1 Introduction

This package has been written to alleviate the task of writing publications containing lots of chemistry. It provides methods for typesetting chemical names, sum formulae and isotopes. It provides the possibility to break very long names even over several lines.

This package also provides a way to automatically enumerate your chemical compounds, allowing for one-level subgrouping.

What this package does not provide: Methods to draw chemical compounds. Although there exist some packages, which were designed for this purpose (e.g. xymtex, PPChTex) they are quite limited once you get to complex organic, or metal organic compounds. I recommend using an external drawing program, possibly in conjunction with psfrag, in these cases.

2 Package options

Currently this package supports only one option:

\texttt{cbgreek}

this option causes the definitions of some macros to be changed to use the cbgreek fonts. As they are not available on all systems, and only in mf format, the default is to use the math fonts for greek symbols.

3 User commands in this package

3.1 Setting chemical sum formulae: \texttt{BPChem<chemical formula>}

\texttt{\textbackslash BPChem} Within this macro you can use \_ and \^ for correct chemical sub- and superscripts. Example:

\begin{verbatim}
\end{verbatim}
\BPChem{C\_2H\_5OH} or \BPChem{SO\_4\^{2-}}

C\textsubscript{2}H\textsubscript{5}OH or SO\textsubscript{4}\textsuperscript{2-}

3.2 Setting long chemical names: IUPAC<formula or name>

\textbf{IUPAC} in addition to sub/superscripts as above, \- is a hyphen which allows further breakpoints, \| is an (invisible) Multibreakpoint.

This environment is especially useful for your long IUPAC-compound names.

Example:

\%\textbf{IUPAC}\{Tetra\|cyclo[2.2.2.1\^{1,4}]\-un\|decane-2\|-dodecyl-5\|(hepta\|decyl\|iso\|dodecyl\|thio\|ester)}

Tetracyclo[2.2.2.1\^{1,4}]-undecane-2-dodecyl-5-(heptadecylisododecyl-thioester)

3.3 Enumerating and referencing chemical compounds: CN-label{<label>}, CNlabelnoref{<label>}, CNref{<label>}

CNlabel defines and use \#1 (via ref) as label for numbering of chemical compounds. If the label has not yet been defined, it is created, otherwise it is just referenced. If you just want to define the label, use CNlabelnoref instead.

If you want to get just the reference, use CNref. This comes handy for figure captions or section titles, as you would get disorder in the numbering due to the moving argument otherwise.

The default style is: \textbf{\textit{\arabic{\counter}}}.

To change, use something like

\renewcommand{\theBPCno}{\textbf{\textit{\arabic{BPCno}}}.

Example:

Alkohol \textbf{CNlabel}{al} is converted to aldehyd \textbf{CNlabel}{ad}. \textbf{CNref}{al} can also be used otherwise, while \textbf{CNref}{ad} cannot.

Alkohol 1 is converted to aldehyd 2. 1 can also be used otherwise, while 2 cannot.

3.4 Using sub-labels for classes of compounds: CNlabel-sub{<label>}{<sublabel>}, CNlabelsubnoref{<label>}{<sublabel>}, CNrefsub{<label>}{<sublabel>}

These commands are the same as above, with additional sub identifier \#2 added. If the primary identifier is not yet used, it will be created and can also be referenced via the normal commands.

The default style is: \textbf{\textit{\arabic{BPCno}\alph{BPCnoa}}}.
To change, use something like
\renewcommand{\theBPCnoa}{\textbf{\arabic{BPCno}\alph{BPCnoa}}}  

To demonstrate the use of sublabels, methanol \CNlabels{alk}{a} and ethanol \CNlabels{alk}{b} are both natural products. The alcohols \CNrefs{alk} can synthesized bio-chemically. \CNrefs{alk}{a} is toxic, while \CNrefs{alk}{b} is only mildly toxic.

To demonstrate the use of sublabels, methanol 3\text{a} and ethanol 3\text{b} are both natural products. The alcohols 3 can synthesized bio-chemically. 3\text{a} is toxic, while 3\text{b} is only mildly toxic.

3.5 Shortcuts for common idioms in chemical literature

1\textsuperscript{H}-NMR: $\delta$  \\HNMR
13\textsuperscript{C}-NMR: $\delta$  \\CNMR
cis \cis
trans \trans
$\alpha$  \\bpalpha
$\beta$  \\bpbeta
$\Delta$  \\bpdelta
$\eta$ \<num> \\hapto{<number>}

Note: Some of these macros are influenced by the \texttt{cbgreek} option! Use is only recommended with the \BPChem and \IUPAC commands. Some will not even work outside those commands.

4 Example

\begin{minipage}{15em}
some normal text and math: $A*B=B$
Test \BPChem{ C\textsubscript{2}H\textsubscript{4}\textsuperscript{+}}
or using math in superscript  \BPChem{ C\textsubscript{2}H\textsubscript{4}\textsuperscript{$+$}}
\BPChem{Example\textsubscript{longer subscript}\textsuperscript{superscript}}
Isotope: \BPChem{\textsubscript{A}\textsuperscript{B}X\textsuperscript{C}\textsubscript{D}}
\IUPAC{Tetra\textmidcyclo[2.2.2.1]\textsuperscript{1,4}\textmid-A
un\textmiddecane-2\textmid-dodecyl-5\textmidheptadecyl\textmidiso\textmiddodecyl\textmidthio\textmidester}}
\end{minipage}
and the resulting output:

some normal text and math: \( A \ast 2 = B \), just to show it.
Test \( \text{C}_2\text{H}_4 \) or using math in superscript \( \text{C}_2\text{H}_4 \)
Example

Isotope: \( \text{H}_{2}\text{A}\text{C} \)

Tetracyclo\( [2.2.2.1^14]\)-undecane-2-dodecyl-5-(heptadecylisododecyl-thioester)

\section{The code}

\texttt{\textsubscript} Define a textsubscript corresponing to textsuperscript. This is now also available as the package textsubscript by D.Arsenau or as part of KOMA-Script2 by M. Kohm.

\texttt{\providecommand\textsubscript\[1\]{\@textsubscript{\selectfont#1}}} a register to save the length to backspace two registers needed to get back to correct working position if one is longer than the other.

\texttt{\newlength{\BPClensub}} \texttt{\newlength{\BPClensuper}} \texttt{\newlength{\BPCdelta}} we are in subscript and maybe the superscript was longer

\texttt{\DeclareRobustCommand{\BPCadjustsub}{\setlength\BPCdelta{\BPClensuper}\addtolength\BPCdelta{-\BPClensub}\ifdim\BPCdelta>0pt{\kern\BPCdelta}\else\relax\fi\setlength{\BPClensub}{0pt}\setlength{\BPClensuper}{0pt}}} we are in superscript and maybe the subscript was longer

\texttt{\DeclareRobustCommand{\BPCadjustsuper}{\setlength\BPCdelta{\BPClensub}\addtolength\BPCdelta{-\BPClensuper}\ifdim\BPCdelta>0pt{\kern\BPCdelta}\else\relax\fi\setlength{\BPClensub}{0pt}\setlength{\BPClensuper}{0pt}}}
make a subscript and remember length in BPClen

\DeclareRobustCommand\BPCsub[1]{% 
  \ifmmode_{#1}\settowidth\BPClensub{_{#1}}\else\textsubscript{#1}\settowidth\BPClensub{\textsubscript{#1}}\fi% 
  \futurelet\next\lookforsuper%
}

make a superscript and remember length in BPClen raise by 0.15 em, else e.g. + collides with subscript

\DeclareRobustCommand\BPCsuper[1]{% 
  \ifmmode^{#1}\settowidth\BPClensuper{^{#1}}\else\raisebox{0.15em}{\textsuperscript{#1}}\settowidth\BPClensuper{\textsuperscript{#1}}\fi% 
  \futurelet\next\lookforsub%
}

see if next token is BPCsuper,

\DeclareRobustCommand\lookforsuper{% 
  \ifx\next\BPCsuper\let\next=\BPCsuperbs% 
  \else\let\next=\BPCadjustsuper\fi\next%
}

see if next token is BPCsub

\DeclareRobustCommand\lookforsub{% 
  \ifx\next\BPCsub\let\next=\BPCsubbs% 
  \else\let\next=\BPCadjustsub\fi\next%
}

backspace BPClen and make superscript eats the old ^

\DeclareRobustCommand\BPCsuperbs[1]{\kern-\BPClensub\BPCsuper}%

backspace and make subscript eats the old _

\DeclareRobustCommand\BPCsubbs[1]{\kern-\BPClensuper\BPCsub}%

needed to get catcodes right

\DeclareRobustCommand\DoBPChem{}{}
\def\DoBPChem#1{% 
  #1\endgroup%
}

\DeclareRobustCommand\BPCSetupCat{}{}
\def\BPCSetupCat{% 
  \catcode`^=\active% 
  \catcode`_=\active% 
  \BPCSetup%
}

\DeclareRobustCommand\BPCSsetup{}{}
\def\BPCSsetup{% 
  \let\_=\BPCsub%
  \let^=\BPCsuper%
  \end BPCSsetup
}
setup for chemical formula

\let\-=\BreakHyph%
\let\|\=\MultiBreak%
\DoIUPAC%
\let\-=\BreakHyph%
\|\=\MultiBreak%
\Prep%
\IUPAC%
\expandafter\expandafter\expandafter\|

Trick by David Kastrup <David.Kastrup@t-online.de> to make non-fragile. Otherwise \| would become \delimiter"026B30D in e.g. the toc Recent \LaTeX releases (starting with <2017-04-15>) define \- robust. This resulted in an infinite loop with older version of bpchem. We could use \IncludeInRelease, but it might be easier to just use the definition from the latest \LaTeX releases.

\let\-=\BreakHyph%
\let\|\=\MultiBreak%
\DoIUPAC%
\Prep%
\IUPAC%
\expandafter\expandafter\expandafter\|

counters for numbering of chemical substances

\newcounter{BPCno}
\renewcommand{\theBPCno}{\textbf{\arabic{BPCno}}}
\newcounter{BPCnoa}[BPCno]
\renewcommand{\theBPCnoa}{\textbf{\arabic{BPCno}\alph{BPCnoa}}}
\renewcommand{\theBPCno}{\arabic{BPCno}}
\renewcommand{\theBPCnoa}{\arabic{BPCnoa}}
\renewcommand{\arabic{BPCno}}{\textbf{\arabic{BPCno}}}
\renewcommand{\arabic{BPCnoa}}{\textbf{\arabic{BPCnoa}}
}\alph{BPCnoa}}
helper functions to mark first definition

\newcommand{\newchems@b}[2]{
\expandafter\gdef\csname cna@#1#2\endcsname{#2}%
}

reference a CNlabel (useful for section titles, captions etc.)

\DeclareRobustCommand*{\CNref}[1]{%
\ref{cn:#1}%
}

reference a CNlabel/sublabel

\DeclareRobustCommand*{\CNrefsub}[2]{%
\ref{cn:#1#2}%
%%\textbf{\csname cna@#1#2\endcsname}%%
}

label a substance and insert the number

\DeclareRobustCommand*{\CNlabel}[1]{%
\CNlabelnoref{#1}\
\CNref{#1}%
}

\DeclareRobustCommand*{\CNlabelnoref}[1]{%
\expandafter\ifx\csname cnd@#1\endcsname\relax%
{\refstepcounter{BPCno}\label{cn:#1}}%
\expandafter\gdef\csname cnd@#1\endcsname{x}%
\fi%
%
}

\DeclareRobustCommand*{\CNlabelsub}[2]{%
\CNlabelsubnoref{#1}{#2}\
\CNrefsub{#1}{#2}%
}

\DeclareRobustCommand*{\CNlabelsubnoref}[2]{%
\CNlabelnoref{#1}\
\expandafter\ifx\csname cna@#1#2\endcsname\relax%
{\refstepcounter{BPCnoa}\label{cn:#1#2}}%
\expandafter\gdef\csname cna@#1#2\endcsname{x}%% \newchems@b{#1}{#2}%% \write\@auxout{\string\newchems@b{#1}{#2}}%
\fi%
%
}

more helper mcors special symbols and macros for math-symbols without math-mode

\DeclareRobustCommand{\HNMR}{\textit{^{1}H-NMR}: $\delta$\xspace}
\DeclareRobustCommand{\CNMR}{\textit{^{13}C-NMR}: $\delta$\xspace}
\DeclareRobustCommand{\cis}{\textit{cis}\xspace}
\DeclareRobustCommand{\trans}{\textit{trans}\xspace}
\DeclareRobustCommand{\R}{\textit{R}}
\DeclareRobustCommand{\S}{\textit{S}}

%%%%%%%%%%%%%%%%%%%%%
\input{lgrenc.def}
\DeclareRobustCommand{\rm@greekletter}{\textfont1%\selectfont%
def\encodingdefault{LGR}#1}
% some examples
\DeclareRobustCommand{\bpalpha}{\rm@greekletter{a}}
\DeclareRobustCommand{\bpbeta}{\rm@greekletter{b}}
\DeclareRobustCommand{\bpDelta}{\rm@greekletter{D}}
\DeclareRobustCommand{\hapto}{\rm@greekletter{h}^{#1}}
% code with standard math greek
\PackageInfo{bpchem}{using default math greek fonts}
\DeclareRobustCommand{\bpalpha}{\ensuremath{\alpha}\xspace}
\DeclareRobustCommand{\bpbeta}{\ensuremath{\beta}\xspace}
\DeclareRobustCommand{\bpDelta}{\ensuremath{\Delta}\xspace}
\DeclareRobustCommand{\hapto}{\ensuremath{\eta^{#1}}}
\\}
\let\talpha\bpalpha
\let\tbeta\bpbeta
%%%%%%
\DeclareRobustCommand*{\dreh}{\lbrack \alpha \rbrack _{\mathrm D}^{#1}}
</bpchem>

Change History

v1.03
General: fixed bug in \IUPAC. \| is not getting translated to \delimiter during \write anymore ..................... 6
re-added lost email-address ... 1
added cbgreek option for using upright greek and fixed namespace, old names will still work .................. 7
v1.04
General: also \- was affected, fixed 6
v1.05
General: changed email ........ 1

\begin{quote}
\begin{itemize}
\item fixed whitespace bug in \DoIUPAC \dotso\dotso 6
\item General: fixed whitespace bug in CNlabel \dotso\dotso 7
\item General: Recent \LaTeX releases make \- robust as well. This results in an infinite loop. \dotso 6
\item Resolved conflict with recent \LaTeX releases (thanks to Ulrike Fischer and Martin Sievers) \dotso\dotso 1
\end{itemize}
\end{quote}