XƔMTEX (Versions 4.05 and 4.06) for Typesetting Chemical Structural Formulas: C. The chemtimes Package for Supporting Times-like Fonts.

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Chapter 1

Introduction

1.1 History

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

Table 1.1: Versions of XΊMTEX

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 XΊM 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 XΊMTEX system (version 4.05) summarized in Table 1.1, this manual is concerned with the release of the chemtimes package (ver 1.00), which allows us to typeset texts and mathematical equations in Times-like fonts. The chemtimes package (ver 1.00) supports two mathversions (chem and boldchem) designed for chemical usage in addition to the original mathversions (normal and bold) of LATEX 2_ε. Moreover,

chemical tools supported by the chmst-ps package (ver 1.02) and the chemist package (ver 4.05) are also available, because the chemtimes package loads these packages (chmst-ps and chemist) automatically. Thus, even in the original mathversions (normal and bold), convenient environments akin to the equation or eqnarray environments of LATEX 2ε can be used just as realized in chemist (chmst-ps). More environments defined in the chemist (chmst-ps) package are also available.

   After publishing the previous online manual named xymtx405C.pdf, the X̄ɪMɪEX (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 6 in the present manual named xymtx405406C.pdf.

1.2   Use of the chemtimes Package

1.2.1   Loading chmst-ps vs. chemist

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

```
¥documentclass{article}
¥usepackage{xymtexps}%XyMTeX (PostScript-compatible mode)
¥usepackage{chemtimes}
¥begin{document}
(text)%default (normal)

¥mathversion{bold}
(text)

¥mathversion{chem}
(text)

¥mathversion{boldchem}
(text)

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

Following this template, the chemtimes package (with no option) loaded the chmst-ps package automatically, where the POSTSCRIPT-compatible mode works.

   The xymtexps package provides the X̄ɪMɪEX 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.

   On the other hand, the [chemist] option of the chemtimes package aims at printing without POSTSCRIPT utilities. This option is not so recommended because of lower quality in printing chemical structural formulas.

```
¥documentclass{article}
¥usepackage{xymtex}%XyMTeX (TeX/LaTeX-compatible mode)
¥usepackage[chemist]{chemtimes}
¥begin{document}
(text)%default (normal)

¥mathversion{bold}
(text)

¥mathversion{chem}
(text)
```

```
¥mathversion{boldchem}
(text)

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

Following this template, the chemtimes package loaded the chemist package automatically, where utilities of POSTSCRIPT are unavailable.

The xymtex package provides the XΥMTEX system of TEX/LATEX mode. Hence, the resulting dvi file would be browsed by an appropriate browser (e.g., dviout).

1.2.2 Mathversions

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 (chmst-ps) package loaded automatically by the present chemtimes 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).

1.3 Fonts

The chemtimes package has been constructed by referring to the times package and the mathptmx package of the PSNFSS system [10]. The chemtimes package sets ptm (Times Roman) for ¥rmdefault, phv (Helvetica) for ¥sfdefault, and cmtt (the Computer Modern Typewriter Type) for ¥ttdefault to print texts. Note that the Computer Modern Typewriter Type (cmtt) of TEX is used as the typewriter text font, whereas the times package uses pcr (Courier). The font setting of math modes in the chemtimes heavily relies on that of the mathptmx package, although the mathversions "bold" (as well as the command ¥boldmath), "chem", and "boldchem" have been introduced as new matters.

1.4 Recent Books Citing the XΥMTEX System

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

Note: This document uses the ¥ symbol to show each control sequence according to Japanese encoding. Because the switching command ¥verbswitchtrue (¥) and ¥verbswitchfalse (\) are provided by the chemist (chmst-ps) package, we can change ¥ into \ easily. For example, the above template is transformed into the one with non-Japanese encoding by declaring ¥verbswitchfalse, as follows:

```
%Note: \verbswitchfalse is declared before entering
%the verbatim environment.
\documentclass{article}
\usepackage{xymtexps}%XyMTeX (PostScript-compatible mode)
\usepackage{chemtimes}
\begin{document}
(text)%default (normal)

\mathversion{bold}
```

```
(text)

\mathversion{chem}
(text)

\mathversion{boldchem}
(text)

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

Chapter 2

Mathematical Equations

The chemtimes supports the mathversions "normal" and "bold", just as the original LaTeX 2ε supports them. Several limitations are present for the mathversion "bold" because there exist no appropriate free fonts for supporting boldfaced Greek letters etc. In the present chapter, we show illustrative examples to exemplify both texts and mathematical equations typeset in Times-like fonts.

2.1 Mathversion "normal"

2.1.1 Examples

Mathematical equations in `equation` and `eqnarray` environments of LaTeX 2ε are typeset in Times-like fonts:

```
¥begin{equation}
¥sin^{-1}x=¥int_{0}^{x}¥frac{1}{¥sqrt{1-t^{2}}}¥,¥mathrm{d}t ¥label{eq:01}
¥end{equation}
¥begin{eqnarray}
¥ln(¥sin¥frac{x}{n})
& = &  ¥ln¥pi - ¥ln¥left(1-¥frac{1}{n^{2}}¥right) ¥nonumber ¥¥
& & {} + ¥ln¥left(1-¥frac{1}{4n^{2}}¥right) + ¥ln¥left(1-¥frac{1}{9n^{2}}¥right)
+ ¥cdots ¥label{eq:02}
¥end{eqnarray}
¥begin{eqnarray}
¥int_{0}^{2¥pi}¥cos^{2}nx¥,¥mathrm{d}x & = &
¥frac{1}{2}¥int_{0}^{2¥pi}(1+¥cos 2nx)¥,¥mathrm{d}x ¥nonumber ¥¥
& = &¥frac{1}{2}¥int_{0}^{2¥pi}1¥:¥mathrm{d}x =
¥frac{1}{4n}¥biggl[¥sin 2nx¥biggr]_{0}^{2¥pi} = ¥pi ¥label{eq:03}
¥end{eqnarray}
```

$$\sin^{-1} x = \int_0^x \frac{1}{\sqrt{1-t^2}} \, \mathrm{d}t \tag{2.1}$$

$$\begin{aligned}
\ln(\sin \frac{x}{n}) &= \ln \pi - \ln\left(1 - \frac{1}{n^2}\right) \\
&\quad + \ln\left(1 - \frac{1}{4n^2}\right) + \ln\left(1 - \frac{1}{9n^2}\right) + \cdots
\end{aligned} \tag{2.2}$$

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$$\int_0^{2\pi} \cos^2 nx \, dx = \frac{1}{2} \int_0^{2\pi} (1 + \cos 2nx) \, dx$$

$$= \frac{1}{2} \int_0^{2\pi} 1 \, dx = \frac{1}{4n} \left[\sin 2nx \right]_0^{2\pi} = \pi \qquad (2.3)$$

where log-type symbols are typeset in upright fonts of the Times Roman family and variables are typeset in Times italic fonts.

The following example shows that the letter d as a variable is differentiated from the letter d as a differential symbol (cf. eqs. 2.1 and 2.3).

```
¥begin{eqnarray}
a(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥alpha_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk}
¥label{eq:4a} ¥¥
c(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥gamma_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk}
¥label{eq:4b} ¥¥
b(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥beta_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk},
¥label{eq:4c}
¥end{eqnarray}
```

$$a(x^d, y^d, z^d) = \sum_{k=0}^{\infty} \left(\sum_{\ell=0}^{\infty} \left(\sum_{m=0}^{\infty} \alpha_{k\ell m} z^{dm} \right) y^{d\ell} \right) x^{dk} \qquad (2.4)$$

$$c(x^d, y^d, z^d) = \sum_{k=0}^{\infty} \left(\sum_{\ell=0}^{\infty} \left(\sum_{m=0}^{\infty} \gamma_{k\ell m} z^{dm} \right) y^{d\ell} \right) x^{dk} \qquad (2.5)$$

$$b(x^d, y^d, z^d) = \sum_{k=0}^{\infty} \left(\sum_{\ell=0}^{\infty} \left(\sum_{m=0}^{\infty} \beta_{k\ell m} z^{dm} \right) y^{d\ell} \right) x^{dk}. \qquad (2.6)$$

Green's equation is typeset by writing the following code:

```
¥[¥int¥mkern-9mu¥int_{¥mathrm{D}}¥left¥{%
u¥mathrm{¥Delta}v - v¥mathrm{¥Delta}u¥right¥}¥mathrm{d}S
=¥oint_{¥mathrm{C}}¥left¥{%
u¥frac{¥partial v}{¥partial n} -
v¥frac{¥partial u}{¥partial n}¥right¥}¥mathrm{d}s¥]
```

$$\iint_D \{ u\Delta v - v\Delta u \} \, dS = \oint_C \left\{ u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right\} ds$$

Note that $\mathrm{¥Delta}$ provides the symbol Δ of upright shape, while $¥Delta$ provides the symbol Δ of slanted shape. Uppercase Greek letters are printed with and without ¥mathrm, as follows:

```
¥[¥Gamma¥Delta¥Theta¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega¥]
¥[¥mathrm{¥Gamma¥Delta¥Theta¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega}¥]
```

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega$$

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega$$

It should be noted that the default setting of LaTeX 2_ε is to print upright uppercase Greek letters in math modes. The present chemtimes package changes the default to print slanted uppercase Greek letters, because new mathversions "chem" and "boldchem" have been created to print upright uppercase Greek letters. Compare these results with the following results due to a ChemEquation environment.

```
¥begin{ChemEquation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega
¥end{ChemEquation}
```

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{2.7}$$

The command ¥mathnormal is used in math modes to print slanted uppercase Greek letters as well as numbers of old type.

```
¥begin{equation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc 0123456789 ¥alpha¥beta¥gamma}
¥end{equation}
¥begin{ChemEquation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc 0123456789 ¥alpha¥beta¥gamma}
¥end{ChemEquation}
```

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc\,0123456789\alpha\beta\gamma \tag{2.8}$$

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc\,0123456789\alpha\beta\gamma \tag{2.9}$$

The commands ¥mathit, ¥mathsf, and ¥mathbf are incapable of printing uppercase Greek letters, although they are effective to alphabets and numbers (with no effects on lowercase Greek letters). The command ¥mathbfit is defined to print alphabets and numbers in boldfaced italic fonts (with no effects on lowercase Greek letters).

- ¥mathit:

  ```
  ¥begin{equation}
  ¥mathit{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{equation}
  ¥begin{ChemEquation}
  ¥mathit{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{ChemEquation}
  ```

  $$abc0123456789\alpha\beta\gamma \tag{2.10}$$

  $$abc0123456789\alpha\beta\gamma \tag{2.11}$$

- ¥mathsf:

  ```
  ¥begin{equation}
  ¥mathsf{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{equation}
  ¥begin{ChemEquation}
  ¥mathsf{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{ChemEquation}
  ```

  $$\mathsf{abc0123456789}\alpha\beta\gamma \tag{2.12}$$

  $$\mathsf{abc0123456789}\alpha\beta\gamma \tag{2.13}$$

- ¥mathbf:

  ```
  ¥begin{equation}
  ¥mathbf{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{equation}
  ¥begin{ChemEquation}
  ¥mathbf{abc 0123456789 ¥alpha¥beta¥gamma}
  ¥end{ChemEquation}
  ```

$$\textbf{abc0123456789}\alpha\beta\gamma \tag{2.14}$$

$$\textbf{abc0123456789}\alpha\beta\gamma \tag{2.15}$$

- ¥mathbfit:

```
¥begin{equation}
¥mathbfit{abc 0123456789 ¥alpha¥beta¥gamma}
¥end{equation}
¥begin{ChemEquation}
¥mathbfit{abc 0123456789 ¥alpha¥beta¥gamma}
¥end{ChemEquation}
```

$$\boldsymbol{abc0123456789}\alpha\beta\gamma \tag{2.16}$$

$$\boldsymbol{abc0123456789}\alpha\beta\gamma \tag{2.17}$$

The command ¥boldmath can be used to print alphabets in boldfaced italic fonts.

```
¥def¥vecLetter#1{¥mbox{¥boldmath $#1$}}
¥[¥int¥!¥!¥!¥int_{¥mathrm{S}}(¥mathrm{rot}¥,¥vecLetter{V})_{n}¥mathrm{d}S
= ¥oint_{¥mathrm{C}}(¥vecLetter{V}, ¥mathrm{d}¥vecLetter{s})¥]
```

$$\iint_{\mathrm{S}}(\mathrm{rot}\,\boldsymbol{V})_n \mathrm{d}S = \oint_{\mathrm{C}}(\boldsymbol{V}, \mathrm{d}\boldsymbol{s})$$

where the command ¥vecLetter is defined to print an alphabet in a boldfaced italic font. The definition can be alternatively given as follows:

```
¥def¥vecLetter#1{¥mbox{¥mathversion{bold}$#1$}}
```

because the ¥boldmath command is synonymous with the declaration ¥mathversion{bold} (cf. Section 2.2). An alternative code $¥mathbfit{V}$ is capable of printing $\boldsymbol{V}$.

2.1.2 Limitations

The commands ¥imath and ¥jmath give fonts of Computer Modern, because they are not available in Times-like families adopted here. Thus, $ij¥imath¥jmath$ provides $ij\imath\jmath$. Similarly, ¥amalg and ¥coprod produce substituted fonts:

```
¥[¥amalg ¥coprod; ¥prod ¥bigcup¥]
```

$$\amalg \coprod; \prod \bigcup$$

2.2 Mathversion "bold"

Throughout the present section, the same examples as shown in the preceding section are again printed, except that ¥mathversion{bold} is declared here.

2.2.1 Examples

Mathematical equations in `equation` and `eqnarray` environments of LaTeX 2_ε are typeset in Times-like fonts according to the mathversion "bold":

```
%¥mathversion{bold} has been declared.
¥begin{equation}
¥sin^{-1}x=¥int_{0}^{x}¥frac{1}{¥sqrt{1-t^{2}}}¥,¥mathrm{d}t ¥label{eq:01x}
¥end{equation}
¥begin{eqnarray}
¥ln(¥sin¥frac{x}{n})
& = &  ¥ln¥pi - ¥ln¥left(1-¥frac{1}{n^{2}}¥right) ¥nonumber ¥¥
& & {} + ¥ln¥left(1-¥frac{1}{4n^{2}}¥right) + ¥ln¥left(1-¥frac{1}{9n^{2}}¥right)
+ ¥cdots ¥label{eq:02x}
¥end{eqnarray}
¥begin{eqnarray}
¥int_{0}^{2¥pi}¥cos^{2}nx¥,¥mathrm{d}x & = &
¥frac{1}{2}¥int_{0}^{2¥pi}(1+¥cos 2nx)¥,¥mathrm{d}x ¥nonumber ¥¥
& = &¥frac{1}{2}¥int_{0}^{2¥pi}1¥:¥mathrm{d}x =
¥frac{1}{4n}¥biggl[¥sin 2nx¥biggr]_{0}^{2¥pi} = ¥pi ¥label{eq:03x}
¥end{eqnarray}
```

$$\sin^{-1} x = \int_0^x \frac{1}{\sqrt{1-t^2}}\, \mathrm{d}t \tag{2.18}$$

$$\ln(\sin \frac{x}{n}) \quad = \quad \ln \pi - \ln\left(1 - \frac{1}{n^2}\right)$$
$$+ \ln\left(1 - \frac{1}{4n^2}\right) + \ln\left(1 - \frac{1}{9n^2}\right) + \cdots \tag{2.19}$$

$$\int_0^{2\pi} \cos^2 nx\, \mathrm{d}x \quad = \quad \frac{1}{2}\int_0^{2\pi}(1 + \cos 2nx)\, \mathrm{d}x$$
$$= \quad \frac{1}{2}\int_0^{2\pi} 1\, \mathrm{d}x = \frac{1}{4n}\left[\sin 2nx\right]_0^{2\pi} = \pi \tag{2.20}$$

where **log**-type symbols are typeset in boldfaced upright fonts of the Times Roman family and variables are typeset in boldfaced Times italic fonts.

The following example shows that the letter d as a variable is differentiated from the letter **d** as a differential symbol (eqs. 2.1 and 2.3).

```
%¥mathversion{bold} has been declared.
¥begin{eqnarray}
a(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥alpha_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk}
¥label{eq:4xa} ¥¥
c(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥gamma_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk}
¥label{eq:4xb} ¥¥
b(x^d, y^d, z^d) & = &
¥sum_{k=0}^{¥infty}¥left(¥sum_{¥ell=0}^{¥infty}
¥left(¥sum_{m=0}^{¥infty}¥beta_{k¥ell m}z^{dm}¥right)y^{d¥ell}¥right)x^{dk}.
¥label{eq:4xc}
¥end{eqnarray}
```

$$a(x^d, y^d, z^d) \;=\; \sum_{k=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\alpha_{k\ell m}z^{dm}\right)y^{d\ell}\right)x^{dk} \tag{2.21}$$

$$c(x^d, y^d, z^d) \;=\; \sum_{k=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\gamma_{k\ell m}z^{dm}\right)y^{d\ell}\right)x^{dk} \tag{2.22}$$

$$b(x^d, y^d, z^d) \;=\; \sum_{k=0}^{\infty}\left(\sum_{\ell=0}^{\infty}\left(\sum_{m=0}^{\infty}\beta_{k\ell m}z^{dm}\right)y^{d\ell}\right)x^{dk}. \tag{2.23}$$

Note that we are forced to use Computer Modern fonts (α, β, and γ) in printing boldfaced lowercase Greek letters because of the absence of appropriate fonts under the mathversion "bold".

Green's equation is typeset by writing the following code:

```
%¥mathversion{bold} has been declared.
¥[¥int¥mkern-9mu¥int_{¥mathrm{D}}¥left¥{%
u¥mathrm{¥Delta}v - v¥mathrm{¥Delta}u¥right¥}¥mathrm{d}S
=¥oint_{¥mathrm{C}}¥left¥{%
u¥frac{¥partial v}{¥partial n} -
v¥frac{¥partial u}{¥partial n}¥right¥}¥mathrm{d}s¥]
```

$$\iint_{\mathbf{D}} \{u\,\Delta v - v\,\Delta u\}\,\mathrm{d}S = \oint_{\mathbf{C}} \left\{ u\,\frac{\partial v}{\partial n} - v\,\frac{\partial u}{\partial n} \right\}\mathrm{d}s$$

Note that $\mathrm{\$¥mathrm\{¥Delta\}\$}$ provides an upright shape $\mathbf{\Delta}$, while $\$¥Delta\$$ provides a slanted shape $\boldsymbol{\Delta}$. Uppercase Greek letters are printed with and without ¥mathrm, as follows:

```
%¥mathversion{bold} has been declared.
¥[¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega¥]
¥[¥mathrm{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega}¥]
```

$$\boldsymbol{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}$$

$$\mathbf{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}$$

Compare these results with the following results due to a ChemEquation environment.

```
%¥mathversion{bold} has been declared.
¥begin{ChemEquation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega
¥end{ChemEquation}
```

$$\mathbf{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{2.24}$$

The command ¥mathnormal in math modes prints slanted uppercase Greek letters (boldfaced), while the output of old-type numbers requires an additional ¥mbox command:

```
%¥mathversion{bold} has been declared.
¥begin{equation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{equation}
¥begin{ChemEquation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{ChemEquation}
```

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc 0123456789\alpha\beta\gamma; \Gamma\Delta \tag{2.25}$$

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc 0123456789\alpha\beta\gamma; \Gamma\Delta \tag{2.26}$$

where the end of each line shows the output of two uppercase Greek letters without ¥mathnormal.

The commands ¥mathit, ¥mathsf, and ¥mathbf are incapable of printing uppercase Greek letters. Although they are used to print alphabets, numbers and lowercase Greek letters, the mathversion "bold" is canceled. Even in the mathversion "bold", the effect of ¥mathbfit is almost equivalent to the one described in the mathversion "normal":

```
%¥mathversion{bold} has been declared.
¥begin{equation}
¥mathbfit{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc 0123456789; ¥mbox{0123456789}; ¥alpha¥beta¥gamma}
¥end{equation}
¥begin{ChemEquation}
¥mathbfit{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc 0123456789; ¥mbox{0123456789}; ¥alpha¥beta¥gamma}
¥end{ChemEquation}
```

$$\boldsymbol{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc0123456789}; 0123456789; \alpha\beta\gamma \tag{2.27}$$

$$\mathbf{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega;} \boldsymbol{abc0123456789}; 0123456789; \alpha\beta\gamma \tag{2.28}$$

As shown in page 12, when we want to print a boldfaced italic letter under the mathversion "normal", the command ¥boldmath is convenient as a shortcut of the declaration ¥mathversion{bold}:

```
{¥mathversion{normal}
%%by using ¥boldmath
¥[¥int¥!¥!¥!¥int_{¥mathrm{S}}(¥mathrm{rot}¥,¥mbox{¥boldmath $V$})_{n}¥mathrm{d}S
= ¥oint_{¥mathrm{C}}(¥mbox{¥boldmath $V$}, ¥mathrm{d}¥vecLetter{s})¥]
%%by using ¥mathversion{bold}
¥def¥vecLetter#1{¥mbox{¥mathversion{bold}$#1$}}
¥[¥int¥!¥!¥!¥int_{¥mathrm{S}}(¥mathrm{rot}¥,¥vecLetter{V})_{n}¥mathrm{d}S
= ¥oint_{¥mathrm{C}}(¥vecLetter{V}, ¥mathrm{d}¥vecLetter{s})¥]
}
```

$$\iint_{\mathrm{S}} (\mathrm{rot}\,\boldsymbol{V})_n \mathrm{d}S = \oint_{\mathrm{C}} (\boldsymbol{V}, \mathrm{d}\boldsymbol{s})$$

$$\iint_{\mathrm{S}} (\mathrm{rot}\,\boldsymbol{V})_n \mathrm{d}S = \oint_{\mathrm{C}} (\boldsymbol{V}, \mathrm{d}\boldsymbol{s})$$

2.2.2 Limitations

The commands ¥imath and ¥jmath give fonts of Computer Modern, because they are not available in Times-like families adopted here. Thus, $ij\imath\jmath$ provides $\boldsymbol{ij\imath\jmath}$. Similarly, ¥amalg and ¥coprod produce substituted fonts:

```
%¥mathversion{bold} has been declared.
¥[¥amalg ¥coprod; ¥prod ¥bigcup¥]
```

$$\amalg \coprod; \prod \bigcup$$

2.3 Use with the amsmath Package

By loading the amsmath package after the present chemtimes package, several useful utilities of the former package can be used continently with those supported by the latter, where Times-like fonts are adopted as default fonts used in math modes. For example, the multline environment of the amsmath package can be used as follows:

```
%the amsmath package has been loaded after the mathtimes package
¥begin{multline}
¥int_{0}^{2¥pi}¥sin mx¥cdot ¥sin nx¥,dx =
¥frac{1}{2}¥left¥{¥int_{0}^{2¥pi}¥cos(m-n)x¥,dx
- ¥int_{0}^{2¥pi}¥cos(m+n)x¥,dx¥right¥} ¥¥
= ¥frac{1}{2}¥frac{1}{(m-n)}¥biggl[¥sin(m-n)x¥biggr]_{0}^{2¥pi}
- ¥frac{1}{2}¥frac{1}{(m+n)}¥biggl[¥sin(m+n)x¥biggr]_{0}^{2¥pi} = 0
¥end{multline}
```

$$\int_0^{2\pi} \sin mx \cdot \sin nx \, dx = \frac{1}{2}\left\{\int_0^{2\pi}\cos(m-n)x\,dx - \int_0^{2\pi}\cos(m+n)x\,dx\right\}$$
$$= \frac{1}{2}\frac{1}{(m-n)}\left[\sin(m-n)x\right]_0^{2\pi} - \frac{1}{2}\frac{1}{(m+n)}\left[\sin(m+n)x\right]_0^{2\pi} = 0 \quad (2.29)$$

The use of the gather environment of the amsmath package is exemplified by the following code:

```
%the amsmath package has been loaded after the mathtimes package
¥begin{gather}
¥int_{-¥pi}^{¥pi}e^{imx}e^{-inx}¥,dx = 2¥pi ¥qquad (¥text{for $m=n$}) ¥¥
¥int_{-¥pi}^{¥pi}e^{imx}e^{-inx}¥,dx = ¥int_{-¥pi}^{¥pi}e^{i(m-n)x}¥,dx
= ¥frac{1}{i(m-n)}¥left[e^{i(m-n)x}¥right]_{-¥pi}^{¥pi}  ¥notag ¥¥
= ¥frac{1}{i(m-n)}¥left(e^{i(m-n)¥pi}-^{-i(m-n)¥pi}¥right) = 0 ¥qquad ¥text{for $m¥neq n$}
¥end{gather}
```

$$\int_{-\pi}^{\pi} e^{imx}e^{-inx}\,dx = 2\pi \qquad (\text{for } m=n) \tag{2.30}$$
$$\int_{-\pi}^{\pi} e^{imx}e^{-inx}\,dx = \int_{-\pi}^{\pi} e^{i(m-n)x}\,dx = \frac{1}{i(m-n)}\left[e^{i(m-n)x}\right]_{-\pi}^{\pi}$$
$$= \frac{1}{i(m-n)}\left(e^{i(m-n)\pi}-^{-i(m-n)\pi}\right) = 0 \qquad (\text{for } m \neq n) \tag{2.31}$$

where the slanted printing of e, i, and π is permitted by the mathematical convention, although upright printing is recommended by the ISO rule (ISO 31/XI-1992).

The align environment of the amsmath package is used as follows:

```
%the amsmath package has been loaded after the mathtimes package
¥begin{align}
e^{-i¥beta¥sigma_{2}/2}
& = ¥sum_{k=0}^{¥infty}%
¥frac{1}{k!}¥left(¥frac{-i¥beta}{2}¥right)^{k}(¥sigma_{2})^{k} ¥notag ¥¥
& = ¥left¥{1+¥frac{1}{2!}¥left(¥frac{-i¥beta}{2}¥right)^{2} +
¥frac{1}{4!}¥left(¥frac{-i¥beta}{2}¥right)^{4} + ¥cdots¥right¥}
¥left(¥begin{array}{cc}
1 & 0 ¥¥ 0 & 1
¥end{array}¥right) ¥notag ¥¥
& = ¥left(¥begin{array}{cc}
¥cos¥frac{¥beta}{2} & -¥sin¥frac{¥beta}{2} ¥¥[5pt]
¥sin¥frac{¥beta}{2} & ¥cos ¥frac{¥beta}{2}
¥end{array}¥right)
¥end{align}
```

$$e^{-i\beta\sigma_2/2} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-i\beta}{2} \right)^k (\sigma_2)^k$$

$$= \left\{ 1 + \frac{1}{2!} \left(\frac{-i\beta}{2} \right)^2 + \frac{1}{4!} \left(\frac{-i\beta}{2} \right)^4 + \cdots \right\} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \tag{2.32}$$

The corresponding equation without equation numbers can be printed out by inputting

```
¥begin{align*}...¥end{align*}
```

where the ¥notag commands are deleted. Then the output is obtained as follows:

$$e^{-i\beta\sigma_2/2} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-i\beta}{2} \right)^k (\sigma_2)^k$$

$$= \left\{ 1 + \frac{1}{2!} \left(\frac{-i\beta}{2} \right)^2 + \frac{1}{4!} \left(\frac{-i\beta}{2} \right)^4 + \cdots \right\} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

The split environment and the align environment can be used in the gather environment as follows:

```
¥def¥antialph#1{¥ensuremath{¥overline{¥mathrm{#1}}}}
¥begin{gather}
¥left.¥begin{split}
¥mbox{CI-CF}^{¥mbox{¥scriptsize (III)}}(¥mathbf{C}_{3}; a_{d},b_{d},c_{d})
& = ¥mbox{CI-CF}^{¥mbox{¥scriptsize (I/III)}}(¥mathbf{C}_{3}; a_{d},c_{d})
- ¥mbox{CI-CF}^{¥mbox{¥scriptsize (I)}}(¥mathbf{C}_{3}; a_{d}) ¥¥
&= ¥frac{1}{3}(b_{1}^3 + 2b_{3})
- ¥frac{1}{3}(a_{1}^3 + 2a_{3})
- (b_{1}b_{2} - a_{1}a_{2})
- (a_{1}c_{2} - a_{1}a_{2}) ¥label{eq:30}
¥end{split}¥qquad¥right¥} ¥¥
¥begin{align}
a_{d} & =  ¥mathrm{A}^d + ¥mathrm{B}^d + ¥mathrm{X}^d  ¥¥
c_{d} & =  ¥mathrm{A}^d + ¥mathrm{B}^d + ¥mathrm{X}^d
+ 2¥mathrm{p}^{d/2}¥antialph{p}^{d/2}
+ 2¥mathrm{q}^{d/2}¥antialph{q}^{d/2}
+ 2¥mathrm{r}^{d/2}¥antialph{r}^{d/2} ¥¥
b_{d} & =  ¥mathrm{A}^d + ¥mathrm{B}^d + ¥mathrm{X}^d
+ ¥mathrm{p}^d + ¥antialph{p}^d
+ ¥mathrm{q}^d + ¥antialph{q}^d
+ ¥mathrm{r}^d + ¥antialph{r}^d.
¥end{align}
¥end{gather}
```

$$\left.\begin{aligned}\text{CI-CF}^{(\text{III})}(\mathbf{C}_3; a_d, b_d, c_d) &= \text{CI-CF}^{(\text{I/III})}(\mathbf{C}_3; a_d, c_d) - \text{CI-CF}^{(\text{I})}(\mathbf{C}_3; a_d) \\ &= \frac{1}{3}(b_1^3 + 2b_3) - \frac{1}{3}(a_1^3 + 2a_3) - (b_1 b_2 - a_1 a_2) - (a_1 c_2 - a_1 a_2)\end{aligned}\right\} \quad (2.33)$$

$$a_d = \text{A}^d + \text{B}^d + \text{X}^d \tag{2.34}$$

$$c_d = \text{A}^d + \text{B}^d + \text{X}^d + 2\text{p}^{d/2}\overline{\text{p}}^{d/2} + 2\text{q}^{d/2}\overline{\text{q}}^{d/2} + 2\text{r}^{d/2}\overline{\text{r}}^{d/2} \tag{2.35}$$

$$b_d = \text{A}^d + \text{B}^d + \text{X}^d + \text{p}^d + \overline{\text{p}}^d + \text{q}^d + \overline{\text{q}}^d + \text{r}^d + \overline{\text{r}}^d. \tag{2.36}$$

These equations are cited from S. Fujita, "Numbers of Achiral and Chiral Monosubstituted Alkanes Having a Given Carbon Content and Given Numbers of Asymmetric and Pseudoasymmetric Centers", *Bull. Chem. Soc. Jpn.*, **81**, 193–219 (2008), which can be downloaded from the following Web page:

> `http://www.jstage.jst.go.jp/article/bcsj/81/2/193/_pdf`

Chapter 3

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), which are automatically loaded by declaring ¥usepackage{chemtimes}. Although such basic functions have once been introduced in Chapters 17 and 19 of the online manual of X$^{\Upsilon}$MTEX version 1.01 (xymtex.pdf, cf. [3]) and Chapter 12 of the online manual of X$^{\Upsilon}$MTEX version 2.00 (xymtx200PS.pdf, cf. [5]), they are discussed again by using commands and environments newly-defined in the latest versions of the chemist and the chmst-ps package loaded automatically from the chemtimes package. In particular, the ¥ChemForm command and three environments (ChemEquation, ChemEqnarray, and ChemEqnarray*) are used to show extensions and improvements achieved by the latest versions, because they provide us with more convenient utilities for drawing chemical equations. This chapter is based on the corresponding one contained in the online manual of the chemist (chmst-ps) package (xymtx405B.pdf).

3.1 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]

3.1.1 Basics Due to the ¥ChemForm Command

TEX supports an in-text (in-line) math mode toggled by $...$. LATEX 2$_\varepsilon$ 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 2$_\varepsilon$) 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 use the command ¥mathrm so as to input a code, $¥mathrm{H}_{2}¥mathrm{O}$ or $¥mathrm{H_{2}O}$, which results in an upright formula H_2O. Although the use of ¥mathrm is not tedious in an in-text math mode, the eqnarray environment of LATEX 2$_\varepsilon$ 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.

---

[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 3.1: 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}	$^{23}Na(\gamma, 3n)\,^{20}Na$	$^{23}¥mathrm{Na(¥gamma,% ¥:3n)¥:^{20}Na}$	$^{23}Na(\gamma, 3n)\,^{20}Na$

$$\text{\$¥mathrm{C}\_{2}¥mathrm{H}\_{3}¥mathrm{O}\_{2}^{-}\$} \qquad C_2H_3O_2^-$$

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 X꙰MTEX 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 3.1 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 3.1. For the solution of No.3, see Subsection 3.1.2.

In order to obtain the formula H_2O, several codes can be written, e.g., ¥ChemForm{H_2O} (in Table 3.1), ¥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 3.1), which provide the same output, $C_2H_3O_2^-$.

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

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

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

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

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 2ε.

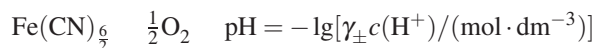|			
¥ChemForm{N_{2(g)}}	$N_{2(g)}$		
¥chemform{N_{2(g)}}	$N_{2(g)}$		
cf. $¥mathrm{N_{2(g)}}$	$N_{2(g)}$	$¥mathit{N_{2(g)}}$	$N_{2(g)}$
		$N_{2(g)}$	$N_{2(g)}$

Finally, the declaration of ¥mathversion{bold} (cf. Chapter 4) 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)}}	$N_{2(g)}$
cf. $¥mathrm{N_{2(g)}}$	$\mathbf{N_{2(g)}}$

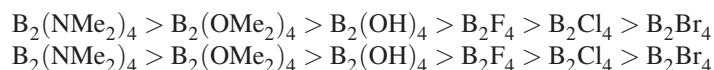### 3.1.3 Using Mathematical Symbols

Mathematical symbols supported by TEX/LATEX 2_ε 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})]}
```

$$\text{Fe(CN)}_{\frac{6}{2}} \quad \tfrac{1}{2}\text{O}_2 \quad \text{pH} = -\lg[\gamma_{\pm} c(\text{H}^+)/(\text{mol} \cdot \text{dm}^{-3})]$$
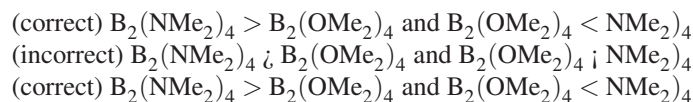
Inequality symbols (> and <) can be used in ¥ChemForm, while they should be replaced by the commands ¥mathgreater and ¥mathless in ¥chemform. Thus, thermal stabilities of boron compounds are typeset as follows:

```
¥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}}
```

$$\text{B}_2(\text{NMe}_2)_4 > \text{B}_2(\text{OMe}_2)_4 > \text{B}_2(\text{OH})_4 > \text{B}_2\text{F}_4 > \text{B}_2\text{Cl}_4 > \text{B}_2\text{Br}_4$$
$$\text{B}_2(\text{NMe}_2)_4 > \text{B}_2(\text{OMe}_2)_4 > \text{B}_2(\text{OH})_4 > \text{B}_2\text{F}_4 > \text{B}_2\text{Cl}_4 > \text{B}_2\text{Br}_4$$

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}}
```

$$(\text{correct}) \; \text{B}_2(\text{NMe}_2)_4 > \text{B}_2(\text{OMe}_2)_4 \text{ and } \text{B}_2(\text{OMe}_2)_4 < \text{NMe}_2)_4$$
$$(\text{incorrect}) \; \text{B}_2(\text{NMe}_2)_4 \; \textit{¿} \; \text{B}_2(\text{OMe}_2)_4 \text{ and } \text{B}_2(\text{OMe}_2)_4 \; \textit{¡} \; \text{NMe}_2)_4$$
$$(\text{correct}) \; \text{B}_2(\text{NMe}_2)_4 > \text{B}_2(\text{OMe}_2)_4 \text{ and } \text{B}_2(\text{OMe}_2)_4 < \text{NMe}_2)_4$$

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}}
```

$$\text{SO}_2 \cdot n\text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{SO}_3(\text{aq}); \quad K \ll 10^{-9} \qquad \text{SO}_2 \cdot n\text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{SO}_3(\text{aq}); \quad K \ll 10^{-9}$$

3.2 Chemical Equations

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

3.2.1 Arrows of Fixed Lengths

Arrows supported by TEX/LATEX 2_ε 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}
```

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

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 3.2.

Table 3.2: 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 3.2) 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 3.2). They can be used in the argument of ¥ChemForm as follows:

```
¥ChemForm{A¥lllongrightarrow B} ¥ChemForm{A¥lllongleftarrow B}
¥ChemForm{A¥lllongleftrightarrow B} ¥ChemForm{A¥lllongleftrightarrow 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.,

$¥Longrightarrow$ ($\Longrightarrow$), $¥Longleftarrow$ ($\Longleftarrow$), and $¥Longleftrightarrow$ ($\Longleftrightarrow$),

a set of longer double-lined arrows and a further longer set are supported by the chemist (chmst-ps) package (Table 3.2). 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}
```

$$A \Longrightarrow B \; A \Longleftarrow B \; A \Longleftrightarrow B$$
$$A \Longrightarrow B \; A \Longleftarrow B \; A \Longleftrightarrow B$$

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

$$A \Longrightarrow B \; A \Longleftarrow B \; A \Longleftrightarrow B$$
$$A \Longrightarrow B \; A \Longleftarrow B \; A \Longleftrightarrow B$$

For arrows of variable lengths, see Section 5.4.

3.2.2 `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}
```

$$\mathrm{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{3.1}$$

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}
```

$$CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{3.2}$$

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}
```

$$\mathrm{CaCO_{3(s)} \longrightarrow Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)}} \tag{3.3}$$

However, the difference between the `ChemEquation` and the `chemeqn` environment becomes obvious, when the mathversion "bold" is used (cf. Subsection 3.1.2 on page 20 and Chapter 4 on page 39):

```
{¥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}
}
```

$$\mathbf{CaCO_{3(s)}} \xrightarrow{\hspace{1.5cm}} \mathbf{Ca^{2+}_{(aq)}} + \mathbf{CO^{2-}_{3(aq)}} \tag{3.4}$$

$$CaCO_{3(s)} \xrightarrow{\hspace{1.5cm}} Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{3.5}$$

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}
}
```

$$CaCO_{3(s)} \xrightarrow{\hspace{1.5cm}} Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{3.6}$$

$$CaCO_{3(s)} \xrightarrow{\hspace{1.5cm}} Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \tag{3.7}$$

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:

$$^{234}_{91}Pa \xrightarrow{\hspace{1.5cm}} ^{0}_{-1}e + ^{234}_{92}U \tag{3.8}$$

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 5.4). 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:

$$HC_2H_3O_2 \rightleftharpoons H^+ + C_2H_3O_2^- \tag{3.9}$$

where the 2nd argument of the ¥reacteqarrow command specifies the length of the resulting arrow. Note that acetic acid ($HC_2H_3O_2$) is written as 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: $\rightleftarrows$ and $\rightleftarrows$ (not systematic)

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

The chmst-ps package supports an equilibrium arrow (right and left arrows) by adopting another 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}
```

$$K_a = \frac{[\mathrm{H^+}][\mathrm{C_2H_3O_2^-}]}{[\mathrm{HC_2H_3O_2}]} = \frac{(6.00\times10^{-4}\,\mathrm{mol/L})(6.00\times10^{-4}\,\mathrm{mol/L})}{1.94\times10^{-2}\,\mathrm{mol/L}} = 1.86\times10^{-5}\,\mathrm{mol/L} \qquad (3.10)$$

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:

$$\mathrm{SF_6 + 2SO_3} \longrightarrow \mathrm{2O_2SF_2}; \qquad \Delta G_{298}^{\circ} = -202\,\mathrm{kJ\cdot mol^{-1}} \qquad (3.11)$$

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}
```

$$\mathrm{CuCl(s)} + \frac{1}{2}\mathrm{Cl_2(g)} \longrightarrow \mathrm{CuCl_2(s)} + 71\,\mathrm{kJ\cdot mol^{-1}} \qquad (3.12)$$

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^{+} ¥equiblongarrow%%in place of ¥rightleftharpoons
¥underset{Magenta}{2MnO_{4}^{-}} + MnO_{2} + 2H_{2}O
¥end{ChemEquation}
```

where the command ¥equiblongarrow supported by the chemist (chmst-ps) package is used to output a longer arrow in place of ¥rightleftharpoons of LATEX 2$_\varepsilon$. Thereby, we obtain the following result:

$$\underset{\mathrm{Green}}{\mathrm{3MnO_4^{2-}}} + \mathrm{4H^+} \xrightleftharpoons{\hspace{1cm}} \underset{\mathrm{Magenta}}{\mathrm{2MnO_4^-}} + \mathrm{MnO_2} + \mathrm{2H_2O} \qquad (3.13)$$

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:

$$2\overset{\text{III}}{\text{S}}_2\text{O}_4^{2-} + \text{H}_2\text{O} \longrightarrow 2\text{H}\overset{\text{IV}}{\text{S}}\text{O}_3^- + \overset{\text{II/VI}}{\text{SSO}}_3^{2-} \tag{3.14}$$

3.2.3 ChemEqnarray **and** ChemEqnarray∗ **Environments**

In a parallel way to the eqnarray and eqnarray∗ environment of LATEX 2ε, 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 ≤ 4.04). The basic functions described above for ¥ChemForm are also effective to the ChemEqnarray and ChemEqnarray∗ environments. The difference between the new environment ChemEqnarray (or ChemEqnarray∗) and the previous environment chemeqnarray (or chemeqnarray∗) 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}
```

$$\text{AgBr} + 2\text{S}_2\text{O}_3^{--} \quad \rightarrow \quad \text{Ag}(\text{S}_2\text{O}_3)_2^{---} + \text{Br}^- \tag{3.15}$$
$$\text{Ag}(\text{S}_2\text{O}_3)_2^{---} \quad \rightarrow \quad \text{Ag}_2\text{S}_2\text{O}_3(\text{s}) + 3\text{S}_2\text{O}_3^{--} \tag{3.16}$$

where the two chemical equations are aligned at the positions of their arrows by placing 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 2ε. 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}
```

$$\text{Fe}^{3+}(\text{aq}) + \tfrac{1}{2}\text{H}_2 \rightleftharpoons \text{Fe}^{2+}(\text{aq}) + \text{H}^+(\text{aq}) \qquad E^\circ = 0.771\,\text{V} \tag{3.17}$$
$$\Delta G^\circ = -74.4\,\text{kJ}\cdot\text{mol}^{-1}$$

Note that the command ¥textstyle is declared to output the fraction $\tfrac{1}{2}$ 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*}
```

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

3.2.4 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:

$$3NaOH + FeCl_3 \rightarrow Fe(OH)_3 + 3NaCl \tag{3.18}$$

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

$$3Na^+(aq) + 3OH^-(aq) + Fe^{3+}(aq) + 3Cl^-(aq)$$
$$\rightarrow \quad Fe(OH)_3(s) + 3Na^+(aq) + 3Cl^-(aq) \tag{3.19}$$

are commonly referred to as follows: Equations 3.18 and 3.19.

3.3 Creation of New Environments for Chemical Equations

As shown in Section 2.3, several environments for printing multiline display equations are available, when the amsmath package is loaded. 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}

3.3.1 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}
```

$$Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^+(aq) + 2OH^-(aq) \rightarrow$$
$$Cu(OH)_2(s) + 2Li^+(aq) + SO_4^{2-}(aq) \tag{3.20}$$

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$_\varepsilon$.

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}
```

$$Cu^{2+}(aq) + SO_4^{2-}(aq) + 2Li^+(aq) + 2OH^-(aq) \rightarrow$$
$$Cu(OH)_2(s) + 2Li^+(aq) + SO_4^{2-}(aq) \quad (3.21)$$

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}
```

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

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. The same code as shown above gives following result after the declaration of `¥let¥ChemEqFont=¥sf`:

```
¥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}
```

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

3.3.2 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}
```
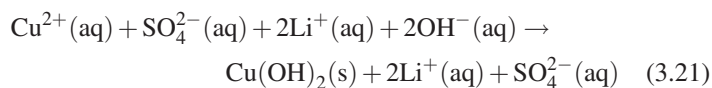
$$Bi(NO_3)_3 \cdot 5H_2O \xrightarrow{50-60^\circ} [Bi_6O_6]_2(NO_3)_{11}(OH) \cdot 6H_2O \xrightarrow{77-130^\circ}$$
$$[Bi_6O_6](NO_3)_6(OH) \cdot 3H_2O \xrightarrow{400-450^\circ} \alpha\text{-}Bi_2O_3 \tag{3.22}$$
$$Bi(NO_3)_3 \cdot N_2O_4 \xrightarrow{200^\circ} Bi_2O(NO_3)_4 \xrightarrow{415^\circ} Bi_4O_5(NO_3)_2 \tag{3.23}$$

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

3.3.3 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}
```

$$
\begin{aligned}
5Fe^{2+} &\longrightarrow 5Fe^{3+} + 5e^- \\
MnO_4^- + 5e^- + 8H^+ &\longrightarrow Mn^{2+} + 4H_2O \\
\hline
MnO_4^- + 5Fe^{2+} + 8H^+ &\longrightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O
\end{aligned}
\tag{3.24}
$$

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*}
```

$$
\text{Co(CN)}_6^{4-} \Longleftrightarrow \text{Co(CN)}_6^{3-} + \text{e}^-
$$
$$
\text{Fe(CN)}_6^{4-} \Longleftrightarrow \text{Co(CN)}_6^{3-} + \text{e}^-
$$

3.3.4 Creation of the `chemalignat` Environment

The `chemalignat` environment can be created as a chemical version of the `alignat` environment of the ams-math 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}
```

$$
\begin{array}{llll}
\text{Solution of zinc oxide:} & \text{ZnO} + 2\text{H}^+ \longrightarrow & \text{Zn}^{2+} + \text{H}_2\text{O} & (3.25) \\
\text{Cathode reaction:} & \text{Zn}^{2+} + 2\text{e}^- \longrightarrow & \text{Zn} & (3.26) \\
\text{Anode reaction:} & \text{H}_2\text{O} \longrightarrow & \tfrac{1}{2}\text{O}_2 + 2\text{H}^+ + 2\text{e}^- & (3.27) \\
\text{Over-all reaction:} & \text{ZnO} \longrightarrow & \text{Zn} + \tfrac{1}{2}\text{O}_2 & (3.28)
\end{array}
$$

3.3.5 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}
```

$$
\begin{aligned}
[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{MnSbPhI}_2] &+ [(\eta^5\text{-C}_5\text{H}_5)\text{Mn(CO)}_2] \cdot \text{THF} \\
&\xrightarrow[\text{[18]crown-6}]{\text{K/THF}} [\text{PhSb}\{\text{Mn(CO)}_2(\eta^5\text{-C}_5\text{H}_5)\}_2] + 2\text{KI} + \cdots \\
&\text{and further lines}
\end{aligned} \tag{3.29}
$$

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{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}
¥makeatother
}
```

$$
[(\eta^5\text{-}C_5H_5)(CO)_2MnSbPhI_2] + [(\eta^5\text{-}C_5H_5)Mn(CO)_2] \cdot THF
$$

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

$$
\text{and further lines} \tag{3.30}
$$

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}
```

$$
H_2O + H_2SO_4 \rightleftharpoons H_3O^+ + HSO_4^-;
$$

$$
K_{H_2O}(25^\circ) = \frac{[H_3O^+][HSO_4^-]}{[H_2O]} \sim 1 \tag{3.31}
$$

$$
SO_3 + H_2SO_4 \rightleftharpoons H_2S_2O_7 \tag{3.32}
$$

$$
H_2S_2O_7 + H_2SO_4 \rightleftharpoons H_3SO_4^+ + HS_2O_7^-;
$$

$$
K_{H_2S_2O_7}(25^\circ) = \frac{[H_3SO_4^+][HS_2O_7^-]}{[H_2S_2O_7]} = 1.4 \times 10^{-2} \tag{3.33}
$$

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}
```

$$
[Cr(CO)_6] \xrightarrow{A} \underset{yellow}{[Cr(CO)_5(AsPhH_2)]} \xrightarrow{B}
$$
$$
\underset{orange}{[Cr(CO)_5(AsPhLi_2)]} \xrightarrow{C} \underset{\text{dark violet (mp 104°)}}{[\{Cr(CO)_5\}_2AsPh]}
$$
$$
\begin{aligned}
A &: \quad PhAsH_2 \\
B &: \quad LiBu \\
C &: \quad \text{cyclohexyl-}NCl_2
\end{aligned}
$$

(3.34)

3.4   Objects Placed Over or Under Arrows

3.4.1   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}
```

$$
CCl_4 + HF \xrightarrow{SbFCl_4} CFCl_3 + HCl
$$

(3.35)

The command ¥stackrel of LATEX 2$_\varepsilon$ 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}
```

$$
CFCl_3 + HF \xrightarrow{SbFCl_4} CF_2Cl_2 + HCl
$$

(3.36)

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}
```

$$
Na + Al + 2H_2 \underset{350\ atom}{\overset{THF/140°/3\,h}{\xrightarrow{\hspace{1cm}}}} NaAlH_4 \quad (99\% \text{ yield})
$$

(3.37)

3.4.2 Application of Arrows for Organic Chemistry

Arrows for organic chemistry (Section 5.4) 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}
```

$$\text{Na} + \text{Al} + 2\text{H}_2 \xrightarrow[\text{350 atom}]{\text{THF}/140°/3\,\text{h}} \text{NaAlH}_4 \quad (99\% \text{ yield}) \tag{3.38}$$

On similar lines, the following set of arrows for organic chemistry (Section 5.4) can be used to draw reaction equations for inorganic chemistry.

$$\texttt{¥reactrarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \xrightarrow[\text{B}]{\text{A}}$$

$$\texttt{¥reactlarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \xleftarrow[\text{B}]{\text{A}}$$

$$\texttt{¥reactlrarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \xrightleftarrows[\text{B}]{\text{A}}$$

$$\texttt{¥reacteqarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \xrightleftharpoons[\text{B}]{\text{A}}$$

Because default positions of objects placed by such arrows for organic chemistry (Section 5.4) 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_20
¥end{ChemEquation}
```

$$\alpha\text{Na(NH}_4)\text{HPO}_4 \xrightarrow{\Delta} (\text{NaPO}_3)_\alpha + \alpha\text{NH}_3 \uparrow + \alpha\text{H}_2\text{O} \tag{3.39}$$

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_20
¥end{ChemEquation}
}
```

$$\alpha\text{Na(NH}_4)\text{HPO}_4 \xrightarrow{\Delta} (\text{NaPO}_3)_\alpha + \alpha\text{NH}_3 \uparrow + \alpha\text{H}_2\text{O} \tag{3.40}$$

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}
```

$$2Ph_3GeBr + 2Na \xrightarrow[\text{xylene}]{\text{boiling}} 2NaBr + Ge_2Ph_6 \quad (mp\,340℃) \tag{3.41}$$

where ¥degC is also defined in the chemist package.

The ChemEquation environment is capable of accommodating structural formulas produced by the XΊMTEX system. The following example shows that the command ¥tetrahedral of the XΊMTEX 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}
```
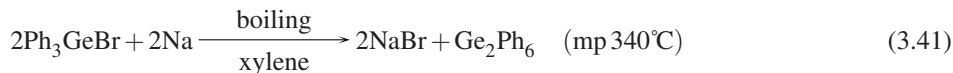
$$Me_3SnCl_2 + 2NaRe(CO)_5 \xrightarrow{\text{Metathesis}} (CO)_5Re\!-\!\underset{\underset{Me}{|}}{\overset{\overset{Me}{|}}{Sn}}\!-\!Re(CO)_5 + 2NaCl \tag{3.42}$$

where the XyMcompd environment is supported in the chemist package (cf. Section 5.3).

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}
```

$$Na[Mn(CO)_5] \xrightarrow{C_3H_5Cl} [Mn(CO)_5(\eta^1\text{-}C_3H_5)] \xrightarrow[\text{or }80℃]{h\nu} [Mn(CO)_4(\eta^3\text{-}C_3H_5)] + CO \tag{3.43}$$

where η^1-allyl (η^1-C_3H_5) is converted into η^3-allyl (η^3-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}}
```

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

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.

3.4.3 Further Commands for Drawing Arrows

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

$$\text{¥reactreqarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \genfrac{}{}{0pt}{}{A}{B}$$

$$\text{¥reactleqarrow\{0pt\}\{1cm\}\{A\}\{B\}} \qquad \genfrac{}{}{0pt}{}{A}{B}$$

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}}

$$\genfrac{}{}{0pt}{}{A}{B} \qquad \genfrac{}{}{0pt}{}{A}{B} \qquad \genfrac{}{}{0pt}{}{A}{B}$$

3.5 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}

$$RC\!\!\equiv\!\!CH + e_{am}^{-} \longrightarrow RC\!\!\equiv\!\!C^{-} + \tfrac{1}{2}H_2 \tag{3.44}$$

where the subscript am of e_{am}^{-} indicates that the electron is solvated by liquid ammonia.

Double bonds are drawn by ¥dbond in a ChemEquation or like environment:
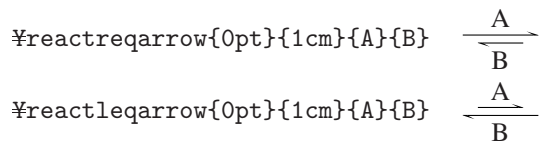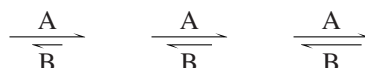
    ¥begin{ChemEquation}
    CH_{2}¥dbond CH_{2} + PhH
    ¥reactrarrow{0pt}{2cm}{¥scriptsize ¥ChemForm{AlCl_{3}}}{¥ChemStrut}
    PhEt
    ¥end{ChemEquation}

$$CH_2\!\!=\!\!CH_2 + PhH \xrightarrow{AlCl_3} PhEt \tag{3.45}$$

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}

$$PhN\!\!=\!\!O + 2e_{am}^{-} \longrightarrow PhN^{-}\!\!-\!\!O^{-} \tag{3.46}$$

Lone pairs around an atom can be typeset by using the ¥lonepairA command, which is supported by X¥!MT$_E$X version 4.05 (the lewisstruc package, cf. the online document (xymtx405A.pdf)). The following example shows that a cuprous chloride ion ($CuCl_2^-$) 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}

$$CuCl_4^{2-} + Cu \longrightarrow 2\bigl[:\ddot{C}l\!\!-\!\!Cu\!\!-\!\!\ddot{C}l:\bigr]^{-} \tag{3.47}$$

Chapter 4

New Mathversions

There are two mathversions ("normal" and "bold") for mathematical usage in LATEX 2ε. The chemist (chmst-ps) package loaded automatically by the chemtimes package provides additional two mathversions ("chem" and "bold-chem") for chemical usage. The latter two mathversions have already been introduced in Chapter 17 of the manual of XΥMTEX version 1.01 (xymtex.pdf). This chapter is devoted to add further comments with examples, where the chemical environments discussed in Chapter 3 are tested under the respective mathversions. This chapter is based on the corresponding one contained in the online manual of the chemist (chmst-ps) package (xymtx405B.pdf).

4.1 Mathversion "normal"

The mathversion "normal" gives outputs of default mode, which are inherent in LATEX 2ε without any declaration or with declaring ¥mathversion{normal}.

4.1.1 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}
```

39

```
¥testmathversion
¥end{tboxscreen}}
```

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

Output A due to "normal"

$abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ$

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

1234567890

1234567890

$\mathscr{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

$\int\Sigma\Pi\amalg\cup\cap\odot\oplus\uplus\otimes$

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

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

Traditional commands are left effective in the chemtimes package. Thus, numbers of old style can be printed by using ¥oldstyle in place of ¥mathnormal. The command ¥cal can be used in place of ¥mathcal:

```
¥begin{eqnarray*}
&& ¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} ¥alpha¥beta¥gamma; ¥¥
&& {¥cal ABCDEFGHIJKLMNOPQRSTUVWXYZ}
¥end{eqnarray*}
```

$$\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc 0123456789 \alpha\beta\gamma;$$
$$\mathscr{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

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:
>
> $$\sum_{a \le k < b} f(k) = \int_a^b f(x)\mathrm{d}x + \sum_{k=1}^{m} \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m. \tag{4.1}$$
>
> The term R_m is represented as follows:
>
> $$\begin{aligned} R_m &=& (-1)^{m+1} \int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)\mathrm{d}x, \\ && a \le b \text{ and } m \ge 1, \end{aligned} \tag{4.2}$$
>
> where the symbols a, b, and m represent integers.

4.1.2 Convenient Environments for Chemical Equations

To test `equation` and `eqnarray` environments containing chemical formulas, the following test command named ¥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 defined above (¥testequationforchemistry) gives the following output.

> **Output C due to "normal"**
>
> An equation environment:
>
> $$2H_2 + O_2 \rightarrow 2H_2O \tag{4.3}$$
>
> An eqnarray environment:
>
> $$\begin{aligned} C + O_2 &\rightarrow& CO_2 \\ Na^+ + Cl^- &\rightarrow& NaCl \downarrow \end{aligned}$$
>
> $$(4.4)$$
> $$(4.5)$$

The chemist (chmst-ps) package defines `chemeqn` and `chemeqnarray` environments in order to support chemical requirements (cf. Subsection 17.1 of the manual of X$\widehat{\text{M}}$T$_{\text{E}}$X 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_20}
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.

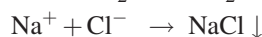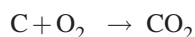---

Output D due to "normal"

A chemeqn environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.6}$$

$$abcdefghijklmnopqrstuvwxyz \imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ \tag{4.7}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.8}$$

A chemeqnarray environment:

$$
\begin{aligned}
C + O_2 &\rightarrow CO_2 \tag{4.9}\\
Na^+ + Cl^- &\rightarrow NaCl \downarrow \tag{4.10}
\end{aligned}
$$

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 addition to the chemeqn and chemeqnarray environments (cf. Subsection 17.1 of the manual of XⒾMTEX 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_20
```

```
¥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 environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.11}$$

$$abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ \tag{4.12}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varsigma\varphi\Gamma\Delta\Theta\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.13}$$

A ChemEqnarray environment:

$$C + O_2 \quad \rightarrow \quad CO_2 \tag{4.14}$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl\downarrow \tag{4.15}$$

A ChemEqnarray$*$ environment:

$$C + O_2 \quad \rightarrow \quad CO_2$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl\downarrow$$

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

4.2   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.

4.2.1   Outputs under Mathversion "bold"

The mathversion "bold" gives outputs of "bold" mode, which are inherent in LATEX 2_ε. 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"

$$abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ$$

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

$$1234567890$$

$$1234567890$$

$$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\int\Sigma\Pi\amalg\cup\cap\odot\oplus\uplus\otimes$$

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

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

The above output shows that the command ¥mathnormal does not work well. To avoid this difficulty, an additional use of ¥mbox or an alternative method of ¥oldstyle is effective.

```
%¥mathversion{bold} has been declared.
¥[¥text{not work:} ¥mathnormal{1234567890}¥]
¥[¥text{success:} ¥mathnormal{¥mbox{1234567890}}¥]
¥[¥text{success:} {¥oldstyle 1234567890}¥]
```

$$\text{not work:}\mathbf{1234567890}$$

$$\text{success:}1234567890$$

$$\text{success:}1234567890$$

Note that the command ¥oldstyle should be used to specify numbers of old style only. Compare the following examples:

```
%¥mathversion{bold} has been declared.
¥begin{equation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{equation}
¥begin{equation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} ¥alpha¥beta¥gamma; ¥Gamma¥Delta
¥end{equation}
```

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc0123456789\alpha\beta\gamma; \Gamma\Delta \tag{4.16}$$

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc0123456789\alpha\beta\gamma; \Gamma\Delta \tag{4.17}$$

The command ¥cal can be used in place of ¥mathcal:

```
¥[ABCDEFGHIJKLMNOPQRSTUVWXYZ {¥cal ABCDEFGHIJKLMNOPQRSTUVWXYZ}¥]
```

ABCDEFGHIJKLMNOPQRSTUVWXYZ𝓐𝓑𝓒𝓓𝓔𝓕𝓖𝓗𝓘𝓙𝓚𝓛𝓜𝓝𝓞𝓟𝓠𝓡𝓢𝓣𝓤𝓥𝓦𝓧𝓨𝓩

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:

$$\sum_{a \leq k_i b} f(k) = \int_a^b f(x)\mathrm{d}x + \sum_{k=1}^m \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m. \tag{4.18}$$

The term R_m is represented as follows:

$$
\begin{aligned}
R_m &= (-1)^{m+1} \int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)\mathrm{d}x, \\
& a \leq b \text{ and } m \geq 1,
\end{aligned}
\tag{4.19}
$$

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:

```
%¥mathversion{bold} has been declared.
¥[¥sum_{a¥leq k ¥mbox{¥scriptsize $¥mathless$} b}f(k)¥]
```

gives the following output:

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

4.2.2 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 environment:
$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.20}$$

An eqnarray environment:
$$
\begin{aligned}
C + O_2 &\rightarrow CO_2 \tag{4.21} \\
Na^+ + Cl^- &\rightarrow NaCl \downarrow \tag{4.22}
\end{aligned}
$$

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".
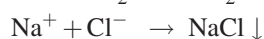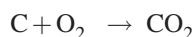

Output D due to "bold"

A chemeqn environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.23}$$

$$\text{abcdefghijklmnopqrstuvwxyz} \iota\jmath \text{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{4.24}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\vartheta\varpi\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.25}$$

A chemeqnarray environment:

$$C + O_2 \quad \rightarrow \quad CO_2 \tag{4.26}$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow \tag{4.27}$$

A chemeqnarray∗ environment:

$$C + O_2 \quad \rightarrow \quad CO_2$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow$$

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 environment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{4.28}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\iota\jmath\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{4.29}$$

$$\boldsymbol{\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega} \tag{4.30}$$

A ChemEqnarray environment:

$$\mathbf{C + O_2} \quad \rightarrow \quad \mathbf{CO_2} \tag{4.31}$$
$$\mathbf{Na^+ + Cl^-} \quad \rightarrow \quad \mathbf{NaCl \downarrow} \tag{4.32}$$

A ChemEqnarray∗ environment:

$$\mathbf{C + O_2} \quad \rightarrow \quad \mathbf{CO_2}$$
$$\mathbf{Na^+ + Cl^-} \quad \rightarrow \quad \mathbf{NaCl \downarrow}$$

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

4.3 Mathversion "chem"

Subsection 17.1 of the manual of XΥMT$_{\!E}$X 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}
```

4.3.1 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

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

1234567890

1234567890

$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

$\int\Sigma\Pi\amalg\cup\cap\odot\oplus\uplus\otimes$

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

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

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

Numbers of old style can not be printed by using ¥mathnormal. They are printed by using the command ¥oldstyle.

```
%mathversion ``chem'' has been declared.
¥begin{equation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} 0123456789 ¥alpha¥beta¥gamma; ¥Gamma¥Delta
¥end{equation}
¥begin{ChemEquation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} 0123456789 ¥alpha¥beta¥gamma; ¥Gamma¥Delta
¥end{ChemEquation}
```

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; \textrm{abc}\,\textit{0123456789}\,0123456789\,\alpha\beta\gamma,\Gamma\Delta \tag{4.33}$$

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; \textrm{abc}\,\textit{0123456789}\,0123456789\,\alpha\beta\gamma,\Gamma\Delta \tag{4.34}$$

An alternative way for printing numbers of old style is the nested use of ¥mathnormal and ¥mbox.

```
%mathversion ``chem'' has been declared.
¥begin{equation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{equation}
¥begin{ChemEquation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{ChemEquation}
```

$$\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}; \mathit{abc}\,\textit{0123456789}\,\alpha\beta\gamma,\Gamma\Delta \tag{4.35}$$

$$\mathit{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega}; \mathit{abc}\,\textit{0123456789}\,\alpha\beta\gamma,\Gamma\Delta \tag{4.36}$$

The command ¥cal can be used in place of ¥mathcal:

```
¥[ABCDEFGHIJKLMNOPQRSTUVWXYZ {¥cal ABCDEFGHIJKLMNOPQRSTUVWXYZ}¥]
```

ABCDEFGHIJKLMNOPQRSTUVWXYZ$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

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:

$$\sum_{a\leq k_{\textrm{i}} b} f(k) = \int_a^b f(x)dx + \sum_{k=1}^m \frac{B_k}{k!} f^{(k-1)}(x)\Big|_a^b + R_m. \tag{4.37}$$

The term R_m is represented as follows:

$$\begin{aligned} R_m &= (-1)^{m+1} \int_a^b \frac{B_m(\{x\})}{m!} f^{(m)}(x)dx, \\ & \qquad a \leq b \text{ and } m \geq 1, \end{aligned} \tag{4.38}$$

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:

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

4.3.2   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.
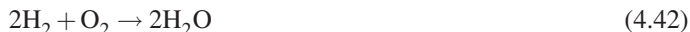

Output C due to "chem"

An equation environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.39}$$

An eqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 \\ Na^+ + Cl^- &\rightarrow NaCl \downarrow \end{aligned} \tag{4.40}$$
$$\tag{4.41}$$

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".

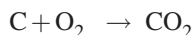---

Output D due to "chem"

A chemeqn environment:
$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.42}$$

$$\text{abcdefghijklmnopqrstuvwxyz}\iota\jmath\text{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{4.43}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\epsilon\vartheta\varpi\rho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.44}$$

A chemeqnarray environment:
$$C + O_2 \quad \rightarrow \quad CO_2 \tag{4.45}$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow \tag{4.46}$$

A chemeqnarray∗ environment:
$$C + O_2 \quad \rightarrow \quad CO_2$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow$$

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 the command ¥ChemForm can be used to 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 environment:
$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.47}$$

$$\text{abcdefghijklmnopqrstuvwxyz}\iota\jmath\text{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{4.48}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\epsilon\vartheta\varpi\rho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.49}$$

A ChemEqnarray environment:
$$C + O_2 \quad \rightarrow \quad CO_2 \tag{4.50}$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow \tag{4.51}$$

A ChemEqnarray∗ environment:
$$C + O_2 \quad \rightarrow \quad CO_2$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow$$

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

4.4   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 X$^?$MT$_E$X version 1.01 (xymtex.pdf)), the latest version of the chemist package

packed in X$^{\widehat{\text{II}}}$MTEX version 4.05 supports the mathversion "boldchem".

This section is typeset after the declaration of

```
¥mathversion{boldchem}
```

4.4.1   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"

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

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

$$\textbf{1234567890}$$

$$\textit{1234567890}$$

$$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$$

$$\int\Sigma\Pi\amalg\cup\cap\odot\oplus\uplus\otimes$$

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

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

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

Numbers of old style can not be printed by using ¥mathnormal. They are printed by using the command ¥oldstyle.

```
%mathversion ''boldchem'' has been declared.
¥begin{equation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} 0123456789 ¥alpha¥beta¥gamma; ¥Gamma¥Delta
¥end{equation}
¥begin{ChemEquation}
¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc {¥oldstyle 0123456789} 0123456789 ¥alpha¥beta¥gamma; ¥Gamma¥Delta
¥end{ChemEquation}
```

$$\boldsymbol{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega};\textbf{abc}0123456789\textbf{0123456789}\alpha\beta\gamma;\boldsymbol{\Gamma\Delta} \qquad (4.52)$$

$$\boldsymbol{\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega};\textbf{abc}0123456789\textbf{0123456789}\alpha\beta\gamma;\boldsymbol{\Gamma\Delta} \qquad (4.53)$$

An alternative way for printing numbers of old style is the nested use of ¥mathnormal and ¥mbox.

```
%mathversion ''boldchem'' has been declared.
¥begin{equation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{equation}
¥begin{ChemEquation}
¥mathnormal{¥Gamma¥Delta¥Theta¥Lambda¥Xi¥Pi¥Sigma¥Upsilon¥Phi¥Psi¥Omega;
abc ¥mbox{0123456789} ¥alpha¥beta¥gamma}; ¥Gamma¥Delta
¥end{ChemEquation}
```

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc\mathit{0123456789}\alpha\beta\gamma; \Gamma\Delta \tag{4.54}$$

$$\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega; abc\mathit{0123456789}\alpha\beta\gamma; \Gamma\Delta \tag{4.55}$$

The command ¥cal can be used in place of ¥mathcal:

```
¥[ABCDEFGHIJKLMNOPQRSTUVWXYZ {¥cal ABCDEFGHIJKLMNOPQRSTUVWXYZ}¥]
```

ABCDEFGHIJKLMNOPQRSTUVWXYZ$\mathcal{ABCDEFGHIJKLMNOPQRSTUVWXYZ}$

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:

$$\sum_{\mathbf{a} \leq \mathbf{k} ; \mathbf{b}} \mathbf{f(k)} = \int_{\mathbf{a}}^{\mathbf{b}} \mathbf{f(x)dx} + \sum_{\mathbf{k=1}}^{\mathbf{m}} \frac{\mathbf{B_k}}{\mathbf{k!}} \mathbf{f}^{(\mathbf{k-1})}\mathbf{(x)} \Big|_{\mathbf{a}}^{\mathbf{b}} + \mathbf{R_m}. \tag{4.56}$$

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

$$\begin{aligned} \mathbf{R_m} &= (-\mathbf{1})^{\mathbf{m+1}} \int_{\mathbf{a}}^{\mathbf{b}} \frac{\mathbf{B_m(\{x\})}}{\mathbf{m!}} \mathbf{f}^{(\mathbf{m})}\mathbf{(x)dx}, \\ & \mathbf{a} \leq \mathbf{b} \text{ and } \mathbf{m} \geq \mathbf{1}, \end{aligned} \tag{4.57}$$

where the symbols $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{m}$ 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:

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

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:

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

4.4.2 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 environment:

$$\mathbf{2H_2 + O_2 \rightarrow 2H_2O} \tag{4.58}$$

An eqnarray environment:

$$\mathbf{C + O_2} \quad \rightarrow \quad \mathbf{CO_2} \tag{4.59}$$
$$\mathbf{Na^+ + Cl^-} \quad \rightarrow \quad \mathbf{NaCl \downarrow} \tag{4.60}$$

A partial mathversion "boldchem" under a mathversion "chem" and a partial mathversion "chem" under a mathversion "boldchem" are available as follows:

```
{
¥mathversion{chem}
¥begin{equation}
2H_{2} + ¥mbox{¥mathversion{boldchem}$O_{2}$} ¥lllongrightarrow 2H_{2}O
¥end{equation}
¥mathversion{boldchem}
¥begin{equation}
2H_{2} + ¥mbox{¥mathversion{chem}$O_{2}$} ¥lllongrightarrow 2H_{2}O
¥end{equation}
}
```

$$2H_2 + \mathbf{O_2} \longrightarrow 2H_2O \tag{4.61}$$

$$\mathbf{2H_2 + O_2} \longrightarrow \mathbf{2H_2O} \tag{4.62}$$

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 environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.63}$$

$$abcdefghijklmnopqrstuvwxyz\imath\jmath ABCDEFGHIJKLMNOPQRSTUVWXYZ \tag{4.64}$$

$$\alpha\beta\gamma\delta\varepsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.65}$$

A chemeqnarray environment:

$$C + O_2 \quad \rightarrow \quad CO_2 \tag{4.66}$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow \tag{4.67}$$

A chemeqnarray∗ environment:

$$C + O_2 \quad \rightarrow \quad CO_2$$
$$Na^+ + Cl^- \quad \rightarrow \quad NaCl \downarrow$$

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 environment:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{4.68}$$

$$\mathbf{abcdefghijklmnopqrstuvwxyz}\imath\jmath\mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \tag{4.69}$$

$$\alpha\beta\gamma\delta\epsilon\zeta\eta\theta\iota\kappa\lambda\mu\nu\xi\pi\rho\sigma\tau\upsilon\phi\chi\psi\omega\varepsilon\vartheta\varpi\varrho\varsigma\varphi\Gamma\Delta\Theta\Lambda\Xi\Pi\Sigma\Upsilon\Phi\Psi\Omega \tag{4.70}$$

A ChemEqnarray environment:

$$\begin{aligned} C + O_2 &\rightarrow CO_2 \tag{4.71}\\ Na^+ + Cl^- &\rightarrow NaCl \downarrow \tag{4.72} \end{aligned}$$

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 $C + O_2 \rightarrow CO_2$

Chapter 5

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 XΥMTEX 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 XΥMTEX 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 XΥMTEX version 2.00 (xymtx200PS.pdf, cf. [5]).

This chapter is based on the corresponding one contained in the online manual of the chemist (chmst-ps) package (xymtx405B.pdf) in order to add further comments with examples.

5.1   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 XΥMTEX 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.

5.2   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.

5.3 Boxes for Chemical Structural Formulas

5.3.1 XyMcompd Environment

Each structural formula drawn by the X$\hat{Y}$MTEX 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 the default value (0.1 pt) as a unit stored in the dimension register ¥unitlength. 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.

5.3.2   Commands for Compound Boxes

The command ¥cdonecell takes three arguments:

$$\text{¥cdonecell\{dimenA\}\{dimenB\}\{formula\}}$$

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.

5.4 Arrows for Organic Chemistry

Arrows due to the chemist package have been introduced in Section 12.2 of the manual of X$^{\text{I}}$MT$_{\text{E}}$X version 2.00 (xymtx200PS.pdf, cf. [5]). The list of arrows of the manual is cited for convenience, as shown in Fig. 5.1, 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 23).

Each command for drawing an arrow listed in Fig. 5.1 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 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:

Figure 5.1: Reaction arrows of various types

```
¥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:

$$CH_3CH_2CH_2CH_2CH_2CH_3 \quad \xrightarrow[\text{heat}]{\text{catalyst}} \quad \bigcirc\!\!\!\!\bigcirc \quad +4H_2 \qquad\qquad (5.1)$$

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_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:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 \xrightarrow[\text{catalyst}]{\text{heat}}$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_2{=}CH_2$$
and
$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH{=}CH_2$$
and
$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3 + CH_3CH_2CH_2CH_2CH{=}CH_2$$
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, i.e., in a text form "and so on" and in a math form "andsoon", where the spaces of the latter are deleted by typesetting mechanism due to the math mode of TeX/LaTeX 2_ε.

```
¥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}
```

$$A \xrightarrow[\text{acid catalysis}]{H^+} B \xleftarrow[CH_3OH]{H^+} C \xleftrightarrow{H^+} D \overset{H^+}{\underset{\text{equilibrium}}{\rightleftarrows}} E \qquad (5.2)$$

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}
```

$$A \xRightarrow[\text{acid catalysis}]{H^+} B \xLeftarrow[CH_3OH]{H^+} C \xLeftrightarrow{H^+} D \qquad (5.3)$$

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

$$A \xRightarrow[\text{acid catalysis}]{H^+} B \xLeftarrow[CH_3OH]{H^+} C \xLeftrightarrow{H^+} D \qquad (5.4)$$

5.5 Framed Boxes

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

5.5.1 Simple Framed Boxes

Chapter 19 of the manual of XˆIMTEX 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 XˆIMTEX 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 XˆIMTEX. The setting ¥let¥substfontsize=¥scriptsize due to XˆIMTEX changes the font size of each substituent. The command ¥centering of LATEX 2$_\varepsilon$ 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.

5.5.2 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}
```

7   **8**

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.

A `tboxscreen` environment provides a frame spreading for ¥textwidth. The following example shows that a `ChemEqnarray∗` environment 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{0pt}{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{0pt}{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{0pt}{1cm}{}{} ¥mskip6mu
¥begin{XyMcompd}(1100,500)(-400,0){}{}
¥dimethylenei{2==¥downnobond{N}{H}}{2W==¥bzdrh{1==(yl)};1W==¥bzdrh{4==(yl)};1D==O}
¥end{XyMcompd}
¥end{ChemEqnarray*}
¥end{tboxscreen}
```

Beckmann Rearrangement

Note that the commands ¥sbond, ¥dbond, and ¥tbond are supported by the chemist packages to draw single (——), double (===), and triple bonds (≡). 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{0pt}{2cm}{[3,3]}{¥strut}
¥begin{XyMcompd}(400,400)(50,-100){}{}
¥sixunitv[df]{}{2==R;3==R}{e}
¥end{XyMcompd}
```

```
¥end{tboxscreen}
```

[3,3]Sigmatropic Rearrangement

5.5.3 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}
```


5.6   Verbatim Environment

A verbatim environment due to the chemist package have been introduced in Section 17.5 of the manual of XᾸMTEX 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 verbatim 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 6

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.

6.1 Harpoons Defined in the chmst-ps Package

6.1.1 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 6.1.

Although a code with the same descriptors (e.g., ¥psline{Hru-Hru}(1.3,0)) works well, a more systematic code described in Table 6.1 (e.g., ¥psline{Hld-Hru}(1.3,0)) is recommended:

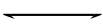| Not Recommended		Recommended (Table 6.1)	
¥psline{Hru-Hru}(1.3,0)		¥psline{Hld-Hru}(1.3,0)	
¥psline{Hld-Hld}(1.3,0)			

The harpoons listed in Table 6.1 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 6.1: 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

(Harpoon head)   (Arrowhead)
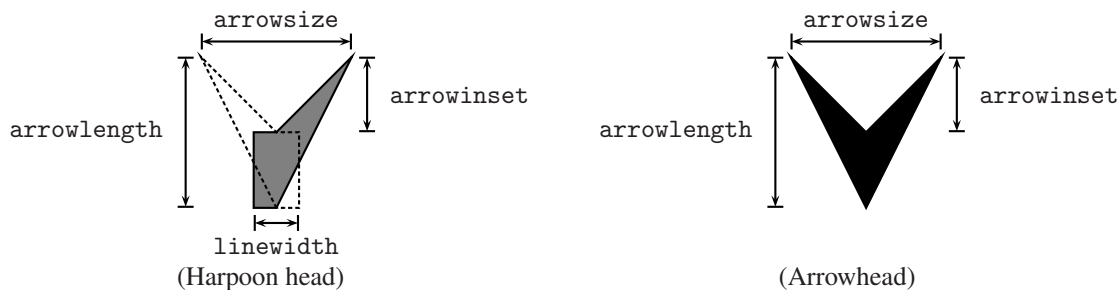
Figure 6.1: Dimensions of a harpoon head (left) and the corresponding arrowhead (right)

6.1.2 Keywords for Harpoons

Dimensions of a harpoon-head is shown in Fig. 6.1. 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 6.2. 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. 6.1 (left) has an additional object for adjusting the terminal of the stem line of a harpoon.
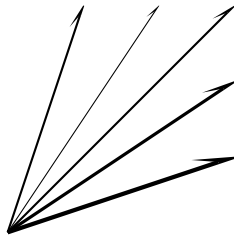
Table 6.2: Keywords for Harpoons (Common to Arrows)

Name	Value Type	Dafault	Explanation
linewidth	*value[unit]*	0.8pt	linewith of a stem, cf. Fig. 6.1
arrows	*style*	–	style of arrows (harpoons)
arrowlength	*value*	1.4	cf. Fig. 6.1
arrowsize	*value[unit] value*	1.5pt 2	cf. Fig. 6.1 (dimension and factor)
arrowinset	*value*	0.4	cf. Fig. 6.1

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 6.2) are used to calculate the arrow size (width) according to the following equation:

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

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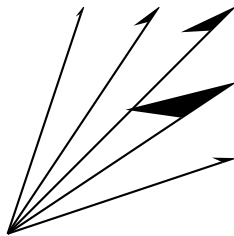
```
¥psset{arrowlength=2,arrowsize=1.5pt 4,arrowinset=0.6}
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[linewidth=0.4pt]{-Hru}(0,0)(2,3)
¥psline[linewidth=0.8pt]{-Hru}(0,0)(3,3)
¥psline[linewidth=1.2pt]{-Hru}(0,0)(3,2)
¥psline[linewidth=1.6pt]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

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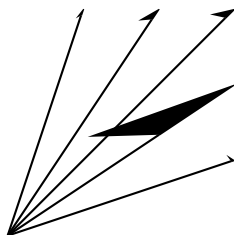
```
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[arrowsize=0pt 10]{-Hru}(0,0)(2,3)
¥psline[arrowsize=10pt]{-Hru}(0,0)(3,3)
¥psline[arrowsize=1]{-Hru}(0,0)(3,2)
¥psline[arrowsize=0.2cm]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

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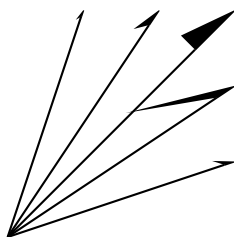
```
¥begin{pspicture}(0,0)(3,3)
¥psline{-Hru}(0,0)(1,3)
¥psline[arrowsize=0pt 10,arrowlength=1]{-Hru}(0,0)(2,3)
¥psline[arrowsize=10pt,arrowlength=0.8]{-Hru}(0,0)(3,3)
¥psline[arrowsize=1,arrowlength=2]{-Hru}(0,0)(3,2)
¥psline[arrowsize=0.2cm,arrowlength=0.4]{-Hru}(0,0)(3,1)
¥end{pspicture}
```

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}
```

6.2   Chemical Conventions for Using Arrows and Harpoons

Chemical conventions use arrows and harpoons differently:

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

2. A right (⇀) or left harpoon (↽) is used to show a shift of an electron, while a right (→) or left arrow (←) is used to show a shift of an electron pair (cf. page 66). 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 3.2.1 and Section 5.4). 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.
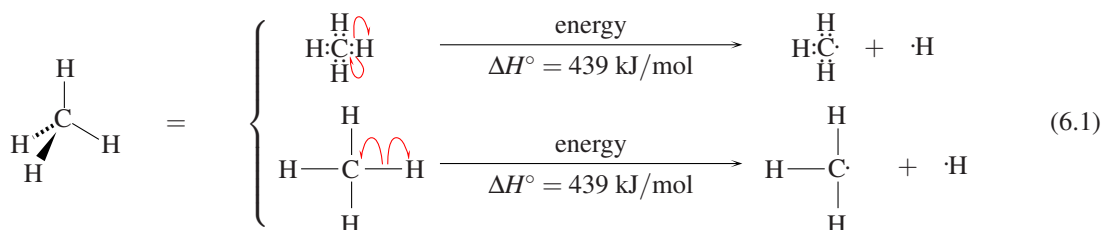
The second convention for using a harpoon is concerned with a radical fission of a covalent bond. For example, the homolysis of the C—H bond of methane is represented by the following scheme.

```
¥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.
```
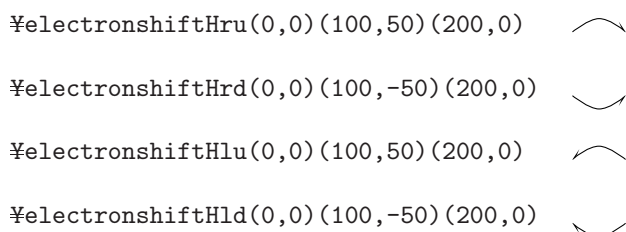
¥end{ChemEquation}

$$
\begin{array}{c}
H \\
| \\
H\!\cdots\!C\!\!-\!\!H \\
| \\
H
\end{array}
\quad = \quad
\left\{
\begin{array}{l}
\begin{array}{c}
H \\
H\!:\!\overset{\cdot\cdot}{C}\!:\!H \\
\overset{\cdot\cdot}{H}
\end{array}
\xrightarrow[\Delta H^\circ = 439\ \mathrm{kJ/mol}]{\text{energy}}
\begin{array}{c}
H \\
H\!:\!\overset{\cdot}{C}\!\cdot \\
\overset{\cdot}{H}
\end{array}
\ + \ \cdot H
\\[2em]
\begin{array}{c}
H \\
| \\
H\!\!-\!\!C\!\!-\!\!H \\
| \\
H
\end{array}
\xrightarrow[\Delta H^\circ = 439\ \mathrm{kJ/mol}]{\text{energy}}
\begin{array}{c}
H \\
| \\
H\!\!-\!\!C\!\cdot \\
| \\
H
\end{array}
\ + \ \cdot H
\end{array}
\right.
\qquad (6.1)
$$

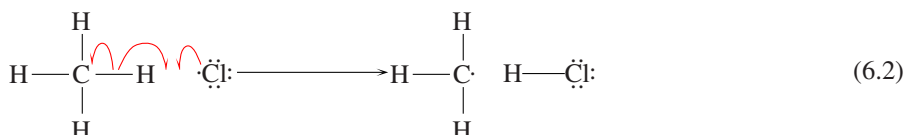Shortcut commands for drawing harpoons are defined as follows:

```
¥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 an internal setting due to ¥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}
```

$$
\begin{array}{c}
H \\
| \\
H\!\!-\!\!C\!\!-\!\!H \\
| \\
H
\end{array}
\ \ddot{\underset{\cdot\cdot}{C}}l\!:
\longrightarrow
H\!\!-\!\!
\begin{array}{c}
H \\
| \\
C\!\cdot \\
| \\
H
\end{array}
\quad H\!\!-\!\!\ddot{\underset{\cdot\cdot}{C}}l\!:
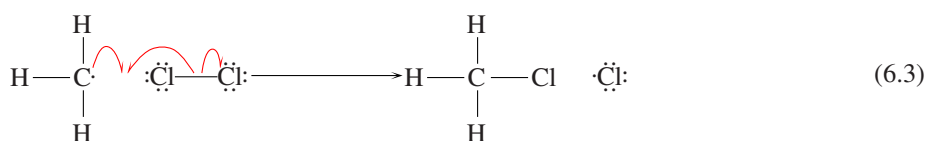\qquad (6.2)
$$

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}
```
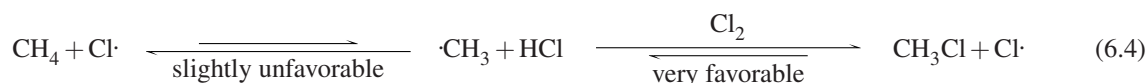
$$(6.3)$$

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}
```

$$(6.4)$$

Note that the steps are linked with right and left harpoons according to the first chemical convention described above (cf. Section 5.4).

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

```
¥def¥electronshiftArrowr{¥electronshiftAH{->}}
¥def¥electronshiftArrowl{¥electronshiftAH{<-}}
```
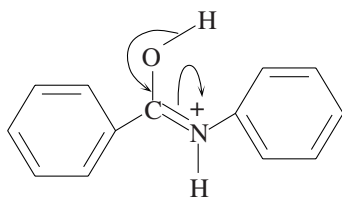
The usage of these commands is exemplified by the following formula:

```
¥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}
```

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