PPCHTex

a macropackage for typesetting
chemical structure formulas

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PPCHTeX is a set of coherent macros that can be used to typeset chemical structure formulas. The macros fall back on PCTeX, a public domain drawing package written by Michael Wichura. Although originally written on top of PCTeX, the second release can cooperate with PSTricks of Timothy Van Zandt, that is, with some limitations. Personally we still prefer the quality of the PCTeX output.

The macros can be used from within several macro packages and fall back on a few generic CONTEXT modules. The macros are written in a way that permits relatively easy upward compatible extensions. The interface is conform the CONTEXT interface.

PPCHTeX was originally meant for typesetting chemical structure formulas like sixrings. At the moment there is also support for reaction mechanisms. Formulas can be typeset at different sizes. Common elements or frequently used formula components can be reused.

Flexibility, simplicity and quality have been prefered over speed. We don’t use the PCTeX option to save pictures, because timing showed that the gain was minimal.

The first version of PPCHTeX was ready for use in 1995. This manual describes the second major release. Thanks to the many suggestions of Tobias Burnus, Dirk Kuypers and Ton Otten, the functionality was extended considerably.
Part 1
Explanation
The number of commands that is used to typeset chemical structure formulas is, apart from some bell and whistle commands, limited to four.\(^1\) In the following example all of these commands are used.

Example 1.1
\begin{verbatim}
\setupchemical[axis=on,frame=on]
\startchemical
  \chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical
\end{verbatim}

With \setupchemical we can influence the makeup of the formulas. These setups influence all the following formulas, unless they are superceded by local setup variables.\(^2\)

The set up variables can be defined right after \startchemical. In that case the set up is only applied to one structure formula.

Example 1.2
\begin{verbatim}
\startchemical[frame=on,width=fit,height=fit]
  \chemical[CARBON,CB1][A,B,C,D,E,F]
\stopchemical
\end{verbatim}

Both examples show that \chemical is the essential command. This command that may be used more than once within a \start--\stop--pair, is accompanied with two arguments. These arguments are written between \[ \]. The first argument is used for defining the chemical bonds, the second argument for the atoms and molecules that make up the structure.

Text is typeset in mathematical mode, this means that you may type anything that normally is allowed between $$.\(^3\)

---

\(^1\) The concept structure in this manual only refers to the chemical structure. It is not related to the document structure.

\(^2\) One can of course limit the scope of the variables by using \{ \} and/or the grouping macros ..group.
We will explain the first example in more detail. The key *SIX* means that we want to draw a sixring. In analogy we could type *ONE*, *THREE*, *FOUR* and *FIVE*, *EIGHT*, *CARBON*, *NEWMAN*, *CHAIR*, some alternatives on these keys and some symbols.

The dimensions of *CHAIR* are somewhat different from the others. This structure is also different in other means. Rotation for example is not possible.

**Example 1.3**

\begin{verbatim}
\startchemical[frame=on,scale=small]
\chemical
[CHAIR,B,+R,-R,
+RZ1,+RZ2,+RZ3,+RZ4,+RZ5,+RZ6,
-RZ1,-RZ2,-RZ3,-RZ4,-RZ5,-RZ6]
[a,b,c,d,e,f,1,2,3,4,5,6]
\stopchemical
\end{verbatim}
Within a structure the chemical bonds between the C-atoms are defined in the same way. In this example we use B and R. Bonds within a structure are numbered and can be defined by:

\chemical[SIX,B1,B2,B3,B4,B5,B6]
\chemical[SIX,B135]
\chemical[SIX,B1..5]

These keys draw parts of a sixring. With R and RZ we place substituents on the ring. The key R draws the bond from a ring corner to the substituent (\( \angle 120^\circ \)). The corner is also identified with a number.

\chemical[SIX,B1..6,R1..6]

The definition above draws the six bonds in the sixring and the bonds to the substituents. The substituents are identified by the key RZ. Again numbers are used to mark the position. The substituents themselves are defined as text in the second argument.

![Chemical structure diagram]

**Example 1.4**

\startchemical[frame=on,width=6000]
\chemical[SIX,B1..6,R1..6,RZ1..3][CH_3,CH_3,OH]
\stopchemical

When the second argument is left out no text (substituents) are placed on the ring and the key RZ1..3 has no effect.
This chapter gives an overview of the bonds you can use in structures. From the examples throughout this manual the use of the different keys will become more meaningful.

Bonds always have two alternatives: a long and a short version. The shortened bonds leave room to place atoms within a structure. A number of bonds can be shortened on both sides left (−) or right (+).

<table>
<thead>
<tr>
<th>B</th>
<th>Bond</th>
<th>SB</th>
<th>Single Bond</th>
</tr>
</thead>
<tbody>
<tr>
<td>BB</td>
<td>Bold Bond</td>
<td>−SB</td>
<td>Left Single Bond</td>
</tr>
<tr>
<td>HB</td>
<td>Hydrogen Bond</td>
<td>+SB</td>
<td>Right Single Bond</td>
</tr>
</tbody>
</table>

**Table 2.1** Single bonds.

The example below shows a number of bonds combined within one structure:

\begin{example}
\begin{chemical}[frame=on]
  \ONE,SD1,SB4,BB2,SB7,Z01247\ [C,H,H,H,H]
\end{chemical}
\end{example}

A bond can be followed by one or more numbers or a range, for example: \texttt{B1, B135} and \texttt{B1..5}. When you want to draw all bonds you can type \texttt{B}.

Within a ring structure you can define extra bonds between atoms, for example a double or triple bond.

<table>
<thead>
<tr>
<th>EB</th>
<th>Extra Bond</th>
<th>DB</th>
<th>Double Bond</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>TB</td>
<td>Triple Bond</td>
</tr>
</tbody>
</table>

**Table 2.2** Multiple bonds.

Free electrons and electron pairs can be defined in different ways. The accompanying keywords start with an \texttt{E}.
The example below shows a carbon atom with 8 outer electrons arranged in a chemically very peculiar way.

<table>
<thead>
<tr>
<th>ES</th>
<th>Extra Single</th>
<th>ED</th>
<th>Extra Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>EP</td>
<td>Extra Pair</td>
<td>ET</td>
<td>Extra Triple</td>
</tr>
</tbody>
</table>

**Table 2.3** Free electrons and electron pairs.

**Example 2.2**

\[
\texttt{\begin{verbatim}
\startchemical[frame=on]
\chemical[ONE,Z0,ES1,ED3,ET5,EP7][C]
\stopchemical
\end{verbatim}}
\]

Within a ring structure you can make a shortcut from one atom to another. In that case the atom that you want to skip has to be identified. As a replacement of the double bonds in an aromatic sixring a circle can be drawn and charges can be placed within the ring.

<table>
<thead>
<tr>
<th>SS</th>
<th>Short Shortcut</th>
<th>S</th>
<th>Shortcut</th>
</tr>
</thead>
<tbody>
<tr>
<td>-SS</td>
<td>Left Short Shortcut</td>
<td>MID</td>
<td>Open Mid Shortcut</td>
</tr>
<tr>
<td>+SS</td>
<td>Right Short Shortcut</td>
<td>MIDS</td>
<td>Closed Mid Shortcut</td>
</tr>
</tbody>
</table>

**Table 2.4** Special bonds.

<table>
<thead>
<tr>
<th>C</th>
<th>Circle</th>
<th>CD</th>
<th>Dashed Circle</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>Shifted Circle</td>
<td>CCD</td>
<td>Dashed Shifted Circle</td>
</tr>
</tbody>
</table>

**Table 2.5** Circle bonds.

An example will explain the use of the circular bond and the use of displaced charges.

**Example 2.3**

\[
\texttt{\begin{verbatim}
\startchemical[frame=on]
\chemical
[SIX,B,ER6,CCD12346,Z0,PB:RZ6,ONE,SB8,EP6,Z0,ZT6,Z8,PE]
[\ominus,O,\oplus,H]
\stopchemical
\end{verbatim}}
\]
Substituents can be connected to all corners of a structure. A substituent can be anything you want. It depends on the presence of atoms or molecules whether the bonds are long or short. In the examples you will see a great number of the keys that are used to define substituents.

<table>
<thead>
<tr>
<th>R</th>
<th>Radical</th>
<th>SR</th>
<th>Single Radical</th>
</tr>
</thead>
<tbody>
<tr>
<td>−R</td>
<td>Left Radical</td>
<td>−SR</td>
<td>Single Left Radical</td>
</tr>
<tr>
<td>+R</td>
<td>Right Radical</td>
<td>+SR</td>
<td>Single Right Radical</td>
</tr>
</tbody>
</table>

**Table 2.6** Bonds to substituents.

There are a few alternatives to draw bridges.

<table>
<thead>
<tr>
<th>RD</th>
<th>Radical Dashed</th>
<th>RB</th>
<th>Radical Bold</th>
</tr>
</thead>
<tbody>
<tr>
<td>−RD</td>
<td>Left Radical Dashed</td>
<td>−RB</td>
<td>Left Radical Bold</td>
</tr>
<tr>
<td>+RD</td>
<td>Right Radical Dashed</td>
<td>+RB</td>
<td>Right Radical Bold</td>
</tr>
</tbody>
</table>

**Table 2.7** Special bonds to substituents.

Radicals can be drawn in three ways. Some alternatives are seldom used.

**Example 2.4**

```latex
\startchemical[frame=on]
  \chemical[SIX,B,R14,RD25,RB36]
\stopchemical
```

<table>
<thead>
<tr>
<th>SD</th>
<th>Single Dashed</th>
<th>LDD</th>
<th>Left Double Dashed</th>
</tr>
</thead>
<tbody>
<tr>
<td>OE</td>
<td>Open Ended</td>
<td>RDD</td>
<td>Right Double Dashed</td>
</tr>
</tbody>
</table>

**Table 2.8** More special bonds to substituents.

An example of an Open Ended is defined below. We see a sixring (SIX) with a number of consecutive ONEs. The use of PB is explained later.

---

3 The word radical schould not be interpreted chemically, but typographically.
It’s obvious that substituents can be attached to the structure by means of double bonds.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
ER & Extra Radical \\
\hline
DR & Double Radical \\
\hline
\end{tabular}
\caption{Double bonds to substituents.}
\end{table}

You can comment on a bond. Text is typed in the second argument of \texttt{\chemical}.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Z & Atom & RZ & Radical Atom \\
CRZ & Center Atom & -RZ & Left Radical Atom \\
MIDZ & Mid Atom & +RZ & Right Radical Atom \\
\hline
\end{tabular}
\caption{Atoms and molecules (radicals).}
\end{table}

From these keys RZ is an addition to the key R. The key MID is only available in combination with a sixring (SIX). In the example below we see the effects of MID and MIDZ. These keys have no positioning parameter.

\begin{example}
\begin{verbatim}
\startchemical[frame=on]
\chemical[SIX,B,MID,MIDZ]\{\SL{CH_2}\}
\stopchemical
\end{verbatim}
\end{example}

Atoms and molecules are numbered clockwise. Combinations are also allowed. Position 0 (zero) is the middle of a structure.

We can attach labels and numbers to an atom or a bond. This is done with ZN and ZT:
Table 2.11  Labels and numbers.

In case of a SIX and a FIVE we can also attach text to radicals. We use RN and RT.

<table>
<thead>
<tr>
<th>RN</th>
<th>Radical Number</th>
<th>RT</th>
<th>Radical Text</th>
</tr>
</thead>
<tbody>
<tr>
<td>RTN</td>
<td>Radical Top Number</td>
<td>RTT</td>
<td>Radical Top Text</td>
</tr>
<tr>
<td>RBN</td>
<td>Radical Bottom Number</td>
<td>RBT</td>
<td>Radical Bottom Text</td>
</tr>
</tbody>
</table>

Table 2.12  Labels and numbers.

The structure ONE has also a top and bottom alternative.

<table>
<thead>
<tr>
<th>ZTN</th>
<th>Atom Top Number</th>
<th>ZTT</th>
<th>Atom Top Text</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZBN</td>
<td>Atom Bottom Number</td>
<td>ZBT</td>
<td>Atom Bottom Text</td>
</tr>
</tbody>
</table>

Table 2.13  Extra labels and numbers.

With the keys ZTN and ZBN numbers are generated automatically. The other keys will use the typed text of the second argument of chemical.

Example 2.7

\startchemical[frame=on]
\chemical[ONE,SB,Z0,ZTT][C,a,b,c,d,e,f,g,h]
\stopchemical

You can also add some symbols to the structure.

<table>
<thead>
<tr>
<th>AU</th>
<th>Arrow Up</th>
<th>AD</th>
<th>Arrow Down</th>
</tr>
</thead>
</table>

Table 2.14  Indications.

The arrows are positioned between the atoms in a structure.
We want to add that while typesetting atoms and molecules the dimensions of these atoms and molecules are taken into account. The width of C and the height of $C_n^m$ play an important role during positioning. This mechanism may be refined in a later stage.
Structures FIVE and SIX can be displayed in a frontview. However there are some limitations. Frontviews can not be rotated. Also the coupling of several structures is limited.

We illustrate the frontview keys in two examples.

**Example 3.1**

\begin{chemical}[height=4500,bottom=2500]
  $\beta$-D-Fructopyranose
  \begin{chemical}
    [SIX,FRONT,BB1236,+SB4,-SB5,Z5][O]
    [SIX,FRONT,+R12346,+RZ12346][\SR{HO},H,H,OH]
    [SIX,FRONT,-R12346,-RZ12346][H,OH,\SR{HO},H,CH_2OH]
  \end{chemical}
\end{chemical}

Positioning the radicals is an optimization of feasibility and quality. The next example will illustrate this.

**Example 3.2**

\begin{chemical}[height=4500,bottom=2500]
  $\alpha$-D-Fructofuranose
  \begin{chemical}
    [FIVE,FRONT,BB125,+SB3,-SB4,Z4][O]
    [FIVE,FRONT,+R1235,+RZ1235][\SR{HO},H,\SR{HOH_2C},CH_2OH]
    [FIVE,FRONT,-R1235,-RZ1235][OH,H,\SR{HO},H,CH_2OH]
  \end{chemical}
\end{chemical}
4 Definitions

It is possible to build a library of structures. These predefined structures can be used in a later stage, for example as a component of a more complex structure. Predefinition can be done with the \TeX--primitive \texttt{\def}.

\begin{verbatim}
\def\sixring{\chemical[SIX,B,R,RZ]}
\end{verbatim}

However it is better to use the command \texttt{\definechemical}. In that case a message will occur during processing if a duplicate name is found.

\begin{verbatim}
\definechemical[sixring]
{\chemical[SIX,B,R,RZ]}
\end{verbatim}

Recalling \texttt{\chemical[sixring]} will display a bare sixring without substituents.

\begin{example}
\texttt{\definechemical[sixring]}
\{\chemical[SIX,B,R,RZ]}
\startchemical[frame=on,width=6000]
\chemical[sixring]
\stopchemical
\end{example}

If we want to attach six substituents in a later stage to a sixring we could type:

\begin{example}
\texttt{\definechemical[sixring]}
\{\chemical[SIX,B,R,RZ]}
\startchemical[frame=on,width=6000]
\chemical[sixring][R_1,R_2,R_3,R_4,R_5,R_6]
\stopchemical
\end{example}

The structure \texttt{sixring} can be defined without substituents (RZ). We could attach them after recalling \texttt{\chemical[sixring]}.
In principal the possibilities are unlimited. However, you should remember that atoms and molecules are selected from the second argument in the order of definition in the first argument.

A definition may contain atoms and molecules (texts).

Example 4.3
\definechemical[sixring]
{\chemical[SIX,B,R]}
\startchemical[frame=on,width=6000]
 \chemical[sixring,RZ][A,B,C,D,E,F]
\stopchemical

In the example above there will always be three substituents. If we want to attach more substituents we have to indicate explicitly that we want to continue with the sixring (SIX).

Example 4.4
\definechemical[sixring]
{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5]}
\startchemical[frame=on,width=6000]
 \chemical[sixring,SIX,RZ246][A,B,C]
\stopchemical

In a definition \texttt{\chemical[]} has a global scope (this means that SIX is remembered) and \texttt{\chemical[]} has a local scope. The idea behind this is that in the first case a range of keys can be added and in the second case a complete structure.

In a definition \texttt{\chemical} may be used more than once. The last example could have been defined thus:
Example 4.5

\definechemical[sixring]  \{\chemical[SIX,B,R,RZ135] [R_{1},R_{3},R_{5}]  \\
\chemical[SIX,RZ246]\}

\startchemical[frame=on,width=6000]  \\
\chemical[sixring][A,B,C] \stopchemical

When \TeX{} announces that an unknown command has occurred, you may have forgotten to type SIX, FIVE or a comparable key.
Structures can be combined to more complex compounds. Moving one structure in relation to another structure is done by MOV, ROT, ADJ and SUB.

<table>
<thead>
<tr>
<th>Key</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOV</td>
<td>Move</td>
</tr>
<tr>
<td>ADJ</td>
<td>Adjace</td>
</tr>
<tr>
<td>SUB</td>
<td>Substitute</td>
</tr>
<tr>
<td>ROT</td>
<td>Rotate</td>
</tr>
</tbody>
</table>

**Table 5.1** Moving and rotating.

The four keys mentioned above have different effects when they are applied to different structures. The angle of rotation in \texttt{\textbackslash chemical[FIVE,ROT1,B]} differs from that in \texttt{\textbackslash chemical[SIX,ROT1,B]}.

With the structure ONE you can use MOV but the key DIR is also available. Both keys have the same effect but differ in spacing. Small adjustments are possible with OFF.

<table>
<thead>
<tr>
<th>Key</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIR</td>
<td>Direction</td>
</tr>
<tr>
<td>OFF</td>
<td>Offset</td>
</tr>
</tbody>
</table>

**Table 5.2** Moving and rotating.

The structure CARBON can be mirrored with MIR.

<table>
<thead>
<tr>
<th>Key</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIR</td>
<td>Mirror</td>
</tr>
</tbody>
</table>

**Table 5.3** Mirroring.

We use a number to indicate the direction of a movement or the level of rotation. These keys are closely related with the structure. Therefore they have to be defined before bonds are drawn and texts are placed. So definition \texttt{\textbackslash chemical[FIVE,B,ROT1,R]} and \texttt{\textbackslash chemical[FIVE,ROT1,B,R]} will not have the same result. The first definition will give an undesirable result.
In this example a sixring is drawn because of SIX,B. Then a movement in the direction of bond 1 takes place and a second sixring is drawn: B (SIX is stil in effect).

A movement with MOV in a sixring can occur in six directions. A movement with ADJ will take place in only four axis–directions ($x$, $-x$, $y$, $-y$). It is a coincidence that in a sixring some of these movements have the same effect. The example above could have been drawn with: [SIX,B,ADJ1,B].

Structures can be combined. It is possible for example to combine structure FIVE with structure SIX in such a way that they have one mutual bond. Luckily the mechanism that takes care of these kinds of combinations is hidden for the user. In the next example you will see a sixring drawn by SIX,B. Then a movement in the positive $x$–direction is done by ADJ1. At last a rotated fivering is drawn: FIVE,ROT3,B.
To go from one structure to an adjacent one is done with **ADJ**. Most of the time one of these structures will have to be rotated to obtain a good attachment. This is done by **ROT**. Rotations are always clockwise in steps of 90°. When a structure is attached with a bond you will have to use **SUB**. Movements with **ADJ** and **SUB** take place in the four directions of the $x$- and $y$-axis.

The next examples illustrate that the dimensions of the smaller structures are determined by the larger structures, especially **SIX**. You will notice that **EIGHT** has fewer possibilities than **SIX**.

**Example 5.4**

```
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,MOV1,B]
\stopchemical
```

**Example 5.5**

```
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,ADJ1,SIX,B]
\stopchemical
```

**Example 5.6**

```
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,ADJ1,FIVE,ROT3,B]
\stopchemical
```

It will be clear by now that the order in which the keys are defined makes a lot of difference. The order should be:
Most of the time putting structures together is done by translating and rotating. You could automate this process. In earlier versions this was done automatically, however this led to misinterpretations of users concerning the positions of bonds, atoms and substituents. A structure that consists of more than one component can best be defined per component, translations included. Rotations should wait until the last step.

A sixring may have substituents consisting of a carbon chain. In those situations we use DIR to build the chain.

```
\startchemical
[structure, % SIX, FIVE, ...
bonds within the structure, % B, C, EB, ...
bonds pointing to substituents, % R, DR, ...
atoms within the structure, % Z
substituents attached to the structure] % RZ, -RZ, ...
[atoms,
substituents]
\stopchemical
```

Because chains have no predefined format the chains are build and positioned as a substructure. For positioning we use the keys PB and PE.

<table>
<thead>
<tr>
<th>PB:..</th>
<th>Picture Begin</th>
<th>beginning a substructure</th>
</tr>
</thead>
<tbody>
<tr>
<td>PE</td>
<td>Picture End</td>
<td>ending a substructure</td>
</tr>
</tbody>
</table>

**Table 5.4** Positioning.

Directly after PB you will have to define the location where the substructure is positioned. The first following atom is centered on that location. Always use a central atom on this location.
These keys were introduced after trying to obtain structures that are typeset in an acceptable quality. There are different ways to define structures. The following alternative would have resulted in:

Example 5.8
\begin{verbatim}
\startchemical
  [scale=small,width=6000,height=6000,frame=on]
  \chemical
    [SIX,SB2356,DB14,Z36,SR36,RZ36][N,C,H,H_2]
  \chemical
    [PB:Z1,ONE,Z0,DIR8,Z0,SB24,DB7,Z27,PE][C,C,CH_3,0]
  \chemical
    [PB:Z5,ONE,Z0,DIR6,Z0,SB24,DB7,Z47,PE][C,C,H_3C,0]
  \chemical
    [PB:Z2,ONE,Z0,DIR2,SB6,CZ0,PE][C,CH_3]
  \chemical
    [PB:Z4,ONE,Z0,DIR4,SB8,CZ0,PE][C,H_3C]
\stopchemical
\end{verbatim}

The most efficient way to define such a structure would be like the example below. Typographically you wouldn’t be satisfied.

Example 5.9
\begin{verbatim}
\startchemical
  [scale=small,width=6000,height=6000,frame=on]
  \chemical
  \chemical
    [PB:RZ1,ONE,Z0,SB2,SB7,Z27,PE][C,CH_3,0]
  \chemical
    [PB:RZ5,ONE,Z0,SB4,SB7,Z47,PE][C,H_3C,0]
\stopchemical
\end{verbatim}

You may have noticed that the measurements of the structure is determined by the substituents. The chains are not taken into account. This leads to a consistent build-up of a structure.

The differences in outcome when using \texttt{SUB} in stead of \texttt{PB} are very small. However compare the following formulas.
Example 5.10
\startchemical
\chemical
[SIX,ROT2,B,C,R236,RZ23,
SUB1,ONE,OFF1,Z0,40OFF1,SB1,Z1]
[HO,HO,CHOH,CH_2NH_2]
\stopchemical

Example 5.11
\startchemical
\chemical
[SIX,ROT2,B,C,R236,RZ23,
P:RZ6,ONE,Z0,3OFF1,SB1,Z1,PE]
[HO,HO,CHOH,CH_2NH_2]
\stopchemical

The use of the key PB: might be somewhat more difficult, but the results are much better. In that case you should define the width yourself, because the substituents are not taken into account when determining the dimensions.

First we will go into the key OFF. In some cases atom (Z0) in ONE can consist of more than one character. The reserved space for these characters would be insufficient and character and bond would overlap. When you need more space for Z0 we can move bond 1, 2 and 8 by means of the key OFF (‘offset’). The example below will illustrate its use.

Example 5.12
\startchemical
\chemical
[SIX,B,C,ADJ1,
FIVE,ROT3,SB34,+SB2,-SB5,Z345,DR35,SR4,CRZ35,SB1,
ONE,OFF1,SB258,Z0,2Z8]
[C,N,C,0,0,
CH,COOC_2H_5,COOC_2H_5]
\stopchemical

Moving the bonds makes room for an extra character. More space was obtained when we would have typed 3OFF1. The example looks rather complex but you can define it rather easy by defining its components first. Rotating should be done in the last stage.
You see a new key: \texttt{CRZ}. This key is used to place the atom or molecule in one line with the bond. You could have used \texttt{RZ}, because you can influence spacing in the second argument with \{\textbackslash, 0\} instead of \texttt{0} (spacing in mathematical mode).

We will show another example, produced in two ways. When choosing a method you should take into account the consistency throughout your document.

Example 5.13

\begin{verbatim}
\startchemical
[width=fit, height=fit, frame=on, scale=small]
\chemical
[ONE, SB15, DB7, Z057, 3OFF1, MOV1, Z0, 3OFF1, MOV1, Z017, SB1357, MOV3, Z0, MOV3, SB1357, Z013, 3OFF5, MOV5, Z0, 3OFF5, SB5, Z5]
[C, H_2N, NH, (CH_2)_3, C, COOH, H, \SL{NH}, C, COOH, H, (CH_2)_2, HOOC]
\stopchemical
\end{verbatim}

Example 5.14

\begin{verbatim}
\startchemical
[width=fit, height=fit, frame=on, scale=small]
\chemical [ONE, SB15, DB7, Z057, 3OFF1][C, H_2N, NH]
\chemical [MOV1, Z0, 3OFF1][(CH_2)_3]
\chemical [MOV1, Z017, SB1357][C, COOH, H]
\chemical [MOV3, Z0][\SL{NH}]
\chemical [MOV3, SB1357, Z013, 3OFF5][C, COOH, H]
\chemical [MOV5, Z0, 3OFF5, SB5, Z5][(CH_2)_2, HOOC]
\stopchemical
\end{verbatim}

Example 5.15

\begin{verbatim}
\startchemical
[width=fit, height=fit, frame=on, scale=small]
\chemical
[ONE, Z0, SAVE, MOV7, SB1357, Z017, 3OFF5, MOV5, Z0, 3OFF5, MOV5, SB15, DB7, Z057, RESTORE, MOV3, SB1357, Z013, MOV5, 3OFF5, Z0, 6OFF5, SB5, Z5]
[\SL{NH}, C, COOH, H, (CH_2)_3, C, H_2N, NH, C, COOH, H, (CH_2)_2, HOOC]
\stopchemical
\end{verbatim}
Notice the use of \texttt{SAVE} and \texttt{RESTORE}. These keys enable you to save a location in a structure and return to that location in another stage.

As an extra we will show you a combination of \texttt{SIX} and \texttt{FIVE}. Be aware of the use of \texttt{SS}.

\textbf{Example 5.17}

\begin{verbatim}
\startchemical
[width=fit,height=fit,frame=on]
\chemical
[SIX, DB135, SB246, Z, SR6, RZ6] [C, C, \SR{HC}, N, C, NH_2]
\chemical
[SIX, MOV1, DB1, SB23, SS6, Z1..5, SR3, RZ3] [N, \SL{CH}, N, C, C, H]
\stopchemical
\end{verbatim}
We can add text and symbols in and around structures. For example:

Example 6.1

```
\startchemical
\[height=4500,top=1250,width=fit,frame=on]\n\bottext
\{2,2-Dimethyl-3-ethylpentane\}
\chemical
\[ONE,Z3570,SB1357]\n\{CH_3,\T{1}\{H_3C\},CH_3,\SR{\LT{2}\{C\}}\}
\chemical
\[MOV1,OFF1,Z0,SB3]\n\{\T{3}\{CH\}\}
\chemical
\[MOV3,Z0,SB3,MOV3,Z0,MOV7,MOV7]\n\{CH_2,CH_3\}
\chemical
\[OFF1,SB1,MOV1,OFF1,Z0,2OFF1,SB1,Z1]\n\{\T{4}\{CH_2\},\T{5}\{CH_3\}\}
\stopchemical
```

There is a range of keys like \T. In a number of cases the arguments are optional. Charges can be displayed in Roman by means of \+ and \- or directly by means of \1 up to \7.

| \+{number}   | positive charge in Roman |
| \-{number}   | negative charge in Roman |
| \1           | I (without sign)          |
| \7           | II, III, IV, V, VI and VII |

Table 6.1  Text: charges.

A charge is centered above the atom. For example:

```
\placeformula
\startformula
\chemical{S}+\chemical{O_2}
\chemical{GIVES}
\chemical{\+{4}\{S\}-\{2\}\{O_2\}}
\stopformula
```
will result in:

\[
S + O_2 \rightarrow S\,O_2^{+IV\,-II}
\]  \(6.1\)

If we want to repeat a number of atoms or molecules we can define an (endless) range with `\[` and `\]`. Both arguments are optional as is shown in the example of PTFE of Polytetrafluorethane, better known as Teflon.

Example 6.2

```
\startchemical[width=fit,frame=on]
\chemical
[ONE,ZT5,SB5,OFF1,Z0,OFF1,SB1,M0V1,SB5,OFF1,Z0,OFF1,SB1,ZT1]
[\{CF_2,CF_2,\}{s1\,n}]
\stopchemical
```

Table 6.2  Text: repeating.

There is no problem of placing texts on the left, right, top or bottom of the atoms or molecules. If we precede the keys `\L`, `\R`, `\T` and `\B` by `\X` the distance from text to atoms is somewhat smaller.

```
\L{text}  text left
\R{text}  text right
\T{text}  text top
\B{text}  text bottom
```

Table 6.3  Text: around an atom.

Logical combinations of these keys are also possible. A key to centre text is also available.

In some cases you will need what we may call smashed text.
An example is given below. The text is centred around the first character.

\begin{chemical}[frame=on]
\chemical[SIX,B,R36,RZ36][\SL{COOH},\SL{COOH}]
\end{chemical}

We can place text above, under or in the middle of structures with the keys \texttt{\textbackslash toptext}, \texttt{\textbackslash midtext} and \texttt{\textbackslash bottext}. The exact position is determined by the height and depth of the structure.

\placeformula
\begin{formula}
\begin{chemical}[width=fit]
\chemical[SIX,B,Z1,MOV1,B][\hbox{$\bullet$}]
\texttt{\textbackslash toptext}{\sl trans}-Decalin
\end{chemical}
\hskip 24pt
\begin{chemical}[width=fit]
\chemical[SIX,B,Z12,MOV1,B][\hbox{$\bullet$},\hbox{$\bullet$}]
\texttt{\textbackslash bottext}{\sl cis}-Decalin
\end{chemical}
\end{formula}

Both \textit{Decalin} formulas look like this:
Explanation

\begin{align*}
\text{trans-Decalin} & \quad \text{cis-Decalin} \\
\end{align*}

(6.2)
Structures can be typeset in a frame that is divided by axis. The dimensions of the axis and the location of the origin can be defined in the set up. The axis and the frame can be made visible.

**Example 7.1**

\begin{chemical}
\[axis=on, \\
width=6000, height=4000\]
\end{chemical}

**Example 7.2**

\begin{chemical}
\[axis=on, \\
left=2000, right=4000\]
\end{chemical}

**Example 7.3**

\begin{chemical}
\[axis=on, \\
width=6000, right=1000\]
\end{chemical}
Example 7.4

\startchemical
[axis=on,
  width=6000,top=1000,bottom=3000]
\stopchemical

The dimensions of the total structure determine the dimensions of the axis. When width=fit and/or height=fit is typed the dimensions are determined by the real dimensions. Your choice will depend on how you want to place the structure in the text. Example 7.1 shows the default set up. Within a \start--\stop–pair you can use PiCTeX–macros. However, be careful.
8 Set ups

After \startchemical and \setupchemical you can type the set up.

<table>
<thead>
<tr>
<th>parameter</th>
<th>values</th>
<th>default</th>
</tr>
</thead>
<tbody>
<tr>
<td>width</td>
<td>number</td>
<td>4000</td>
</tr>
<tr>
<td>height</td>
<td>number</td>
<td>4000</td>
</tr>
<tr>
<td>left</td>
<td>number</td>
<td></td>
</tr>
<tr>
<td>right</td>
<td>number</td>
<td></td>
</tr>
<tr>
<td>top</td>
<td>number</td>
<td></td>
</tr>
<tr>
<td>bottom</td>
<td>number</td>
<td></td>
</tr>
<tr>
<td>resolution</td>
<td>number</td>
<td>\outputresolution</td>
</tr>
<tr>
<td>bodyfont</td>
<td>8pt 9pt 10pt etc.</td>
<td>\bodyfontsize</td>
</tr>
<tr>
<td>character</td>
<td>\rm \bf etc.</td>
<td>\rm</td>
</tr>
<tr>
<td>scale</td>
<td>number</td>
<td>medium</td>
</tr>
<tr>
<td>size</td>
<td>small medium big</td>
<td>medium</td>
</tr>
<tr>
<td>state</td>
<td>start stop</td>
<td>start</td>
</tr>
<tr>
<td>option</td>
<td>test</td>
<td></td>
</tr>
<tr>
<td>axis</td>
<td>on off</td>
<td>off</td>
</tr>
<tr>
<td>frame</td>
<td>on off</td>
<td>off</td>
</tr>
<tr>
<td>alternative</td>
<td>1 2</td>
<td>1</td>
</tr>
<tr>
<td>offset</td>
<td>HIGH LOW</td>
<td>LOW</td>
</tr>
</tbody>
</table>

Table 8.1 Set ups for structures.

The axis range from $-2000$ upto $+2000$, height as well as width. The parameter $Z_0$ is at $(0,0)$. Other divisions can be set up with \textit{left, right, top} and/or \textit{bottom} in combination with \textit{width} and \textit{height}.

You can use the key \texttt{size} to set up the bodyfont. In doing so the \TeX–primitives \texttt{textsize, scriptsize} and \texttt{scripts dataSnapshot} are used. With \texttt{scale} you can set up the dimensions of the structure itself. The scale is determined by the parameter \texttt{bodyfont}. The values \texttt{small, medium} and \texttt{big} are proportionally related.
The set up of the parameter \texttt{bodyfont} is used for calculations and has no consequences for the text. In \LaTeX{} and \texttt{PPCH\TeX} this set up parameter is coupled to the mechanism that sets the bodyfont.

In \TeX{} and \texttt{CON\TeX} you can use commands like \texttt{\textbackslash\rm}, \texttt{\textbackslash\bf} and \texttt{\textbackslash\sl} in mathematical mode. \texttt{PPCH\TeX} uses default \texttt{\rm}. With the parameter \texttt{character} another alternative can be chosen. In \texttt{example 8.1} the substituents are typeset \textit{slanted}.

**Example 8.1**

```latex
\texttt{\startchemical[frame=on,character=\sl]
\chemical[SIX,B,R,RZ][A,B,C,D,E,F]
\stopchemical}
```

The set up of \texttt{character} is valid for chemical structures in a picture and in the text. The sub- and superscripts are changed accordingly. This is illustrated in CH$_4$, CH$_4$, and CH$_4$, in which the set ups are \texttt{\rm}, \texttt{\bf} and \texttt{\sl}. Italic \texttt{\it} formulas lead to a bigger linewidth. In \texttt{CON\TeX} default bold–slanted (\texttt{\bs}) and bold–italic (\texttt{\bi}) are available. These commands adjust automatically to the actual fontstyle: CH$_4$, CH$_4$, CH$_4$ etc. (\texttt{\ss}, \texttt{\rm}, \texttt{\tt}).

It is also possible to set the characters at the instant you type them in the argument.

**Example 8.2**

```latex
\texttt{\startchemical[frame=on]
\chemical[SIX,B,R,RZ][\tf a,\bf b,\it c,\sl d,\bi e,\bs f]
\stopchemical}
```

With parameter \texttt{state} calculations can be shortcut. The parameters \texttt{frame} and \texttt{axis} need no further explanation. With \texttt{option=test} frames are drawn around the texts in a structure. In this way you can see how the text is aligned.\footnote{In \texttt{CON\TeX} you can activate the visual debugger. When activated the baseline is a dotted line. The module \texttt{supp-vis} can be used in other systems.} With the parameter
alternative you can set up the quality of the lines. Default PCTeX uses a 5 point . to draw lines. When option 2 is chose a thinner line is drawn.

Example 8.3
\startchemical[frame=on,option=test,alternative=2]
\chemical[SIX,B,R,RZ][R_1,R_2,R_3,R_4,R_5,R_6]
\stopchemical

The offset relates to the position of the sub- and superscripts. With HIGH the subscripts are placed high (H\textsubscript{2}O) and with LOW somewhat lower (H\textsubscript{2}O).

A structure can be displayed in different sizes. This is done with formaat and scale.

Example 8.4
\startchemical[frame=on,scale=small,size=small]
\chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical

Example 8.5
\startchemical[frame=on,scale=medium,size=medium]
\chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical
Example 8.6

\begin{verbatim}
\startchemical[frame=on,scale=big,size=big]
\chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical
\end{verbatim}

You can also type a number between 1 and 1000 in \texttt{scale}. The values belonging to \texttt{small}, \texttt{medium} or \texttt{big} are proportionally related.
There are some symbols that can be used to display reactions. The reaction below is typed by:

```
\setupchemical
  [size=small,
   scale=small,
   width=fit,
   height=5500,
   bottom=1500]
\hbox
{\startchemical
  \chemical[SIX,B,ER6,RZ6][O]
\stopchemical
\startchemical
  \chemical[SPACE,PLUS,SPACE]
\stopchemical
\startchemical
  \chemical[FIVE,ROT4,B125,+SB3,-SB4,Z4,SR4,RZ4][N,H]
\stopchemical
\startchemical
  \chemical[SPACE,GIVES,SPACE][?]
\stopchemical
\startchemical
  \chemical[SIX,B,EB6,R6,SUB4,FIVE,ROT4,B125,+SB3,-SB4,Z4][N]
\stopchemical
\startchemical
  \chemical[SPACE,PLUS,SPACE,CHEM][H_2O]
\stopchemical}
```

The \hbox is necessary to align the structures. The symbols \texttt{GIVES} and \texttt{PLUS} need no further explanation. With \texttt{SPACE} more room can be created between the structures and symbols.
An equilibrium can be displayed with \texttt{EQUILIBRIUM}. Over \texttt{GIVES} and \texttt{EQUILIBRIUM} you can place text. In the example the text is just a ‘?’. In addition \texttt{MESOMERIC} is also available. Braces used for displaying complexes can be created with \texttt{OPENCOMPLEX} and \texttt{CLOSECOMPLEX}. 
10 | Positioning

When you are combining atoms or molecules, for example with \texttt{SUB}, some positions and dimensions change their value. To overcome this problem it is possible to save a location with \texttt{SAVE} and return to that location with \texttt{RESTORE}.

<table>
<thead>
<tr>
<th>SAVE</th>
<th>Save Status</th>
<th>save actual status</th>
</tr>
</thead>
<tbody>
<tr>
<td>RESTORE</td>
<td>Restore Status</td>
<td>restore actual status</td>
</tr>
</tbody>
</table>

Table 10.1  Positioning.

The keys \texttt{SAVE} and \texttt{RESTORE} are used with substituents. When placing radicals we use \texttt{PB} and \texttt{PE}. This example also illustrates the possibility to create chains.

\definechemical[molecule]
{\chemical
  [\texttt{ONE},\texttt{Z0},\texttt{SB1357},
   \texttt{SAVE},\texttt{SUB2},\texttt{SIX},\texttt{B},\texttt{R6},\texttt{C},\texttt{RESTORE},
   \texttt{MOV1},\texttt{Z0},\texttt{SB137},
   \texttt{MOV1},\texttt{Z0},\texttt{SB37},
   \texttt{MOV1}]
  [\texttt{C},\texttt{C},\texttt{C}]}\stopchemical

\startchemical[width=fit,height=fit]
  \chemical[molecule,molecule,molecule]\stopchemical

The example below is more complicated and show a complete reaction. The set up of bottom and top is essential in this example.
\placeformula 
\setupchemical 
[width=fit,top=2000,bottom=2000, 
scale=small,size=small] 
\startchemical 
\chemical 
[ONE, 
SAVE, 
Z0,SB7,SB3,SB1,MOV1,Z0,SB1,MOV1,Z0,DB8,CZ8,SB1,Z1, 
RESTORE, 
SAVE, 
SUB4,ONE,Z0,SB3,SB1,MOV1,Z0,SB1,MOV1,Z0,DB8,CZ8,SB1,Z1, 
RESTORE, 
SUB2,ONE,Z0,SB7,SB1,MOV1,Z0,SB1,MOV1,Z0,DB8,CZ8,SB1,Z1] 
[\SR{HC},O,C,O,C_{19}H_{39}, 
\SR{H_{2}C},O,C,O,C_{17}H_{29}, 
\SR{H_{2}C},O,C,O,C_{21}H_{41}] 
\stopchemical 
\startchemical 
\chemical [SPACE,PLUS,SPACE] 
\stopchemical 
\startchemical [right=600] 
\chemical [ONE,CZ0][3CH_{3}OH] 
\stopchemical 
\startchemical 
\chemical [SPACE,GIVES,SPACE,SPACE][H^+/H_2O] 
\stopchemical 
\startchemical 
\chemical 
[ONE, 
SAVE, 
Z0,SB7,SB3,SB1,Z1, 
RESTORE, 
SAVE, 
SUB4,ONE,Z0,SB3,SB1,Z1, 
RESTORE, 
SUB2,ONE,Z0,SB7,SB1,Z1] 
[\SR{HC},OH, 
\SR{H_{2}C},OH, 
\SR{H_{2}C},OH]
This definition might have been more compact if we would have typed \texttt{SB731} in stead of \texttt{SB7,SB3,SB1}. But in this way the definition is readable. Complex structures can best be defined in its respective components.

\begin{equation}
\frac{H_2C\; O\; C\; C_{19}H_{39} + 3CH_3OH}{H^+ / H_2O} \rightarrow \frac{H_2C\; OH\; C\; O\; C_{17}H_{29}}{C\; O\; C_{17}H_{30}\; C\; O\; CH_3}
\end{equation}

Just two more examples where we place text under a structure.
The use of OFF can be very subtle. The examples below illustrate this and show minor shifts of ONE.

**Example 10.1**

```
\startchemical[height=fit,frame=on]
  \chemical[ONE,SB]
\stopchemical
```

**Example 10.2**

```
\startchemical[height=fit,frame=on]
  \chemical[ONE,3OFF1,SB]
\stopchemical
```
The next example shows the definition of complexes. Pay special attention to the use of \texttt{RBT}. Normally an extra spacing is not necessary but we use here —the command is not visible— a smaller bodyfont to prevent the structure to run in the margin.

\begin{verbatim}
\startformula
\setupchemical[scale=small,width=fit]
\startchemical
\stopchemical
\end{verbatim}
Without the use of `SPACE` the separate structures would merge. Most of the time the optimization of such a reaction is an iterative process.
Explanation
Not only the typesetting of chemical structures is supported but also the typesetting of normal reactions. The command \texttt{\textbf{\textbackslash chemical}} has three other appearances:

- \texttt{\textbackslash chemical\{formula\}}
- \texttt{\textbackslash chemical\{formula\}\{bottom text\}}
- \texttt{\textbackslash chemical\{formula\}\{top text\}\{bottom text\}}

This command adapts itself to text mode. That means that it 'knows' whether it is used in:

- text--mode
- mathematical text--mode
- mathematical display--mode

When the command is used in running text it will automatically be surrounded by $$. Typing \texttt{\textbackslash chemical\{NH\_4\^+\}} will result in NH$_4^+$.

The result would be the same if we would place the command between $$. In both cases the second and third argument can be left out. If we place the command between $$ $$ (or \texttt{\textbackslash startformula} and \texttt{\textbackslash stopformula}) both arguments do have a function. First a simple example. The command \texttt{\textbackslash placeformula} is a \texttt{CONTeX} command and handles the positioning and numbering of the formula.

\begin{verbatim}
\placeformula
   \startformula
   \texttt{\textbackslash chemical\{2H\_2\} \textbackslash chemical\{PLUS\} \textbackslash chemical\{O\_2\} \texttt{\textbackslash chemical\{GIVES\} \textbackslash chemical\{2H\_2O\}}
   \stopformula

   2H\_2 + O\_2 \longrightarrow 2H\_2O \quad (11.1)
\end{verbatim}

The definition of the chemical part could be somewhat shorter:

\begin{verbatim}
\texttt{\textbackslash chemical\{2H\_2,PLUS,O\_2,GIVES,2H\_2O\}}
\end{verbatim}

or even:

\begin{verbatim}
\texttt{\textbackslash chemical\{2H\_2,+,O\_2,->,2H\_2O\}}
\end{verbatim}
A \LaTeX--addict will notice from these examples that the plus sign and the arrow are on the baseline. Compare for example + and +. In the reaction you will see that the + and the $\rightarrow$ are vertically aligned.

You can use PLUS, GIVES and EQUILIBRIUM \(<\rightarrow\) in this command. With MESOMERIC or <> you will get $\leftarrow$.

The reaction can be placed in the text. In that case a more compact display is used: $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$. Some finetuning with $\backslash$, would result in $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$.

It is also possible to display bonds in textmode. For example if you want $\text{H}--\text{CH}--\text{HC}--\text{H}$ you should type \chemical{H,SINGLE,CH,Doble,HC,SINGLE,H} or something like this \chemical{H,CH,HC,H}. A triple bond can be defined as TRIPLE or ---: HC\equiv CH.

We return two the display--mode. The second and third argument can be used to add text to the reaction:

\begin{verbatim}
\placeformula
\startformula
\chemical{2\text{H}_2}{hydrogen} \chemical{PLUS} \chemical{\text{O}_2}{oxygen} \chemical{GIVES}{heat} \chemical{2\text{H}_2\text{O}}{water}
\stopformula
\end{verbatim}

So we can also place text over and under symbols!

$$2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} \quad (11.2)$$

The last argument is placed under the compound.

\begin{verbatim}
\placeformula
\startformula
\chemical{\text{H}_2\text{O}}{\text{liquid}}{\text{water}} \hbox{c.q.} \chemical{\text{H}_2\text{O}}{\text{water}}
\stopformula
\end{verbatim}

\begin{verbatim}
\placeformula
\startformula
\hbox{liquid} \chemical{\text{H}_2\text{O}}{\text{c.q.}} \chemical{\text{H}_2\text{O}}{\text{water}}
\stopformula
\end{verbatim}

The formula above is defined with:

The size of the formulas or reactions in the running text can be set up with:
**Table 11.1** Set up in text formulas.

The definition \( \text{chemical}\{H,\text{SINGLE,CH,DOUBLE,HC,SINGLE,H}\} \) result with big, medium and small in the following formulas:

\[
\begin{align*}
H &\text{--CH=HC--H} \\
H &\text{--CH=HC--H} \\
H &\text{--CH=HC--H}
\end{align*}
\]
Sub- and superscripts are placed somewhat lower as is recommended by Knuth in the TeXBook. The rather strange chemical compound that is shown on page 179 of the TeXBook is defined with \chemical{Fe_{2}^{+2}Cr_{2}O_{4}}. This will result in Fe_{2}^{+2}Cr_{2}O_{4}. Without correction it would have been: Fe_{2}^{+2}Cr_{2}O_{4}.

The position of the subscript is determined by the parameter offset: HIGH or LOW. This position can be influenced locally (per substituent) as is shown in the example below.

Example 12.1

\begin{verbatim}
\startchemical[frame=on,option=test,alternative=2]
\chemical[SIX,B,R13,HIGH,RZ1,LOW,RZ3][NH_3,NH_3]
\stopchemical
\end{verbatim}

However, it is recommended to set up this parameter globally to obtain consistent formulas.

The values LOW and HIGH can also be used in text formulas. For example if you type \chemical{HIGH,H_{2}O} then you will get H_{2}O and \chemical{LOW,H_{2}O} will become H_{2}O.
Part 2
Backgrounds
1 Installation

The package PPCHTEX is developed for use in combination with CONTEX. PPCHTEX is activated in CONTEX by:

\usemodule[pictex,chemic]

This command loads the PICTEX macros so PPCHTEX knows what output is needed. The chemical macros are not automatically available.

The package can be used in combination with PLAIN TeX or \LaTeX. In that case the file m-chemie.sty is also used. PPCHTEX is then activated by \documentstyle:

\documentstyle[m-pictex,m-chemie]{}

In \LaTeX it is somewhat different:

\usepackage{m-pictex}
\usepackage{m-chemie}

The file m-pictex takes care of an efficient loading of PICTEX. This is necessary because \LaTeX allocates a lot of \texttt{dimen}s. Because of the user interface a big version of \TeX is needed to run PPCHTEX.

PPCHTEX can be used in three languages. The actual language can be activated by:

<table>
<thead>
<tr>
<th>language</th>
<th>files</th>
</tr>
</thead>
<tbody>
<tr>
<td>dutch</td>
<td>m-che-nl = m-chemie.sty</td>
</tr>
<tr>
<td>english</td>
<td>m-che-en = m-chemic.sty</td>
</tr>
<tr>
<td>german</td>
<td>m-che-de = m-chemie.sty</td>
</tr>
</tbody>
</table>

In the file ppchtex.noc you can see the coupling between CONTEX and macropackage. This file also loads the system modules of CONTEX.

The total distribution consists of the definition files ppchtex.tex and ppchtex.noc the starting files m-che-nl.tex, m-che-en.tex and m-che-de.tex and the alternative starting files m-chemie.tex and m-chemic.tex.

\footnote{The macros in file ppchtex.tex, are loaded by typing m-chemic.tex (the m stands for module).}
2 | Extensions

Users of PPCH\TeX{} are free to use and alter the macros. However one should be careful because most macros are still under development. Some macros may look more complex than necessary, but this is due to the userfriendly interface of CON\TeX{} and PPCH\TeX{}.

Commands like \texttt{\setup...} make it possible to make readable ASCII–layouts. Compare for example:

\begin{verbatim}
\setupchemical[size=small]
\end{verbatim}

and:

\begin{verbatim}
\setupchemical
[size=small, \\
scale=500, \\
textsize=big]
\end{verbatim}

The set up can be defined in a random order and newlines and spaces are not interpreted.

Originally PPCH\TeX{} was meant to be a module in CON\TeX{}, therefore the package is multilingual.

If you study the file \texttt{ppchtex.tex} you may notice that \texttt{\processaction} macros are being used while interpreting the keys in \texttt{\chemical}. These kind of macros are relatively slow but then the PPCH\TeX{} interface is very flexible.
The macros are in mathematical mode and therefore use \textfont, \scriptfont and \scriptscriptfont. When needed the \fontdimens 14, 16 and 17 of \font2 are adapted. The size of the actual font is derived from x height (\fontdimen5).

Changes in \fontdimen s have are global, so grouping makes no sense. The dimensions are therefore continually set and reset. This solution may seem poor but alternatives are not failsave and will result in problems with scaled fonts.

Typesetting atoms and molecules (text) during processing are rather time consuming. Speed depends on the complexity of the macro \textit{rm}.
The interface of PPCH\TeX is derived from the CON\TeX XT interface. This means that the interface is multi langual. The advantage is that one can use PPCH\TeX in his or her own language. The disadvantage is the fact that macros have to be shared between languages.

At this moment the CON\TeX XT commands and parameters are dutch. PPCH\TeX however has english commands.

\startchemical
  \chemical[SIX,B,C]
\stopchemical

Set ups are more difficult. We use system constants and variables that are dutch. In due time these will be translated. Adaption of these constants and variables is not too difficult.

\setupchemical[\c!breed=10cm, \c!height=\v!passend]

Parameters are preceded by \c! and set ups by \v!. This only works when ! is a character. That is the reason that these set ups have to be surrounded by \unprotect and \protect.

For example:

\unprotect
\setupchemical[\c!width=10cm, \c!height=\v!passend]
\startchemical
  \chemical[SIX,B,C]
\stopchemical
\protect

More information on the interface can be found in the documentation of the CON\TeX XT modules from the mult group.
In CONTeXT you can colorize parts of a structure. In example 5.1 the substituent as well as the bond are colored red.

Example 5.1
\startchemical[axis=on,frame=on,width=5000]
  \chemical[SIX,B]
  \color[red]{\chemical[SIX,R1,RZ1][COOH]}
\stopchemical

First the color mechanism has to be activated by \setupcolors[state=start].
6 Interaction

In combination with CON\text{\textsc{\texttt{f}}xt} PPCH\text{\textsc{t}}\text{\texttt{e}}\text{\textsc{x}} supports interactive texts. An interactive text is a text that can be consulted on a computerscreen and contains many hyperlinked textareas. This means that clicking on such an area will result in a jump to the target area.

**Example 6.1**
\begin{verbatim}
\startchemical[axis=on,frame=on,width=5000]
\chemical[SIX,B]
\chemical[sub:cooh][SIX,R1,RZ1][COOH]
\stopchemical
\end{verbatim}

We see a new argument: the reference \texttt{[sub:cooh]}. This means that we can refer from the text COOH to the structure with:

\begin{verbatim}
... text \goto\chemical{COOH}\texttt{[sub:cooh]} ... text ...
\end{verbatim}

In this definition \texttt{\goto} is a CON\text{\textsc{f}}xt--command. We can also refer from the structure to a particular part of the text.

Clicking in COOH in the structure results in a jump to the text that is marked with:

\begin{verbatim}
\paragraph[txt:cooh]{Substituents}
\end{verbatim}

\begin{verbatim}
... text \chemical{COOH} ... text ...
\end{verbatim}

A combination is also possible. In that case it is necessary to mark the reference with \texttt{\chemical} and to refer in the text with \texttt{\gotochemical}.

The coupling of the interaction mechanism is done with macros:

\begin{verbatim}
\localgotochemical \{reference\} \{text\}
\localthisischemical \{reference\}
\end{verbatim}

You can see the CON\text{\textsc{f}}xt sources for more information.
Part 3
Overview
1  One

SB  DB  TB

EP  ES  ED  ET

SD  LDD  RDD

HB  BB  OE

Overview
Overview

2 | Three

B

SB | −SB | +SB

MOV | ROT

R | −R | +R
Overview
3 | Four

B

EB

SB

−SB

+SB

MOV

ROT

R

−R

+R
Overview

ROT1

+RZ4
+RZ3
+RZ2
+RZ1

ROT2

+RZ4
+RZ3
+RZ2
+RZ1

ROT3

+RZ2
+RZ1
+RZ4
+RZ3

ROT4

+RZ1
+RZ4
+RZ3
4 | Five

Overview
Overview
Overview

5 | Six

B

EB

MID

MIDS

MIDZ

B

EB

MID

MIDZ

S

SS

-SS

+SS
Overview

SB

-SB

+SB

MOV

ROT

C

CD

CC

CCD

R

-R

+R
Overview

SR

-SR

+SR

ER

DB

DR

ZN

ZT

AU

AD

RD

-RD

+RD
Overview

CRZ

MOV1

MOV2

MOV3

MOV4

MOV5

MOV6

ROT1

ROT2

ROT3

ROT4
6 Eight

B

SB

-SB

+SB

Z
7 Five Front

B

BB

R

-R

+R

SB

-SB

+SB

Z

-RZ

+RZ
8 Six Front

B

BB

R

-R

+R

SB

-SB

+SB

Z

-Z

+Z

PPCTeX
9 | Carbon
10 | Newman Stagger

B

C

CB

MOV

ROT

Z

MOV1

MOV2

MOV3

MOV4

ROT1

ROT2

ROT3

ROT4
11 Newman Eclipse

Overview
Overview

12 | Symbol

GIVES  EQUILIBRIUM  MESOMERIC

PLUS  MINUS

OPENCOMPLEX  CLOSECOMPLEX

SPACE