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**PPCH $\TeX$ : typesetting chemical formulas in  $\TeX$** 

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**Abstract**

This article is about a package for typesetting chemical formulas. The primary interface of this package is in the Dutch language. Because PPCH $\TeX$  has a multilingual interface, all commands and keywords can be toggled to English. The Dutch version of this article is published in *N $\mathcal{T}G$ 's MAPS* (94.2) and is translated to English by H. de Weert.

**1 Introduction**

The macro-package PPCH $\TeX$  can be used to typeset chemical formulas. The macros are based on P $\mathcal{I}$ C $\TeX$ , a macropackage that was created to facilitate the drawing of graphics and other line diagrams. P $\mathcal{I}$ C $\TeX$  was brought to the public domain by M.J. Wichura. We are considering a second implementation, using T. van Zandt's PSTRICKS.

The macros can be used within different  $\TeX$ -environments because they only depend on Knuth's plain  $\TeX$ . In addition, some general macros of our Con $\TeX$ t-library are utilized. Macros are written in such a way that further development is quite easy.

At first, macros are created to typeset chemical structure formulas. Moreover, reaction mechanisms can be reflected. Chemical structures can be typeset in different sizes and comparable formulas can be linked optically. Structures of frequent occurrence can be predefined and recalled.

During the development of the macros, processing speed is subordinated to flexibility, simplicity and quality. No use has been made of the mechanism (available in P $\mathcal{I}$ C $\TeX$ ) to store parts of figures in a file. It turned out that this mechanism does not produce a gain of time.

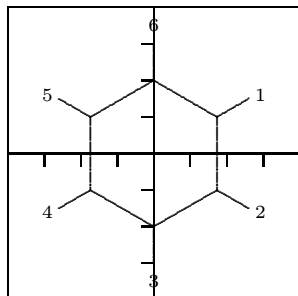
*The macros are still being developed. For example, the mechanism to place texts still has to be refined and some structures like CHAIR still have to be added.*

**2 Structures**

The number of commands that is used to typeset chemical structure formulas is reduced to four.<sup>1</sup> In the following example all of these commands are used.

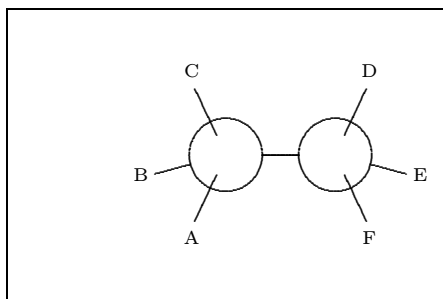
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<sup>1</sup> The concept structure in this manual only refers to the chemical structure. It is not related to the structure of the text that is used to typeset the formula.

**Example 1**

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

Different features of the typesetting can be set up with `\setupchemical`. If something is set up in this way, the setups are valid for all the following formulas.<sup>2</sup>

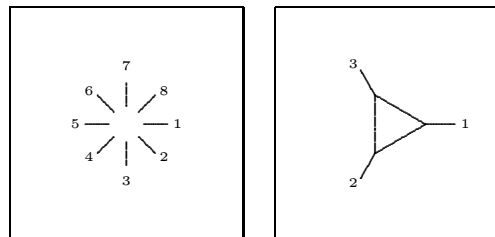
**Example 2**

```
\startchemical[border=on,width=6000]
  \chemical[CARBON,CB1][A,B,C,D,E,F]
\stopchemical
```

As can be seen from both examples, `\chemical` is the central command. This command, that can be typed many times within a `\start`-`\stop`-pair, gets one or two arguments. These arguments are given between `[ ]`. The first argument refers to the bonds that are to be drawn. The second argument contains the atoms or molecules that are to be reflected. Text is typesetted in a mathematical mode, so everything that is normally allowed between `$ $` can be given.

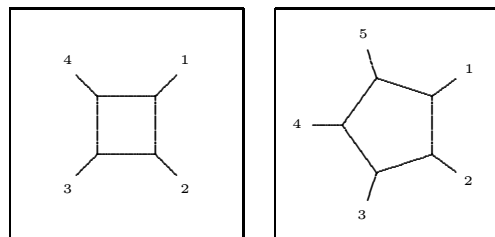
We work out the first example. First of all the keyword `SIX` is given. By using this word we can indicate that we want to draw a sixring structure. In the same way we can use the keywords `ONE`, `THREE`, `FOUR`, `FIVE`, `NEWMAN` and `CARBON`.

<sup>2</sup> Obviously the scope can be confined by using `{ }` and the grouping macros `..group`. The setups can also be given immediately after `\startchemical`. In that case the setups are applied to one formula.



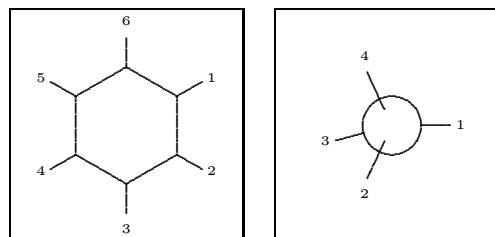
One

Three



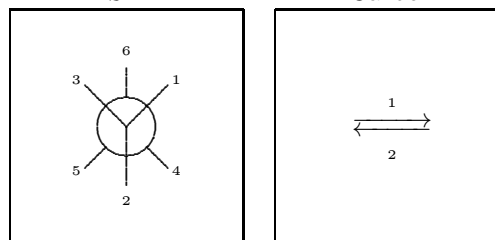
Four

Five



Six

Carbon



Newman

Symbol

Within these structures chemical bonds between C-atoms can be indicated in a comparable way. For instance, in this example we use B and R. Bonds are numbered and can be indicated in different ways:

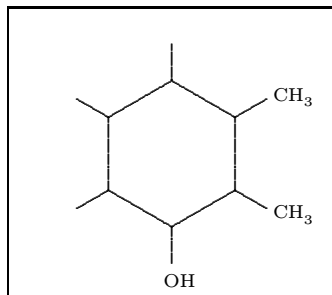
```
\chemical[SIX,B1,B2,B3,B4,B5,B6]
\chemical[SIX,B135]
\chemical[SIX,B1..5]
```

These commands create parts of a sixring structure. `R` enables us to add substituents to the sixring structure. The command `R` draws the beginning of a bond with a substituent from an angular point in the sixring structure ( $\angle 120^\circ$ ). The concerning angular point is indicated with a number.

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

The above mentioned command only places bonds to substituents. Substituents themselves are indicated with `RZ`. Therefore in this case, numbers

are being used to mark the position. In the second optional argument substituents are given as text.



### Example 3

```
\startchemical[border=on,width=4500]
\chemical[SIX,B1..6,R1..6,RZ1..3][CH_3,CH_3,OH]
\stopchemical
```

If the second argument is omitted, no text is placed, so the command `RZ1..3` has no effect.

### 3 Definitions

It is possible to build a library of structures. As we wish, we can recall these structures at a later point of time and provide them with extra components. Furthermore they can serve as building blocks for more complex structures. Structures can be predefined with the  $\TeX$ -primitive `\def`.

If a structure, for example `[SIX,B,R,RZ]`, is often used, it is practical to predefine this structure.

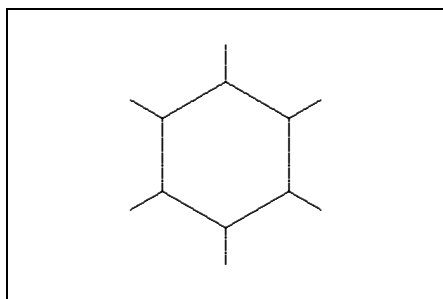
```
\def\sixring{\chemical[SIX,B,R,RZ]}
```

Instead of `\def` the following command can be used. In this case an already existing definition will be announced.

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

Although both ways of defining are allowed, the second way is more robust. Protective measures are taken to avoid conflicts with existing commands.

The command `\chemical[sixring]` provides a sixring structure without substituents. No second argument is given.

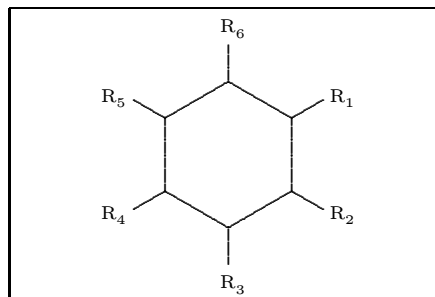


### Example 4

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

```
\startchemical[border=on,width=6000]
\chemical[sixring]
\stopchemical
```

If we want to add six substituents, we have to carry out the following actions:

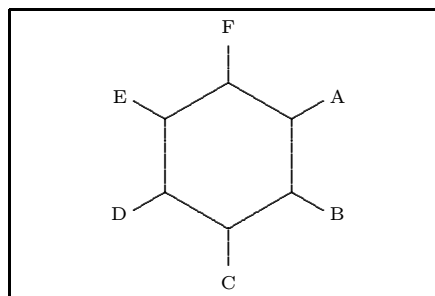


### Example 5

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

\startchemical[border=on,width=6000]
\chemical[sixring]%
[R_1,R_2,R_3,R_4,R_5,R_6]
\stopchemical
```

The sixring structure can also be defined without substituents (`RZ`). In this case no substituents are expected if the command `\chemical` is given. Even now substituents can be placed, as is shown by the following example.



### Example 6

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

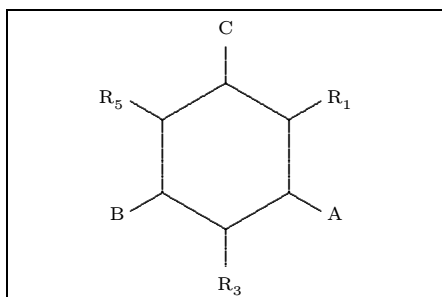
\startchemical[border=on,width=6000]
\chemical[sixring,RZ][A,B,C,D,E,F]
\stopchemical
```

Essentially the number of possibilities is unlimited. One should be aware of the fact that the atoms and molecules of the second argument are raised in the sequence of the first argument.

In a definition atoms and molecules (texts) can also be placed.

```
\definechemical[sixring]
{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5]}
```

So in this definition always three substituents are added. If we decide to add more substituents, we have to explicitly state that we are dealing with a sixring structure (SIX).



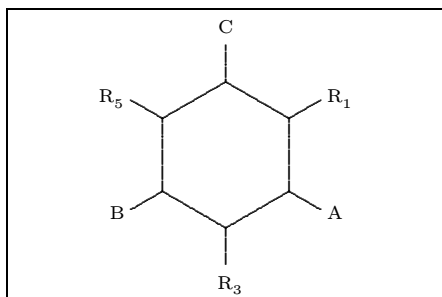
#### Example 7

```
\definechemical[sixring]
{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5]}
```

```
\startchemical[border=on,width=6000]
\chemical[sixring,SIX,RZ246][A,B,C]
\stopchemical
```

So in definitions, the command `\chemical` has a global character and the command `\chemical[] []` has a local character. The idea behind this is that in the first case a series of commands is inserted and in the second case a complete independent structure is inserted.

In a definition the command `\chemical` can occur more than once. The last example can also be recalled with:



#### Example 8

```
\definechemical[sixring]
{\chemical[SIX,B,R,RZ135][R_1,R_3,R_5]
\chemical[SIX,RZ246]}
```

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

If PPCH<sub>T</sub>E<sub>X</sub> makes mention of an unknown command, one has probably forgotten to type a structure command, like `SIX` or `FIVE`.

## 4 Bonds

In this section we show the bonds that can be found in the different chemical structures. The meaning of the commands will be explained by the reviews that are stated further in this article.

In the left column the complete bonds are shown, in the right column only the shortened bonds. Due to these shortened bonds, atoms and molecules can be attached to a bond. Bonds can be shortened on both sides, left (-) as well as right (+).

B	Bond	SB	Single Bond
		-SB	Left Single Bond
		+SB	Right Single Bond

Table 1: Saturated bonds

A bond can be followed by one or more numbers or a range, for instance: `B1`, `B135` and `B1..5`. If all bonds are necessary, only `B` can be given.

In a ring structure an extra bond can be given and furthermore double or triple bonds can be introduced between atoms and molecules.

EB	Extra Bond	DB	Double Bond
		TB	Triple Bond

Table 2: Unsaturated bonds

A bond, in a sixring structure for example, can be shortcut. In this case the atom is given that has to be omitted, therefore a circle can be drawn in a sixring structure.

S	Shortcut	C	Circle
---	----------	---	--------

Table 3: Special bonds

Substituents can be attached to the angular points and depending on the presence of atoms and molecules the bonds can be short or long.

It is possible to bind substituents to the structure by double bonds.

Text can be linked to bonds. These texts are collected from the second set behind `\chemical` in the sequence that is given.

The atoms—/—molecules are numbered clockwise. In this case, combinations are allowed. With `Z0` (z zero) a text can be placed in the middle of a structure.

R	Radical
SR	Single Radical
-R	Left Radical
-SR	Single Left Radical
+R	Right Radical
+SR	Single Right Radical

Table 4: Bonds to substituents

ER	Extra Radical	DR	Double Radical
----	---------------	----	----------------

Table 5: Double bonds to substituents

While positioning the atoms and molecules in the text, their (possible) dimensions are taken into account. In this case the width of  $C$  and the height of  $C_m^n$  play a prominent role. However, this mechanism can still be refined.

## 5 Combinations

Structures can be combined to complex compounds and can be moved to other structures by using MOV, ROT, ADJ and SUB.

These four commands have another effect within the different structures. For example, the angle used to rotate at `\chemical[FIVE,ROT1,B]` differs from the angle that is used at `\chemical[SIX,ROT1,B]`.

In addition, within CARBON it is possible to mirror a structure. This can be done with MIR.

The direction of a displacement or the amount of the rotation is indicated by a number. Since these commands are closely related to the actual structure, they must be given before bonds and texts are drawn. It makes a difference whether one gives the command `\chemical[FIVE,B,ROT1,R]` or `\chemical[FIVE,ROT1,B,R]`. The first call delivers an unwanted result.

Z	Atom	RZ	Radical Atom
		-RZ	Left Radical Atom
		+RZ	Right Radical Atom

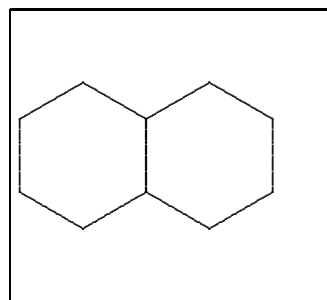
Table 6: Atoms and molecules (radicals)

MOV	Move	move the same kind of structure in the direction of a bond
ADJ	Adjacent	move a different kind of structure in the direction of the $x$ - or $y$ -axis, linked to a bond
SUB	Substitute	move a structure relative to another one in the direction of the $x$ - or $y$ -axis
ROT	Rotate	rotate a structure

Table 7: Displacements and rotations.

MIR	Mirror	mirror a structure
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Table 8: Mirroring

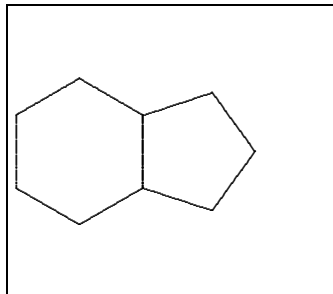


### Example 9

```
\startchemical[border=on,width=4500,right=3500]
\chemical[SIX,B,MOV1,B]
\stopchemical
```

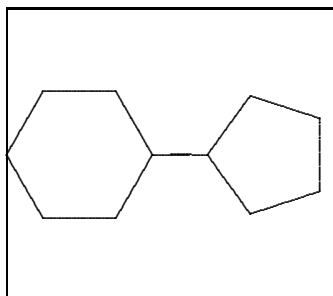
Successively a sixring structure is drawn: SIX,B, a displacement is realized in the direction of bond 1: MOV1, and a second sixring structure is drawn: B. A displacement with MOV concerning a sixring structure can be realized in six directions, as opposed to a displacement with ADJ, which is realized in the four axis-directions ( $x$ ,  $-x$ ,  $y$ ,  $-y$ ). In a sixring structure some of these displacements coincide. The above example also could have been achieved with: [SIX,B,ADJ1,B].

It is also possible to combine different structures. For instance, SIX can be linked to a structure FIVE. The mechanism that is responsible for this linking is for the greater part hidden from the user. In the following example a sixring structure is successively drawn: SIX,B, a displacement along the positive  $x$ -axis is achieved: ADJ1, and a rotated fiveing structure is drawn: FIVE,ROT3,B.

**Example 10**

```
\startchemical[border=on,width=4500,right=3500]
  \chemical[SIX,B,ADJ1,FIVE,ROT3,B]
\stopchemical
```

A transition to a connected structure can be achieved with ADJ. To get a good connection, one of the two structures have to be rotated with ROT. If a structure is not directly linked, but through a bond, one uses SUB. Rotations are made in steps of 90 degrees, clockwise. Displacements with ADJ and SUB are achieved in the four axis-directions.

**Example 11**

```
\startchemical[border=on,width=4500,right=3500]
  \chemical[SIX,ROT2,B,R6,SUB1,FIVE,B,R4]
\stopchemical
```

We can therefore conclude that the sequence of the given commands is very important. An obvious sequence of commands is as follows:

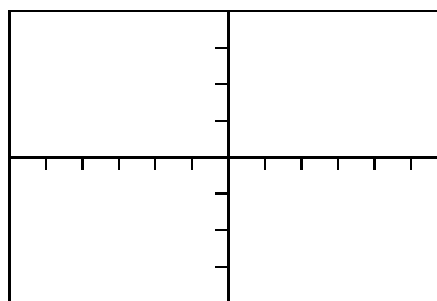
```
\chemical
[structure,           % SIX,FIVE,...
 bonds inside the structure,% B,C,EB,...
 bonds outside the structure,% R,DR,...
 locations of atoms,   % Z
 locations of substituents] % RZ,-RZ,...
[atoms,
 substituents]
```

As a rule, the connection of structures is reduced to some translations and rotations. Although it may not seem so, a certain systematic is enclosed. In fact, the process could be simplified. The automation that was already achieved in former versions has been undone: it turned out that 'hidden' rotations induce misunderstandings with regard to

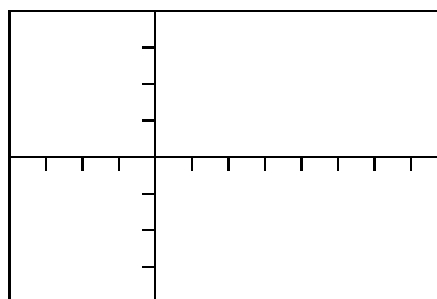
the place of bonds. Furthermore, it is easier to provide a structure that is not rotated with bonds, atoms and molecules than to provide a rotated structure. It is better to define the parts of a complex structure first, possibly with translations, and to rotate the complete complex structure later.

**6 Axis**

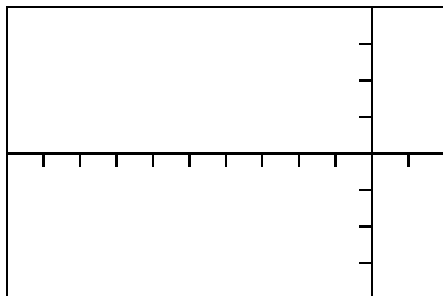
Structures are typeset in a bounded space, for convenience indicated by axis. The dimensions of the axis and the location of the origin can be defined in the setup. In addition the axis can be made visible (for the sake of the location in the text) and a border can be drawn.

**Example 12**

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

**Example 13**

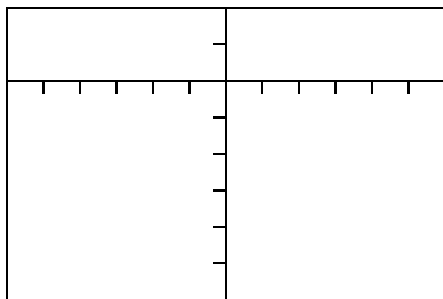
```
\startchemical
  [axis=on,
   left=2000,right=4000]
...
...
\stopchemical
```

**Example 14**

```
\startchemical
[axis=on,
width=6000,right=1000]
...
...
\stopchemical
```

The dimensions of the structure are determined by the dimensions of the axis. However, if at least one of following two options `width=fit` and `height=fit` is given, the dimensions of the total structure are determined by the real dimensions. Whatever is chosen is depending on the way structures are placed in the text. Side by side, on top of each other, etc. Example 12 shows the standard setups.

Within a `\start-\stop`-pair P<sub>T</sub>CT<sub>E</sub>X-macros can be used. Of course, some caution must be taken into account.

**Example 15**

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

**7 Setups**

The behavior of the macros and the layout of the formulas can be adapted to one's personal needs. After both `\startchemical` and `\setupchemical` setups can be given.

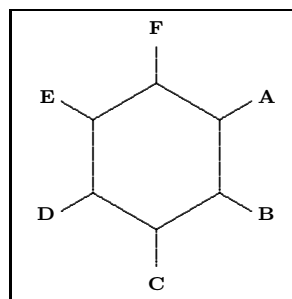
variable	values	default
width	number	4000
height	number	4000
left	number	
right	number	
top	number	
bottom	number	
resolution	number	see manual
corps	8pt 9pt 10pt etc.	see manual
style	<code>\rm</code> <code>\bf</code> etc.	see manual
scale	number small medium big	medium
size	small medium big	medium
status	start stop	start
option	test	
axis	on off	off
border	on off	off
alternative	1 2	1
offset	HIGH LOW	LOW

Table 9: Setups for structures

The axis reaches from  $-2000$  to  $+2000$ , in height as well as in width. The point Z<sub>0</sub> is situated at (0,0). Other setups can be set up with `left`, `right`, `above` and/or `under` in combination with `width` and `height`.

The dimensions of the characters can be set up with `size`. In doing so, the T<sub>E</sub>X-primitives `\textsize`, `\scriptsize` and `\scriptscriptsize` are used. The dimensions of the structure itself can be set up with `scale` (1..1000). The scale is also determined by `corps`. The keywords `small`, `medium` and `big` are attuned.

In the mathematical mode commands like `\rm`, `\bf` and `\sl` can be utilized in T<sub>E</sub>X as well as in ConT<sub>E</sub>Xt. PPCHT<sub>E</sub>X by default uses `\rm`. An alternative command can be set up with `style`. For instance in example 16 the substituents are typeset **bold**.

**Example 16**

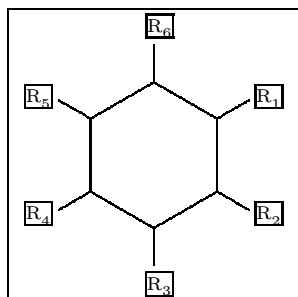
```
\startchemical[border=on,style=\bf]
```

```
\chemical[SIX,B,R,RZ][A,B,C,D,E,F]
\stopchemical
```

For the time being `style` is valid for chemical formulas in the text as well as in a figure. The sub- and superscripts also change, as can be seen from:  $CH_4$ ,  $\overset{H}{C}H_4$  and  $\overset{H}{\underset{H}{C}}H_4$ . Successively the setups are: `\rm`, `\bf` and `\sl`. When formulas are typeset in italic (`\it`), baseline-distances can be greater than normal. Within ConT<sub>E</sub>Xt bold-slanted (`\bs`) and bold-italic (`\bi`) are also available. All these commands automatically adjust to the actual style (`\ss`, `\rm`, `\tt`):  $CH_4$ ,  $\overset{H}{C}H_4$  etc.

The time-consuming calculations can be short-circuited with `status`. The variables `border` and `axis` speak for themselves. A border round a text can be drawn with `option=test`. By doing so, one can see how things are aligned. The quality of the lines is set up with `alternative`. By default, P<sub>l</sub>CT<sub>E</sub>X uses a 5 point period to draw the lines. As one chooses alternative 2 smaller points are used. Therefore thinner lines are drawn.

The offset refers to the position of the sub- and superscripts. By using `HIGH` the subscripts are positioned high ( $H_2O$ ). Obviously, with `LOW`, the subscripts are positioned a little lower ( $H_2O$ ).

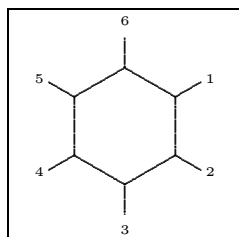


### Example 17

```
\startchemical[border=on,option=test,%
alternative=2]
\chemical[SIX,B,R,RZ][R_1,R_2,R_3,R_4,R_5,R_6]
\stopchemical
```

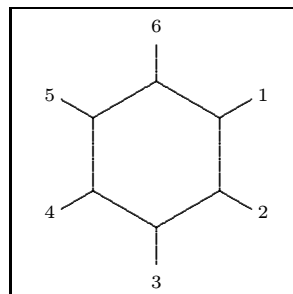
## 8 Dimensions

A structure can be shown in different sizes. Dimensions can be set up with `size` and `scale`.



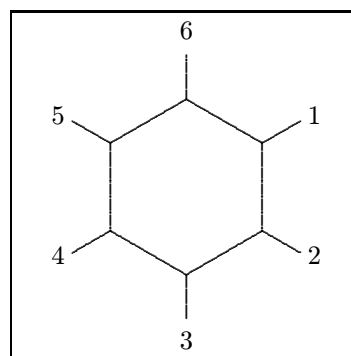
### Example 18

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



### Example 19

```
\startchemical[scale=medium,size=medium]
\chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical
```



### Example 20

```
\startchemical[scale=big,size=big]
\chemical[SIX,B,R,RZ][1,2,3,4,5,6]
\stopchemical
```

Scaling can take place between 1 and 1000. The values belonging to the keywords `small`, `medium` and `big` are attuned.

## 9 Symbols

To typeset reaction equations some symbols are available. In the following figure an equation is shown. This equation is defined as follows:

```
\setupchemical
[width=fit,
height=5500,
under=1500]
\hbox
{\startchemical
\chemical[SIX,B,ER6,RZ6][0]
\stopchemical
\startchemical
```

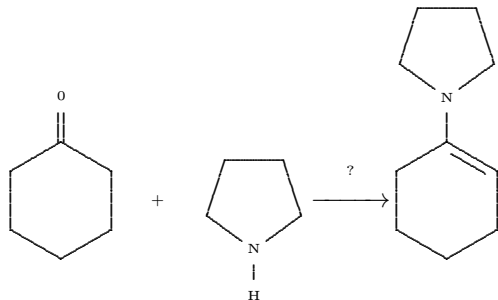


```

\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

```

The command `\hbox` is necessary to position the structures behind each other. The symbols `GIVES` and `PLUS` speak for themselves. Extra space can be achieved with `SPACE`.



An equilibrium can be shown with `EQUILIBRIUM`. A text can be set above `GIVES` and `EQUILIBRIUM`. In the example this text is a question mark.

## 10 Special features

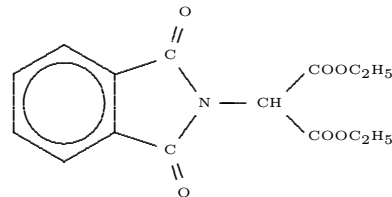
By using `ONE`, `ZO` can consist of more than one atom. In this case, the reserved space is insufficient. If more space is needed for the command `ZO`, the bonds 1, 2 and 8 can be moved with the command `OFF`, which means ‘offset’. Below, an example of the use of this command is given.

```

\startchemical[width=fit]
\chemical
[SIX,B,C,ADJ1,
FIVE,ROT3,SB34,+SB2,-SB5,Z345,DR35,SR4,%
CRZ35,SUB1,ONE,OFF1,SB258,ZO,Z28]
[C,N,C,O,O,
CH,COOC_2H_5,COOC_2H_5]
\stopchemical

```

In this case the offset is 1, which means that we use one extra character. Though definitions appear to be quite complicated at first, they can best be constructed by defining the separate parts first. The rotation can best be made last.



A new command is seen in the above example: `CRZ`. This command can be used to position an atom or a molecule in line with a bond, which is desirable in this case. This positioning could have been achieved with the command `RZ`, since one can influence the spacing with the second set: `{\,0}` instead of `{0}`.

OFF	Offset	CRZ	Centered Radical Atom
-----	--------	-----	-----------------------

Table 10: Special commands

## 11 Text formulas

Along with the typesetting of structure formulas, the typesetting of reaction equations is supported too. Therefore, the previously described command `\chemical` has another two versions:

```

\chemical{formula}
\chemical{formula}{text}

```

This command will fit to the position in the text. This means that a difference is made between:

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

If the command is given in the current text, automatically `$$` are set round the command. In this way the command `\chemical{NH_4^+}` delivers the formula  $NH_4^+$ .

The same result is achieved by placing the command between `$$`. Therefore in both cases the second argument is omitted. If we type the command between `$$$ $$$`, the second argument is obliged. The second argument may be empty:

```

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

```

gives:



This formula can also be defined in a shorter way:

```

$$$ \chemical{2H_2,PLUS,0_2,GIVES,2H_2O}{ } $$$

```

or even:

```
$$\chemical{2H_2,+ ,O_2,->,2H_2O}{}$$
```

The more experienced T<sub>E</sub>X user will notice that the plus-sign as well as the arrow are located at the baseline; i.e., just compare + and +. Independent of the size of reflection, the + and the  $\longrightarrow$  are aligned.

In addition to PLUS and GIVES, EQUILIBRIUM can be given, which delivers double arrows ( $\longleftrightarrow$ ).

This formula can also be typeset in the current text, where a smaller layout is chosen:  $2H_2 + O_2 \longrightarrow 2H_2O$ . It is also possible to show bonds. For example, the rather long sequence

```
\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}
```

gives  $H-CH=HC-H$ .

This can also be achieved in a shorter way:

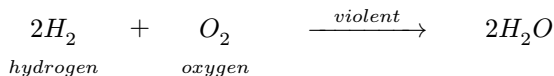
```
\chemical{H,-,CH--,HC-, -,H}
```

A triple bond can be called with TRIPLE or --:  $HC\equiv CH$ .

Now we just return to the display mode. The second argument can be used to give an explanation of the formula:

```
$$
\chemical{2H_2}{hydrogen} \chemical{PLUS}{ }
\chemical{O_2}{oxygen}
\chemical{GIVES}{violent} \chemical{2H_2O}{ }
$$
```

gives:



The size of the formulas that are placed in the text can be set up with the setup-command:

variable	values	default
textsize	small medium big	big

Table 11: Setups for text formulas

When big, medium or small is used,

```
\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}
```

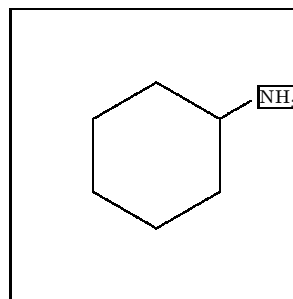
gives the successive formulas:



## 12 Subscripts

Sub- and superscripts are placed a little lower, as is recommended by Knuth in the T<sub>E</sub>Xbook. As such, the example on page 179 in the T<sub>E</sub>Xbook (that is chemically a bit strange) can be typeset by typing the command `\chemical{Fe_2^{+2}Cr_2O_4}`. This command gives  $Fe_2^{+2}Cr_2O_4$ . Without a correction, the command would have given the result:  $Fe_2^{+2}Cr_2O_4$ .

The location of the subscript is by default determined by the `offset`: HIGH or LOW. The `offset` can be overruled by the commands of the same name.



## Example 21

```
\startchemical[border=on,option=test,%
alternative=2]
\chemical[SIX,B,R1,HIGH,RZ1][NH_3]
\stopchemical
```

Although the location of the subscript can be set up by substituent, it is advisable to do this with the command `\setupchemical`. By doing so, all the formulas will be set up in the same way.

The keywords LOW and HIGH can also be used in text formulas, although this may lead to inconsistencies in layout. We can see that `\chemical{HIGH,H_2O}` results in  $H_2O$  and `\chemical{LOW,H_2O}` results in  $H_2O$ .

## 13 Installation

The package PPCHT<sub>E</sub>X is developed as an extension to ConT<sub>E</sub>Xt but can be used with other packages. The macros can be found in the file `m-chemie.tex`, with the m standing for module. Therefore the macros are not standardly available.

Furthermore, the package can be used in combination with L<sup>A</sup>T<sub>E</sub>X. In this case the file `m-chemie.sty` is used too.<sup>3</sup> PPCHT<sub>E</sub>X can be activated by means of `\documentstyle`:

```
\documentstyle[m-chemie]{}
```

In addition to the English interface that was described earlier, a Dutch interface is available. The Dutch version is loaded with:

```
\documentstyle[m-chemie]{}
```

## 14 Some Dutch

The original interface of PPCHT<sub>E</sub>X is Dutch. One can switch back to Dutch with:

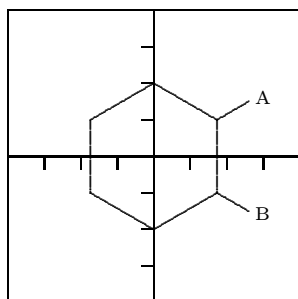
```
\resetinterface
```

Switching back to English can be done with:

```
\setinterface[english]
```

<sup>3</sup> The Dutch word chemie stands for chemistry in English.

Although more interfaces are possible, only the Dutch and English are implemented. In the file `m-chemie.sty` the interfaces are defined.



### Example 22

```
\startchemie[assenstelsel=aan,kader=aan]
  \chemie[SIX,B,R12,RZ12][A,B]
\stopchemie
```

### 15 Extensions

All T<sub>E</sub>X-users are allowed to use the PPCHT<sub>E</sub>X-macros in another, non-commercial, way. However, some caution has to be taken into account, since the macros are still being developed, optimized and made more robust. Some macros may seem quite complicated, but appearances are deceptive. For example, commands in the shape of `\setup...` utilize the macros that support nesting and different ASCII-layouts. Compare for instance:

```
\setupchemical[size=small]
```

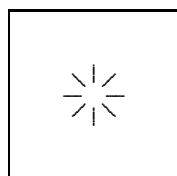
with:

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

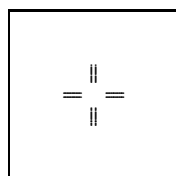
Setups can be given in an arbitrary sequence. When possible, spaces and newline-characters are suppressed and errors are announced.

*The following overview shows the available structures. We use a somewhat smaller corps to save space. The manual of PPCHT<sub>E</sub>X is a bit more extensive in its overviews.*

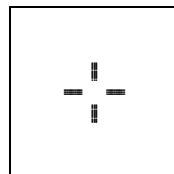
### 16 One



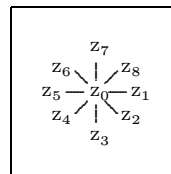
SB



DB

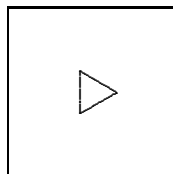


TB

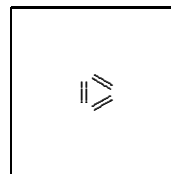


Z

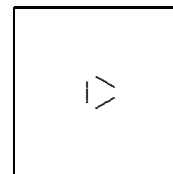
### 17 Three



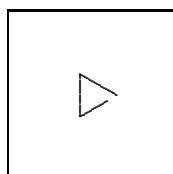
B



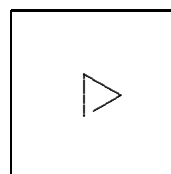
DB



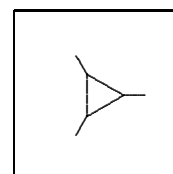
SB



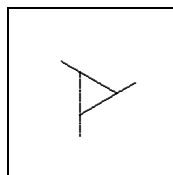
-SB



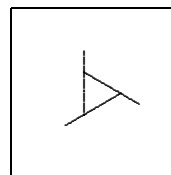
+SB



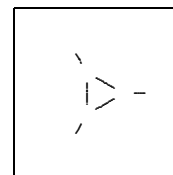
R



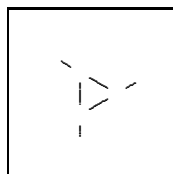
-R



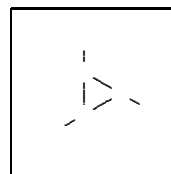
+R



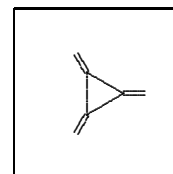
SR



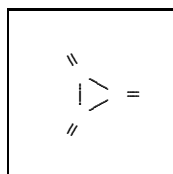
-SR



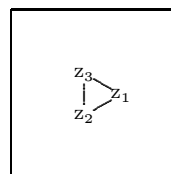
+SR



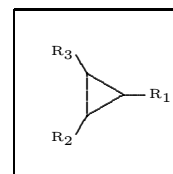
ER



DR

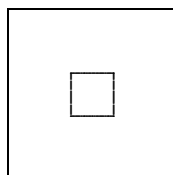


Z

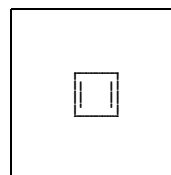


RZ

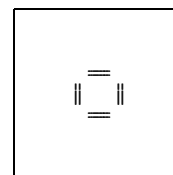
### 18 Four



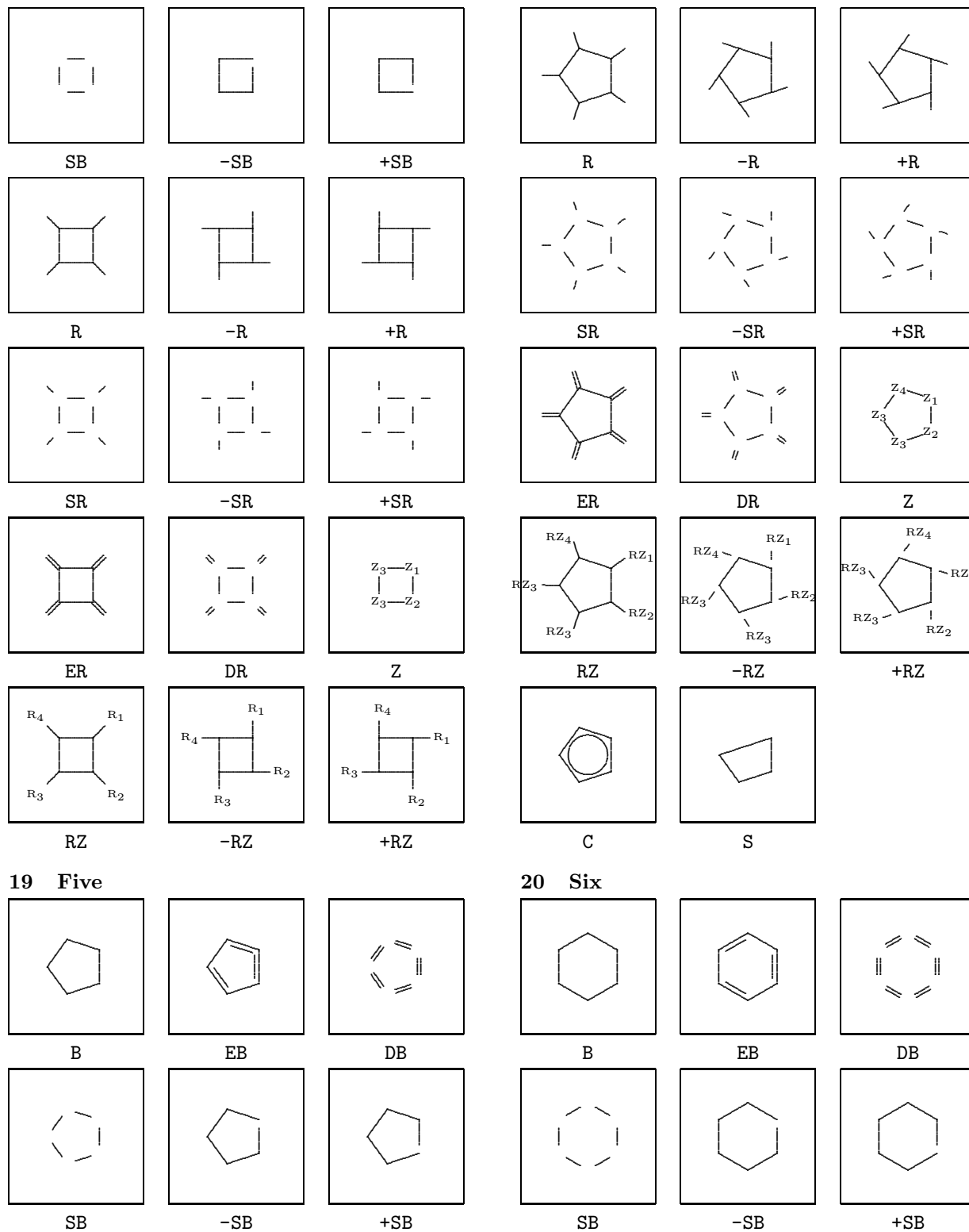
B

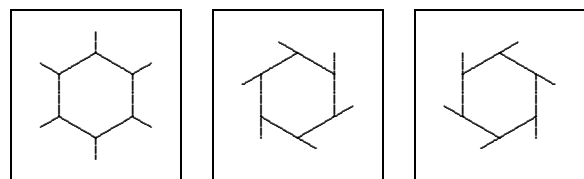


EB



DB

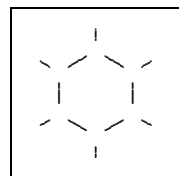




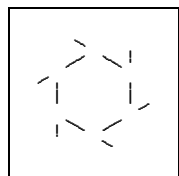
R

-R

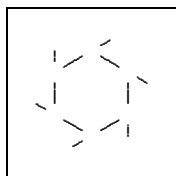
+R



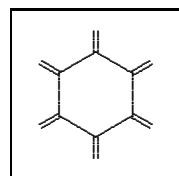
R



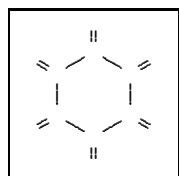
-R



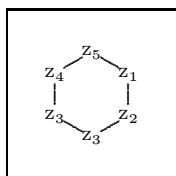
+R



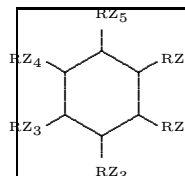
ER



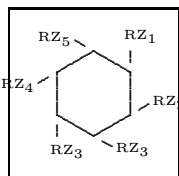
DR



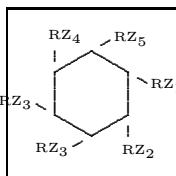
Z



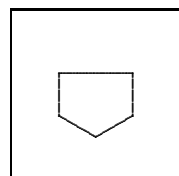
RZ



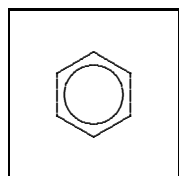
-RZ



+RZ

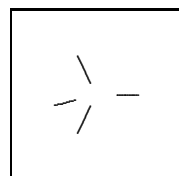


S

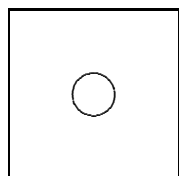


C

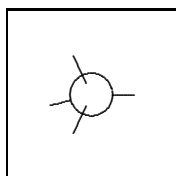
## 21 Carbon



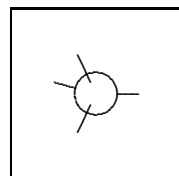
B



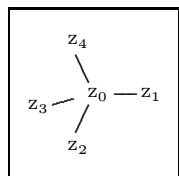
C



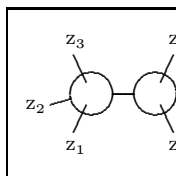
CB



MIR

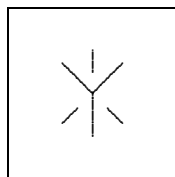


Z

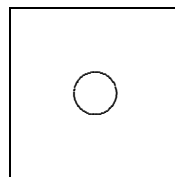


CB3

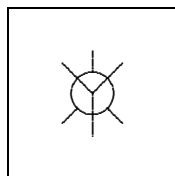
## 22 Newman



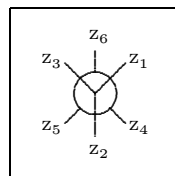
B



C

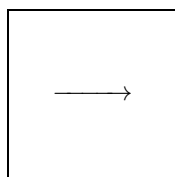


CB

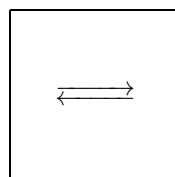


Z

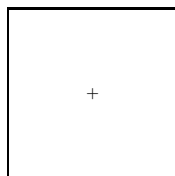
## 23 Symbol



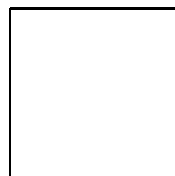
GIVES



EQUILIBRIUM



PLUS



SPACE

## 24 Other features

The following features of PPCHTEX are not described here, but one can find more on them in the manual.

- coloring parts of formulas
- active formulas in interactive texts
- automatic adapting to the corps size
- adapting to the resolution of printers
- the multilingual interface
- manipulating super- en subscripts

Also, the manual is a bit more extensive in its overview of the rotations and displacements.

◇ J. Hagen and A.F. Otten  
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8000 AC Zwolle  
The Netherlands