SUBSTANCES

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A Chemical Database

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English documentation

The SUBSTANCES package allows you to create a database like file that contains data of various chemicals. These data can be retrieved in the document and an index of the chemicals used in the document can be created.

Contents

1 Licence and Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the LaTeX Project Public License, version 1.3 or later (http://www.latex-project.org/lppl.txt). The package has the status "maintained."

SUBSTANCES loads and needs the following packages: expl3,[1] xparse,[2] xtemplate[3] and l3keys2e.[4] It also needs the chemistry package chemmacros.[5]

[1] CTAN: expl3 [2] CTAN: xparse [3] CTAN: xtemplate [4] CTAN: l3keys2e [5] CTAN: chemmacros

2 About

The SUBSTANCES package allows you to create a database like file that contains data of various chemicals. These data can be retrieved in the document and an index of the chemicals used in the document can be created.

3 Options

SUBSTANCES has only a few options:

▸ `draft = true|false` Default: `false`
If set to true all warnings will be errors.

▸ `final = true|false` Default: `true`
The opposite of `draft`.

▸ `index = true|false` Default: `false`
Add index entries when `\chem` is called, see section 6.

▸ `style = <style>` Default: `default`
Load specific style, see section 4.3.

▸ `strict = true|false` Default: `false`
If set to true all warnings will be errors. This option overwrites any `draft` or `final` option that is passed on by the document class.

4 The Database

4.1 Declaring the Chemicals

The data about substances are stored via the command

▸ `\DeclareSubstance{<id>}{<list of properties>}`

An entry could look like this:

```
\DeclareSubstance{NaCl}{
  name    = Sodiumchloride ,
  sum     = NaCl ,
  CAS     = 7647-14-5,
  mass    = 58.44 ,
  mp      = 801 ,
  bp      = 1465 ,
  phase   = solid ,
  density = 2.17
}
```

Such entries can either be declared in the document preamble or probably more useful in a file with the ending `.sub`. Such a file can be input in the document via

▸ `\LoadSubstances{<filename>}` ⟶ input the file *without* specifying the file ending.

Suppose you have the file `mysubstances.sub` then you input it in the document preamble via `\LoadSubstances{mysubstances}`.

4.2 Available Fields

4.2.1 Always Defined Fields

Below all fields defined by SUBSTANCES are listed.[6]

▸ `name` required
The IUPAC name of the substance. This is the only field that *has* to be used. The field's input is parsed with chemmacros' command `\iupac`.

▸ `alt` optional
An alternative name. The field's input is parsed with chemmacros' command `\iupac`.

▸ `CAS` optional
The Chemical Abstract Service (CAS) number. The input needs to be input in the form `<num>-<num>-<num>`.

▸ `PubChem` optional
The PubChem number.

4.2.2 Style-dependend Fields

SUBSTANCES defines the style 'default' which is loaded if no other style has been specified. It defines the following additional fields and loads the packages chemfig[7] and siunitx.[8]

▸ `formula` optional
The molecular formula of the substance. The field's input is parsed with chemmacros' command `\ch`.

▸ `structure` optional
The structural formula of the substance. The field's input is parsed with chemfig's command `\chemfig`.

▸ `mp` optional
The boiling point. The field's entry is input into the siunitx command `\SI` in the following way: `\SI{<field>}{\celsius}`.

[6] Look in the file `substances-examples.sub` which is part of this package and should be in the same place as this documentation for example uses. [7] CTAN: chemfig [8] CTAN: siunitx

▸ bp optional
The melting point. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\celsius}.

▸ density optional
The density. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\gram\per\cmc}.

▸ phase optional
The state of aggregation.

▸ pKa optional
The pK_A value. The field's entry is input into the siunitx command \num.

▸ pKa1 optional
The first of several pK_A values. The field's entry is input into the siunitx command \num.

▸ pKa2 optional
The second of several pK_A values. The field's entry is input into the siunitx command \num.

▸ pKb optional
The pK_B values. The field's entry is input into the siunitx command \num.

▸ pKb1 optional
The first of several pK_B values. The field's entry is input into the siunitx command \num.

▸ pKb2 optional
The second of several pK_B values. The field's entry is input into the siunitx command \num.

▸ pictograms optional
The GHS pictograms. This field takes a list of pictogram names as they're input into chemmacros' command \ghspic.

▸ H optional
The H statements. This field takes a list of numbers as they're input into chemmacros' command \ghs{h}{<number>}.

▸ P optional
The P statements. This field takes a list of pictogram names as they're input into chemmacros' command \ghs{p}{<number>}.

▸ EUH optional
The EUH statements. This field takes a list of pictogram names as they're input into chemmacros' command \ghs{h}{<number>}.

▸ LD50 optional
The Median Lethal Dose (LD50) in mg kg^{-1}. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\milli\gram\per\kilo\gram}.

4.3 Define Custom Styles

4.3.1 Background

You might have other needs for fields than the ones defined by SUBSTANCES and the 'default' style. You can easily define your own style which means that you save a file with the name `substances_<style>.def`. In it you save the commands you need and use the command `\DeclareSubstanceProperty`, which is explained in the next section, to declare your own fields.

Please beware that this style file is loaded by the package when the `expl3` namespace is active. This means that all spaces are ignored and you need to use `~` if you need a space. It also means that `_` and `:` are letters (as is `@`). Should you ever decide to call `\ExplSyntaxOff` to turn off the `expl3` namespace *don't* forget to use `\ExplSyntaxOn` at the end of the file!

4.3.2 Declare New Fields or Change Existing Fields

You might want other fields or change the definition of the predefined ones. For this there's

▸ `\DeclareSubstanceProperty*{<field name>}[<pre code>][<post code>]`

This command declares a new property field for a substance. The star makes the property a required one which means an error will be issued if a substance is declared without it. The optional arguments `<pre code>` and `<post code>` specify any code that should be input directly before or after the field entry, respectively. The `<pre code>` may end with a command that takes one mandatory argument. In this case the field entry will be its argument.

The following example would define a field `EC` which uses a custom command to parse the field entry. The European Commission Number (EC) is assigned to chemical substances for regulatory purposes within the European Union by the regulatory authorities.

```
\makeatletter
\def\@EC#1-#2-#3{#1-#2-#3}
\newcommand*\EC[1]{\@EC#1}
\makeatother
\DeclareSubstanceProperty{EC}[\EC]
```

For further examples of the usage of pre and post code look at the definition of the `name` and the `mp` field:

```
\DeclareSubstanceProperty*{name}[\iupac]
\DeclareSubstanceProperty{mp}[\SI][{\celsius}]
```

5 Retrieving the Data

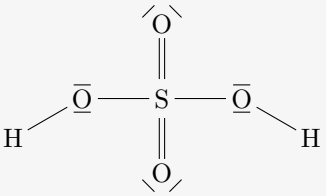
There are two commands defined by SUBSTANCES that allow the retrieving of the data. The command `\chem` is intended as user command, the command `\GetSubstanceProperty` can be used to define your own user command (perhaps in your own style file, see section 4.3).

- `\chem*[<pre>][<post>]{<id>}[<property>]`
- `\GetSubstanceProperty{<id>}{<property>}`

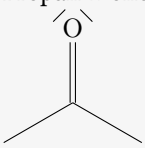
If the command `\chem` is called without the `[<property>]` argument the `name` entry will be called. The starred version calls the `alt` entry if it is defined and the `name` entry otherwise. The arguments `[<pre>]` and `[<post>]` add arbitrary input before or after the output, respectively.

All of the next examples use the data defined in the file `substances-examples.sub` that is part of this package, see section 7.

```
\chem{H2SO4}[structure] \newline
\chem{H2SO4} has the boiling point \(\chem[T_b =]{H2SO4}[bp]\) and a
density of \(\chem[\rho =]{H2SO4}[density]\).

Compare the melting points of methane and ethane,
\(\chem[T_m=]{methane}[mp]\) and \(\chem[T_m=]{ethane}[mp]\),
with the boiling points \(\chem[T_b=]{methane}[bp]\) and
\(\chem[T_b=]{ethane}[bp]\).

\chem{NaCl} has the \ac{CAS} number \chem{NaCl}[CAS].

\chem{acetone} (\chem*{acetone}) is the most simple ketone:

\chem{acetone}[structure]
```



Sulfuric Acid has the boiling point $T_b = 279.6\,°C$ and a density of $\rho = 1.8356\,g\,cm^{-3}$.
Compare the melting points of methane and ethane, $T_m = -182\,°C$ and $T_m = -183\,°C$, with the boiling points $T_b = -162\,°C$ and $T_b = -89\,°C$.
Sodiumchloride has the CAS number 7647-14-5.
Propan-2-one (Acetone) is the most simple ketone:



The following code creates table 1.

```
\begin{table}[htp]
\centering\chemsetup[ghsystem]{hide}
\sisetup{scientific-notation=fixed,fixed-exponent=0,per-mode=
  symbol}
\begin{tabular}{l>{\raggedright\arraybackslash}p{.6\linewidth}}
 \toprule
  name               & \chem{methane} \\
  formula            & \chem{methane}[formula] \\
                     & \chem{methane}[structure] \\
 \midrule
  CAS                & \chem{methane}[CAS] \\
  PubChem            & \chem{methane}[PubChem] \\
 \midrule
  boiling point      & \chem{methane}[bp] \\
  melting point      & \chem{methane}[mp] \\
  density            & \chem{methane}[density] \\
  molar mass         & \chem{methane}[mass] \\
 \midrule
                     & \chem{methane}[pictograms] \\
  H statements       & \chem{methane}[H] \\
  P statements       & \chem{methane}[P] \\
 \bottomrule
\end{tabular}
\caption{\label{tab:methane}All properties of \chem{methane} that
  have been
saved in the example database.}
\end{table}
```

6 Create an Index

7 The Example Database

The following code shows the example database that is part of this package.

```
% ------------------------------------------------------------------------
% substances-examples.sub
% example database to the package ‘substances’
%
% Clemens Niederberger
% 2012/07/19
%
\DeclareSubstance{NaCl}{
  name    = Sodiumchloride ,
  formula = NaCl ,
  CAS     = 7647-14-5,
  mass    = 58.44 ,
  mp      = 801 ,
  bp      = 1465 ,
```

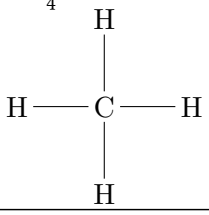
name	Methane
formula	CH_4
	
CAS	74-82-8
PubChem	297
boiling point	−162 °C
melting point	−182 °C
density	0.000 72 g/cm^3
molar mass	16.04 g/mol
	
H statements	H220
P statements	P210, P377, P381, P410 + P403

Table 1: All properties of Methane that have been saved in the example database.

```
  phase   = solid ,
  density = 2.17
}

\DeclareSubstance{H2SO4}{
  name       = Sulfuric Acid ,
  formula    = H2SO4 ,
  structure  = {H-[:30]\Lewis{26,O}-S(=[2]\Lewis{13,O})(=[6]\Lewis{57,O})-\Lewis{26,
  O}-[:-30]H} ,
  CAS        = 7664-93-9 ,
  PubChem    = 1118 ,
  mass       = 98.08 ,
  density    = 1.8356 ,
  mp         = 10.38 ,
  bp         = 279.6 ,
  phase      = liquid ,
  pKa        = -3.0 ,
  pKa1       = -3.0 ,
  pKa2       = 1.9 ,
  pictograms = acid ,
  H          = 314 ,
  P          = {280,301+330+331,309,310,305+351+338} ,
  LD50       = 510
}

```

```
\DeclareSubstance{methane}{
  name       = Methane ,
  formula    = CH4 ,
  structure  = H-C(-[2]H)(-[6]H)-H ,
  CAS        = 74-82-8 ,
  PubChem    = 297 ,
  pictograms = {flame,bottle} ,
  H          = 220 ,
  P          = {210,377,381,410+403} ,
  mass       = 16.04 ,
  density    = 0.72e-3 ,
  mp         = -182 ,
  bp         = -162 ,
  phase      = gaseous
}

\DeclareSubstance{ethane}{
  name       = Ethane ,
  formula    = C2H6 ,
  structure  = H-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-H ,
  CAS        = 74-84-0 ,
  PubChem    = 6324 ,
  pictograms = {flame,bottle} ,
  H          = 220 ,
  P          = {210,377,381,403} ,
  mass       = 30.07 ,
  density    = 0.72e-3 ,
  mp         = -183 ,
  bp         = -89 ,
  phase      = gaseous
}

\DeclareSubstance{acetone}{
  name      = Propan\-2\-one ,
  alt       = Acetone ,
  formula   = C3H6O ,
  structure = {-[:30](=[2]\Lewis{13,O})-[:-30]} ,
  CAS       = 67-64-1 ,
  PubChem   = 180 ,
  mass      = 58.08 ,
  density   = 0.79 ,
  mp        = -95 ,
  bp        = 56 ,
  LD50      = 5800
}
```

Chemicals

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