

chemmacros v1.0

2011/05/15

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‘chemmacros’ is a collection of macros and commands which are intended to make typesetting chemistry documents faster and more convenient. This includes some nomenclature commands, oxidation numbers, thermodynamic data, newman projections...

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1 Licence, Requirements

chemmacros v1.0 underlies the The L^AT_EX project public license (<http://www.latex-project.org/lppl.txt>).

chemmacros internally loads the packages ‘xkeyval’¹, ‘amsmath’² and ‘tikz’ (Ti \boldsymbol{k} Z = ‘pgf’³). If they’re missing it will cause an error.

The definition of some commands depends on which packages have been loaded *before* chemmacros was loaded. Some commands are only defined if a certain package has

¹<http://www.ctan.org/pkg/xkeyval>

²<http://www.ctan.org/pkg/amsmath>

³<http://www.ctan.org/pkg/pgf>

been loaded. This concern the packages ‘mhchem’⁴, ‘siunitx’⁵ and ‘chemstyle’⁶ and the commands from section 2, `\ox` (section 4.2), the commands from section 6 and the environments from section 7.

The package option `xspace` (section 10) needs the package ‘xspace’⁷ to be available.

If the user loads ‘mhchem’ *before* chemmacros, the packages ‘mathtools’⁸ and ‘environ’⁹ are needed.

The `\redox` command (section 5) and the `\newman` command (section 8) need the tikz library ‘calc’ to be loaded.

The full functionality should be guaranteed with a preamble like this:

```
1 \usepackage{siunitx,chemstyle}
2 \usepackage[version=3,arrows=pgf]{mhchem}
3 \usepackage[xspace=true]{chemmacros}
4 \usetikzlibrary{calc}
```

2 Particles, Ions and a Symbol

Some simple macros for displaying often needed particles and a symbol:

- `\Hp1` H^{\oplus} (proton)
- `\Hyd` OH^{\ominus} (hydroxide)
- `\Ht0` $\text{H}_3\text{O}^{\oplus}$ (oxonium)
- `\el` e^{\ominus} (electron)
- `\prt` p^{\oplus} (proton)
- `\ntr` n^0 (neutron)
- `\transitionstatesymbol` \neq transition state symbol (uses `TikZ`)

⁴<http://www.ctan.org/pkg/mhchem>

⁵<http://www.ctan.org/pkg/siunitx>

⁶<http://www.ctan.org/pkg/chemstyle>

⁷<http://www.ctan.org/pkg/xspace>

⁸<http://www.ctan.org/pkg/mathtools>

⁹<http://www.ctan.org/pkg/environ>

These commands are working both in text mode and math mode. Depending on whether ‘mhchem’ has been loaded, the first three particles are defined with the `\cf{}` command or with `\ensuremath{\text{}}`.

3 Stereo Descriptors, Nomenclature

The following macros are intended to make the writing of IUPAC names more convenient:

- Cahn-Ingold-Prelog:

- `\Rcip` (*R*)
- `\Scip` (*S*)
- `\cip{<conf>}` e. g.: `\cip{R,S}` (*R,S*)

- Fischer:

- `\Dfi` *D*
- `\Lfi` *L*





- cis/trans & zusammen/entgegen:

- `\Z` (*Z*)
- `\E` (*E*)
- `\cis` *cis*
- `\trans` *trans*

- ortho/meta/para:

- `\ortho` *o*
- `\meta` *m*
- `\para` *p*

absolute configuration (uses **TikZ**):

- `\Rconf[<letter>]` `\Rconf:`  `\Rconf[]:` 
 - `\Sconf[<letter>]` `\Sconf:`  `\Sconf[]:` 
- ```

1 \Dfi-Weinsäure = \cip{2S,3S}-Weinsäure, \Dfi-($-)-
 Threose = \cip{2S,3R}-($-)-2,3,4-Trihydroxybutanal\
2 \cis-2-Buten = \Z-2-Butene, \cip{2E,4Z}-Hexadiene\
3 \meta-Xylol = 1,3-Dimethylbenzene
4
5 % with 'bpchem' command \IUPAC:
6 \IUPAC{\Dfi-Wein\|säure} = \IUPAC{\cip{2S,3S}-Wein\|säure
 }, \IUPAC{\Dfi-($-)-Threose} = \IUPAC{\cip{2S,3R
 }-($-)-2,3,4-Tri\|hydroxy\|butanal}

```

D-Weinsäure = (2*S*,3*S*)-Weinsäure, D-(*-*)-Threose = (2*S*,3*R*)-(*-*)-2,3,4-Trihydroxybutanal  
*cis*-2-Buten = (*Z*)-2-Butene, (2*E*,4*Z*)-Hexadiene  
*m*-Xylol = 1,3-Dimethylbenzene

D-Weinsäure = (2*S*,3*S*)-Weinsäure, D-(*-*)-Threose = (2*S*,3*R*)-(*-*)-2,3,4-Trihydroxybutanal

The last example uses the `\IUPAC` command, which is provided by the 'bpchem'<sup>10</sup> package.

## 4 Oxidation Numbers and (real) Charges

### 4.1 Ion Charges

Simple displaying of charges:

- `\pch[<number>]` positive charge (**plus** + **charge**), `\pch`, `Na\pch`, `Ca\pch[2]` <sup>⊕</sup>, `Na⊕`, `Ca2⊕`
- `\mch[<number>]` negative charge (**minus** + **charge**), `\mch`, `F\mch`, `S\mch[2]` <sup>⊖</sup>, `F⊖`, `S2⊖`

<sup>10</sup><http://www.ctan.org/pkg/bpchem>

## 4.2 Oxidation Numbers

Typesetting oxidation numbers:

- `\ox{<number>,<atom>}` places <number> above <atom>; `\ox{+1,Na}`, `\ox{+I,Na}`,  
`\ox{-2,S}`, `\ox{-II,S}`  $\overset{+1}{\text{Na}}$ ,  $\overset{+I}{\text{Na}}$ ,  $\overset{-2}{\text{S}}$ ,  $\overset{-II}{\text{S}}$

If the package ‘mhchem’ has been loaded <atom> is set inside the `\ce` command: `\ox{+II,Ca}\ox{-I,F2}`  $\overset{+II}{\text{Ca}}\overset{-I}{\text{F}_2}$ . Without ‘mhchem’ this isn’t working this way ( $\overset{+II}{\text{Ca}}\overset{-I}{\text{F}2}$ ) and you need to use the math way: `\ox{+II,Ca}\ox{-I,F$_2$}`  $\overset{+II}{\text{Ca}}\overset{-I}{\text{F}_2}$ .

## 4.3 Partial Charges and similar Stuff

The next ones probably are seldomly needed but nevertheless useful:

- `\delp  $\delta^+$`  (`delta` + `plus`)
- `\delm  $\delta^-$`  (`delta` + `minus`)

These macros for example can be used with the `\ox` command or with the ‘chemfig’<sup>11</sup> package:

```
1 \ox{\delp,H}\ox{\delm,Cl}\par
2 \chemfig{\chemabove[3pt]{\lewis{246,Br}}{\delm}-\chemabove[3pt]{H}{\delp}}
```



Also the following macros are useful together with ‘chemfig’.

- `\scrip  $\oplus$`  (`scriptstyle` + `plus`)
- `\scrm  $\ominus$`  (`scriptstyle` + `minus`)

For example:

---

<sup>11</sup><http://www.ctan.org/pkg/chemfig>

```

1 {\setatomsep{1.8em}\chemfig{CH_3-CH_2-\chemabove{\lewis
 {026,0}}{\hspace{5mm}\scrm}}}

```



## 5 Redox Reactions

chemmacros provides two commands <sup>12</sup> to visualize the transfer of electrons in redox reactions. Both commands are using ‘TikZ’, the second also needs the tikz library ‘calc’, **which thus must be loaded in the preamble.**

```

1 \OX{<name>,<atom>}
2 \redox(<name1>,<name2>)[<tikz>][<dim>]{<text>}

```

\OX places <atom> into a node, which is named with <name>. If you have set two \OX, they can be connected with a line using \redox. To do so the names of the two nodes that shall be connected are written in the round braces. Since \redox draw a tikzpicture with options remember picture, overlay, the document needs to be *compiled at least two times*.

```

1 \OX{a,Na} \rightarrow \OX{b,Na}\pch\redox(a,b){
 oxidation}

```

$$\text{Na} \rightarrow \text{Na}^\oplus$$

This line can be customized using TikZ keys in <tikz>:

```

1 \OX{a,Na} \rightarrow \OX{b,Na}\pch\redox(a,b)[->,red]{
 ox}

```

$$\text{Na} \rightarrow \text{Na}^\oplus$$

<dim> can be used to adjust the length of the vertical line. The default value is .6em. If you use a negative value the line is placed *below* the text.

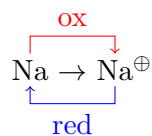
```

1 \begin{center}
2 \OX{a,Na} \rightarrow \OX{b,Na}\pch\redox(a,b)[->,red
]{ox}\redox(a,b)[<-,blue][-.6em]{red}
3 \end{center}

```

---

<sup>12</sup>Thanks to [Peter Cao](#) who suggested the feature.

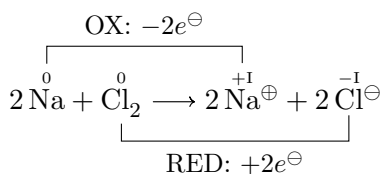
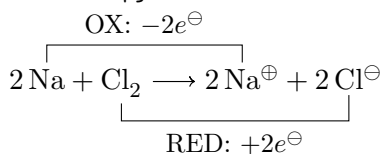


Both commands also can be used with the ‘mhchem’ command `\ce` and with the `\ox` command (section 4.2).

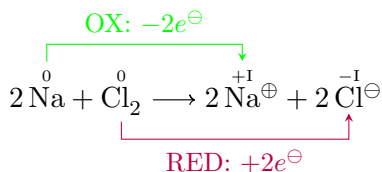
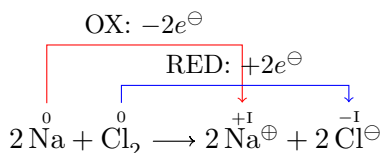
```

1 \ce{ 2 \OX{o1,Na} + \OX{r1,Cl2} -> 2 \OX{o2,Na}\pch + 2 \
 \OX{r2,Cl}\mch }
2 \redox(o1,o2){\small OX: $- 2\el$}
3 \redox(r1,r2)[][-.6em]{\small RED: $+ 2\el$}
4
5 \vskip2cm
6 \ce{ 2 \OX{o1,\ox{0,Na}} + \OX{r1,\ox{0,Cl2}} -> 2 \OX{o
 2,\ox{+I,Na}}\pch + 2 \OX{r2,\ox{-I,Cl}}\mch }
7 \redox(o1,o2){\small OX: $- 2\el$}
8 \redox(r1,r2)[][-.6em]{\small RED: $+ 2\el$}
9
10 \vskip3cm
11 \ce{ 2 \OX{o1,\ox{0,Na}} + \OX{r1,\ox{0,Cl2}} -> 2 \OX{o
 2,\ox{+I,Na}}\pch + 2 \OX{r2,\ox{-I,Cl}}\mch }
12 \redox(o1,o2)[draw=red,->][2em]{\small OX: $- 2\el$}
13 \redox(r1,r2)[draw=blue,->]{\small RED: $+ 2\el$}
14
15 \vskip1cm
16 \ce{ 2 \OX{o1,\ox{0,Na}} + \OX{r1,\ox{0,Cl2}} -> 2 \OX{o
 2,\ox{+I,Na}}\pch + 2 \OX{r2,\ox{-I,Cl}}\mch }
17 \redox(o1,o2)[green,-stealth]{\small OX: $- 2\el$}
18 \redox(r1,r2)[purple,-stealth][-.6em]{\small RED: $+ 2\el
 $}

```







## 6 (Standard) State, Thermodynamics

### 6.1 With ‘siunitx’

If the package ‘siunitx’ has been loaded, the following commands are available:

- `\Enthalpy[<kind>,<exponent>,<unit>]{<value>}`
- `\Entropy[<kind>,<exponent>,<unit>]{<value>}`
- `\Gibbs[<kind>,<exponent>,<unit>]{<value>}`

Their usage is pretty much self-explaining: `\Enthalpy{-123.4}` gives  $\Delta H^{\ominus} = -123.4 \text{ kJ mol}^{-1}$ .

If you want to specify what kind of enthalpy (reaction, formation,...) is meant Möchte you can use the first optional argument:

`\Enthalpy[r]{-123.4}`  $\Delta_r H^{\ominus} = -123.4 \text{ kJ mol}^{-1}$ .

The standard state symbol can be replaced by the second optional argument...

`\Enthalpy[,o]{-123.4}`  $\Delta H^{\circ} = -123.4 \text{ kJ mol}^{-1}$

...and is anyway only set as standard state if the package ‘chemstyle’ has been loaded, see section 6.2.

The third optional argument can be used to change the unit:

`\Enthalpy[,kcal/mol]{-123.4}`  $\Delta H^{\ominus} = -123.4 \text{ kcal/mol}$

The unit is set corresponding to the rules of ‘siunitx’ and depends on its settings:

```

1 \Enthalpy{-1234.56e3}\par
2 \sisetup{per-mode=symbol,exponent-product=\cdot,output-
 decimal-marker={,},group-four-digits=true}
3 \Enthalpy{-1234.56e3}

```

$$\Delta H^{\ominus} = -1234.56 \times 10^3 \text{ kJ mol}^{-1}$$

$$\Delta H^{\ominus} = -1\,234,56 \cdot 10^3 \text{ kJ/mol}$$

The other two commands work exactly the same way.

```
1 \Entropy{12.3}, \Gibbs{-12.3}.
```

$$S^\ominus = 12.3 \text{ J K}^{-1} \text{ mol}^{-1}, \Delta G^\ominus = -12.3 \text{ kJ mol}^{-1}.$$

You can use the command `\setnewstate[<standard exponent>,<Delta symbol>]{<name>}{<symbol>}{<unit>}` to create new corresponding commands:

```
1 \setnewstate{Helmholtz}{A}{\kilo\joule\per\mole}
2 \setnewstate{ElPot}{E}{Volt}
3 \Helmholtz{123.4} \ElPot{-1.1}
```

$$\Delta A^\ominus = 123.4 \text{ kJ mol}^{-1} \quad \Delta E^\ominus = -1.1 \text{ Volt}$$

Indeed, the commands

```
1 \Enthalpy, \Entropy, \Gibbs
```

are defined as follows:

```
1 \setnewstate{Enthalpy}{H}{\kilo\joule\per\mole}
2 \setnewstate[,]{Entropy}{S}{\joule\per\kelvin\per\mole}
3 \setnewstate{Gibbs}{G}{\kilo\joule\per\mole}
```

With `\setnewstate` you also can redefine the existing commands:

```
1 \setnewstate{Enthalpy}{X}{\joule\per\mole}
2 \Enthalpy[f]{12.5}
```

$$\Delta_f X^\ominus = 12.5 \text{ J mol}^{-1}$$

## 6.2 State

The commands presented in section 6.1 internally all use the command

```
1 \State[<exponent>,<Delta symbol>]{<symbol>}{<kind>}
```

which also is available without ‘siunitx’. It can be used to write the thermodynamic variables without value and unit.

```
1 \State{G}{f}, \State[]{E}{}, \State[\SI{1000}{\celsius}
]{H}{f}, \State[,\delta]{+}{}
```

$\Delta_f G^\ominus$ ,  $\Delta E$ ,  $\Delta_f H^{1000^\circ\text{C}}$ ,  $\delta+$

The standard state symbol  $\ominus$  is only used, if the ‘chemstyle’ package has been loaded, which provides it through the command `\standardstate`. With ‘chemstyle’: `\State{A}{b}`  $\Delta_b A^\ominus$ , without:  $\Delta_b A$ .

## 7 Environments for ‘mhchem’

If the package ‘mhchem’ has been loaded the environments

```
1 \begin{reaction}
2 <mhchem code>
3 \end{reaction}
4 \begin{reactions}
5 <mhchem code>
6 \end{reactions}
```

and the starred versions

```
1 \begin{reaction*}
2 <mhchem code>
3 \end{reaction*}
4 \begin{reactions*}
5 <mhchem code>
6 \end{reactions*}
```

are defined. `reaction/reaction*` uses the math environment `equation/equation*` and `reactions/reactions*` uses the math environment `align/align*` to display the reactions.

```
1 reaction with counter:
2 \begin{reaction}
3 H2 + 1/2 O2 -> H2O
4 \end{reaction}
5 reaction without counter:
6 \begin{reaction*}
7 C + O2 -> CO2
8 \end{reaction*}
9 several aligned reactions with counter:
10 \begin{reactions}
11 Cl2 &-> 2 Cl. \\
12 Cl.{ } + CH4 &-> HCl + { }.CH3\\
```

```

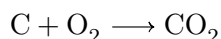
13 {}{} .CH3 + Cl2 &-> CH3Cl + Cl.
14 \end{reactions}
15 several aligned reactions without counter:
16 \begin{reactions*}
17 \Hpl + \Hyd &=> H2O\\
18 SO4 \mch[2] + Ba \pch[2] &-> BaSO4 v
19 \end{reactions*}

```

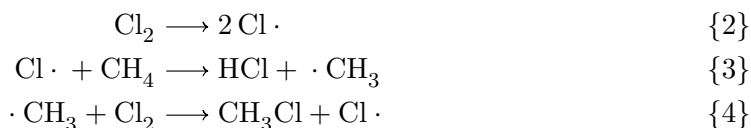
reaction with counter:



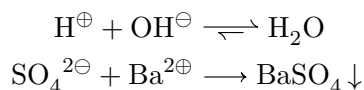
reaction without counter:



several aligned reactions with counter:



several aligned reactions without counter:



If you want to change the layout of the counter tags, you can use `\renewtagform{<tagname>}[<format>]{<right delim>}{<left delim>}`<sup>13</sup>.

```

1 \renewtagform{CMreaction}[R \textbf]{[]{}
2 \begin{reaction}
3 H2O + CO2 <=> H2CO3
4 \end{reaction}

```



## 8 Newman Projections

The command

```

1 \newman[<angle>,<scale>,<tikz>]{<1>,<2>,<3>,<4>,<5>,<6>}

```

---

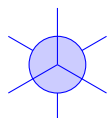
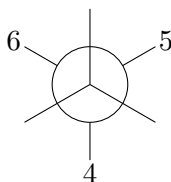
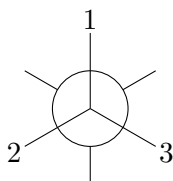
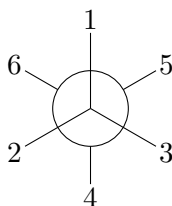
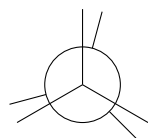
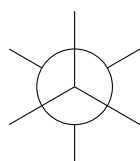
<sup>13</sup>provided by the package ‘mathtools’

allows you to create newman projections (uses *TikZ*). You need to load the *tikz* library ‘calc’ for that:

```
1 \usetikzlibrary{calc}
```

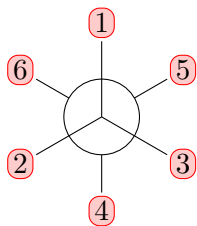
Examples:

```
1 \newman{}\par% default: staggered
2 \newman[165]{}\par% rotated by 165 degrees => eclipsed
3 \newman{1,2,3,4,5,6} \newman{1,2,3} \newman{,,4,5,6}\par
% with atoms
4 \newman[,.75,draw=blue,fill=blue!20]{}% scaled and
customized with TikZ
```



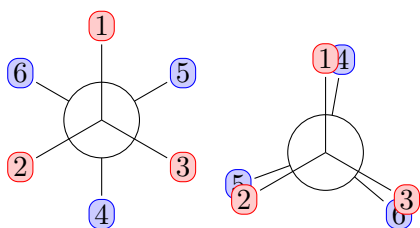
Another option allows you to customize the nodes within which the atoms are placed:

```
1 \newman[[][<tikz nodes>]{<1>,<2>,<3>,<4>,<5>,<6>}
2 % example:
3 \newman[[][draw=red,fill=red!20,inner sep=2pt,rounded
corners]{1,2,3,4,5,6}
```



If you want to display the "frontatoms differently from the "backatoms, you can use a third option:


```
1 \newman[<tikz front nodes>][<tikz back nodes>]{<1>,<2>,<3>,<4>,<5>,<6>}
2 % example:
3 \newman[draw=red,fill=red!20,inner sep=2pt,rounded corners][draw=blue,fill=blue!20,inner sep=2pt,rounded corners]{1,2,3,4,5,6} \newman[170][draw=red,fill=red!20,inner sep=2pt,rounded corners][draw=blue,fill=blue!20,inner sep=2pt,rounded corners]{1,2,3,4,5,6}
```




## 9 p-Orbitals

chemmacros provides commands to visualize p-orbitals.

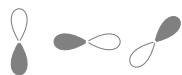
```
1 \porb[<size factor>,<color>,<angle>]
2 \phorb[<size factor>,<color>,<angle>]
3 \setorbheight{<length>}
```

This displays a horizontal orbital or one rotated by <angle>: `\porb \quad \porb [,,30]` 

`\phorb` only displays one half orbital: `\phorb[,red,90]` 

There are shortcuts for the *x*-, *y*- and *z*-orbitals:

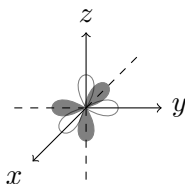
```
1 \pzorb \quad \pyorb \quad \pxorb
```



With suitable shifting you can display them all on one spot:

```

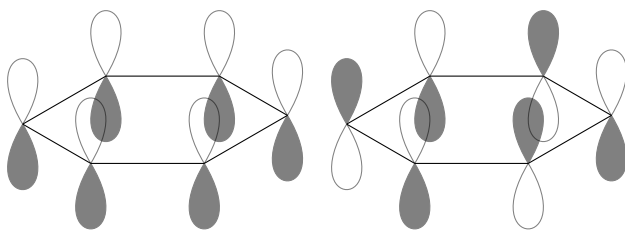
1 \hspace{2cm}\pxorb\hspace{-.3em}\pyorb\hspace{-.3em}\
 pzorb
2 \tikz[overlay]{
3 \draw[>](0,0)--(1,0)node[right]{y};
4 \draw[dashed](0,0)--(-1,0);
5 \draw[>](0,0)--(0,1)node[above]{z};
6 \draw[dashed](0,0)--(0,-1);
7 \draw[>](0,0)--(-.707,-.707)node[below left]{x};
8 \draw[dashed](0,0)--(.707,.707);
9 }
```



The orbitals also can be used together with ‘chemfig’:

```

1 \setorbheight{2em}\setbondoffset{0pt}
2 \chemfig{?\pzorb-[1.3]\pzorb-[:30,1.1]\pzorb-[:150,.9]\
 pzorb-[4,1.3]\pzorb-[: -150,1.1]\pzorb?}\quad
3 \chemfig{?\pzorb-[1.3]{\porb[,,-90]}-[:30,1.1]\pzorb
 -[:150,.9]{\porb[,,-90]}-[4,1.3]\pzorb-[: -150,1.1]{\
 porb[,,-90]}?}
```



## 10 Package Options

chemmacros has two package options:

- `xspace=<boolean>` With the option `xspace=true` the commands `\Hyd`, `\HtO` Text `\Hyd`, `\HtO`, Text  $\text{OH}^\ominus$   $\text{H}_3\text{O}^\oplus$  Text  $\text{OH}^\ominus$ ,  $\text{H}_3\text{O}^\oplus$ , Text

get a `\xspace`.  
 Default: `xspace=false`

- `circled=<boolean>` not everybody likes circled charge symbols ( $\oplus$  and  $\ominus$ ). Some prefer them without circles (+ and -). This can be chosen this option. With `circled=false` all chemmacros commands are set without circles.  
 Default: `circled=true`

## 11 List of Commands

|                                                                                                                                                                                                                                                                                                   |                                                 |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| <code>\el</code> , <code>\prt</code> , <code>\ntr</code><br><code>\HtO</code> , <code>\Hpl</code> , <code>\Hyd</code><br><code>\transitionstatesymbol</code>                                                                                                                                      | section 2: Particles, Ions and a Symbol         |
| <code>\cip</code> , <code>\Rcip</code> , <code>\Scip</code><br><code>\Dfi</code> , <code>\Lfi</code><br><code>\E</code> , <code>\Z</code> , <code>\cis</code> , <code>\trans</code><br><code>\Rconf</code> , <code>\Sconf</code><br><code>\ortho</code> , <code>\meta</code> , <code>\para</code> | section 3: Stereo Descriptors, Nomenclature     |
| <code>\delm</code> , <code>\delp</code><br><br><code>\mch</code> , <code>\pch</code><br><code>\ox</code><br><code>\scrm</code> , <code>\scrip</code>                                                                                                                                              | section 4: Oxidation Numbers and (real) Charges |
| <code>\Enthalpy</code> , <code>\Entropy</code> , <code>\Gibbs</code><br><code>\setnewstate</code><br><code>\State</code>                                                                                                                                                                          | section 6: (Standard) State, Thermodynamics     |
| <code>\newman</code>                                                                                                                                                                                                                                                                              | section 8: Newman Projections                   |
| <code>\redox</code> , <code>\OX</code>                                                                                                                                                                                                                                                            | section 5: Redox Reactions                      |
| <code>\begin{reaction}</code> ,<br><code>\begin{reaction*}</code> ,<br><code>\begin{reactions}</code> ,<br><code>\begin{reactions*}</code>                                                                                                                                                        | section 7: Environments for ‘mhchem’            |
| <code>\phorb</code> , <code>\porb</code> , <code>\pxorb</code> ,<br><code>\pyorb</code> , <code>\pzorb</code><br><code>\setorbheight</code>                                                                                                                                                       | section 9: p-Orbitals                           |