairA[12]{O}}{¥strut}
¥begin{XyMcompd}(700,500)(150,150){}{}
¥put(0,0){¥sixheterovi[ace]{1==¥lonepairA[3]{N}}{%
2==¥lonepairA[1]{N}H$_{2}$}}
¥end{XyMcompd}
+ H¥lonepairA[123]{O}$^{¥:-}$
¥end{center}
```
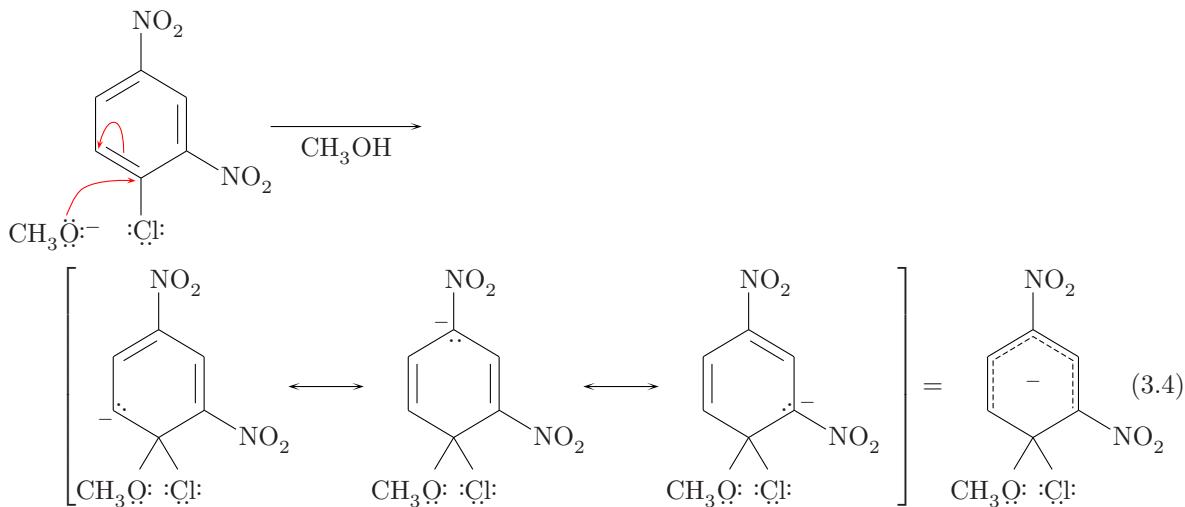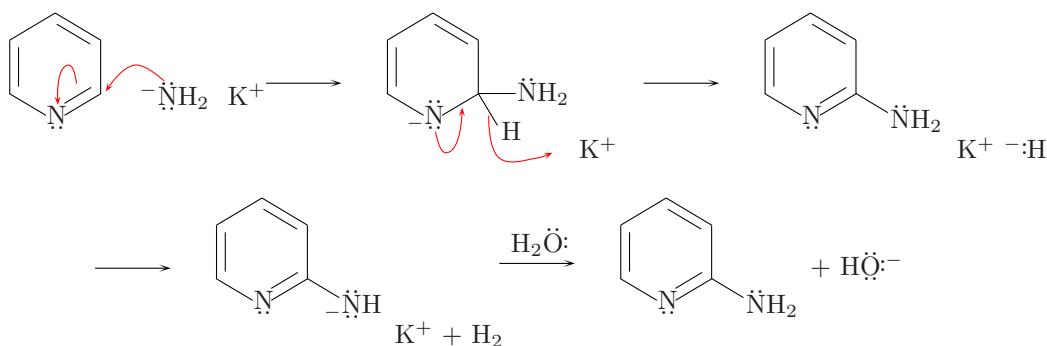

3.7   Further Reactions

3.7.1   Formation and Reactions of Diazoketones

The reaction of diazomethane with an acid chloride results in subsequent processes of addition, elimination, and deprotonation so as to give a diazoketone as follows:

```
¥begin{quote}
```

```
¥begin{XyMcompd}(700,600)(100,0){}{}
¥put(0,0){¥Dtrigonal{O==C;1D==¥lonepairB[14]{O};3==R;2==¥lonepairA[123]{Cl}}}
¥put(171,-50){$^{-}$¥lonepairA[1]{C}H$_{2}$¥sbond N$^{+}$¥tbond¥lonepairA[2]{N}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(220,50)(180,150)(300,250)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(350,400)(400,450)(350,500)%
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{addition}{¥strut}
¥begin{XyMcompd}(800,500)(100,50){}{}
¥put(0,0){¥tetrahedral{O==C;1==¥lonepairA[124]{O}$^{-}$;2==R;4==¥lonepairA[123]{Cl};%
3==CH$_{2}$¥sbond N$^{+}$¥tbond¥lonepairA[2]{N}}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(400,310)(450,400)(550,360)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(300,400)(400,450)(350,500)%
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{elimination}{¥strut}
¥begin{XyMcompd}(800,600)(100,-50){}{}
¥put(0,0){¥Dtrigonal{O==C;1D==¥lonepairB[14]{O};3==R;%
2==¥squareplanar{4==(yl);O==C;1==H;3==H;2==N$^{+}$¥tbond¥lonepairA[2]{N}}}}
¥put(600,450){¥lonepairA[1234]{Cl}$^{¥:-}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(500,180)(540,300)(600,250)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(680,360)(750,400)(700,450)%
¥end{XyMcompd} ¥¥
¥vskip10pt
¥reactrarrow{0pt}{2cm}{deprotonation}{¥strut}
¥begin{XyMcompd}(900,400)(100,150){}{}
¥put(0,0){¥Dtrigonal{O==C;1D==¥lonepairB[14]{O};3==R;%
2==¥llap{$_{-}$}¥lonepairA[3]{C}H¥sbond N$^{+}$¥tbond¥lonepairA[2]{N}}}
¥end{XyMcompd}
+ H¥sbond¥lonepairA[123]{Cl}
¥end{quote}
```
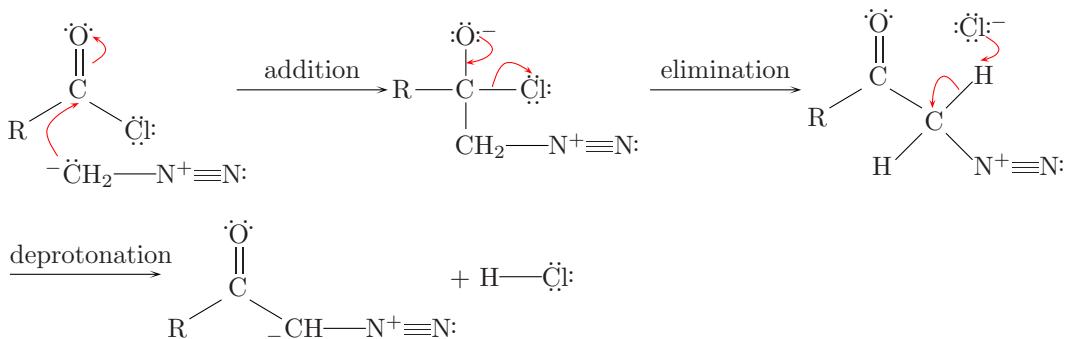

The resulting diazoketone is decomposed via thermolysis or photosisis to release a ketocarbene and nitrogen. The ketocarbene adds to an olefin to produce a cyclopropane, undergoes insertion into a C–H bond, or rearranges into a ketene (Wolff rearrangement). Among these subsequent processes, the following scheme shows a Wolff rearrangement.

```
¥begin{XyMcompd}(900,400)(100,150){}{}
¥put(0,0){¥Dtrigonal{O==C;1D==¥lonepairB[14]{O};3==R;%
2==¥llap{$_{-}$}¥lonepairA[1]{C}H¥sbond N$^{+}$¥tbond¥lonepairA[2]{N}}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
```

```
(700,160)(750,250)(830,200)%
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{$¥Delta$ or $h¥nu$}{¥strut}
¥begin{XyMcompd}(400,400)(100,150){}{}
¥put(0,0){¥Dtrigonal{0==C;1D==¥lonepairB[14]{O};3==R;2==¥lonepairA[1]{C}H}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(180,200)(350,80)(520,100)%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{<-}%
(400,220)(480,320)(510,200)%
¥end{XyMcompd}
+ ¥lonepairA[4]{N}¥tbond¥lonepairA[2]{N}¥quad
¥reactrarrow{0pt}{3cm}{Wolff}{Rearrangement}
¥begin{XyMcompd}(500,400)(-100,100){}{}
¥Rtrigonal{0==C;2==R;3==H;1D==¥lonepairA[34]{O}¥dbond C}
¥end{XyMcompd}
```
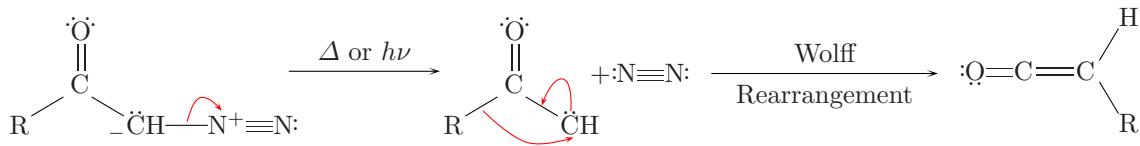

3.7.2   Williamson Ether Synthesis

Williamson Ether Synthesis is a typical S_N2 reaction to produce an ether by starting from an alcohol and an halide (or sulfonate).

```
¥begin{XyMcompd}(1800,700)(200,300){}{}
¥put(0,0){¥cyclopentanevi{1Sb==H;1Sa==¥lonepairA[124]{O}$^{¥:-}$Na$^{+}$}}
¥put(650,500){+}
¥put(800,500){%
CH$_{3}$(CH$_{2}$)$_{15}$CH$_{2}$¥sbond¥lonepairA[13]{O}SO$_{2}$CH$_{3}$}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(500,900)(900,1000)(1300,900)(1400,580)
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{->}%
(1630,550)(1680,700)(1740,600)%
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{DMSO}{¥strut}
¥begin{XyMcompd}(1000,700)(200,300){}{}
¥put(0,0){¥cyclopentanevi{1Sb==H;1Sa==%
¥lonepairA[14]{O}CH$_{2}$(CH$_{2}$)$_{15}$CH$_{3}$}}
¥end{XyMcompd} ¥kern-1cm
+ Na$^{+}$ $^{-¥:}$$¥lonepairA[134]{O}SO$_{2}$CH$_{3}$
```
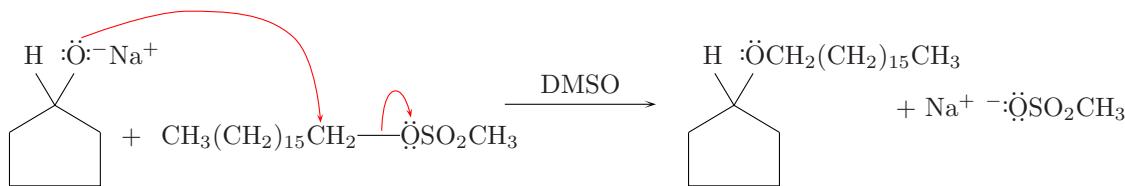
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