Bijlage 17

**PPCHTeX**

*a macropackage for typesetting chemical structure formulas with \TeX{} — release 2*

**Keywords**

PPCHTeX, chemical formulas, graphics

**abstract**

A few years ago **PPCHTeX** was introduced. This generic macro package can be used to typeset chemical structure formulas. Currently the **NTG** supports a dedicated mailing list, to which quite some users subscribed. Although **PPCHTeX** is used all over the world, the main body of users lives in Germany. Thanks to the input of Tobias Burnus and Dirk Kuypers the second release of **PPCHTeX** doubles the functionality of the first and also supports PSTricks. Currently Tobias is coordinating the wish-list for the third release and Tobias and Dirk are collecting predefined structure formulas for a future database.

We’re also considering a **METAPOST** backend.

Here we present the long awaited for English update of the manual. The Dutch and German manuals were already available for about a year and can be uploaded from the **NTG** server.

Before we go to the the manual, we present the content of **readme.en**. This file shows how the current distribution is packaged.

**PPCHTeX**

This macropackage can be used to typeset chemical structure formulas. **PPCHTeX** is applicable with **LaTeX**, **CONTeXT**, **L\LaTeX{}** etc. The next files are part of this distribution:

- `ppchtex.tex`: the typesetting macros
- `ppchtex.noc`: the interface to **CONTeXT**
- `m-ch-nl.tex`, `m-ch-nl.sty`: Dutch version
- `m-ch-de.tex`, `m-ch-de.sty`: German version
- `m-ch-en.tex`, `m-ch-en.sty`: English version

For historic reasons we still got:

- `m-chemie.sty`: Dutch version
- `m-chemie.sty`: English version

Within **CONTeXT** one needs:

- `m-chemie.tex`: automatic interface

The package **PPCHTeX** falls back on one of the system modules of **CONTeXT**.

- `syst-gen.tex`: general interface macros

Voorjaar 1998
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Introduction

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

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

PPCH\TeX{} 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 preferred over speed. We don’t use the P\TeX{} option to save pictures, because timing showed that the gain was minimal.

The first version of PPCH\TeX{} 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
1 Structures

The number of commands that is used to typeset chemical structure formulas is, apart from some bell and whistle commands, limited to four. In the following example all of these commands are used.

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

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.

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
\startchemical[frame=on,width=fit,height=fit]
  \chemical[CARBON,CB1][A,B,C,D,E,F]
\stopchemical

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 \$ \$.

---

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

```
\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
```
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.

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:

**Example 2.1**

```
\startchemical[frame=on]
\chemical[ONE,SD1,SB4,BB2,SB7,Z01247][C,H,H,H,H]
\stopchemical
```

A bond can be followed by one or more numbers or a range, for example: B1, B135 and B1..5. When you want to draw all bonds you can type 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>TB</td>
<td>Triple Bond</td>
<td></td>
<td></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 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>
</tr>
</thead>
<tbody>
<tr>
<td>EP</td>
<td>Extra Pair</td>
</tr>
<tr>
<td>ED</td>
<td>Extra Double</td>
</tr>
<tr>
<td>ET</td>
<td>Extra Triple</td>
</tr>
</tbody>
</table>

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

**Example 2.2**

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

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>
</tr>
</thead>
<tbody>
<tr>
<td>-SS</td>
<td>Left Short Shortcut</td>
</tr>
<tr>
<td>+SS</td>
<td>Right Short Shortcut</td>
</tr>
<tr>
<td>S</td>
<td>Shortcut</td>
</tr>
<tr>
<td>MID</td>
<td>Open Mid Shortcut</td>
</tr>
<tr>
<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>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>Shifted Circle</td>
</tr>
<tr>
<td>CD</td>
<td>Dashed Circle</td>
</tr>
<tr>
<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**

\[ \text{\texttt{\startchemical[frame=on]}} \]
\[ \text{\texttt{\chemical}} \]
\[ \text{\texttt{[SIX,B,ER6,CCD12346,Z0,PB:RZ6,ONE,SB8,EP6,Z0,2T6,2B,PE]}} \]
\[ \text{\texttt{[\ominus,0,\oplus,H]}} \]
\[ \text{\texttt{\stopchemical}} \]
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

\begin{chemical}[frame=on]
  \SIX, B, R14, RD25, RB36
\end{chemical}

<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.

---

\footnote{The word radical should not be interpreted chemically, but typographically.}
It’s obvious that substituents can be attached to the structure by means of double bonds.

<table>
<thead>
<tr>
<th>ER</th>
<th>Extra Radical</th>
<th>DR</th>
<th>Double Radical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z</td>
<td>Atom</td>
<td>RZ</td>
<td>Radical Atom</td>
</tr>
<tr>
<td>CRZ</td>
<td>Center Atom</td>
<td>−RZ</td>
<td>Left Radical Atom</td>
</tr>
<tr>
<td>MIDZ</td>
<td>Mid Atom</td>
<td>+RZ</td>
<td>Right Radical Atom</td>
</tr>
</tbody>
</table>

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

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.

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 \texttt{ZN} and \texttt{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.
Example 2.8

\startchemical[frame=on]
\chemical[SIX,B,AU]
\stopchemical

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.
3 Frontviews

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

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

Example 3.2

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

\texttt{\def\sixring{\chemical[SIX,B,R,RZ]}}

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.

\texttt{\definechemical[sixring]}
{\chemical[SIX,B,R,RZ]}

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

**Example 4.1**

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

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

**Example 4.2**

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

The structure \texttt{sixring} can be defined without substituents (RZ). We could attach them after recalling \texttt{\chemical[sixring]}. 
Example 4.3

\begin{verbatim}
\definechemical[sixring]
\{chemical[SIX,B,R] \}
\suitablechemical[frame=on,width=6000]
\chemical[sixring,RZ][A,B,C,D,E,F]
\stopchemical
\end{verbatim}

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).

\begin{verbatim}
\definechemical[sixring]
\{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5] \}
\suitablechemical[frame=on,width=6000]
\chemical[sixring,SIX,RZ246][A,B,C]
\stopchemical
\end{verbatim}

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

\begin{verbatim}
\definechemical[sixring]
\{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5] \}
\suitablechemical[frame=on,width=6000]
\chemical[sixring,SIX,RZ246][A,B,C]
\stopchemical
\end{verbatim}

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>MOV</th>
<th>Move</th>
<th>moving a comparable structure structure in the direction of a bond</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADJ</td>
<td>Adjace</td>
<td>moving another structure in the direction of the x– or y–axis, adjacent to a bond</td>
</tr>
<tr>
<td>SUB</td>
<td>Substitute</td>
<td>moving one structure in relation to another in the direction of the x– or y–axis</td>
</tr>
<tr>
<td>ROT</td>
<td>Rotate</td>
<td>rotating a structure</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>DIR</th>
<th>Direction</th>
<th>moving a structure in a diagonal direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>OFF</td>
<td>Offset</td>
<td>moving atoms and molecules over small distances</td>
</tr>
</tbody>
</table>

Table 5.2 Moving and rotating.

The structure CARBON can be mirrored with MIR.

| MIR | Mirror | mirroring a structure |

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.
Example 5.1

\begin{verbatim}
\startchemical[frame=on,width=4000,right=3000]
  \chemical[SIX,B,MOV1,B]
\stopchemical
\end{verbatim}

In this example a sixring is drawn because of \texttt{SIX,B}. Then a movement in the direction of bond 1 takes place and a second sixring is drawn: \texttt{B} (\texttt{SIX} is still in effect).

A movement with \texttt{MOV} in a sixring can occur in six directions. A movement with \texttt{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: \texttt{[SIX,B,ADJ1,B]}.

Structures can be combined. It is possible for example to combine structure \texttt{FIVE} with structure \texttt{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 \texttt{SIX,B}. Then a movement in the positive $x$--direction is done by \texttt{ADJ1}. At last a rotated fivering is drawn: \texttt{FIVE,ROT3,B}.

Example 5.2

\begin{verbatim}
\startchemical[frame=on,width=4000,right=3000]
  \chemical[SIX,B,ADJ1,FIVE,ROT3,B]
\stopchemical
\end{verbatim}

Example 5.3

\begin{verbatim}
\startchemical[frame=on,width=5000,right=4500]
  \chemical[SIX,ROT2,B,R6,SUB1,FIVE,B,R4]
\stopchemical
\end{verbatim}
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 90º. 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**
\begin{verbatim}
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,MOV1,B]
\stopchemical
\end{verbatim}

**Example 5.5**
\begin{verbatim}
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,ADJ1,SIX,B]
\stopchemical
\end{verbatim}

**Example 5.6**
\begin{verbatim}
\startchemical[width=6000,left=1500,frame=on]
  \chemical[EIGHT,B,ADJ1,FIVE,ROT3,B]
\stopchemical
\end{verbatim}

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.

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

```
Example 5.7
\startchemical
  \[scale=small,width=6000,height=6000,frame=on\]
  \chemical[SIX,SB2356,DB14,22346,SR36,RZ36]
  \[C,N,C,C,H,H_2\]
  \chemical[PB:Z1,ONE,Z0,DIR8,Z0,SB24,DB7,227,PE]
  \[C,C,H_3C,0\]
  \chemical[PB:Z5,ONE,Z0,DIR6,Z0,SB24,DB7,247,PE]
  \[C,C,H_3C,0\]
  \chemical[SR24,RZ24]
  \[CH_3,H_3C\]
\stopchemical
```

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**

```latex
\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
```

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

**Example 5.9**

```latex
\startchemical
  [scale=small,width=6000,height=6000,frame=on]
  \chemical [SIX,SB2356,DB14,Z,SR36,SR1245,RZ24]
  [C,C,N,C,C,H,H_2,CH_3,H_3C]
  \chemical [PB:RZ1,ONE,Z0,SB2,DB7,Z27,PE]
  [C,CH_3,0]
  \chemical [PB:RZ5,ONE,Z0,SB4,DB7,Z47,PE]
  [C,H_3C,0]
\stopchemical
```

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 `SUB` in stead of `PB` are very small. However compare the following formulas.
Example 5.10
\startchemical
   [width=fit,frame=on,scale=small]
   \chemical
       [SIX,ROT2,B,C,R236,RZ23,
        SUB1,ONE,OFF1,Z0,40FF1,SB1,Z1]
       [HO,HO,CHOH,CH_2NH_2]
\stopchemical

Example 5.11
\startchemical
   [width=fit,frame=on,scale=small]
   \chemical
       [SIX,ROT2,B,C,R236,RZ23, 
        PB: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
   [width=fit,size=small,scale=small,frame=on]
   \chemical
       [SIX,B,C,ADJ1, 
        FIVE,ROT3,SB34,+SB2,SB5,2345,DR35,SR4,CRZ35,SB1, 
        ONE,OFF1,SB258,Z0,Z28]
       [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 \texttt{\{,0\}} in stead off 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.

\begin{example}
\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}
\end{example}
Example 5.16

\textbf{Example 5.16}

\begin{verbatim}
\startchemical
[width=fit,height=fit,frame=on,scale=small]
\chemical
[ONE,Z0,MOV7,SB1357,Z017,3OFF5,MOV5,Z0,
3OFF5,MOV5,SB15,Db7,Z057,MOV0,MOV3,SB1357,
Z013,MOV5,3OFF5,Z0,6OFF5,SB5,Z5]
[\SL{NH},C,COOH,H,(CH_2)_3,C,H,\SL{H},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}.

Example 5.17

\begin{verbatim}
\startchemical
[width=fit,height=fit,frame=on]
\chemical
[SIX,Db135,SB246,Z,SR6,RZ6][C,C,N,\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]
\bottext
{2,2-Dimethyl-3-ethylpentane}
\chemical
[ONE,Z3570,SB1357]
[CH_3,\T{1}{H_3C},CH_3,\SR{\LT{2}{C}}]
\chemical
[MOV1,OFF1,Z0,SB3]
[\T{3}{CH}]
\chemical
[MOV3,Z0,SB3,MOV3,Z0,MOV7,MOV7]
[CH_2,CH_3]
\chemical
[OFF1,SB1,MOV1,OFF1,Z0,2OFF1,SB1,Z1]
[\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`.

<table>
<thead>
<tr>
<th>Key</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>\+{number}</code></td>
<td>positive charge in Roman</td>
</tr>
<tr>
<td><code>\-{number}</code></td>
<td>negative charge in Roman</td>
</tr>
<tr>
<td><code>\1</code></td>
<td>I (without sign)</td>
</tr>
<tr>
<td><code>\7</code></td>
<td>II, III, IV, V, VI and VII</td>
</tr>
</tbody>
</table>

**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
```
Explanation

will result in:

\[ S + O_2 \rightarrow S^\text{+IV} O_2 \quad (6.1) \]

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

Example 6.2

\[
\begin{align*}
\text{Example 6.2} \\
\text{Table 6.2 Text: repeating.}
\end{align*}
\]

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

\[
\begin{align*}
\text{Table 6.3 Text: around an atom.}
\end{align*}
\]

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 \textit{smashed} text.
An example is given below. The text is centred around the first character.

Example 6.3

```
\startchemical[frame=on]
  \chemical[SIX,B,R36,RZ36][\SL{COOH},\SL{COOH}]
\stopchemical
```

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

```
\placeformula
  \startformula
    \startchemical[width=fit]
      \chemical[SIX,B,Z1,MOV1,B][\hbox{$\bullet$}]
      \toptext{\sl trans}-Decalin
    \stopchemical
    \hskip 24pt
    \startchemical[width=fit]
      \chemical[SIX,B,Z12,MOV1,B][\hbox{$\bullet$},\hbox{$\bullet$}]
      \bottext{\sl cis}-Decalin
    \stopchemical
  \stopformula
```

Both Decalin formulas look like this:
trans-Decalin

cis-Decalin

Explanation

(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
\startchemical
[axis=on,
width=6000,height=4000]
\stopchemical

Example 7.2
\startchemical
[axis=on,
left=2000,right=4000]
\stopchemical

Example 7.3
\startchemical
[axis=on,
width=6000,right=1000]
\stopchemical
Example 7.4
\startchemical
[\text{axis}=on,\
  \text{width}=6000,\text{top}=1000,\text{bottom}=3000]\
\stopchemical

The dimensions of the total structure determine the dimensions of the axis. When \text{width}=\text{fit} and/or \text{height}=\text{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 \texttt{\start--\stop} pair you can use \texttt{PCTeX} 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 size</td>
<td>number</td>
<td>medium</td>
</tr>
<tr>
<td>state option</td>
<td>start stop</td>
<td>start</td>
</tr>
<tr>
<td>axis 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 \texttt{left}, \texttt{right}, \texttt{top} and/or \texttt{bottom} in combination with \texttt{width} and \texttt{height}.

You can use the key \texttt{size} to set up the bodyfont. In doing so the \TeX-primatives \texttt{textsize}, \texttt{scriptsize} and \texttt{scriptsamplesize} 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}, \texttt{medium} and \texttt{big} are proportionally related.
The set up of the parameter `bodyfont` is used for calculations and has no consequences for the text. In **\LaTeX** and **\TEX** this set up parameter is coupled to the mechanism that sets the bodyfont.

In **\TEX** and **\LaTeX** you can use commands like `\rm`, `\bf` and `\sl` in mathematical mode. **PPCHTEX** uses default `\rm`. With the parameter `character` another alternative can be chosen. In **example 8.1** the substituents are typeset *slanted*.

```
Example 8.1
\startchemical[frame=on,character=\sl]
  \chemical[SIX,B,R,RZ][A,B,C,D,E,F]
\stopchemical
```

The set up of `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 `\rm`, `\bf` and `\sl`. Italic `\it` formulas lead to a bigger linewidth. In **\LaTeX** default bold–slanted (`\bs`) and bold–italic (`\bi`) are available. These commands adjust automatically to the actual fontstyle: `CH_4`, `CH_4`, `CH_4` etc. (`\ss`, `\rm`, `\tt`).

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

```
Example 8.2
\startchemical[frame=on]
  \chemical[SIX,B,R,RZ][\tf a,\bf b,\it c,\sl d,\bi e,\bs f]
\stopchemical
```

With parameter `state` calculations can be shortcut. The parameters `frame` and `axis` need no further explanation. With `option=test` frames are drawn around the texts in a structure. In this way you can see how the text is aligned.\footnote{In **\LaTeX** you can activate the visual debugger. When activated the baseline is a dotted line. The module `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 chosen 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$_2$O) and with **LOW** somewhat lower (H$_2$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
You can also type a number between 1 and 1000 in `scale`. The values belonging to `small`, `medium` or `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 GIVES and PLUS need no further explanation. With 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 '?'\texttt{.} In addition \texttt{MESOMERIC} is also available. Braces used for displaying complexes can be created with \texttt{OPENCOMPLEX} and \texttt{CLOSECOMPLEX}.
When you are combining atoms or molecules, for example with \textit{SUB}, some positions and dimensions change their value. To overcome this problem it is possible to save a location with \textit{SAVE} and return to that location with \textit{RESTORE}.

<table>
<thead>
<tr>
<th>SAVE</th>
<th>Restore Status</th>
<th>save actual status</th>
<th>restore actual status</th>
</tr>
</thead>
</table>

\begin{table}[h]
\centering
\caption{Positioning.}
\begin{tabular}{|c|c|}
\hline
SAVE & Save Status \tabularnewline
\hline
RESTORE & Restore Status \tabularnewline
\hline
\end{tabular}
\end{table}

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

\begin{verbatim}
\definechemical[molecule]
  \chemical
    [\text{O,2,SB1357,}
     \text{SAVE,SB2,SIX,B,R6,C,RESTORE,}
     \text{MOV1,2,SB137,}
     \text{MOV1,2,SB37,}
     \text{MOV1}]
  [\text{C,C,C}]
\end{verbatim}

\begin{verbatim}
\startchemical[width=fit,height=fit]
  \chemical[molecule,molecule,molecule]
\stopchemical
\end{verbatim}

The example below is more complicated and show a complete reaction. The set up of bottom and top is essential in this example.
Explanation

\placeformula
\startformula
\setupchemical
[width=fit,top=2000,bottom=2000,
scale=small,size=small]
\startchemical
\chemical
[ONE,
SAVE,
Z0,SB7,SB3,SB1,M0V1,Z0,SB1,M0V1,Z0,DB8,CZ8,SB1,Z1,
RESTORE,
SAVE,
SUB4,ONE,Z0,SB3,SB1,M0V1,Z0,SB1,M0V1,Z0,DB8,CZ8,SB1,Z1,
RESTORE,
SUB2,ONE,Z0,SB7,SB1,M0V1,Z0,SB1,M0V1,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_{2}O]
\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 SB731 in stead of SB7,SB3,SB1. But in this way the definition is readable. Complex structures can best be defined in its respective components.

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

**Example 10.1**

\begin{verbatim}
\startchemical[height=fit,frame=on]
\chemical[ONE,SB]
\stopchemical
\end{verbatim}

**Example 10.2**

\begin{verbatim}
\startchemical[height=fit,frame=on]
\chemical[ONE,3OFF1,SB]
\stopchemical
\end{verbatim}
The next example shows the definition of complexes. Pay special attention to the use of \textbf{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.

\startformula
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical

\stopchemical
\setupchemical[\textcolor{black}{\texttt{scale=small}},\texttt{width=fit}]
\startchemical
\endformula
Without the use of \texttt{SPACE} the separate structures would merge. Most of the time the optimization of such a reaction is an iterative process.
11 Reactions

Not only the typesetting of chemical structures is supported but also the typesetting of normal reactions. The command \chemical has three other appearances:

- \chemical{formula}
- \chemical{formula}{bottom text}
- \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 \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 \startformula and \stopformula) both arguments do have a function. First a simple example. The command \placeformula is a CONTiXT command and handles the positioning and numbering of the formula.

\placeformula
\startformula
\chemical{2H_2} \chemical{PLUS} \chemical{O_2} \chemical{GIVES} \chemical{2H_2O}
\stopformula

\[ 2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} \quad (11.1) \]

The definition of the chemical part could be somewhat shorter:

\chemical{2H_2,PLUS,O_2,GIVES,2H_2O}

or even:

\chemical{2H_2,+,O_2,->,2H_2O}
A \TeX-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 \texttt{PLUS}, \texttt{GIVES} and \texttt{EQUILIBRIUM} \(<\rightarrow\) in this command. With \texttt{MESOMERIC} or \texttt{<>} you will get \(\leftarrow\).

The reaction can be placed in the text. In that case a more compact display is used: \[ 2\text{H}_2+\text{O}_2\rightarrow2\text{H}_2\text{O}. \]
Some finetuning with \backslash{}, would result in \[ 2\text{H}_2 + \text{O}_2 \rightarrow \text{2H}_2\text{O}. \]

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 \texttt{\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}} or something like this \texttt{\chemical{H,-,CH,--,HC,-,H}}. A triple bond can be defined as \texttt{TRIPLE} or \texttt{---}: \texttt{HC=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!

\begin{verbatim}
2\text{H}_2 + \text{O}_2 \rightarrow \text{2H}_2\text{O} \hspace{1cm} (11.2)
\end{verbatim}

The last argument is placed under the compound.

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

The formula above is defined with:

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

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 \texttt{\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}} result with big, medium and small in the following formulas:

\begin{align*}
H &\rightleftharpoons CH \rightleftharpoons HC \rightleftharpoons H \\
H &\rightleftharpoons CH \rightleftharpoons HC \rightleftharpoons H \\
H &\rightleftharpoons CH \rightleftharpoons HC \rightleftharpoons 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 $\text{chemical}{Fe_2^{+2}Cr_2O_4}$. This will result in $Fe_2^{+2}Cr_2O_4$. Without correction it would have been: $Fe_2^{+2}Cr_2O_4$.

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.

\begin{center}
\begin{verbatim}
Example 12.1
\startchemical[frame=on,option=test,alternative=2]
  \chemical[SIX,B,R13,HIGH,RZ1,LOW,RZ3][NH_3,NH_3]
\stopchemical
\end{verbatim}
\end{center}

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 $\text{chemical}{HIGH,H_2O}$ then you will get $H_2O$ and $\text{chemical}{LOW,H_2O}$ will become $H_2O$. 
Part 2
Backgrounds
1 Installation

The package PPCHTEX is developed for use in combination with CONTEX. PPCHTEX is activated in CONTEX by:\n
\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 \LaTeX2ε 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 userinterface 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 \setup... make it possible to make readable ASCII–layouts. Compare for example:

\setupchemical[size=small]

and:

\setupchemical
  [size=small, scale=500, textsize=big]

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 ppchtex.tex you may notice that \processaction macros are being used while interpreting the keys in \chemical[]. These kind of macros are relatively slow but then the PPCH\TeX{} interface is very flexible.
3 | Fonts

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 \textit{x} height (\fontdimens5).

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 failsafe 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}. 
4 Definitions

The interface of PPCH\TeX is derived from the CON\TeX 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 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 modules from the mult group.
5 Color

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 CONITTEx PPCHiTEx supports interactive texts. An interactive text is a text that can be consulted on a computer screen 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**

\startchemical[axis=on, frame=on, width=5000]
  \chemical[SIX,B]
  \chemical[sub:cooh][SIX,R1,RZ1][COOH]
\stopchemical

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

```latex
... text ... \goto{\chemical{COOH}}[sub:cooh] ... text ...
```

In this definition \goto is a CONITTEx–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:

```latex
\paragraph[txt:cooh]{Substituents}

... text ... \chemical{COOH} ... text ...
```

A combination is also possible. In that case it is necessary to mark the reference with \chemical and to refer in the text with \go\toco\mehemical.

The coupling of the interaction mechanism is done with macros:

```latex
\localgotochemical \{reference\} \{text\}
\localthisischemical \{reference\}
```

You can see the CONITTEx sources for more information.
Part 3
Overview
Overview

1 One

SB   DB   TB

EP   ES   ED   ET

SD   LDD   RDD

HB   BB   OE

PPCHT_{\text{EX}}
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

SR

- SR

+ SR

ER

DB

DR

ZN

A

B C

D

ZT

Z1

Z2 Z3

Z4

Z

R1

R2 R3

R1

R2

R3

R4

-RZ

R1

R2

R3

R4

+ RZ

PPCHTeX 3–7
Five
Overview

5  Six

B  EB
MID  MIDS  MIDZ
S  SS  -SS  +SS
Overview
Overview

ROT1

ROT2

ROT3

ROT4

ROT1

ROT2

ROT3

ROT4
6 | Eight

Overview

B

SB

−SB

+SB

Z
7 Five Front

Overview

B

BB

R

-R

+R

SB

-SB

+SB

Z

-Z

+Z

PPCHTEX 3–22
8 Six Front

\begin{align*}
\text{B} & \quad \text{BB} \\
\text{R} & \quad -\text{R} \quad +\text{R} \\
\text{SB} & \quad -\text{SB} \quad +\text{SB} \\
\text{Z} & \quad -\text{RZ} \quad +\text{RZ}
\end{align*}
Overview

9 Carbon

B
C
CB
MOV
ROT
MIR
Z
MOV1
MOV2
MOV3
MOV4
10 Newman Stagger
Overview

11 Newman Eclipse

B

C

CB

MOV

ROT

Z

MOV1

MOV2

MOV3

MOV4

ROT1

ROT2

ROT3

ROT4
Overview

12 Symbol

GIVES

EQUILIBRIUM

MESOMERIC

PLUS

MINUS

OPENCOMPLEX

CLOSECOMPLEX

SPACE