XƎMTEX (Versions 4.05 and 4.06) for Typesetting Chemical Structural Formulas: B. Extension and Improvement of the **chemist** Package and the **chmst-ps** Package.

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Chapter 1

Introduction

1.1 History

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

Table 1.1: Versions of XyMTEX

version	package files and comments
1.00 (1993)	(for LaTeX2.09) See Ref. [1, 2]. aliphat.sty, carom.sty, lowcycle.sty, hetarom.sty, hetaromh.sty, hcycle.sty, chemstr.sty, locant.sty, xymtex.sty
1.01 (1996)	(for LaTeX 2_ε) See Ref. [3]. ccycle.sty, polymers.sty, chemist.sty
1.02 (1998)	(not released) Nested substitution by 'yl'-function.
2.00 (1998)	Enhanced version based on the XyM Notation. See Ref. [4, 5]. fusering.sty, methylen.sty
2.01 (2001)	(not released) Size reduction, sizeredc.sty (version 1.00)
3.00 (2002)	Size reduction (sizeredc.sty, version 1.01), and reconstruction of the command system. See Ref. [6]
4.00 (2002)	(not released) PostScript printing (xymtx-ps.sty, version 1.00 and chmst-ps.sty, version 1.00)
4.01 (2004)	PostScript printing and length-variable central atoms
4.02 (2004)	PostScript printing and wedges bonds for stereochemistry
4.03 (2005)	PostScript printing and wavy bonds for stereochemistry
4.04 (2009)	Macros for drawing steroids (steroid.sty, ver 1.00)
4.05 (2009)	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)
4.06 (2009)	(The present version) the chmst-ps package (ver 1.03) for supporting bent (curved) harpoons.

Among the new matters of the XyMTEX system (versions 4.05) summarized in Table 1.1, this manual is concerned with revised and improved macros added to the chemist package (ver 4.05) as well as the chmst-ps package (ver 1.02). In particular, the chemist package (ver 4.05) [and the chmst-ps package (ver 1.02)] supports two mathversions (chem and boldchem) designed for chemical usage in addition to the

original mathversions (normal and bold) of LaTeX 2ε. Even in the original mathversions (normal and bold), convenient environments akin to the `equation` or `eqnarray` environments of LaTeX 2ε have been developed. More environments are defined in the present chemist (chmst-ps) package. After publishing the previous online manual named xymtx405B.pdf, the XyMTEX (version 4.06) has developed a utility for supporting bent (curved) harpoons, which is stored in the chmst-ps package (version 1.03). The explanation of the utility is added to renew the previous online manual so as to serve as Chapter 5 in the present manual named xymtx405406B.pdf.

1.2 Use of chemist and chmst-ps Packages

1.2.1 chemist vs. chmst-ps

The chemist package is read by a command `¥usepackage` declared in the preamble of a tex file, as shown in the following template:

```
¥documentclass{article}
¥usepackage{xymtexps}
¥usepackage{chemist}
¥begin{document}
(text)%default (normal)

¥mathversion{bold}
(text)

¥mathversion{chem}
(text)

¥mathversion{boldchem}
(text)

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

Alternatively, the chmst-ps package is read to meet PostScript requirements, where the chemist package is automatically loaded.

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

¥mathversion{bold}
(text)

¥mathversion{chem}
(text)

¥mathversion{boldchem}
(text)

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

The xymtexps package provides the X^^MTEX system of PostScript-compatible mode. Hence, the resulting dvi file should be converted into a PostScript file by means of an appropriate converter (e.g., dvips(k)). The resulting PostScript file can be browsed by GSview/Ghostscript.

1.2.2 Mathverstions

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

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:

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

\mathversion{bold}
(text)

\mathversion{chem}
(text)

\mathversion{boldchem}
(text)

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

1.3 Recent Books Citing the X^^MTEX System

Recent books on LaTeX 2_ε have referred to the X^^MTEX system, e.g., pages 520–540 of [11] and pages 551–598 of Vol. II of [12].

Chapter 2

New Commands and Environments for Chemical Equations

This chapter is devoted to introduce basic functions supported by the chemist package and the PostScript counterpart package (the chmst-ps package). Although such basic functions have once been introduced in Chapters 17 and 19 of the online manual of X̃MTEX version 1.01 (xymtex.pdf, cf. [3]) and Chapter 12 of the online manual of X̃MTEX version 2.00 (xymtx200PS.pdf, cf. [5]), they are discussed again by using commands and environments newly-defined in the present versions of the chemist and the chmst-ps package. In particular, the `¥ChemForm` command and three environments (`ChemEquation`, `ChemEqnarray`, and `ChemEqnarray*`) are used to show extensions and improvements achieved by the present versions, because they provide us with more convenient utilities for drawing chemical equations.

2.1 Basic Utilities for Writing Chemical Formulas

Basic utilities are exemplified by using `¥ChemForm`. They are common to the three environments (ChemEquation, ChemEqnarray, and ChemEqnarray*) supported by the chemist (chmst-ps) package.[1]

2.1.1 Basics Due to the `¥ChemForm` Command

TEX supports an in-text (in-line) math mode toggled by `$...$`. LATEX 2ε provides us with a facility of the same kind, i.e., `¥(...¥)`. These in-text math modes (as well as the `equation` environment etc. supported by LATEX 2ε) have the following difficulties in representing molecular formulas.

1. Each text letter in these in-text math modes is typeset in italic form, which is unsuitable to represent molecular formulas. For example, `$H_{2}O$` results in H_2O. Hence, we should input `$¥mathrm{H}_{2}¥mathrm{O}$` or `$¥mathrm{H_{2}O}$` to output an upright formula H_2O. Although the use of `¥mathrm` is not tedious in an in-text math mode, the `eqnarray` environment of LATEX 2ε requires a more complicated treatment. Hence, a simpler and integrated method of inputting chemical formulas would be desirable for convenience.

2. In these in-text math modes, the depth of a subscript depends on the presence or absence of the coexisting superscript. For example, the depth of the subscript 2 of C_2 is different from the subscript 2 of O_2^-, as found in the following output.

```
$¥mathrm{C}_{2}¥mathrm{H}_{3}¥mathrm{O}_{2}^{-}$
```
$C_2H_3O_2^-$

[1] Because the chmst-ps package loads the chemist package automatically, descriptions on the chemist package are also useful to the chmst-ps package throughout the present manual.

Table 2.1: Outputs Due to the ¥ChemForm Command

¥ChemForm		$...$	
¥ChemForm{H_2O}	H_2O	$¥mathrm{H_2O}$	H_2O
¥ChemForm{N_{2(g)}}	$N_{2(g)}$	$¥mathrm{N_{2(g)}}$	$N_{2(g)}$
¥ChemForm{CrO_{4}^{2-}}	CrO_4^{2-}	$¥mathrm{CrO}_{4}^{2-}$	CrO_4^{2-}
¥ChemForm{C_{2}H_{3}% O_{2}^{-}}	$C_2H_3O_2^-$	¥(¥mathrm{C_{2}H_{3}% O_{2}^{-}}¥)	$C_2H_3O_2^-$
¥ChemForm{CuSO_4¥cdot% 5H_2 O}	$CuSO_4 \cdot 5H_2O$	$¥mathrm{CuSO_4¥cdot % 5H_2O}$	$CuSO_4 \cdot 5H_2O$
¥ChemForm{Pb_{2}^{II}% Pb^{IV}O_{4}}	$Pb_2^{II}Pb^{IV}O_4$	$¥mathrm{Pb_{2}^{II}% Pb^{IV}O_{4}}$	$Pb_2^{II}Pb^{IV}O_4$
¥ChemForm{^{79}Br^{-}	$^{79}Br^-$	$^{79}¥mathrm{Br}^{-}$	$^{79}Br^-$
¥ChemForm{¥rho(H_{2}SO_{4})}	$\rho(H_2SO_4)$	$¥rho(¥mathrm{H_{2}% SO_{4}})$	$\rho(H_2SO_4)$
¥ChemForm{^{23}Na(¥gamma,% ¥:3n)¥:^{20}Na}	$^{23}Na(\gamma,\ 3n)\ ^{20}Na$	$^{23}¥mathrm{Na(¥gamma,% ¥:3n)¥:^{20}Na}$	$^{23}Na(\gamma,\ 3n)\ ^{20}Na$

3. The fonts used in such an in-text math mode are italics (for the mathversion normal) or bold italics (for mathversion bold). The use of other fonts (e.g., san serif) would be desirable by a means of a simpler and integrated method.

To avoid such difficulties, the previous chemist package (packed in the XƎMTEX system ≤ version 4.04) has supported the ¥chemform command (as well as the chemeqn and the chemeqnarray environments). Although this command has cleared Nos. 1 and 2 of the above difficulties, it has not yet cleared difficulty No. 3.

The present version of the chemist (chmst-ps) package supports the ¥ChemForm command, which gives sufficient results with respect to the difficulties described above. Table 2.1 summarizes examples which show that the ¥ChemForm command solves difficulties Nos. 1 and 2. With respect to difficulty No. 2 in particular, refer to the rows for $C_2H_3O_2^-$ and $Pb_2^{II}Pb^{IV}O_4$ in Table 2.1. For the solution of No.3, see Subsection 2.1.2.

To obtain the formula H_2O, several codes can be written, e.g., ¥ChemForm{H_2O} (in Table 2.1), ¥ChemForm{H_2␣O} (the symbol ␣ represents a space), and ¥ChemForm{H_{2}O}. Although the first input obeys a TEX standard, it is not so easy to find pauses. The second or third one is redundant but easy to find pauses. For a more complicated example, compare ¥ChemForm{C_2H_3O_2^-} and ¥ChemForm{C_2␣H_3␣O_2^-} (as well as the counterpart listed in Table 2.1), which provide the same output, $C_2H_3O_2^-$.

2.1.2 Fonts

In a normal situation of LATEX 2ε, ¥ChemForm and ¥chemform give equivalent outputs as follows:

¥ChemForm{N_{2(g)}}	$N_{2(g)}$
¥chemform{N_{2(g)}}	$N_{2(g)}$
cf. $¥mathrm{N_{2(g)}}$	$N_{2(g)}$

In order to change math fonts into san serif fonts, a command ¥let¥ChemEqFont=¥sf is declared at any place in a tex file. For example, the source code represented by

```
{¥let¥ChemEqFont=¥sf
¥begin{tabular}{lclc}
¥verb/¥ChemForm{N_{2(g)}}/ & ¥ChemForm{N_{2(g)}} & & ¥¥
¥verb/¥chemform{N_{2(g)}}/ & ¥chemform{N_{2(g)}} & & ¥¥
¥hline cf.¥ %
¥verb/$¥mathrm{N_{2(g)}}$/ & $¥mathrm{N_{2(g)}}$ &
¥verb/$¥mathsf{N_{2(g)}}$/ & $¥mathsf{N_{2(g)}}$ ¥¥
¥end{tabular}
}
```

produces the following output:

¥ChemForm{N_{2(g)}}	$\mathsf{N_{2(g)}}$		
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
cf. $¥mathrm{N_{2(g)}}$	$\mathrm{N_{2(g)}}$	$¥mathsf{N_{2(g)}}$	$\mathsf{N_{2(g)}}$

It should be noted that the output due to ¥ChemForm obeys the declaration of ¥let¥ChemEqFont=¥sf, while the output due to ¥chemform does not follow the declaration.

In a similar way, the declaration of ¥let¥ChemEqFont=¥tt changes fonts due to ¥ChemForm into typewriter fonts.

¥ChemForm{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
cf. $¥mathrm{N_{2(g)}}$	$\mathrm{N_{2(g)}}$	$¥mathtt{N_{2(g)}}$	$\mathrm{N_{2(g)}}$

By the declaration of ¥let¥ChemEqFont=¥bf, fonts due to ¥ChemForm are changed into boldfaced fonts.

¥ChemForm{N_{2(g)}}	$\mathbf{N_{2(g)}}$		
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
cf. $¥mathrm{N_{2(g)}}$	$\mathrm{N_{2(g)}}$	$¥mathbf{N_{2(g)}}$	$\mathbf{N_{2(g)}}$

The declaration of ¥let¥ChemEqFont=¥sl results in slanted fonts printed by ¥ChemForm, although a LaTeX font warning (Command ¥sl invalid in math mode) appears.

¥ChemForm{N_{2(g)}}	$N_{2(g)}$		
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
cf. $¥mathrm{N_{2(g)}}$	$\mathrm{N_{2(g)}}$	${¥@nomath¥sl N_{2(g)}}$	$N_{2(g)}$

By declaring ¥let¥ChemEqFont=¥it, fonts due to ¥ChemForm are changed into italic fonts, which are slightly different from the default fonts for the math modes of LaTeX 2_ε.

¥ChemForm{N_{2(g)}}	$N_{2(g)}$		
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$		
cf. $¥mathrm{N_{2(g)}}$	$\mathrm{N_{2(g)}}$	$¥mathit{N_{2(g)}}$	$N_{2(g)}$
		$N_{2(g)}$	$N_{2(g)}$

Finally, the declaration of ¥mathversion{bold} (cf. Chapter 3) changes the output of ¥ChemForm as well as that of the in-text math mode.

¥mathversion{bold}	
¥ChemForm{N_{2(g)}}	$\mathbf{N_{2(g)}}$
¥chemform{N_{2(g)}}	$\mathrm{N_{2(g)}}$
cf. $¥mathrm{N_{2(g)}}$	$\mathbf{N_{2(g)}}$

2.1.3 Using Mathematical Symbols

Mathematical symbols supported by TEX/LATEX 2ε can be used in the argument of ¥ChemForm. The following examples show the use of of ¥frac and ¥lg in the argument of ¥ChemForm.

```
¥ChemForm{Fe(CN)_{¥frac{6}{2}}} ¥quad
¥ChemForm{¥frac{1}{2}O_{2}} ¥quad
¥ChemForm{pH=-¥lg[¥gamma_{¥pm}¥mathit{c}(H^{+})/(mol¥cdot dm^{-3})]}
```

$$\mathrm{Fe(CN)}_{\frac{6}{2}} \quad \tfrac{1}{2}\mathrm{O}_2 \quad \mathrm{pH} = -\lg[\gamma_{\pm} c(\mathrm{H}^+)/(\mathrm{mol}\cdot\mathrm{dm}^{-3})]$$

Inequality symbols (> and <) can be used in ¥ChemForm, while they should be replaced by the commands ¥mathgreater and ¥mathless in ¥chemform. Thus, thermal stabilities of boron compounds are typeset as follows:

```
¥ChemForm{B_{2}(NMe_{2})_{4}>B_{2}(OMe_{2})_{4}>B_{2}(OH)_{4}
>B_{2}F_{4}>B_{2}Cl_{4}>B_{2}Br_{4}} ¥¥
¥chemform{B_{2}(NMe_{2})_{4}¥mathgreater B_{2}(OMe_{2})_{4}¥mathgreater B_{2}(OH)_{4}
¥mathgreater B_{2}F_{4}¥mathgreater B_{2}Cl_{4}¥mathgreater B_{2}Br_{4}}
```

$$\mathrm{B_2(NMe_2)_4} > \mathrm{B_2(OMe_2)_4} > \mathrm{B_2(OH)_4} > \mathrm{B_2F_4} > \mathrm{B_2Cl_4} > \mathrm{B_2Br_4}$$
$$\mathrm{B_2(NMe_2)_4} > \mathrm{B_2(OMe_2)_4} > \mathrm{B_2(OH)_4} > \mathrm{B_2F_4} > \mathrm{B_2Cl_4} > \mathrm{B_2Br_4}$$

Compare the following examples:

```
(correct) ¥ChemForm{B_{2}(NMe_{2})_{4}>B_{2}(OMe_{2})_{4}} and
¥ChemForm{B_{2}(OMe_{2})_{4}<NMe_{2})_{4}} ¥¥
(incorrect) ¥chemform{B_{2}(NMe_{2})_{4}>B_{2}(OMe_{2})_{4}} and
¥chemform{B_{2}(OMe_{2})_{4}<NMe_{2})_{4}} ¥¥
(correct) ¥chemform{B_{2}(NMe_{2})_{4}¥mathgreater B_{2}(OMe_{2})_{4}} and
¥chemform{B_{2}(OMe_{2})_{4}¥mathless NMe_{2})_{4}}
```

(correct) $\mathrm{B_2(NMe_2)_4} > \mathrm{B_2(OMe_2)_4}$ and $\mathrm{B_2(OMe_2)_4} < \mathrm{NMe_2)_4}$
(incorrect) $\mathrm{B_2(NMe_2)_4}$ ¿ $\mathrm{B_2(OMe_2)_4}$ and $\mathrm{B_2(OMe_2)_4}$ ¡ $\mathrm{NMe_2)_4}$
(correct) $\mathrm{B_2(NMe_2)_4} > \mathrm{B_2(OMe_2)_4}$ and $\mathrm{B_2(OMe_2)_4} < \mathrm{NMe_2)_4}$

Double inequality symbols (¥gg and ¥ll) can be used in both ¥ChemForm and ¥chemform.

```
¥ChemForm{SO_{2}¥cdot ¥mathit{n}H_{2}O ¥rightleftharpoons H_{2}SO_{3}(aq);%
¥quad ¥mathit{K} ¥ll 10^{-9}} ¥qquad
¥chemform{SO_{2}¥cdot ¥mathit{n}H_{2}O ¥rightleftharpoons H_{2}SO_{3}(aq);%
¥quad ¥mathit{K} ¥ll 10^{-9}}
```

$$\mathrm{SO_2}\cdot n\mathrm{H_2O} \rightleftharpoons \mathrm{H_2SO_3(aq)}; \quad K \ll 10^{-9} \qquad \mathrm{SO_2}\cdot n\mathrm{H_2O} \rightleftharpoons \mathrm{H_2SO_3(aq)}; \quad K \ll 10^{-9}$$

2.2 Chemical Equations

The command ¥ChemForm (or ¥chemform) corresponds to the in-text math mode represented by $...$ (TEX) or ¥(...¥) (LATEX 2ε). On the other hand, ChemEquation and like environments correspond to equation and like environments of LATEX 2ε.

2.2.1 Arrows of Fixed Lengths

Arrows supported by TEX/LATEX 2$_\varepsilon$ can be used in `¥ChemForm`, as shown in the following examples:

```
¥ChemForm{H_{2}+Br_{2} ¥rightarrow 2HBr} ¥qquad
¥ChemForm{H_{2}+Br_{2} ¥longrightarrow 2HBr} ¥¥
¥ChemForm{H_{2}+Br_{2} ¥leftarrow 2HBr} ¥qquad
¥ChemForm{H_{2}+Br_{2} ¥longleftarrow 2HBr} ¥¥
¥ChemForm{H_{2}+Br_{2} ¥rightleftharpoons 2HBr}
```

$$\mathrm{H_2 + Br_2 \rightarrow 2HBr} \qquad \mathrm{H_2 + Br_2 \longrightarrow 2HBr}$$
$$\mathrm{H_2 + Br_2 \leftarrow 2HBr} \qquad \mathrm{H_2 + Br_2 \longleftarrow 2HBr}$$
$$\mathrm{H_2 + Br_2 \rightleftharpoons 2HBr}$$

Because longer arrows of fixed lengths are frequently used in chemical equations, they are supported by the chemist (chmst-ps) package. Such commands for drawing longer arrows should be used in an in-text or display math mode (e.g., `$¥¥llongrightarrow$` and `¥ChemForm{¥¥llongrightarrow}`), because they are defined as relational operators. The appearances of arrows produced by a command of the same name in chemist and chmst-ps are different, as summarized in Table 2.2.

Table 2.2: Arrows of Fixed Lengths Supported by chemist and chmst-ps

command	chemist	chmst-ps	comment
`¥¥llongrightarrow`	⟶	⟶	
`¥¥llongleftarrow`	⟵	⟵	
`¥¥llongleftrightarrow`	⟷	⟷	
`¥¥Llongrightarrow`	⟹	⟹	
`¥¥Llongleftarrow`	⟸	⟸	
`¥¥Llongleftrightarrow`	⟺	⟺	
`¥¥llongleftharpoondown`	↽	↽	
`¥¥llongrightharpoonup`	⇀	⇀	
`¥¥llongleftharpoonup`	(↼)	↼	not supported by chemist
`¥¥llongrightharpoondown`	(⇁)	⇁	not supported by chemist
`¥¥equilibarrow`	⇌	⇌	
`¥¥Equilibarrow`	⇌	⇌	
`¥¥lllongrightarrow`	⟶	⟶	
`¥¥lllongleftarrow`	⟵	⟵	
`¥¥lllongleftrightarrow`	⟷	⟷	
`¥¥Lllongrightarrow`	⟹	⟹	
`¥¥Lllongleftarrow`	⟸	⟸	
`¥¥Lllongleftrightarrow`	⟺	⟺	
`¥¥lllongleftharpoondown`	↽	↽	
`¥¥lllongrightharpoonup`	⇀	⇀	
`¥¥lllongleftharpoonup`	(↼)	↼	not supported by chemist
`¥¥lllongrightharpoondown`	(⇁)	⇁	not supported by chemist
`¥¥equiliblongarrow`	⇌	⇌	
`¥¥Equiliblongarrow`	⇌	⇌	

These commands for drawing arrows (Table 2.2) can be used in `¥ChemForm` as part of a chemical equation. The following list shows several examples, where horizontal spaces before and after each arrow (as a relational operator) are placed automatically.

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

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

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

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

Further longer arrows are also supported by the chemist (chmst-ps) package (Table 2.2). They can be used in the argument of ¥ChemForm as follows:

```
¥ChemForm{A¥lllongrightarrow B} ¥ChemForm{A¥lllongleftarrow B}
¥ChemForm{A¥llongleftrightarrow B} ¥ChemForm{A¥llongleftrightarrow B}
¥ChemForm{A¥equiliblongarrow B} ¥ChemForm{A¥Equiliblongarrow B}
```

$$A \longrightarrow B \quad A \longleftarrow B \quad A \longleftrightarrow B \quad A \longleftrightarrow B \quad A \rightleftharpoons B \quad A \rightleftharpoons B$$

In a parallel way to double-lined arrows supported by TEX/LATEX 2ε, i.e., $¥Longrightarrow$ ($\Longrightarrow$) $¥Longleftarrow$ ($\Longleftarrow$) $¥Longleftrightarrow$ ($\Longleftrightarrow$), a set of longer double-lined arrows and a further longer set are supported by the chemist (chmst-ps) package (Table 2.2). They can be used in the argument of ¥ChemForm as follows:

```
¥ChemForm{A ¥Llongrightarrow B}
¥ChemForm{A ¥Llongleftarrow B}
¥ChemForm{A ¥Llongleftrightarrow B} ¥¥
¥ChemForm{A¥Lllongrightarrow B}
¥ChemForm{A¥Lllongleftarrow B}
¥ChemForm{A¥Lllongleftrightarrow B}
```

$$\mathrm{A} \Longrightarrow \mathrm{B}\ \mathrm{A} \Longleftarrow \mathrm{B}\ \mathrm{A} \Longleftrightarrow \mathrm{B}$$
$$\mathrm{A} \Longrightarrow \mathrm{B}\ \mathrm{A} \Longleftarrow \mathrm{B}\ \mathrm{A} \Longleftrightarrow \mathrm{B}$$

If the switching command `¥chemistsw` is declared, the same commands for drawing double-lined arrows give the corresponding arrows of different appearances:

$$\mathrm{A} \Longrightarrow \mathrm{B}\ \mathrm{A} \Longleftarrow \mathrm{B}\ \mathrm{A} \Longleftrightarrow \mathrm{B}$$
$$\mathrm{A} \Longrightarrow \mathrm{B}\ \mathrm{A} \Longleftarrow \mathrm{B}\ \mathrm{A} \Longleftrightarrow \mathrm{B}$$

For arrows of variable lengths, see Section 4.4.

2.2.2 `ChemEquation` Environment

In parallel with the `equation` environment of LaTeX 2_ε, the chemist package (version 4.05, also chmst-ps version 1.02) supports the `ChemEquation` environment in addition to the `chemeqn` environment defined previously (version $\leq$ 4.04). The basic functions described above for `¥ChemForm` are also effective to the `ChemEquation` environment.

The following code is a typical example containing a chemical compound and ionic species. Thus, solid limestone ($CaCO_3$) is almost water insoluble, but a very small quantity dissolves in water according to the following process:

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

$$\mathrm{CaCO_{3(s)}} \longrightarrow \mathrm{Ca^{2+}_{(aq)}} + \mathrm{CO^{2-}_{3(aq)}} \tag{2.1}$$

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

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

$$CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{2.2}$$

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

The `chemeqn` environment defined previously (version $\leq$ 4.04) can be also used equivalently when we work in a usual condition, i.e., in the mathversion "normal":

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

$$\mathrm{CaCO_{3(s)}} \longrightarrow \mathrm{Ca^{2+}_{(aq)}} + \mathrm{CO^{2-}_{3(aq)}} \tag{2.3}$$

However, the difference between the `ChemEquation` and the `chemeqn` environment becomes obvious, when the mathversion "bold" is used (cf. Subsection 2.1.2 on page 10 and Chapter 3 on page 29):

```
{¥mathversion{bold}
¥begin{ChemEquation}
 CaCO_{3(s)} ¥llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
¥end{ChemEquation}
¥begin{chemeqn}
 CaCO_{3(s)} ¥llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
¥end{chemeqn}
}
```

$$\mathbf{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{2.4}$$

$$\mathrm{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{2.5}$$

On a similar line, when fonts are changed by declaring `¥let¥ChemEqFont=¥sf` for example, the following difference emerges:

```
{¥let¥ChemEqFont=¥sf
¥begin{ChemEquation}
 CaCO_{3(s)} ¥llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
¥end{ChemEquation}
¥begin{chemeqn}
 CaCO_{3(s)} ¥llongrightarrow Ca_{(aq)}^{2+} + CO_{3(aq)}^{2-}
¥end{chemeqn}
}
```

$$\mathsf{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{2.6}$$

$$\mathrm{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{2.7}$$

Isotopes can be written in a `ChemEquation` environment. For example, the code:

```
¥begin{ChemEquation}
{}_{~91}^{234}Pa ¥llongrightarrow {}^{~~0}_{-1}e + {}^{234}_{~92}U
¥end{ChemEquation}
```

typesets the following equation:

$$\mathrm{{}^{234}_{91}Pa \longrightarrow {}^{0}_{-1}e + {}^{234}_{92}U} \tag{2.8}$$

In addition to arrows of fixed lengths, another set of arrows of variable lengths (for organic structural formulas) is supported by the chemist (chmst-ps) package (cf. Section 4.4). Such arrows can be also used in chemical equations of inorganic chemistry. For example, the code:

```
¥begin{ChemEquation}
 HC_2H_3O_2 ¥reacteqarrow{0pt}{3cm}{}{} H^+ + C_2H_3O_2^-
¥end{ChemEquation}
```

typesets the following equation:

$$\mathrm{HC_2H_3O_2 \rightleftharpoons H^+ + C_2H_3O_2^-} \tag{2.9}$$

where the 2nd argument of the `¥reacteqarrow` command specifies the length of the resulting arrow. Note that acetic acid ($\mathrm{HC_2H_3O_2}$) is written as $\mathrm{CH_3COOH}$ in organic chemistry.

The chemist package itself supports an equilibrium arrow (right and left arrows), while the chmst-ps package supports an equilibrium harpoon (right and left harpoons) by the same name `¥reacteqarrow`. They are exchanged by declaring `¥chemstsw` or `¥chmstpssw` as follows, when the chmst-ps package is loaded (the PSTricks package is necessary but automatically loaded).

```
¥textsf{chemist}: {¥chemistsw ¥reacteqarrow{0pt}{3cm}{}{}
and ¥reactEqarrow{0pt}{3cm}{}{} (not systematic)}¥¥
¥textsf{chmst-ps}: {¥chmstpssw ¥reacteqarrow{0pt}{3cm}{}{}
and ¥reactEqarrow{0pt}{3cm}{}{} (systematic)}
```

chemist: $\rightleftharpoons$ and $\rightleftharpoons$ (not systematic)

chmst-ps: $\rightleftharpoons$ and $\rightleftharpoons$ (systematic)

The chmst-ps package supports an equilibrium arrow (right and left arrows) by the command name ¥reactEqarrow. Strictly speaking, a more systematic naming is desirable for the chemist package, just as the chmst-ps package has already realized.

The ChemEquation environment can be used to write the calculation of an equilibrium constant as follows:

```
¥begin{ChemEquation}
¥mathit{K_a} = ¥frac{[H^+][C_2H_3O_2^-]}{[HC_2H_3O_2]}
= ¥frac{(6.00¥times10^{-4}¥:mol/L)(6.00¥times10^{-4}¥:mol/L)}{1.94¥times10^{-2}¥:mol/L}
= 1.86¥times10^{-5}¥:mol/L
¥end{ChemEquation}
```

$$K_a = \frac{[\mathrm{H^+}][\mathrm{C_2H_3O_2^-}]}{[\mathrm{HC_2H_3O_2}]} = \frac{(6.00\times10^{-4}\,\mathrm{mol/L})(6.00\times10^{-4}\,\mathrm{mol/L})}{1.94\times10^{-2}\,\mathrm{mol/L}} = 1.86\times10^{-5}\,\mathrm{mol/L} \tag{2.10}$$

It should be noted that the unit (mol/L) is written directly (i.e., without using the ¥mathrm command) in the ChemEquation environment. Moreover, the arguments of ¥frac (i.e., $[\mathrm{H^+}][\mathrm{C_2H_3O_2^-}]$ and $[\mathrm{HC_2H_3O_2}]$) are written directly without toggling by $...$. The corresponding output by an in-text math mode can be obtained by the following code, ¥ChemForm{¥frac{[H^+][C_2H_3O_2^-]}{[HC_2H_3O_2]}}, which produces $\frac{[\mathrm{H^+}][\mathrm{C_2H_3O_2^-}]}{[\mathrm{HC_2H_3O_2}]}$.

The following example shows a chemical equation with information on ΔG:

```
¥begin{ChemEquation}
SF_{6} + 2SO_{3} ¥llongrightarrow 2O_{2}SF_{2}; ¥qquad
¥Delta¥mathit{G}_{298}^{¥circ}=-202¥:kJ¥cdot mol^{-1}
¥end{ChemEquation}
```

where such information (as well as a unit) is written directly in the ChemEquation environment. The code typesets as follows:

$$\mathrm{SF_6 + 2SO_3 \longrightarrow 2O_2SF_2;} \qquad \Delta G^\circ_{298} = -202\,\mathrm{kJ\cdot mol^{-1}} \tag{2.11}$$

The heat of formation can be directly written in the ChemEquation environment as follows:

```
¥begin{ChemEquation}
CuCl(s) + ¥frac{1}{2}Cl_2(g) ¥llongrightarrow CuCl_2(s) + 71¥:kJ¥cdot mol^{-1}
¥end{ChemEquation}
```

$$\mathrm{CuCl(s)} + \frac{1}{2}\mathrm{Cl_2(g)} \longrightarrow \mathrm{CuCl_2(s)} + 71\,\mathrm{kJ\cdot mol^{-1}} \tag{2.12}$$

After declaration of ¥usepackage{amsmath} in a preamble, the command ¥underset supported by the amsmath package can be used.

```
¥begin{ChemEquation}
¥underset{Green}{3MnO_{4}^{2-}} + 4H^{+} ¥equiliblongarrow%%in place of ¥rightleftharpoons
¥underset{Magenta}{2MnO_{4}^{-}} + MnO_{2} + 2H_{2}O
¥end{ChemEquation}
```

where the command ¥equiliblongarrow supported by the chemist (chmst-ps) package is used to output a longer arrow in place of ¥rightleftharpoons of LaTeX 2_ε. Thereby, we obtain the following result:

$$\underset{\text{Green}}{3\mathrm{MnO_4^{2-}}} + 4\mathrm{H^+} \rightleftharpoons \underset{\text{Magenta}}{2\mathrm{MnO_4^-}} + \mathrm{MnO_2} + 2\mathrm{H_2O} \tag{2.13}$$

The counterpart command ¥overset for writing an object over a math object is also defined in the amsmath package. Thereby, the disproportionation of dithionates $\mathrm{S_2O_4^{2-}}$ in the presence of water is typeset as follows:

```
¥begin{ChemEquation}
2¥overset{III}{S}_{2}O_{4}^{2-} + H_{2}O ¥llongrightarrow
2H¥overset{IV}{S}O_{3}^{-} +
¥overset{II/VI¥mkern-15mu}{SS}O_{3}^{2-}
¥end{ChemEquation}
```

where the oxidation state of sulfur in each species is specified explicitly. Thereby, the following output is obtained:

$$\overset{\text{III}}{2\,\text{S}}{}_2\text{O}_4^{2-} + \text{H}_2\text{O} \longrightarrow 2\text{H}\overset{\text{IV}}{\text{S}}\text{O}_3^{-} + \overset{\text{II/VI}}{\text{SS}}\text{O}_3^{2-} \tag{2.14}$$

2.2.3 ChemEqnarray and ChemEqnarray∗ Environments

In a parallel way to the eqnarray and eqnarray∗ environment of LaTeX 2_ε, the chemist package (version 4.05, also chmst-ps version 1.02) supports the ChemEqnarray and ChemEqnarray∗ environments in addition to the chemeqnarray and chemeqnarray∗ environments defined previously (version $\leq$ 4.04). The basic functions described above for ¥ChemForm are also effective to the ChemEqnarray and ChemEqnarray∗ environments. The difference between the ChemEqnarray (or ChemEqnarray∗) environment and the chemeqnarray (or chemeqnarray∗) environment is parallel to the difference between the ChemEquation environment and the chemeqn environment (for the mathversions "normal" and "bold").

The following example shows a typical output due to the ChemEqnarray environment:

```
¥begin{ChemEqnarray}
AgBr + 2S_{2}O_{3}^{--} & ¥rightarrow & Ag(S_{2}O_{3})_{2}^{---} + Br^{-} ¥¥
Ag(S_{2}O_{3})_{2}^{---} & ¥rightarrow & Ag_{2}S_{2}O_{3}(s) + 3S_{2}O_{3}^{--}
¥end{ChemEqnarray}
```

$$\begin{aligned} \text{AgBr} + 2\text{S}_2\text{O}_3^{--} &\rightarrow \text{Ag}(\text{S}_2\text{O}_3)_2^{---} + \text{Br}^- && (2.15)\\ \text{Ag}(\text{S}_2\text{O}_3)_2^{---} &\rightarrow \text{Ag}_2\text{S}_2\text{O}_3(\text{s}) + 3\text{S}_2\text{O}_3^{--} && (2.16) \end{aligned}$$

where the positions of the two chemical equations are aligned at their arrows by using two ampersands (...&...&...).

When a chemical equation number is unnecessary partly, the command ¥nonumber is declared in a similar way to an eqnarray environment of LaTeX 2_ε. For example, we obtain:

```
¥begin{ChemEqnarray}
Fe^{3+}(aq) + {¥textstyle ¥frac{1}{2}}H_{2} ¥equiliblongarrow  Fe^{2+}(aq) + H^{+}(aq)
&& ¥mathit{E}^{¥circ} = 0.771¥:V ¥¥
&& ¥Delta ¥mathit{G}^{¥circ} = -74.4¥:kJ¥cdot mol^{-1} ¥nonumber
¥end{ChemEqnarray}
```

$$\begin{aligned} \text{Fe}^{3+}(\text{aq}) + \tfrac{1}{2}\text{H}_2 \rightleftharpoons \text{Fe}^{2+}(\text{aq}) + \text{H}^+(\text{aq}) \qquad & E^\circ = 0.771\ \text{V} \\ & \Delta G^\circ = -74.4\ \text{kJ}\cdot\text{mol}^{-1} \end{aligned} \tag{2.17}$$

Note that the command ¥textstyle is declared to output the fraction $\frac{1}{2}$ in an in-text mode.

When all chemical equation numbers are unnecessary, the ChemEqnarray∗ environment can be used as follows:

```
¥begin{ChemEqnarray*}
{¥textstyle ¥frac{1}{2}}I_{2} + e^{-} & ¥rightleftharpoons &   I^{-}
¥mskip36mu ¥mathit{E}^{¥circ} = 0.536¥:V; ¥quad
¥Delta ¥mathit{G}^{¥circ} = -51.5¥:kJ¥cdot mol^{-1} ¥¥
I_{2} + 2e^{-} & ¥rightleftharpoons&   2I^{-}
¥mskip28mu ¥mathit{E}^{¥circ} = 0.536¥:V; ¥quad
¥Delta ¥mathit{G}^{¥circ} = -103.0¥:kJ¥cdot mol^{-1}
¥end{ChemEqnarray*}
```

$$\begin{aligned} \tfrac{1}{2}\mathrm{I}_2 + \mathrm{e}^- &\rightleftharpoons \mathrm{I}^- \qquad E^\circ = 0.536\,\mathrm{V}; \quad \Delta G^\circ = -51.5\,\mathrm{kJ}\cdot\mathrm{mol}^{-1} \\ \mathrm{I}_2 + 2\mathrm{e}^- &\rightleftharpoons 2\mathrm{I}^- \qquad E^\circ = 0.536\,\mathrm{V}; \quad \Delta G^\circ = -103.0\,\mathrm{kJ}\cdot\mathrm{mol}^{-1} \end{aligned}$$

2.2.4 Cross References

The equation numbers of the `ChemEquation` (`chemeqn`) and `ChemEqnarray` (`chemeqnarray`) environments supported by the chemist (chmst-ps) package are given by using the `equation` counter which is used in the `equation` and `eqnarray` environments of LaTeX 2_ε. They are all referred to by means of the cross reference mechanism of LaTeX 2_ε (`¥label` and `¥ref`).

```
A chemical equation which is produced by a ¥texttt{ChemEquation} environment
to represent balanced molecular formulas in the both sides:
¥begin{ChemEquation}
3NaOH + FeCl_{3} ¥rightarrow Fe(OH)_{3} + 3NaCl ¥label{ce:01}
¥end{ChemEquation}
and a balanced complete ionic equation which is
produced by a ¥texttt{ChemEqnarray} environment:
¥begin{ChemEqnarray}
¥lefteqn{3Na^{+}(aq) + 3OH^{-}(aq) + Fe^{3+}(aq) + 3Cl^{-}(aq)} && ¥nonumber ¥¥
& ¥rightarrow & Fe(OH)_{3}(s) + 3Na^{+}(aq) + 3Cl^{-}(aq) ¥label{ce:02}
¥end{ChemEqnarray}
are commonly referred to as follows: Equations ¥ref{ce:01} and ¥ref{ce:02}.
```

A chemical equation having balanced molecular equations which is produced by a `ChemEquation` environment:

$$3\mathrm{NaOH} + \mathrm{FeCl}_3 \rightarrow \mathrm{Fe(OH)}_3 + 3\mathrm{NaCl} \tag{2.18}$$

and a balanced complete ionic equation which is produced by a `ChemEqnarray` environment:

$$\begin{aligned} &3\mathrm{Na}^+(\mathrm{aq}) + 3\mathrm{OH}^-(\mathrm{aq}) + \mathrm{Fe}^{3+}(\mathrm{aq}) + 3\mathrm{Cl}^-(\mathrm{aq}) \\ &\quad\rightarrow\quad \mathrm{Fe(OH)}_3(\mathrm{s}) + 3\mathrm{Na}^+(\mathrm{aq}) + 3\mathrm{Cl}^-(\mathrm{aq}) \end{aligned} \tag{2.19}$$

are commonly referred to as follows: Equations 2.18 and 2.19.

2.3 Creation of New Environments for Chemical Equations

When the amsmath package is loaded, several environments for printing multiline display equations are available. These mathematical environments can be converted into chemical versions by using the `¥newchemenvironment` command supported by the present chemist (chmst-ps) package.

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

2.3.1 Creation of the `chemmultline` Environment

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

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

$$Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq) \quad (2.20)$$

Note that the `minipage` environment reduces the text width to emphasize the function of the `multiline` environment. Each molecular formula in the `multline` environment is printed in italic fonts on a similar line to `equation` and like environments of LaTeX 2_ε.

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

```
¥newchemenvironment{chemmultline}{multline}
```

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

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

$$\mathrm{Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq) \rightarrow Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq)} \quad (2.21)$$

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

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

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

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

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

$$\begin{aligned}\mathsf{Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^{+}(aq) + 2OH^{-}(aq)} &\rightarrow \\ &\mathsf{Cu(OH)_2(s) + 2Li^{+}(aq) + SO_4^{2-}(aq)}\end{aligned}$$

2.3.2 Creation of the chemgather Environment

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

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

$$\begin{aligned}\mathrm{Bi(NO_3)_3 \cdot 5H_2O} &\xrightarrow{50-60^\circ} \mathrm{[Bi_6O_6]_2(NO_3)_{11}(OH) \cdot 6H_2O} \xrightarrow{77-130^\circ} \\ \mathrm{[Bi_6O_6](NO_3)_6(OH) \cdot 3H_2O} &\xrightarrow{400-450^\circ} \alpha\text{-}\mathrm{Bi_2O_3} \qquad (2.22)\\ \mathrm{Bi(NO_3)_3 \cdot N_2O_4} &\xrightarrow{200^\circ} \mathrm{Bi_2O(NO_3)_4} \xrightarrow{415^\circ} \mathrm{Bi_4O_5(NO_3)_2} \qquad (2.23)\end{aligned}$$

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

2.3.3 Creation of the chemalign Environment

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

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

$$\begin{aligned}5\mathrm{Fe^{2+}} &\longrightarrow 5\mathrm{Fe^{3+}} + 5\mathrm{e^-} \\ \mathrm{MnO_4^-} + 5\mathrm{e^-} + 8\mathrm{H^+} &\longrightarrow \mathrm{Mn^{2+}} + 4\mathrm{H_2O} \\ \hline \mathrm{MnO_4^-} + 5\mathrm{Fe^{2+}} + 8\mathrm{H^+} &\longrightarrow \mathrm{Mn^{2+}} + 5\mathrm{Fe^{3+}} + 4\mathrm{H_2O} \qquad (2.24)\end{aligned}$$

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

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

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

2.3.4 Creation of the chemalignat Environment

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

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

$$\begin{aligned}
\text{Solution of zinc oxide:}\qquad & \mathrm{ZnO + 2H^+ \longrightarrow Zn^{2+} + H_2O} && (2.25)\\
\text{Cathode reaction:}\qquad & \mathrm{Zn^{2+} + 2e^- \longrightarrow Zn} && (2.26)\\
\text{Anode reaction:}\qquad & \mathrm{H_2O \longrightarrow \tfrac{1}{2}O_2 + 2H^+ + 2e^-} && (2.27)\\
\text{Over-all reaction:}\qquad & \mathrm{ZnO \longrightarrow Zn + \tfrac{1}{2}O_2} && (2.28)
\end{aligned}$$

2.3.5 The Use of the split Environment

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

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

$$[(\eta^5\text{-}C_5H_5)(CO)_2MnSbPhI_2] + [(\eta^5\text{-}C_5H_5)Mn(CO)_2]\cdot THF \xrightarrow[\text{[18]crown-6}]{\text{K/THF}} [PhSb\{Mn(CO)_2(\eta^5\text{-}C_5H_5)\}_2] + 2KI + \cdots \quad (2.29)$$

and further lines

where an ampersand is used to mark an alignment point.

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

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

$$[(\eta^5\text{-}C_5H_5)(CO)_2MnSbPhI_2] + [(\eta^5\text{-}C_5H_5)Mn(CO)_2]\cdot THF \xrightarrow[\text{[18]crown-6}]{\text{K/THF}} [PhSb\{Mn(CO)_2(\eta^5\text{-}C_5H_5)\}_2] + 2KI + \cdots$$

and further lines (2.30)

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

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

$$\begin{aligned} H_2O + H_2SO_4 &\rightleftharpoons H_3O^+ + HSO_4^-; \\ K_{H_2O}(25^\circ) &= \frac{[H_3O^+][HSO_4^-]}{[H_2O]} \sim 1 \end{aligned} \quad (2.31)$$

$$SO_3 + H_2SO_4 \rightleftharpoons H_2S_2O_7 \quad (2.32)$$

$$\begin{aligned} H_2S_2O_7 + H_2SO_4 &\rightleftharpoons H_3SO_4^+ + HS_2O_7^-; \\ K_{H_2S_2O_7}(25^\circ) &= \frac{[H_3SO_4^+][HS_2O_7^-]}{[H_2S_2O_7]} = 1.4 \times 10^{-2} \end{aligned} \quad (2.33)$$

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

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

$$
\begin{aligned}
[\mathrm{Cr(CO)_6}] &\xrightarrow{\mathrm{A}} \underset{\text{yellow}}{[\mathrm{Cr(CO)_5(AsPhH_2)}]} \xrightarrow{\mathrm{B}} \\
[\mathrm{Cr(CO)_5(AsPhLi_2)}] &\xrightarrow[\text{orange}]{\mathrm{C}} \underset{\text{dark violet (mp 104°)}}{[\{\mathrm{Cr(CO)_5}\}_2\mathrm{AsPh}]}
\end{aligned}
\tag{2.34}
$$

A : $\mathrm{PhAsH_2}$
B : LiBu
C : cyclohexyl-$\mathrm{NCl_2}$

2.4 Objects Placed Over or Under Arrows

2.4.1 Combination of Commands

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

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

$$\mathrm{CCl_4 + HF \xrightarrow{SbFCl_4} CFCl_3 + HCl} \tag{2.35}$$

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

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

$$\mathrm{CFCl_3 + HF \xrightarrow{SbFCl_4} CF_2Cl_2 + HCl} \tag{2.36}$$

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

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

$$\mathrm{Na + Al + 2H_2} \xrightarrow[350\ \mathrm{atom}]{\mathrm{THF/140^\circ/3\,h}} \mathrm{NaAlH_4} \quad (99\%\ \text{yield}) \tag{2.37}$$

2.4.2 Application of Arrows for Organic Chemistry

Arrows for organic chemistry (Section 4.4) can also be used for outputting objects over or below arrows in inorganic chemical equations. An equivalent result is obtained by using `¥reactrarrow`, where `¥scriptsize` is declared to adjust the sizes of objects over and below an arrow:

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

$$\mathrm{Na + Al + 2H_2} \xrightarrow[350\ \mathrm{atom}]{\mathrm{THF/140^\circ/3\,h}} \mathrm{NaAlH_4} \quad (99\%\ \text{yield}) \tag{2.38}$$

On similar lines, the following set of arrows for organic chemistry (Section 4.4) can be used to draw reaction equations for inorganic chemistry.

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

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

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

¥reacteqarrow{0pt}{1cm}{A}{B} $\underset{\mathrm{B}}{\overset{\mathrm{A}}{\rightleftharpoons}}$

Because default positions of objects placed by such arrows for organic chemistry (Section 4.4) are adjusted to meet large structural formulas in organic chemistry, they are sometimes unsuitable if they are combined with rather small inorganic formulas, as found in the following equation:

```
¥begin{ChemEquation}
¥alpha Na(NH_4)HPO_4
¥reactrarrow{0pt}{1cm}{¥scriptsize $¥Delta$}{¥ChemStrut}
(NaPO_3)_{¥alpha }
+ ¥alpha NH_3¥uparrow + ¥alpha H_2O
¥end{ChemEquation}
```

$$\alpha\mathrm{Na(NH_4)HPO_4} \xrightarrow{\Delta} (\mathrm{NaPO_3})_\alpha + \alpha\mathrm{NH_3}\uparrow + \alpha\mathrm{H_2O} \tag{2.39}$$

The position of Δ over an arrow is adjustable by means of `¥reactarrowsep` in the chemist package (version 4.05).

```
{¥reactarrowsep=-2pt
¥begin{ChemEquation}
¥alpha Na(NH_4)HPO_4
¥reactrarrow{0pt}{1cm}{¥scriptsize $¥Delta$}{¥ChemStrut}
(NaPO_3)_{¥alpha }
+ ¥alpha NH_3¥uparrow + ¥alpha H_2O
¥end{ChemEquation}
}
```

$$\alpha\mathrm{Na(NH_4)HPO_4} \xrightarrow{\Delta} (\mathrm{NaPO_3})_\alpha + \alpha\mathrm{NH_3}\uparrow + \alpha\mathrm{H_2O} \tag{2.40}$$

Note that `¥ChemStrut` is used to adjust the up and down position of the arrow.

The following example shows texts over and under an arrow:

```
¥begin{ChemEquation}
2Ph_{3}GeBr + 2Na
¥reactrarrow{0pt}{2cm}{boling}{xylene}
2NaBr + Ge_{2}Ph_{6} ¥quad (mp¥: 340¥degC)
¥end{ChemEquation}
```

$$2\mathrm{Ph_3GeBr} + 2\mathrm{Na} \xrightarrow[\text{xylene}]{\text{boling}} 2\mathrm{NaBr} + \mathrm{Ge_2Ph_6} \quad (\text{mp } 340^\circ\mathrm{C}) \tag{2.41}$$

where `¥degC` is also defined in the chemist package.

The `ChemEquation` environment is capable of accommodating structural formulas produced by the XƎMTEX system. The following example shows that the command `¥tetrahedral` of the XƎMTEX system is used to demonstrate an organo-metallic compound of rhenium:

```
¥begin{ChemEquation}
Me_{3}SnCl_{2} + 2NaRe(CO)_{5}
¥reactrarrow{0pt}{3cm}{Metathesis}{¥ChemStrut} ¥quad
¥begin{XyMcompd}(1050,400)(-200,100){}{}
¥tetrahedral{0==Sn;1==Me;2==(CO)$_{5}$Re;3==Me;4==Re(CO)$_{5}$}
¥end{XyMcompd}
+ 2NaCl
¥end{ChemEquation}
```

$$\mathrm{Me_3SnCl_2} + 2\mathrm{NaRe(CO)_5} \xrightarrow{\text{Metathesis}} (\mathrm{CO})_5\mathrm{Re}\text{—}\underset{\displaystyle\mathrm{Me}}{\overset{\displaystyle\mathrm{Me}}{\mathrm{Sn}}}\text{—}\mathrm{Re(CO)_5} + 2\mathrm{NaCl} \tag{2.42}$$

where the `XyMcompd` environment is supported in the chemist package (cf. Section 4.3).

The following example shows the use of `¥ChemForm` in an argument of the `¥reactrarrow`:

```
¥begin{ChemEquation}
Na[Mn(CO)_{5}]
¥reactrarrow{0pt}{2cm}{¥ChemForm{C_{3}H_{5}Cl}}{¥ChemStrut}
[Mn(CO)_{5}(¥eta^{1}¥mbox{-}C_{3}H_{5})]
¥reactrarrow{0pt}{2cm}{$¥mathit{h}¥nu$}{or 80¥degC}
[Mn(CO)_{4}(¥eta^{3}¥mbox{-}C_{3}H_{5})] + CO
¥end{ChemEquation}
```

$$\mathrm{Na[Mn(CO)_5]} \xrightarrow{\mathrm{C_3H_5Cl}} [\mathrm{Mn(CO)_5}(\eta^1\text{-}\mathrm{C_3H_5})] \xrightarrow[\text{or } 80^\circ\mathrm{C}]{h\nu} [\mathrm{Mn(CO)_4}(\eta^3\text{-}\mathrm{C_3H_5})] + \mathrm{CO} \tag{2.43}$$

where η^1-allyl (η^1-$\mathrm{C_3H_5}$) is converted into η^3-allyl (η^3-$\mathrm{C_3H_5}$).

If fine tuning is necessary with respect vertical spaces, the following examples would be helpful:

```
¥reactrarrow{0pt}{1cm}{A}{A}
¥reactrarrow{0pt}{1cm}{A}{a}
¥reactrarrow{0pt}{1cm}{a}{a}
{¥reactarrowsep=-1pt ¥def¥reactarrowseprate{1.8}
¥reactrarrow{0pt}{1cm}{A}{a}}
{¥reactarrowsep=-1pt ¥def¥reactarrowseprate{1.8}
¥reactrarrow{0pt}{1cm}{a}{a}}
```

$$\xrightarrow[\mathrm{A}]{\mathrm{A}} \quad \xrightarrow[\mathrm{a}]{\mathrm{A}} \quad \xrightarrow[\mathrm{a}]{\mathrm{a}} \quad \xrightarrow[\mathrm{a}]{\mathrm{A}} \quad \xrightarrow[\mathrm{a}]{\mathrm{a}}$$

where ¥reactarrowsep is an adjustment value between an upper object and an arrow, while the corresponding value between an arrow and a lower object is determined by multiplying the ratio stored as a letter string (¥reactarrowseprate), i.e., ¥reactarrowseprate × ¥reactarrowsep.

2.4.3 Further Commands for Drawing Arrows

New commands ¥reactreqarrow and ¥reactleqarrow have been defined to show unbalanced equilibrium:

¥reactreqarrow{0pt}{1cm}{A}{B} $\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$

¥reactleqarrow{0pt}{1cm}{A}{B} $\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$

The ratio of the length of the shorter arrow to that of the longer arrow is specified by ¥eqlbarrowstretch, which is 0.6 for a default setting. To change the ratio, the following declaration is necessary:

```
{¥def¥eqlbarrowstretch{0.4} ¥reactreqarrow{0pt}{1cm}{A}{B}} ¥qquad
{¥def¥eqlbarrowstretch{0.6} ¥reactreqarrow{0pt}{1cm}{A}{B}} ¥qquad
{¥def¥eqlbarrowstretch{0.8} ¥reactreqarrow{0pt}{1cm}{A}{B}}
```

$\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$ $\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$ $\xrightleftharpoons[\mathrm{B}]{\mathrm{A}}$

2.5 Bonds and Relevant Representations

Triple bonds are drawn by ¥tbond in a ChemEquation or like environment:

```
¥begin{ChemEquation}
RC¥tbond CH + e_{am}^{-} ¥llongrightarrow RC¥tbond C^{-} +
{¥textstyle ¥frac{1}{2}}H_{2}
¥end{ChemEquation}
```

$$\mathrm{RC{\equiv}CH} + \mathrm{e^-_{am}} \longrightarrow \mathrm{RC{\equiv}C^-} + \tfrac{1}{2}\mathrm{H_2} \tag{2.44}$$

where the subscript am of $\mathrm{e^-_{am}}$ indicates that the electron is solvated by liquid ammonia.

Double bonds are drawn by ¥dbond in a ChemEquation or like environment:

```
¥begin{ChemEquation}
CH_{2}¥dbond CH_{2} + PhH
¥reactrarrow{0pt}{2cm}{¥scriptsize ¥ChemForm{AlCl_{3}}}{¥ChemStrut}
PhEt
¥end{ChemEquation}
```

$$\mathrm{CH_2{=}CH_2} + \mathrm{PhH} \xrightarrow{\mathrm{AlCl_3}} \mathrm{PhEt} \tag{2.45}$$

Single bonds are drawn by ¥sbond in a ChemEquation or like environment:

```
¥begin{ChemEquation}
PhN¥dbond O + 2e_{am}^{-} ¥llongrightarrow PhN^{-}¥sbond O^{-}
¥end{ChemEquation}
```

$$\mathrm{PhN{=}O} + 2\mathrm{e^-_{am}} \longrightarrow \mathrm{PhN^-{-}O^-} \tag{2.46}$$

Lone pairs around an atom can be typeset by using the ¥lonepairA command, which is supported by XY-MTEX version 4.05 (the lewisstruc package, cf. on-line document (xymtx405A.pdf)). The following example shows that a cuprous chloride ion ($\mathrm{CuCl_2^-}$) involves two covalent bonds between Cu and Cl and lone pairs around each chlorine atom.

```
¥begin{ChemEquation}
CuCl_{4}^{2-} + Cu ¥llongrightarrow
2¥bigl[¥:¥lonepairA[134]{Cl}¥sbond Cu¥sbond¥lonepairA[123]{Cl}¥:¥bigr]^{-}
¥end{ChemEquation}
```

$$\mathrm{CuCl_4^{2-}} + \mathrm{Cu} \longrightarrow 2\left[:\ddot{\underset{\cdot\cdot}{\mathrm{C}}}\mathrm{l}\text{—}\mathrm{Cu}\text{—}\ddot{\underset{\cdot\cdot}{\mathrm{C}}}\mathrm{l}:\right]^{-} \tag{2.47}$$

Chapter 3

New Mathversions

There are two mathversions ("normal" and "bold") for mathematical usage in LaTeX 2$_\varepsilon$. The chemist (chmst-ps) package provides additional two mathversions ("chem" and "boldchem") for chemical usage. The latter two mathversions have already been introduced in Chapter 17 of the manual of XyMTeX version 1.01 (xymtex.pdf). This chapter is devoted to add further comments with examples, where the chemical environments discussed in Chapter 2 are tested under the respective mathversions.

3.1 Mathversion "normal"

The mathversion "normal" gives outputs of default mode, which are inherent in LaTeX 2$_\varepsilon$without any declaration or with declaring `¥mathversion{normal}`.

3.1.1 Default Outputs

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

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

Thereby, the following code using `¥testmathversion`:

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

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

Output A due to "normal"

$$abcdefghijklmnopqrstuvwxyzıȷABCDEFGHIJKLMNOPQRSTUVWXYZ$$

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

$$1234567890$$

$$1234567890$$

$$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

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

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

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

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

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

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

Output B due to "normal"

Euler's summation:

$$\sum_{a\leq k<b} f(k) = \int_a^b f(x)\mathrm{d}x + \sum_{k=1}^{m} \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m. \tag{3.1}$$

The term R_m is represented as follows:

$$\begin{aligned} R_m &= (-1)^{m+1} \int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)\mathrm{d}x, \\ &\quad a \leq b \text{ and } m \geq 1, \end{aligned} \tag{3.2}$$

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

3.1.2 Convenient Environments for Chemical Equations

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

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

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

Output C due to "normal"

An equation enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.3}$$

An eqnarray environment:

$$C + O_2 \rightarrow CO_2 \tag{3.4}$$
$$Na^+ + Cl^- \rightarrow NaCl\downarrow \tag{3.5}$$

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

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

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

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

Output D due to "normal"

A chemeqn enviroment:

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O} \tag{3.6}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.7}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.8}$$

A chemeqnarray environment:

$$\begin{aligned} \mathrm{C} + \mathrm{O}_2 &\rightarrow \mathrm{CO}_2 && (3.9)\\ \mathrm{Na}^+ + \mathrm{Cl}^- &\rightarrow \mathrm{NaCl}\downarrow && (3.10) \end{aligned}$$

A chemeqnarray$*$ environment:

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

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

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

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

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

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

Output E due to "normal"

A ChemEquation enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.11}$$

$$\text{abcdefghijklmnopqrstuvwxyz}\imath\jmath\text{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.12}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.13}$$

A ChemEqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.14)\\ Na^+ + Cl^- &\rightarrow NaCl\downarrow && (3.15) \end{aligned}$$

A ChemEqnarray$*$ environment:

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

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

3.2 Mathversion "bold"

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

```
¥mathversion{bold}
```

according to LaTeX 2_ε.

3.2.1 Outputs under Mathversion "bold"

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

Output A due to "bold"

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

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

$$\boldsymbol{1234567890}$$

$$\boldsymbol{1234567890}$$

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

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

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

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

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

Output B due to "bold"

Euler's summation:

$$\sum_{a\le k<b} \boldsymbol{f(k)} = \int_a^b \boldsymbol{f(x)}\mathrm{d}\boldsymbol{x} + \sum_{k=1}^{m} \frac{\boldsymbol{B_k}}{\boldsymbol{k!}} \boldsymbol{f^{(k-1)}(x)}\Big|_a^b + \boldsymbol{R_m}. \tag{3.16}$$

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

$$\begin{aligned} \boldsymbol{R_m} &= (-\boldsymbol{1})^{m+1} \int_a^b \frac{\boldsymbol{B_m(\{x\})}}{\boldsymbol{m!}} \boldsymbol{f^{(m)}(x)}\mathrm{d}\boldsymbol{x}, \\ & \qquad \boldsymbol{a \le b} \text{ and } \boldsymbol{m \ge 1}, \end{aligned} \tag{3.17}$$

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

3.2.2 Environments and Commands for Chemistry

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

Output C due to "bold"

An equation enviroment:

$$\boldsymbol{2H_2 + O_2 \rightarrow 2H_2O} \tag{3.18}$$

An eqnarray environment:

$$\begin{aligned} \boldsymbol{C + O_2} &\rightarrow \boldsymbol{CO_2} && (3.19) \\ \boldsymbol{Na^+ + Cl^-} &\rightarrow \boldsymbol{NaCl\downarrow} && (3.20) \end{aligned}$$

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

Output D due to "bold"

A chemeqn enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.21}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.22}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.23}$$

A chemeqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.24)\\ Na^+ + Cl^- &\rightarrow NaCl\downarrow && (3.25) \end{aligned}$$

A chemeqnarray∗ environment:

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

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

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

Output E due to "bold"

A ChemEquation enviroment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{3.26}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.27}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{3.28}$$

A ChemEqnarray environment:

$$\begin{aligned} \mathbf{C + O_2} &\rightarrow \mathbf{CO_2} && (3.29)\\ \mathbf{Na^+ + Cl^-} &\rightarrow \mathbf{NaCl}\downarrow && (3.30) \end{aligned}$$

A ChemEqnarray∗ environment:

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

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

3.3 Mathversion "chem"

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

This section is typeset after the declaration of

```
¥mathversion{chem}
```

3.3.1 Outputs under Mathversion "chem"

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

Output A due to "chem"

abcdefghijklmnopqrstuvwxyz$\imath\jmath$ABCDEFGHIJKLMNOPQRSTUVWXYZ

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

1234567890

$\mathbf{1234567890}$

$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

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

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

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

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

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

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

Output B due to "chem"

Euler's summation:

$$\sum_{a\leq k¡b} f(k) = \int_a^b f(x)dx + \sum_{k=1}^{m} \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m. \tag{3.31}$$

The term R_m is represented as follows:

$$\begin{aligned} R_m &= (-1)^{m+1} \int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)dx, \\ &\quad a \leq b \text{ and } m \geq 1, \end{aligned} \tag{3.32}$$

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

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

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

gives the following output:

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

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

```
{¥mathversion{normal}
```

```
¥[¥sum_{a¥leq k < b}f(k)¥]
}
```

which gives the following output:

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

3.3.2 Environments and Commands for Chemistry

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

Output C due to "chem"

An equation enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.33}$$

An eqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.34)\\ Na^+ + Cl^- &\rightarrow NaCl \downarrow && (3.35) \end{aligned}$$

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

Output D due to "chem"

A chemeqn enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.36}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.37}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.38}$$

A chemeqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.39)\\ Na^+ + Cl^- &\rightarrow NaCl \downarrow && (3.40) \end{aligned}$$

A chemeqnarray$*$ environment:

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

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

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

Output E due to "chem"

A ChemEquation enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.41}$$

$$\mathrm{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathrm{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.42}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.43}$$

A ChemEqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.44)\\ Na^+ + Cl^- &\rightarrow NaCl\downarrow && (3.45) \end{aligned}$$

A ChemEqnarray∗ environment:

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

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

3.4 Mathversion "boldchem"

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

This section is typeset after the declaration of

```
¥mathversion{boldchem}
```

3.4.1 Outputs under Mathversion "boldchem"

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

Output A due to "boldchem"

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

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

$$\mathbf{1234567890}$$

$$\mathbf{1234567890}$$

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

$$\boldsymbol{\int\sum\prod\coprod\cup\cap\odot\oplus\uplus\otimes}$$

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

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

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

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

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

Output B due to "boldchem"

Euler's summation:

$$\sum_{\mathbf{a\leq k¡b}} \mathbf{f(k)} = \int_{\mathbf{a}}^{\mathbf{b}} \mathbf{f(x)dx} + \sum_{\mathbf{k=1}}^{\mathbf{m}} \frac{\mathbf{B_k}}{\mathbf{k!}} \mathbf{f^{(k-1)}(x)} \Big|_{\mathbf{a}}^{\mathbf{b}} + \mathbf{R_m}. \tag{3.46}$$

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

$$\begin{aligned} \mathbf{R_m} &= \mathbf{(-1)^{m+1}} \int_{\mathbf{a}}^{\mathbf{b}} \frac{\mathbf{B_m(\{x\})}}{\mathbf{m!}} \mathbf{f^{(m)}(x)dx}, \\ &\quad \mathbf{a \leq b} \text{ and } \mathbf{m \geq 1}, \end{aligned} \tag{3.47}$$

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

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

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

gives the following output:

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

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

```
{¥mathversion{normal}
¥[¥sum_{a¥leq k < b}f(k)¥]
}
```

which gives the following output:

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

3.4.2 Environments and Commands for Chemistry

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

Output C due to "boldchem"

An equation enviroment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{3.48}$$

An eqnarray environment:

$$\begin{aligned} \mathbf{C + O_2} &\rightarrow \mathbf{CO_2} && (3.49) \\ \mathbf{Na^+ + Cl^-} &\rightarrow \mathbf{NaCl\downarrow} && (3.50) \end{aligned}$$

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

Output D due to "boldchem"

A chemeqn enviroment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{3.51}$$

$$\text{abcdefghijklmnopqrstuvwxyz}\imath\jmath\text{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.52}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{3.53}$$

A chemeqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 && (3.54)\\ Na^+ + Cl^- &\rightarrow NaCl\downarrow && (3.55) \end{aligned}$$

A chemeqnarray$*$ environment:

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

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

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

Output E due to "boldchem"

A ChemEquation enviroment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{3.56}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{3.57}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{3.58}$$

A ChemEqnarray environment:

$$\begin{aligned} \mathbf{C + O_2} &\rightarrow \mathbf{CO_2} && (3.59)\\ \mathbf{Na^+ + Cl^-} &\rightarrow \mathbf{NaCl}\downarrow && (3.60) \end{aligned}$$

A ChemEqnarray$*$ environment:

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

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

Chapter 4

Chemical Schemes

This chapter is partly based on Chapter 9 of "LaTeX for (Bio)Chemists" [14] by Shinsaku Fujita. The previous manuals have already discussed functions provided by the the chemist package:

1. Chapter 17 of the online manual of XyMTeX version 1.01 (xymtex.pdf, cf. [3]) has discussed tools for drawing chemical schemes, which are supported by the chemist package, e.g., arrows for chemical equations (Section 17.2); boxes for chemical formulas (Section 17.3); as well as compounds number and cross-references (Section 17.4).

2. Chapter 19 of the online manual of XyMTeX version 1.01 (xymtex.pdf, cf. [3]) has discussed tools for drawing frames, which are supported by the chemist package, e.g., environments for drawing framed boxes (Section 19.1) and environment for drawing shadow boxes (Section 19.2).

3. Reaction schemes due to the chemist package have already been introduced in Chapter 12 of the online manual of XyMTeX version 2.00 (xymtx200PS.pdf, cf. [5]).

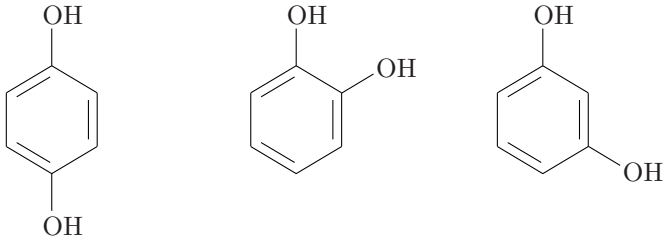
This chapter is devoted to add further comments with examples.

4.1 Compound Numbers and Cross-References

After the chemist (chmst-ps) package is loaded, the command `¥compd` can be used to print out a sequential compound number. The compound number is capable of usual cross reference of LaTeX 2_ε, where `¥label` and `¥ref` is used. To print a boldfaced number, the chemist (chmst-ps) package supports `¥cref` command. For example, structural formulas due to the XyMTeX system are numbered sequentially by writing the following code:

```
¥begin{tabular}{ccc}
¥bzdrv{1==OH;4==OH} & ¥bzdrv{1==OH;2==OH} & ¥bzdrv{1==OH;3==OH} ¥¥
¥compd¥label{cpd:1} & ¥compd¥label{cpd:2} & ¥compdlabel{cpd:3} ¥¥
¥multicolumn{3}{l}{Compound ¥cref{cpd:1} is called hydroquinone
or 1,4-dihyroxybenzene.} ¥¥
¥multicolumn{3}{l}{Compound ¥cref{cpd:2} is called catechol
or 1,2-dihyroxybenzene.} ¥¥
¥multicolumn{3}{l}{Compound ¥cref{cpd:3} is called resorcinol
or 1,3-dihydroxybenzene.} ¥¥
¥end{tabular}
```

which results in the following output:



1 **2** **3**

Compound **1** is called hydroquinone or 1,4-dihyroxybenzene.
Compound **2** is called catechol or 1,2-dihyroxybenzene.
Compound **3** is called resorcinol or 1,3-dihydroxybenzene.

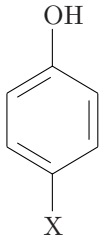
The `¥compdlabel{...}` command can be used in place of `¥compd¥label{...}`, where ... is a reference key.

4.2 Derivative Numbers and Cross-References

The command `¥nocompd` gives a sequential compound number to a compound, but the compound number is not output. The compound number can be referred by using `¥label` and `¥cref` (or `¥ref`). The command `¥nocompd` is combined with the `¥deriv` command as shown in the following code:

```
¥begin{tabular}{cll}
¥multicolumn{3}{c}{%
¥bzdrv{1==OH;4==X}¥nocompd¥label{cpd:4} }¥¥
¥deriv¥label{cpd:4a} & ¥chemform{X = OH} & hydroquinone ¥¥
¥deriv¥label{cpd:4b} & ¥chemform{X = F}  & 4-fluorophenol ¥¥
¥deriv¥label{cpd:4c} & ¥chemform{X = Cl} & 4-chlorophenol ¥¥
¥derivlabel{cpd:4d}  & ¥chemform{X = Br} & 4-bromophenol ¥¥
¥derivlabel{cpd:4e}  & ¥chemform{X = NO_2} & 4-nitrophenol ¥¥
¥derivlabel{cpd:4f}  & ¥chemform{X = NH_3^+ClO_4^-} &
4-hydroxy-1-anilinium perchlorate ¥¥
¥end{tabular}
```

which results in the following output:

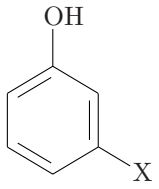


4a	X = OH	hydroquinone
4b	X = F	4-fluorophenol
4c	X = Cl	4-chlorophenol
4d	X = Br	4-bromophenol
4e	X = NO_2	4-nitrophenol
4f	X = $NH_3^+ClO_4^-$	4-hydroxy-1-anilinium perchlorate

The `¥deriv` command gives a derivative number such as **4a**, in which the number **4** stems from the "compd" counter in the setting due to `¥nocompd` and the alphabet **a** stems from the "deriv" counter in the setting due to `¥deriv`. Each derivative is referred to by `¥label` and `¥cref`. For example, `¥cref{cpd:4b}` outputs a derivative number **4b**, while `¥cref{cpd:4}` output the group number **4** of the derivatives.

On the other hand, the `¥derivnum` command is used in combination with `¥compd` as follows:

```
¥begin{tabular}{cll}
¥multicolumn{2}{c}{¥bzdrv{1==OH;3==X}}&¥¥[-15pt]
¥multicolumn{2}{c}{¥compd¥label{cpd:5}}&¥¥[10pt]
¥derivnum¥label{cpd:5a} & ¥chemform{X = OH} & resorcinol ¥¥
¥derivnum¥label{cpd:5b} & ¥chemform{X = F}  & 3-fluorophenol ¥¥
¥derivnum¥label{cpd:5c} & ¥chemform{X = Cl} & 3-chlorophenol ¥¥
¥derivnum¥label{cpd:5d}  & ¥chemform{X = Br} & 3-bromophenol ¥¥
¥derivnum¥label{cpd:5e}  & ¥chemform{X = NO_2} & 3-nitrophenol ¥¥
¥derivnum¥label{cpd:5f}  & ¥chemform{X = NH_3^+ClO_4^-} &
3-hydroxy-1-anilinium perchlorate ¥¥
¥end{tabular}
```



5

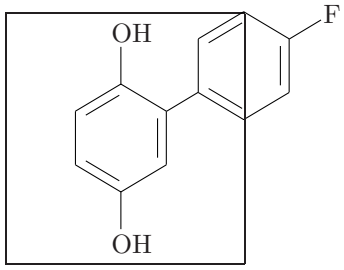
a	X = OH	resorcinol
b	X = F	3-fluorophenol
c	X = Cl	3-chlorophenol
d	X = Br	3-bromophenol
e	X = NO_2	3-nitrophenol
f	X = $NH_3^+ClO_4^-$	3-hydroxy-1-anilinium perchlorate

The `¥derivnum` command gives a derivative number as a sequential alphabet (**a** etc.) which stems from the "deriv" counter in the setting due to `¥derivnum`. Each derivative is referred to by `¥label` and `¥cref`. For example, `¥cref{cpd:5a}` outputs a derivative number **5a**, while `¥cref{cpd:5}` output the group number **5** of the derivatives.

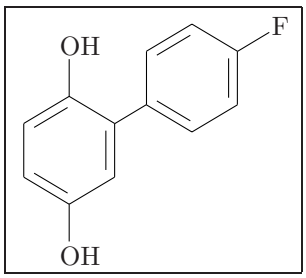
4.3 Boxes for Chemical Structural Formulas

4.3.1 XyMcompd Environment

Each structural formula drawn by the XyMTEX system has its drawing domain, which is decided by its main skeleton. This means that a large substituent sticks out from the domain, as shown in the following formula:



where the domain is surrounded by a frame due to `¥fbox`. To adjust such a drawing domain to cover the net formula, we use a XyMcompd environment as follows:



which is drawn by the following code:

```
¥fbox{%
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}
}
```

The first argument `(900,900)` indicates the (width, height) of the domain which is measured by using `¥unitlength` (default 0.1 pt) as a unit. The 2nd argument `(250,50)` represents a shift value of x, y-coordinates. The 3rd argument is a key for compound number if necessary. The 4th argument is a derivative alphabet if necessary.

4.3.2 Commands for Compound Boxes

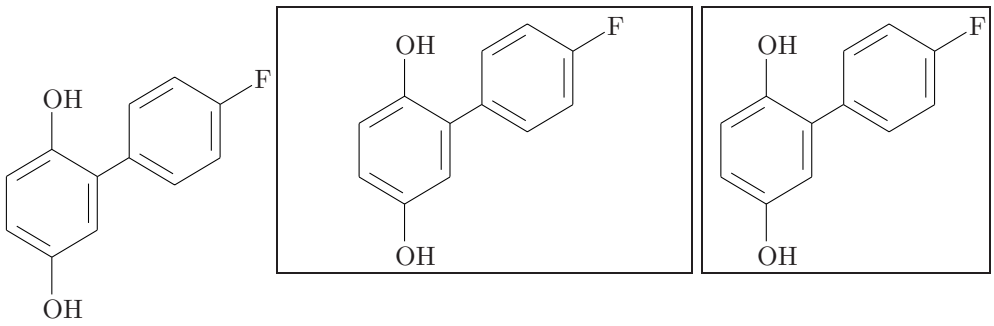
The command `¥cdonecell` takes three arguments:

```
¥cdonecell{dimenA}{dimenB}{formula}
```

to draw the structure of the 3rd argument `formula` with a width of the 2nd argument `dimenB` at a raised position decided by the 1st argument `dimenA`. A similar raised structural formula can be drawn by using the `¥raisebox` command of the graphicx package. For example, the following code:

```
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}
¥fbox{%
¥cdonecell{20pt}{150pt}{%
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}}}
¥fbox{%
¥raisebox{20pt}{%
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}}}
```

gives the following result:

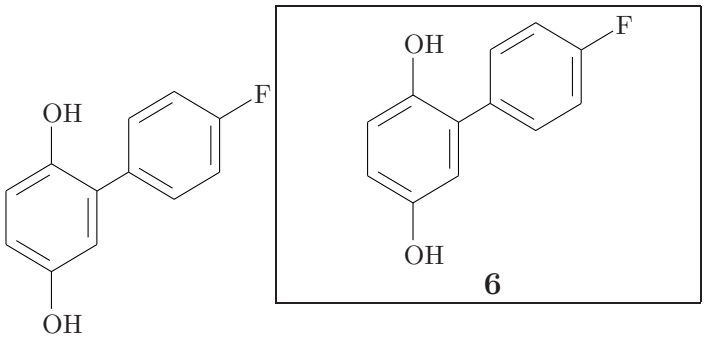


where the frame of the latter formula is drawn by the ¥fbox command.

The command ¥cdtwocell{dimenA}{dimenB}{formula}{labels} draws the structure of the 3rd argument formula with a width of the 2nd argument dimenB at a raised position decided by the 1st argument dimenA, where compound labels are written as the fourth argument labels. For example, the following code:

```
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}
¥fbox{%
¥cdtwocell{20pt}{150pt}{%
¥begin{XyMcompd}(900,900)(250,50){}{}
¥bzdrv{1==OH;4==OH;2==¥bzdrv{5==(yl);2==F}}
¥end{XyMcompd}}{¥compd¥label{cpd:7}}}
```

gives the following result:



where the frame of the latter formula is drawn by the ¥fbox command.

4.4 Arrows for Organic Chemistry

Arrows due to the chemist package have been introduced in Section 12.2 of the manual of XyMTEX version 2.00 (xymtx200PS.pdf, cf. [5]). The list of arrows of the manual is cited for convenience, as shown in Fig. 4.1, where the four arrows for representing equilibriums in the fourth row are new matters in the present version of chemist (chmst-ps) package. The arrows in the fifth row have been renamed into the present names in order to assign the previous names to the arrows in the fourth row. Note that a combination of left and right arrows is used to represent a forward and reverse reaction, while a combination of left and right harpoons is used to represent an equilibrium (cf. page 13).

Each command for drawing an arrow listed in Fig. 4.1 is used in the following format:

```
¥ARROWNAME[xshift]{yshift}{length}{itemover}{itemunder}
```

where ¥ARROWNAME represents a command name; xshift is an optional argument to show a horizontal adjustment value; yshift is an argument to show a vertical adjustment value; length is an argument to designate the length of the arrow; and the arguments itemover and itemunder represent items placed over and under the arrow. The name (¥ARROWNAME) of each reaction arrow take the format of ¥react...arrow in which ... is selected from the following list: r = right arrow, l = left arrow, d = down arrow, u = up arrow; sw = southwest arrow, se = southeast arrow, nw = northwest arrow, ne = northeast arrow; du = down up arrow, lr = leftright arrow, dlr = down leftright arrow, ulr = up leftright arrow; eq = equilibrium arrow, deq = down equilibrium arrow, leq = up equilibrium arrow, veq = vertical equilibrium arrow; Eq = forward-reverse arrow, DEq = down forward-reverse arrow, LEq = up forward-reverse arrow, and VEq = vertical forward-reverse arrow.

For example, the ¥reactrarrow{dimenA}{dimenB}{textA}{textB} gives a chemical arrow of length ¥dimenB (the 2nd argument) at a position raised by the first argument dimenA, where textA of the 3rd

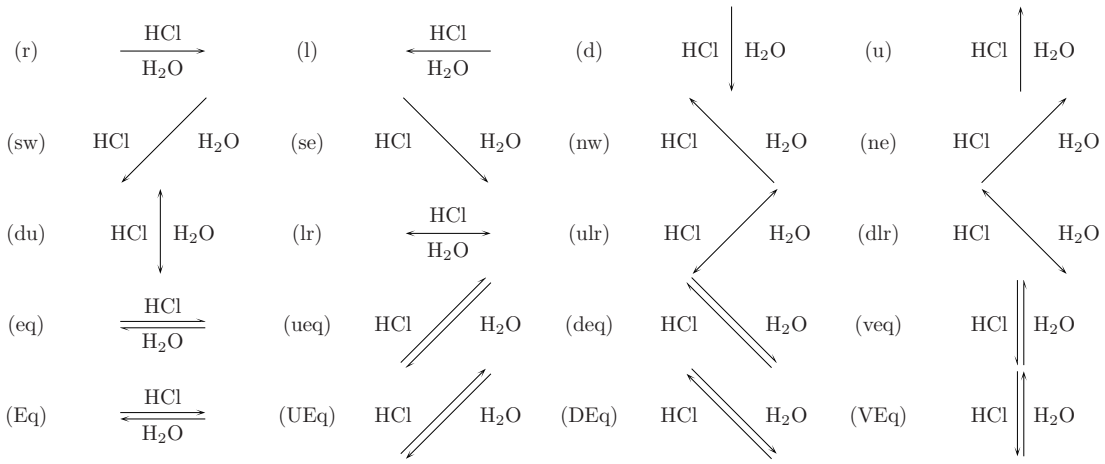


Figure 4.1: Reaction arrows of various types

argument is printed over the arrow and `textB` of the 4th argument is printed below the arrow. For example, the following code for writing catalytic reforming:

```
¥begin{ChemEquation}
CH_3CH_2CH_2CH_2CH_2CH_3 ¥quad
¥reactrarrow{0pt}{2cm}{catalyst ¥¥[-5pt]}{{}¥¥[-15pt]heat}
¥quad
¥begin{XyMcompd}(200,350)(300,280){}{}
¥bzdrv[A]{}
¥end{XyMcompd} ¥quad + 4H_2
¥end{ChemEquation}
```

gives the following output:

$$\mathrm{CH_3CH_2CH_2CH_2CH_2CH_3} \xrightarrow[\text{heat}]{\text{catalyst}} \bigcirc + 4\mathrm{H_2} \tag{4.1}$$

where the `¥reactrarrow` command is used in a `ChemEquation` environment.

Another example is shown as follows:

```
¥begin{ChemEqnarray*}
¥lefteqn{%
CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 ¥qquad
¥reactrarrow{0pt}{2cm}{heat¥¥[-5pt]}{{}¥¥[-15pt]catalyst}} && ¥¥[10pt]
&¥hskip40pt& CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_2¥dbond CH_2 ¥¥
&& ¥hskip120pt¥mbox{and} ¥¥
&& CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH¥dbond CH_2 ¥¥
&& ¥hskip120pt¥mbox{and} ¥¥
&& CH_3CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH_2CH_2CH_2CH¥dbond CH_2 ¥¥
&& ¥hskip120pt¥mbox{and so on}
¥end{ChemEqnarray*}
```

where the `¥reactrarrow` command is used in a `ChemEqnarray`$*$ environment. This code results in the

following output:

$$\mathrm{CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3} \xrightarrow[\text{catalyst}]{\text{heat}}$$

$$\mathrm{CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_2{=}CH_2}$$
and
$$\mathrm{CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH{=}CH_2}$$
and
$$\mathrm{CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH_2CH_2CH_2CH{=}CH_2}$$
and so on

It should be noted that `¥ChemForm{¥mbox{and}}` and `¥ChemForm{and}` give equivalent outputs, "and" and "and". In contrast, `¥ChemForm{¥mbox{and so on}}` and `¥ChemForm{and so on}` give different outputs, "and so on" and "andsoon", where the spaces of the latter are deleted by typesetting mechanism due to the math mode of TEX/LATEX 2ε.

```
¥begin{ChemEqnarray}
A ¥reactrarrow{0pt}{3cm}{¥ChemForm{H^+}}{acid catalysis}
B ¥reactlarrow{0pt}{2cm}{¥ChemForm{H^+}}{¥ChemForm{CH_3OH}}
C ¥reactlrarrow{0pt}{2cm}{¥ChemForm{H^+}}{¥strut}
D ¥reacteqarrow{0pt}{2cm}{¥ChemForm{H^+}}{equilibrium}  E
¥end{ChemEqnarray}
```

$$\mathrm{A} \xrightarrow[\text{acid catalysis}]{\mathrm{H^+}} \mathrm{B} \xleftarrow[\mathrm{CH_3OH}]{\mathrm{H^+}} \mathrm{C} \xleftrightarrow{\mathrm{H^+}} \mathrm{D} \underset{\text{equilibrium}}{\overset{\mathrm{H^+}}{\rightleftharpoons}} \mathrm{E} \tag{4.2}$$

Arrows with a double line are drawn by using `¥schemerarrow`, `¥schemelarrow`, and `¥schemelrarrow`. When the chmst-ps package is loaded after the loading of the chmemist package, the PSTricks package becomes effective so as to print arrows due to PostScript utilities, as shown in the following examples.

```
¥begin{ChemEqnarray}
A ¥schemerarrow{0pt}{3cm}{¥ChemForm{H^+}}{acid catalysis}
B ¥schemelarrow{0pt}{2cm}{¥ChemForm{H^+}}{¥ChemForm{CH_3OH}}
C ¥schemelrarrow{0pt}{2cm}{¥ChemForm{H^+}}{¥strut} D
¥end{ChemEqnarray}
```

$$\mathrm{A} \xRightarrow[\text{acid catalysis}]{\mathrm{H^+}} \mathrm{B} \xLeftarrow[\mathrm{CH_3OH}]{\mathrm{H^+}} \mathrm{C} \xLeftrightarrow{\mathrm{H^+}} \mathrm{D} \tag{4.3}$$

If the chmst-ps package is not loaded, the following output is obtained by means of the same code shown above:

$$\mathrm{A} \xRightarrow[\text{acid catalysis}]{\mathrm{H^+}} \mathrm{B} \xLeftarrow[\mathrm{CH_3OH}]{\mathrm{H^+}} \mathrm{C} \xLeftrightarrow{\mathrm{H^+}} \mathrm{D} \tag{4.4}$$

4.5 Framed Boxes

Framed boxes due to the chemist package have been introduced in Chapter 19 of the manual of XYMTEX version 1.01 (xymtex.pdf).

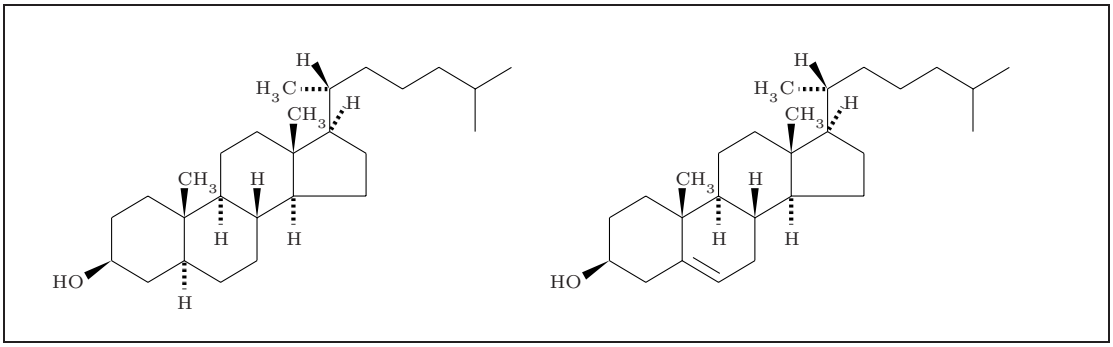
4.5.1 Simple Framed Boxes

Chapter 19 of the manual of XyMTEX version 1.01 (xymtex.pdf) has discussed tools for drawing frames, which are supported by the chemist package, e.g., environments for drawing framed boxes (Section 19.1) and environment for drawing shadow boxes (Section 19.2).

The `frameboxit` environment of the chemist (chmst-ps) package has one argument (for specifying the width of the resulting box.

```
¥begin{frameboxit}{0.9¥textwidth}
¥changeunitlength{0.08pt}
¥let¥substfontsize=¥scriptsize
¥centering
¥cholestaneAlpha{3B==HO}
¥cholestane[e]{3B==HO}
¥end{frameboxit}
```

Then, you obtain the following result.



Note that each structural formula drawn by XyMTEX has a space around itself, which will be used for typesetting possible substituents. The dimension register `¥textwidth` stores the width of the printed domain of a page. The command `¥changeunitlength{0.08pt}` reduces the size of each structural formulas drawn by XyMTEX. The setting `¥let¥substfontsize=¥scriptsize` due to XyMTEX changes the font size of each substituent. The command `¥centering` of LaTeX 2ε results in the centering of objects within the `frameboxit` environment.

The `frameboxit` environment is based on the `fr@meboxit` environment of the chemist package, which can specify the line thickness of the frame (`line_thickness`) and the margin (`frame_sep`) around the text included in addition to the with of the resulting box (`box_width`):

```
¥begin{fr@meboxit}{line_thickness}{frame_sep}{box_width}}
(text)
¥end{fr@meboxit}
```

The default values of them are equal to those of the `¥fbox` command of LaTeX.

The following example shows the use of the `fr@meboxit` environment with changes of such parameters.

```
¥makeatletter
¥begin{frameboxit}{5cm}
Default Parameters are selected to be 0.4pt for the line thickness and
3pt for the margin space.
The box width can be selected according to your choice.
¥end{frameboxit}
¥begin{fr@meboxit}{1pt}{10pt}{7cm}
Parameters are changed into 1pt for the line thickness and
10pt for the margin space.
The box width can be selected according to your choice.
```

```
¥end{fr@meboxit}
¥makeatother
```

Note that the commands ¥makeatletter and ¥makeatother should be used for the special treatment of the @ character. This statement produces the following result.

Default Parameters are selected to be 0.4pt for the line thickness and 3pt for the margin space. The box width can be selected according to your choice.

Parameters are changed into 1pt for the line thickness and 10pt for the margin space. The box width can be selected according to your choice.

4.5.2 Oval Boxes

The miniscreen environment of the chemist package has one argument specifying the width of the resulting box. For example, by writing a statement such as

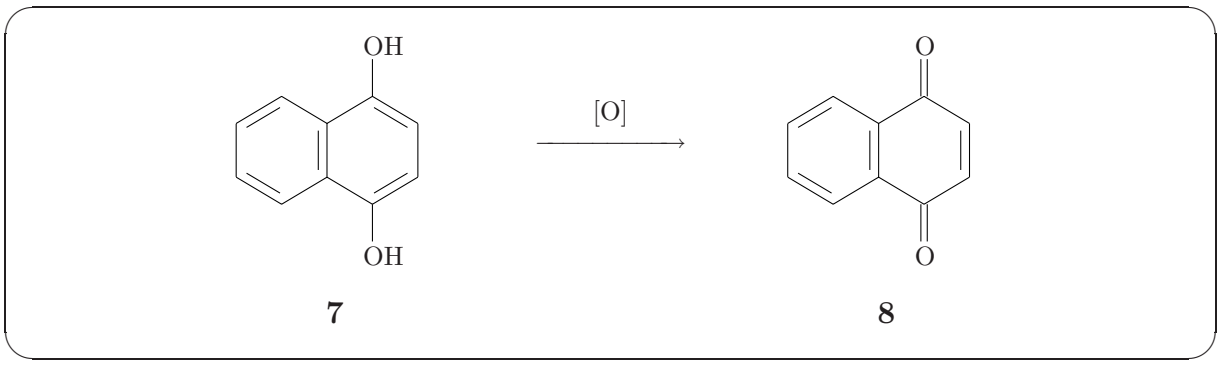
```
¥begin{miniscreen}{7cm}
¥begin{center}
$¥displaystyle e^{x}  =  1 + ¥frac{x}{1!} + ¥frac{x^{2}}{2!} +
¥frac{x^{3}}{3!} + ¥cdots$ ¥qquad
$¥displaystyle ¥sin x  =  ¥frac{x}{1!} - ¥frac{x^{3}}{3!} +
¥frac{x^{5}}{5!} - ¥frac{x^{7}}{7!} + ¥cdots$
¥end{center}
¥end{miniscreen}
```

you obtain the following result.

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$
$$\sin x = \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots$$

When the argument of the miniscreen environment is specified to be ¥textwidth, the resulting box generated a framed text of width ¥textwidth. The resulting frame is equivalent to the one generated by the screen environment of the package ascmac.sty. It follows that the screen environment can be redefined on the basis of the definition of the miniscreen environment described above. The redefined screen environment can be used as follows.

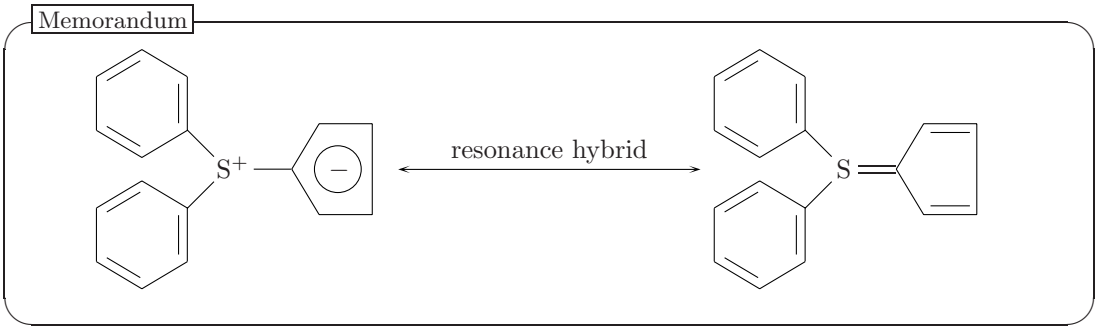
```
¥begin{screen}
¥begin{center}
¥begin{tabular}{c}
¥naphdrv{1==OH;4==OH} ¥¥[.3cm] ¥compd ¥label{box:a2} ¥¥
¥end{tabular}
¥begin{tabular}{c}
[O] ¥¥ ¥parbox{2cm}{¥rightarrowfill} ¥¥[1cm] ¥mathstrut ¥¥
¥end{tabular}
¥begin{tabular}{c}
¥naphdrv[p]{1D==O;4D==O} ¥¥[.3cm] ¥compd ¥label{box:a3} ¥¥
¥end{tabular}
¥end{center}
¥end{screen}
```



The tboxminiscreen environment of the chemist package is used to generate a box with a heading title (the default title is "Memorandum"), where the width of the generated box can be specified by its argument. For example, by writing such a statement as

```
¥begin{tboxminiscreen}{0.9¥textwidth}
¥begin{center}
¥begin{XyMcompd}(1000,900)(-150,-150){}{}
¥ltrigonal{0==S$^{+}$;2==¥bzdrv{3==(yl)};3==¥bzdrv{2==(yl)};
1==¥cyclopentanehi[A{0{$-$}}]{1==(yl)}}
¥end{XyMcompd}
¥reactlrarrow{0pt}{4cm}{resonance hybrid}{¥strut}
¥begin{XyMcompd}(1000,900)(-150,-150){}{}
¥ltrigonal{0==S;2==¥bzdrv{3==(yl)};3==¥bzdrv{2==(yl)};
1D==¥cyclopentanehi[bd]{1==(yl)}}
¥end{XyMcompd}
¥end{center}
¥end{tboxminiscreen}
```

you obtain the following result.



For changing the heading title, you redefine the control sequence ¥tboxtitle by means of the command ¥def or ¥renewcommand. For example, the statement

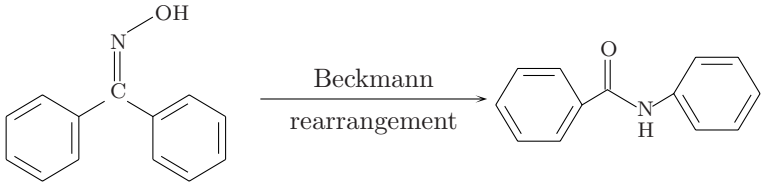
```
¥def¥tboxtitle{¥bf Summary Notes}
¥begin{tboxminiscreen}{0.8¥textwidth}
The Beckmann rearrangement is a transformation of
an oxime into an amide under an acidic condition.
Since a substrate oxime can be easily obtained from
a ketone (or aldehyde) and hydroxylamine,
the Beckmann rearrangement is important as one of
valuable industrial processes.
¥par ¥medskip
¥begin{center}
```

```
¥changeunitlength{0.08pt}
¥begin{XyMcompd}(1000,850)(-150,-150){}{}
¥Ethylenev{1==C;2==N}{3==OH;2==¥bzdrv{6==(yl)};1==¥bzdrv{2==(yl)}}
¥end{XyMcompd}
¥reactrarrow{0pt}{3cm}{Beckmann}{rearrangment}
¥begin{XyMcompd}(1100,500)(-400,0){}{}
¥dimethylenei{2==¥downnobond{N}{H}}{2W==¥bzdrh{1==(yl)};1W==¥bzdrh{4==(yl)};1D==O}
¥end{XyMcompd}
¥end{center}
¥end{tboxminiscreen}
```

typesets the following miniscreen box with a changed title.

Summary Notes

The Beckmann rearrangement is a transformation of an oxime into an amide under an acidic condition. Since a substrate oxime can be easily obtained from a ketone (or aldehyde) and hydroxylamine, the Beckmann rearrangement is important as one of valuable industrial processes.

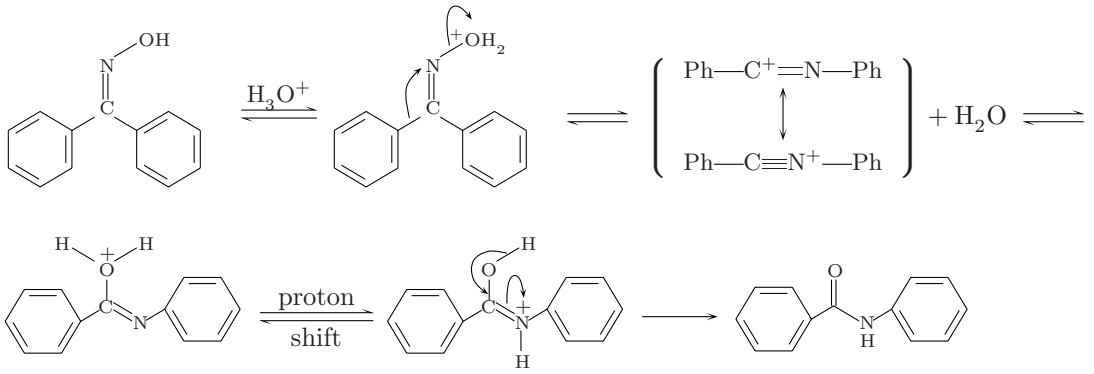


A `tboxscreen` environment provides a frame spreading for `¥textwidth`. The following example shows that a `ChemEqnarray*` enviroment can be used in a `tboxscreen` environment to give a reaction scheme exhibiting the multistep mechanism of the Beckmann Rearrangement.

```
¥def¥tboxtitle{¥bf Beckmann Rearrangement}
¥begin{tboxscreen}
¥changeunitlength{0.07pt}
¥begin{ChemEqnarray*}
&&
¥begin{XyMcompd}(1000,850)(-150,-150){}{}
¥Ethylenev{1==C;2==N}{3==OH;2==¥bzdrv{6==(yl)};1==¥bzdrv{2==(yl)}}
¥end{XyMcompd}
¥mskip6mu ¥reacteqarrow{0pt}{1cm}{¥small H$_{3}$O$^{+}$}{¥strut} ¥mskip6mu
¥begin{XyMcompd}(1000,850)(-150,-150){}{}
¥Ethylenev{1==C;2==N;%
1==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(-85,-20)(-100,150)(-20,250);%
2==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(130,140)(150,350)(250,280)%
}{3==¥llap{$^{+}$}OH$_{2}$;2==¥bzdrv{6==(yl)};1==¥bzdrv{2==(yl)}}
¥end{XyMcompd}
¥mskip6mu ¥reacteqarrow{0pt}{0.8cm}{}{} ¥mskip6mu
¥left¥lgroup
¥begin{tabular}{c}
¥small Ph¥sbond C$^{+}$¥dbond N¥sbond Ph ¥¥
¥reactduarrow{0pt}{20pt}{}{} ¥¥
¥small Ph¥sbond C¥tbond N$^{+}$¥sbond Ph ¥¥
¥end{tabular}
¥right¥rgroup
```

```
+ H_{2}O
¥mskip6mu ¥reacteqarrow{Opt}{0.8cm}{}{}
¥¥ ¥noalign{¥vskip20pt}
& &
¥begin{XyMcompd}(1100,500)(-400,0){}{}
¥dimethylenei[a]{1==C;2==N}{2W==¥bzdrh{1==(yl)};1W==¥bzdrh{4==(yl)};%
1==¥Utrigonal{0==¥upnobond{O}{+};3==H;2==H;1==(yl)}}
¥end{XyMcompd}
¥mskip6mu ¥reacteqarrow{Opt}{1.5cm}{proton}{shift} ¥mskip6mu
¥begin{XyMcompd}(1100,500)(-400,0){}{}
¥dimethylenei[a]{1==C;2==¥upnobond{N}{+};%
1==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{<-}%
(-40,100)(-120,180)(-120,280)(-40,330)(60,320);%
1==¥pscurve[unit=¥unitlength,linewidth=0.4pt]{->}%
(60,50)(100,200)(150,80)%
}%
{2==H;2W==¥bzdrh{1==(yl)};1W==¥bzdrh{4==(yl)};%
1==¥Utrigonal{0==O;2==H;1==(yl)}}
¥end{XyMcompd}
¥mskip6mu ¥reactrarrow{Opt}{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

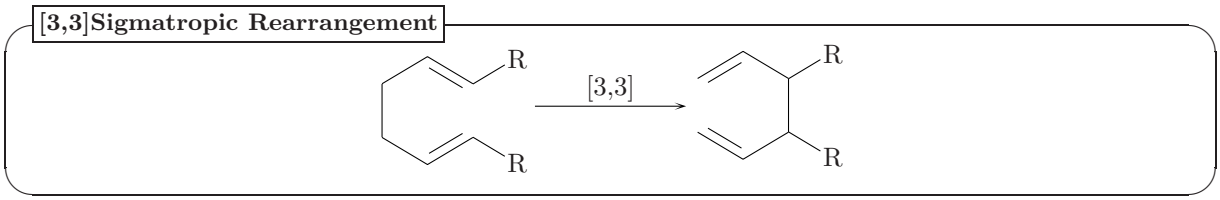


Note that the commands ¥sbond, ¥dbond, and ¥tbond are supported by the chemist packages to draw single (——), double (═), and triple bonds (≡). The command ¥pscurve is supported by the PSTricks package to draw curved lines or arrows.

Another example using a tboxscreen environment is shown as follows:

```
¥def¥tboxtitle{¥bf [3,3]Sigmatropic Rearrangement}
¥begin{tboxscreen}
¥centering
¥begin{XyMcompd}(400,400)(-260,-280){}{}
¥sixunitv[ac]{}{2==R;3==R}{b}
¥end{XyMcompd}
¥reactrarrow{Opt}{2cm}{[3,3]}{¥strut}
¥begin{XyMcompd}(400,400)(50,-100){}{}
¥sixunitv[df]{}{2==R;3==R}{e}
¥end{XyMcompd}
```

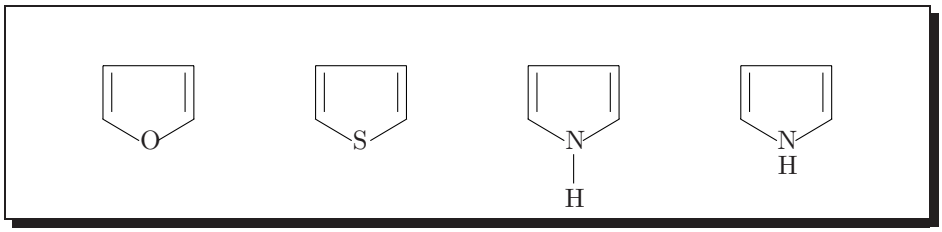
```
¥end{tboxscreen}
```



4.5.3 Frames with Shadows

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

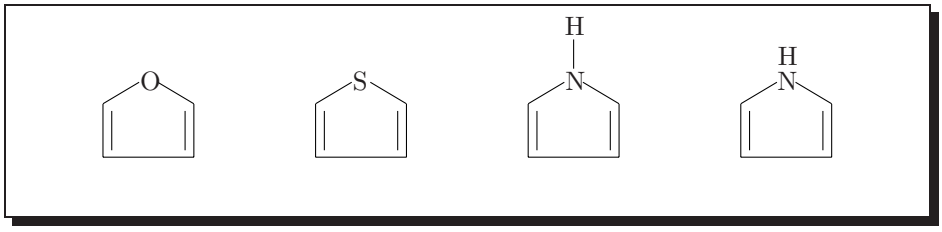
```
¥begin{rshfboxit}{12cm}
¥centering
¥vspace*{-15pt}
¥furanv{} ¥thiophenev{} ¥pyrrolev{1==H}
¥fiveheterov[bd]{1==¥downnobond{N}{H}}{}
¥end{rshfboxit}
```



In a similar way, an `lshfboxit` (left-shadow-frame-box-it) environment provides a framed box with left and bottom shadows, where the width of the box can be specified by its argument. The following example shows another list of commands for drawing five-membered heterocycles, which is surrounded by such a framed box.

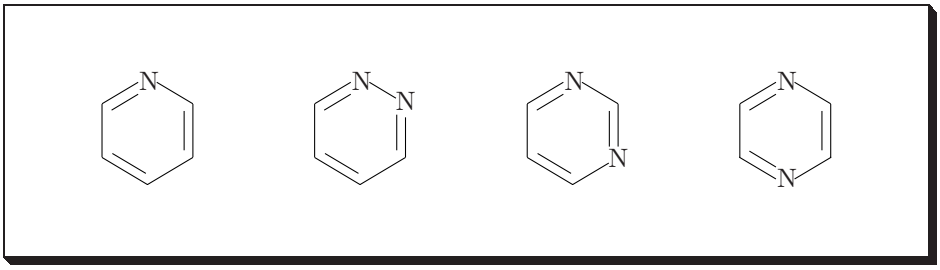
```
¥begin{rshfboxit}{12cm}
¥centering
¥furanvi{} ¥thiophenevi{} ¥pyrrolevi{1==H}
¥fiveheterovi[bd]{1==¥upnobond{N}{H}}{}

¥vspace*{-15pt}
¥end{rshfboxit}
```



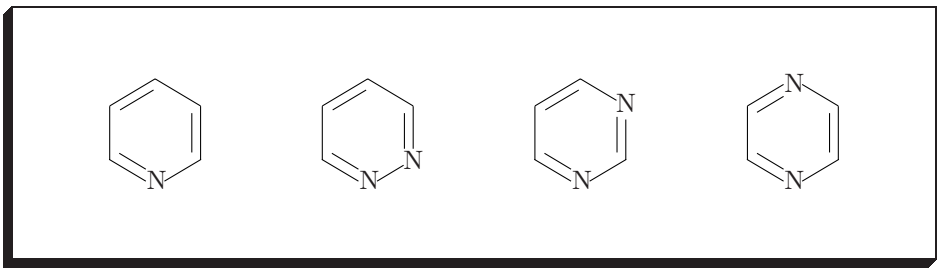
A `grshfboxit` (gradient-right-shadow-frame-box-it) environment provides a framed box with right and bottom gradient shadows, where the width of the box can be specified by its argument. The following example shows a list of commands for drawing six-membered heterocycles, which is surrounded by such a framed box.

```
¥begin{grshfboxit}{12cm}
¥centering
¥pyridinev{} ¥pyridazinev{} ¥pyrimidinev{} ¥pyrazinev{}
¥end{grshfboxit}
```



In a similar way, a `glshfboxit` (gradient-left-shadow-frame-box-it) environment provides a framed box with gradient shadows locating at left and bottom positions, where the width of the box can be specified by its argument. The following example shows another list of commands for drawing six-membered heterocycles, which is surrounded by such a framed box.

```
¥begin{glshfboxit}{12cm}
¥centering
¥pyridinevi{} ¥pyridazinevi{} ¥pyrimidinevi{} ¥pyrazinevi{}
¥end{glshfboxit}
```



4.6 Verbatim Enviroment

A `verbatim` enviroment due to the chemist package have been introduced in Section 17.5 of the manual of XyMTEX version 1.01 (xymtex.pdf). Because Japanese encoding has adopted the symbol ¥ (ASCII character code "5C) in place of the symbol \, the the symbol ¥ has been adopted as a default top letter of each command (control sequence) of TEX/LATEX 2_ε in Japanese applications. Hence, the `varbatim` environment supported by the chemist package has adopted the symbol ¥ as its default output, where the switch `¥verbswitchtrue` is declared initially. The symbol can be changed into \ by declaring `¥verbswitchfalse`, as found in the following output.

The present document has declared `\verbswitchtrue` in its preamble so as to adopt ¥ in place of \. If we declare `\verbswitchfalse` here, we can go back to default expressions with the symbol \, e.g.,

```
\begin{glshfboxit}{12cm}
\centering
\pyridinevi{} \pyridazinevi{} \pyrimidinevi{} \pyrazinevi{}
\end{glshfboxit}
```

(Note that this paragraph is output under the declaration of `\verbswitchfalse`.)

Chapter 5

Harpoons

The chmst-ps package after version 1.03 (the PostScript-compatible version of the chemsit package) supports arrows with arrowheads of harpoon type. They can be used on a similar line to the standard arrows of the pstricks package, because they are defined according to the setting of the pstricks package, which is loaded automatically by the chmst-ps package.

5.1 Harpoons Defined in the chmst-ps Package

5.1.1 Harpoons of Four Kinds

After loading the chmst-ps package,[1] four kinds of harpoons can be used, where they are specified by shortcut descriptors, i.e., Hru (right upward harpoon), Hrd (right downward harpoon), Hlu (left upward harpoon), and Hld (left downward harpoon). They are used in combination with `¥psline`, `¥pscurve`, etc. of the PSTricks system, as shown in Table 5.1.

Although a code with the same descriptors (e.g., `¥psline{Hru-Hru}(1.3,0)`) works well, a more systematic code described in Table 5.1 (e.g., `¥psline{Hld-Hru}(1.3,0)`) is recommended:

Not Recommended		Recommended (Table 5.1)	
`¥psline{Hru-Hru}(1.3,0)`		`¥psline{Hld-Hru}(1.3,0)`	
`¥psline{Hld-Hld}(1.3,0)`			

The harpoons listed in Table 5.1 can be combined with descriptors defined in the pstricks package, e.g.,

`%¥usepackage{chmst-ps}` (loading the pstricks package automatically)

`¥psline{|-Hru}(1.3,0)`	
`¥psline{Hld-|}(1.3,0)`	
`¥psline{*-Hru}(1.3,0)`	
`¥psline{Hld-*}(1.3,0)`	
`¥psline{**-Hrd}(1.3,0)`	
`¥psline{Hlu-**}(1.3,0)`	
`¥psline{o-Hru}(1.3,0)`	
`¥psline{Hld-o}(1.3,0)`	
`¥psline{oo-Hrd}(1.3,0)`	
`¥psline{Hlu-oo}(1.3,0)`	

As for the standard descriptors defined for arrows and like in the pstricks package, see [11].

[1] The chmst-ps package loads the chemist package and the pstricks package automatically.

Table 5.1: List of Harpoons

Value	Code	Example	Explanation
-Hru	¥psline{-Hru}(1.3,0)		right upward harpoons
-Hrd	¥psline{-Hrd}(1.3,0)		right downward harpoons
Hlu-	¥psline{Hlu-}(1.3,0)		left upward harpoons
Hld-	¥psline{Hld-}(1.3,0)		left downward harpoons
Hld-Hru	¥psline{Hld-Hru}(1.3,0)		left-down right-up harpoons
Hlu-Hrd	¥psline{Hlu-Hrd}(1.3,0)		left-up right-down harpoons
Hlu-Hru	¥psline{Hlu-Hru}(1.3,0)		left-up right-up harpoons
Hld-Hrd	¥psline{Hld-Hrd}(1.3,0)		left-down right-down harpoons
cf.			
->	¥psline{->}(1.3,0)		right arrows
<-	¥psline{<-}(1.3,0)		left arrows
<->	¥psline{<->}(1.3,0)		leftright arrows

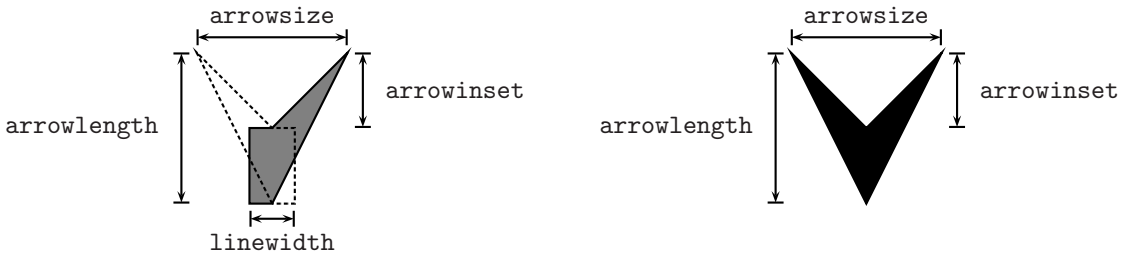


Figure 5.1: Dimensions of a harpoon head (left) and the corresponding arrowhead (right)

5.1.2 Keywords for Harpoons

Dimensions of a harpoon-head is shown in Fig. 5.1. They are consistent with those of the standard arrows of the pstricks package, where the keywords (`arrowlength`, `arrowsize`, and `arrowinset`) are common to those of the pstricks package, while the key word, `linewidth`, is concerned with the stem of an arrow of harpoon type (i.e., the linewidth of a line drawn by `¥psline` etc.).

The keywords for harpoons, which are common to those of arrows set in the pstricks package, are shown in Table 5.2. The other keywords for arrows (e.g., `arrowscale`, cf. Table 5.11 of [11]) are not effective (or harmful) to draw harpoons, because the harpoon head shown in Fig. 5.1 (left) has an additional object for adjusting the terminal of the stem line of a harpoon.

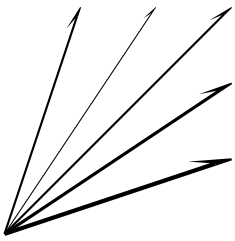
If the keyword `linewidth` is set to be an appropriate value, the value is stored in `¥pslinewidth`. Then, the dimension [unit] and the factor set by the `arrowsize` keyword (default: 1.5pt 2 listed in Table 5.2) are used to calculate the arrow size (width) according to the following equation:

$$\text{arrow width} = \text{dimension [unit]} + \text{factor} \times \texttt{¥pslinewidth}$$

The half of this value is adopted in drawing a harpoon. When `linewidth` is varied, the width of a harpoon head is varied, as found in the following examples:

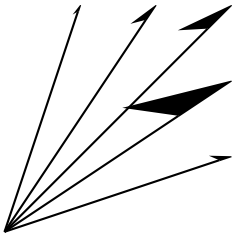
Table 5.2: Keywords for Harpoons (Common to Arrows)

Name	Value Type	Dafault	Explanation
`linewidth`	*value[unit]*	0.8pt	linewith of a stem, cf. Fig. 5.1
`arrows`	*style*	–	style of arrows (harpoons)
`arrowlength`	*value*	1.4	cf. Fig. 5.1
`arrowsize`	*value[unit] value*	1.5pt 2	cf. Fig. 5.1 (dimension and factor)
`arrowinset`	*value*	0.4	cf. Fig. 5.1



```
¥psset{arrowlength=2,arrowsize=1.5pt 4,arrowinset=0.6}
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[linewidth=0.4pt]{-Hru}(0,0)(2,3)
¥psline[linewidth=0.8pt]{-Hru}(0,0)(3,3)
¥psline[linewidth=1.2pt]{-Hru}(0,0)(3,2)
¥psline[linewidth=1.6pt]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

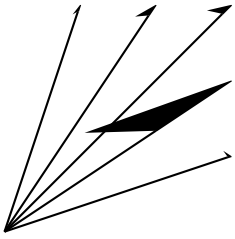
When the default value (0.8pt) of the keyword `linewidth` (`¥pslinewidth`) is used as a fixed line width, the effect of varying `arrowsize` is exemplified as follows:



```
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[arrowsize=0pt 10]{-Hru}(0,0)(2,3)
¥psline[arrowsize=10pt]{-Hru}(0,0)(3,3)
¥psline[arrowsize=1]{-Hru}(0,0)(3,2)
¥psline[arrowsize=0.2cm]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

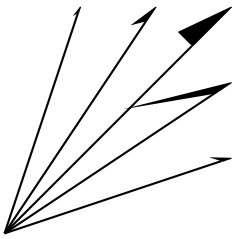
It should be noted that, when the first value (dimension) of the keyword `arrowsize` is 0pt, the second value is regarded as a factor. Hence, "factor × `¥pslinewidth`" is applied to the drawing of a harpoon. When a unit is absent, the default unit (stored in `¥psunit`) is applied; thus the setting `arrowsize=1` is regarded as being `arrowsize=1cm` in the present case (0.5cm for the corresponding harpoon head). On the other hand, when the second value (factor) of the keyword `arrowsize` is 0 (or absent), the first value (with a unit) is adopted in drawing a harpoon.

The value of `arrowlength` is a factor to calculate the arrow length according to the equation "factor × arrow width". The effect of `arrowlength` is exemplified as follows:



```
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[arrowsize=0pt 10,arrowlength=1]{-Hru}(0,0)(2,3)
¥psline[arrowsize=10pt,arrowlength=0.8]{-Hru}(0,0)(3,3)
¥psline[arrowsize=1,arrowlength=2]{-Hru}(0,0)(3,2)
¥psline[arrowsize=0.2cm,arrowlength=0.4]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

The value of `arrowinset` is a factor to make a notch of an arrowhead. Thus, the notch is calculated according to the equation "factor × arrow length". The effect of `arrowinset` is exemplified as follows:



```
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[arrowsize=0pt 10,arrowinset=0.4]{-Hru}(0,0)(2,3)
¥psline[arrowsize=15pt,arrowinset=0]{-Hru}(0,0)(3,3)
¥psline[arrowsize=1,arrowinset=0.8]{-Hru}(0,0)(3,2)
¥psline[arrowsize=0.2cm,arrowinset=0.5]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

5.2 Chemical Conventions for Using Arrows and Harpoons

Chemical conventions use arrows and harpoons differently:

1. A composite of right and left harpoons ($\rightleftharpoons$) is used to specify an equilibrium equation, while a composite of right and left arrows ($\rightleftarrows$) is used to specify a forward-reverse reaction.

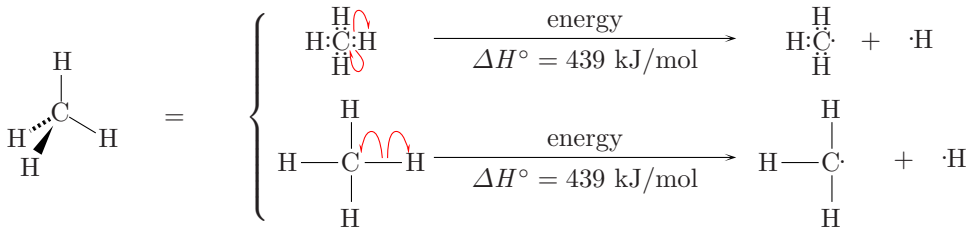
2. A right ($\rightharpoonup$) or left harpoon ($\leftharpoondown$) is used to show a shift of an electron, while a right ($\rightarrow$) or left arrow ($\leftarrow$) is used to show a shift of an electron pair (cf. page 52). These harpoons or arrows are frequently printed in bent (curved) styles to visualize a path of moving an electron or an electron pair.

The first convention can be fulfilled, because the chmst-ps (chemist) package has defined harpoons and arrows for using equilibrium equations and forward-reverse reactions (Subsection 2.2.1 and Section 4.4). The harpoons defined by the old version of the chmst-ps (chemist) package have been replaced by the newly-defined harpoons in the present version.

The second convention for using a harpoon is concerned with a radical fission of a covalent bond. For example, the homolysis of the C—H bond of methane is represented by the following scheme.

```
¥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){¥LewistetrahedralA{0==C;1==H;2==H;3==H;4==H}}
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{-Hru}%
(185,70)(200,150)(240,80)
¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{Hlu-}%
(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]{Hlu-}%
(40,70)(80,150)(120,50);%
0==¥pscurve[unit=¥unitlength,linewidth=0.4pt,linecolor=red]{-Hru}%
```

```
(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}
```



(5.1)

Shortcut commands for drawing harpoons are defined as follows:

```
¥def¥electronshiftAH#1{%
¥pscurve[unit=¥unitlength,linewidth=0.4pt,arrowsize=2pt 2,%
arrowlength=1.6,arrowinset=0.6]{#1}}
¥def¥electronshiftHru{¥electronshiftAH{-Hru}}
¥def¥electronshiftHrd{¥electronshiftAH{-Hrd}}
¥def¥electronshiftHlu{¥electronshiftAH{Hlu-}}
¥def¥electronshiftHld{¥electronshiftAH{Hld-}}
```

These commands print harpoons as shown below:

```
¥electronshiftHru(0,0)(100,50)(200,0)
¥electronshiftHrd(0,0)(100,-50)(200,0)
¥electronshiftHlu(0,0)(100,50)(200,0)
¥electronshiftHld(0,0)(100,-50)(200,0)
```

The commands defined above for drawing electron shifts are used in the following equation, where `¥psset{linecolor=red}` is declared to print red harpoons.

```
¥begin{ChemEquation}
¥begin{XyMcompd}(700,450)(100,100){}{}
¥put(0,0){¥tetrahedral{0==C;%
0=={¥psset{linecolor=red}¥electronshiftHlu(40,70)(80,150)(120,50)};%
0=={¥psset{linecolor=red}¥electronshiftHru(140,50)(200,140)(280,140)(320,50)};%
0=={¥psset{linecolor=red}¥electronshiftHlu(370,50)(400,140)(450,70)};%
1==H;2==H;3==H;4==H}}
¥put(750,270){¥lonepairA[123]{¥chemradicalA[4]{Cl}}}
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{}{}
¥begin{XyMcompd}(600,450)(100,100){}{}
```

```
¥put(0,0){¥tetrahedral{0==¥chemradicalA[2]{C};1==H;2==H;3==H}}
¥put(450,270){H¥sbond¥lonepairA[123]{Cl}}
¥end{XyMcompd}
¥end{ChemEquation}
```

(5.2)

The subsequent propagation step is represented by the following equation:

```
¥begin{ChemEquation}
¥begin{XyMcompd}(750,450)(100,100){}{}
¥put(0,0){¥tetrahedral{0==¥chemradicalA[2]{C};1==H;2==H;3==H;%
0=={¥psset{linecolor=red}¥electronshiftHru(40,70)(90,150)(150,50)};%
0=={¥psset{linecolor=red}¥electronshiftHlu(170,50)(260,140)(340,140)(420,50)};%
0=={¥psset{linecolor=red}¥electronshiftHru(450,50)(490,140)(520,70)}%
}}
¥put(550,270){¥lonepairA[134]{Cl}¥sbond¥lonepairA[123]{Cl}}
¥end{XyMcompd}
¥reactrarrow{0pt}{2cm}{}{}
¥begin{XyMcompd}(700,450)(100,100){}{}
¥put(0,0){¥tetrahedral{0==C;1==H;2==H;3==H;4==Cl}}
¥put(750,270){¥lonepairA[123]{¥chemradicalA[4]{Cl}}}
¥end{XyMcompd}
¥end{ChemEquation}
```

(5.3)

The radical chain mechanism for chlorination of methane is explained by the following equilibrium equations:

```
¥begin{ChemEquation}
CH_{4} + ¥chemradicalA[2]{Cl}
¥quad ¥reactleqarrow{0pt}{3.5cm}{¥ChemStrut}{slightly unfavorable} ¥quad
¥chemradicalA[4]{C}H_{3} + HCl
¥quad¥reactreqarrow{0pt}{3.5cm}{¥ChemForm{Cl_{2}}¥¥[3pt]}{very favorable} ¥quad
CH_{3}Cl + ¥chemradicalA[2]{Cl}
¥end{ChemEquation}
```

$$\mathrm{CH_4 + Cl\cdot} \underset{\text{slightly unfavorable}}{\overset{}{\rightleftharpoons}} \mathrm{\cdot CH_3 + HCl} \xrightarrow[\text{very favorable}]{\mathrm{Cl_2}} \mathrm{CH_3Cl + Cl\cdot} \tag{5.4}$$

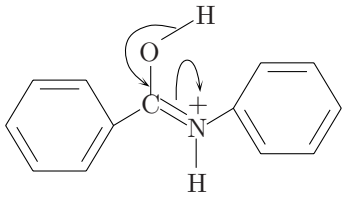
Note that the steps are linked with right and left harpoons according to the first chemical convention described above (cf. Section 4.4).

Incidentally, arrows for representing an elenctron-pair shift can be drawn by creating commands `¥electronshiftArrowr` and `¥electronshiftArrowr`, both of which are defined also by the command `¥electronshiftAH` defined above.

```
¥def¥electronshiftArrowr{¥electronshiftAH{->}}
¥def¥electronshiftArrowl{¥electronshiftAH{<-}}
```

The usage of these commands is exemplified by the following formula:

```
¥begin{XyMcompd}(1100,700)(-400,0){}{}
¥dimethylenei[a]{1==C;2==¥upnobond{N}{+};%
1==¥electronshiftArrowl%
(-40,100)(-120,180)(-120,280)(-40,330)(60,320);%
1==¥electronshiftArrowr(60,50)(100,200)(150,80)%
}%
{2==H;2W==¥bzdrh{1==(yl)};1W==¥bzdrh{4==(yl)};%
1==¥Utrigonal{0==O;2==H;1==(yl)}}
¥end{XyMcompd}
```



Bibliography

[1] Fujita S., "Typesetting structural formulas with the text formatter TEX/LATEX", *Comput. Chem.*, **18**, 109 (1994).

[2] Fujita S., "XYMTEX for Drawing Chemical Structural Formulas", *TUGboat*, **16** (1), 80 (1995).

[3] Fujita, S., *XYMTEX—Typesetting Chemical Structural Formulas*, Addison-Wesley, Tokyo (1997). The book title is abbreviated as "XYMTEXbook" in the present manual.

[4] Fujita, S., Tanaka, N., "XYM Notation for Electronic Communication of Organic Chemical Structures", *J. Chem. Inf. Comput. Sci.*, **39**, 903 (1999).

[5] Fujita, S., Tanaka, N., "XYMTEX (Version 2.00) as Implementation of the XYM Notation and the XYM Markup Language", *TUGboat*, **21** (1), 7 (2000).

[6] Fujita, S., Tanaka, N., *TUGboat*, **22** (4), 285 (2001).

[7] Fujita, S., "XYMTEX (Version 4.01) for Typesetting Chemical Structural Formulas. A Tool for DVI- and PostScript-Typsetting", On-line manual (2004).

[8] Fujita, S., "XYMTEX (Version 4.02, 4.03) for Typesetting Chemical Structural Formulas. An Extension for Stereochemistry According to PostScript", On-line manual (2004, 2005).

[9] Fujita, S., "XYMTEX (Version 4.04) for Typesetting Chemical Structural Formulas. An Extension for Drawing Steroid Derivatives", On-line manual (2009).

[10] Schmidt, W., "Using Common PostScript fonts with LATEX", On-line manual for Version 9.2: http://ctan.org/tex-archive/macros/latex/required/psnfss/psnfss2e.pdf

[11] For graphic applications of TEX, LATEX and relevant systems, see Goossens, M., Mittelbach, F., Rahtz, S., Roegel, D., Voß, H., *The LATEX Graphics Companion*, 2nd Ed., Addison Wesley, Upper Saddle River (2008).

[12] Fujita, S., *LATEX 2ε Kaitei*, 3rd Ed., Volumes I and II, Pearson Educ. Japan, Tokyo (2009).

[13] van Zandt, T., Girou, D., "Inside PSTricks", *TUGboat*, **15** (3), 239 (1995).

[14] Fujita, S., *Kagakusha, Seikagakusha no tame no LATEX* (LATEX for Organic Chemists and Biochemists), Tokyo Kagaku Dojin, Tokyo (1993).