

PPCH_{TEX}

a macropackage
for typesetting
chemical structure-
formulas with $\text{T}_{\text{E}}\text{X}$

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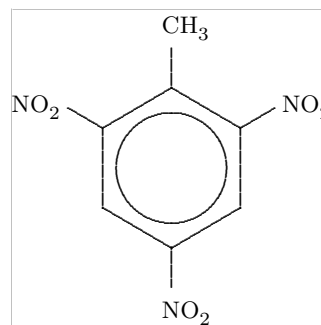
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Part 1 Explanation



Introduction

The macro-package `PPCHTEX` can be used to typeset chemical formulas. The macros are based on `PICTEX`, a macropackage that was created to facilitate the drawing of graphics and other linediagrams. `PICTEX` was brought to the public domain by M.J. Wichura. We consider a second implementation, using `PSTRICKS` of T. van Zandt.

The macros can be used within different `TEX`-environments and only depend on Knuth's plain `TEX`. In addition, some general macros of our `CONTEXT`-library are utilized. Besides, macros are typeset 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 `PICTEX`) to store parts of figures in a file. It turned out that this mechanism does not produce a gain of time.

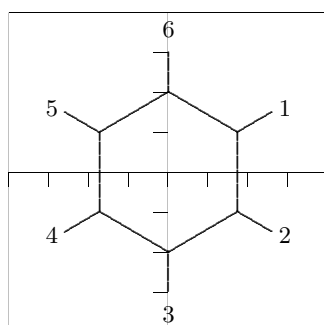
The macros are still being developed. For example, the mechanism to place texts still has to be refined. Also, the precise form of the commands will be recalculated. Finally, some structures like `CHAIR` still have to be added.

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1 | Structures

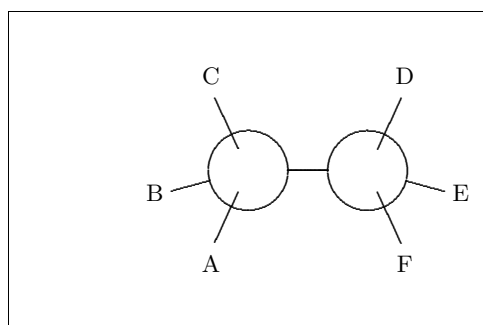
The number of commands that is used to typeset chemical structure formulas is reduced to four.¹ In the following example all of these commands are used.



Example 1.1

```
\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.²



Example 1.2

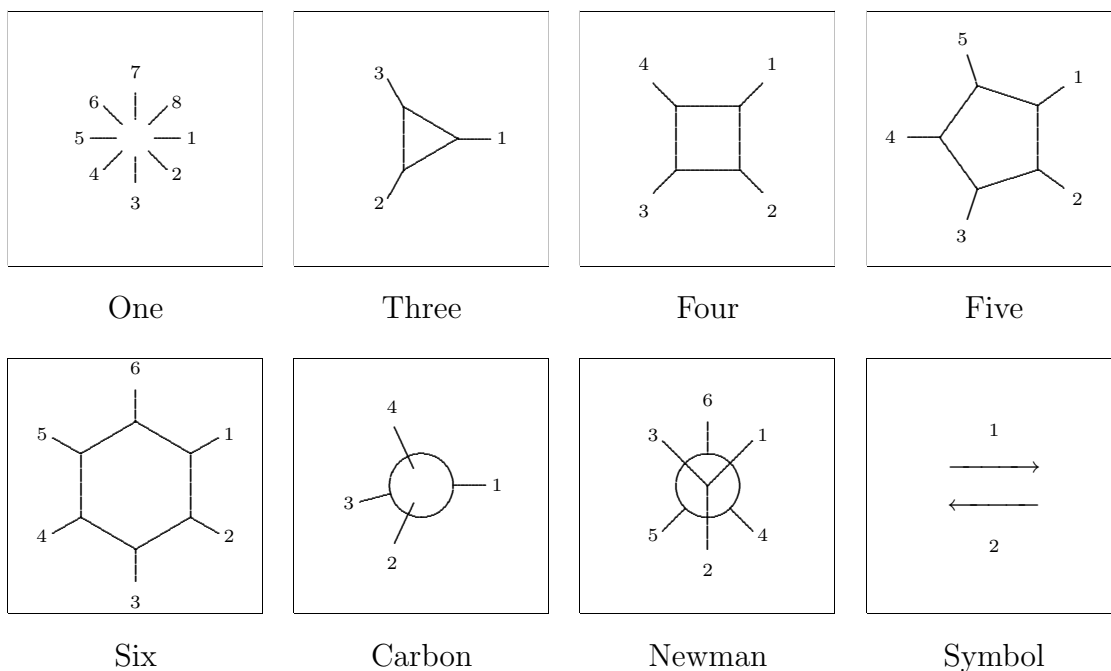
```
\startchemical[border=on,width=6000]
  \chemical[CARBON,CB1][A,B,C,D,E,F]
\stopchemical
```

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`.

¹ 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.

² 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.



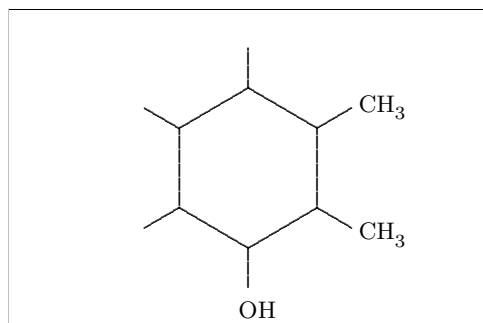
Within these structures chemical bonds between C-atoms can be indicated in a comparable way. For instance, in this example we use **B** and **R**. Bonds are numbered and can be indicated in different ways:

```
\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 1.3**

```
\startchemical[border=on,width=6000]
  \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.

2 | 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.

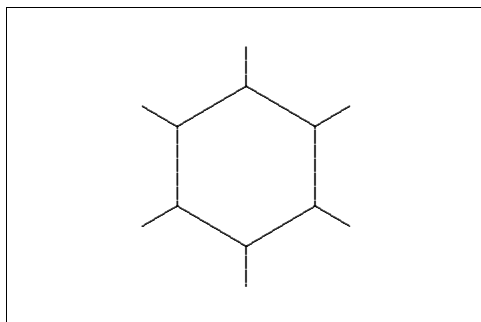
```
\def\sixring{\chemical[SIX,B,R,RZ]}
```

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

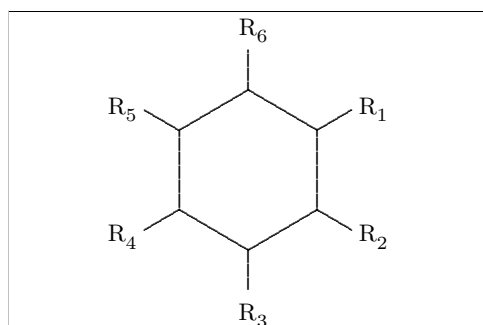


Example 2.1

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

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

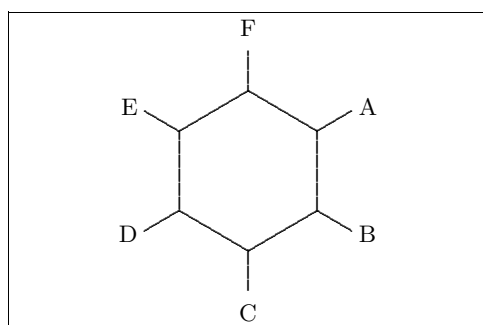
If we want to add six substituents, we have to carry out the following actions:

**Example 2.2**

```
\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 2.3**

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

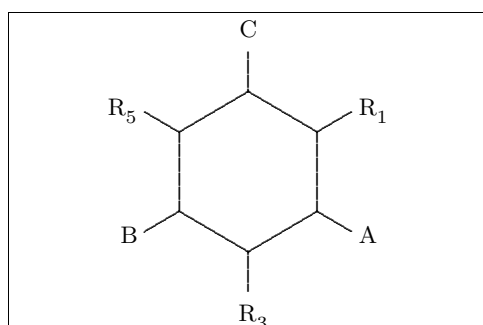
\startchemical[border=on,width=6000]
  \chemical[sixring,RZ][A,B,C,D,E,F]
\stopchemical
```

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).

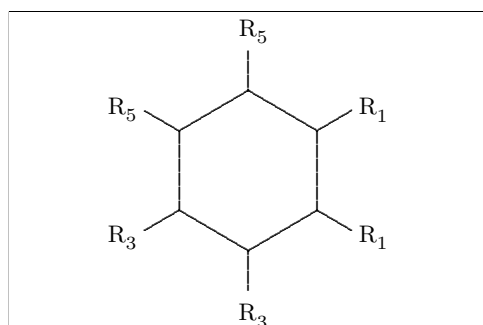
**Example 2.4**

```
\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 2.5

```
\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 `PPCHTEX` makes mention of an unknown command, one has probably forgotten to type a structure command, like `SIX` or `FIVE`.

3 | Bonds

In this chapter 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 manual.

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 3.1 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 3.2 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 3.3 Special bonds.

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

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

Table 3.4 Bonds to substituents.

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

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

Table 3.5 Double bonds to substituents.

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

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

Table 3.6 Atoms and molecules (radicals).

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.

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.

4 | Combinations

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

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

Table 4.1 Displacements and rotations.

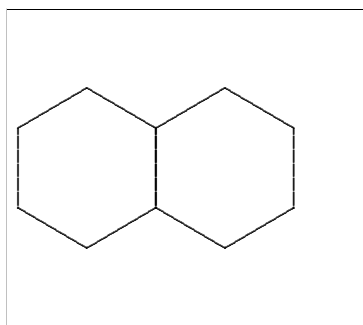
These four commands have another effect within the different structures. For example, the angle that can be used to rotate at `\chemical[FIVE,ROT1,B]` differs from the angle that is used at `\chemical[SIX,ROT1,B]`.

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

<code>MIR</code>	Mirror	mirror a structure
------------------	--------	--------------------

Table 4.2 Mirroring.

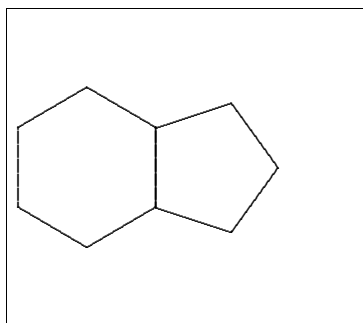
The direction of a displacement or the amount of the rotation is indicated by a number. Since these commands are closely related to the actual structure, they must be given before bonds and texts are drawn. It makes a difference whether `\chemical[FIVE,B,ROT1,R]` is given or `\chemical[FIVE,ROT1,B,R]`.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

**Example 4.1**

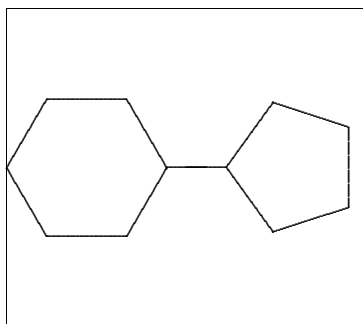
```
\startchemical[border=on,width=4500,right=3500]
\chemical[SIX,B,MOV1,B]
\stopchemical
```

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 fivering structure is drawn: **FIVE,ROT3,B**.

**Example 4.2**

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

**Example 4.3**

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

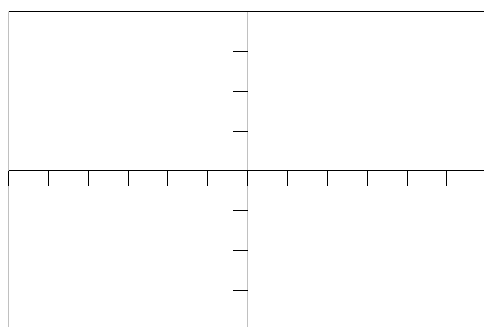
We can therefore conclude that the sequence of the given commands is very important. An obvious sequence of commands is as follows:

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

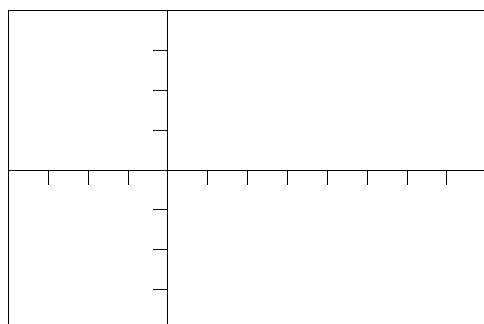
5 | Axis

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.



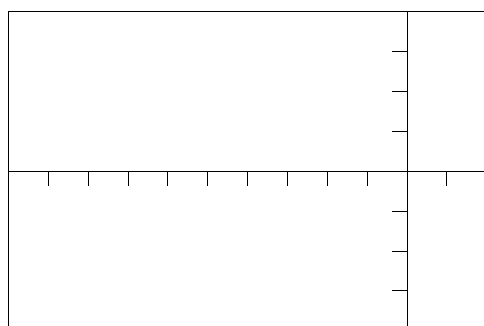
Example 5.1

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



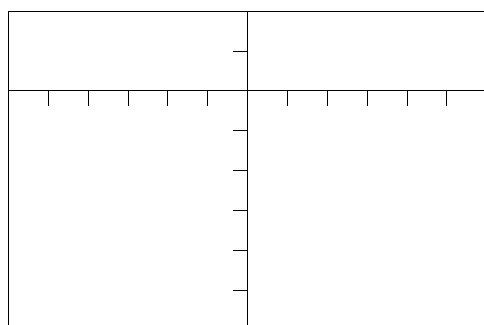
Example 5.2

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



Example 5.3

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


**Example 5.4**

```

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

```

The dimensions of the total structure are determined by the dimensions of the axis. However, if `width=fit` and/or `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 5.1 shows the standard setups.

Within a `\start`–`\stop`–pair P₁CT_EX–macros can be used. Of course, some caution must be taken into account.

6 | Setups

The behaviour of the macro's and the layout of the formulas can be adapted to 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	<code>\systeemresolutie</code>
corps	8pt 9pt 10pt etc.	<code>\systeemkorps</code>
style	<code>\rm \bf</code> etc.	<code>\rm</code>
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

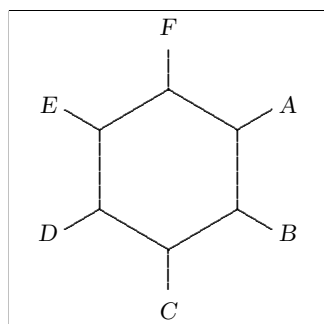
Table 6.1 Setups for structures.

The axis reaches from -2000 till $+2000$, in height as well as in width. The point Z0 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 \TeX -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.

Standard, a coupling to the actual corps is made. This coupling is achieved by the (dutch) `CONTEXT`-variable `\systeemkorps`. As one wishes to maintain the coupling, the variable must be adjusted at every change in corps setup (of the current text). The corps is used for calculations and has no effect on the current text. Within `CONTEXT`, the coupling is automatically achieved.³

In the mathematical mode commands like `\rm`, `\bf` and `\sl` can be utilized in `TEX` as well as in `CONTEXT`. `PPCHTEX` standardly uses `\rm`. An alternative command can be set up with `style`. For instance in example 6.1 the substituents are typeset *slanted*.

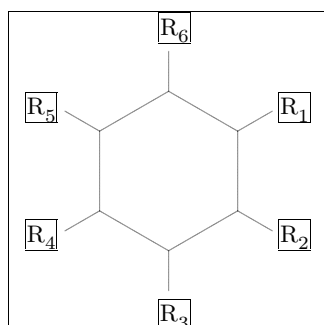


Example 6.1

```
\startchemical [border=on, style=\sl]
\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 , CH_4 and CH_4 . Successively the setups are: `\rm`, `\bf` and `\sl`. When formulas are typeset in italic (`\it`), baseline-distances can be greater than normal. Within `CONTEXT` bold-slanted (`\bs`) and bold-italic (`\bi`) are also available. All these commands automatically adjust to the actual style (`\ss`, `\rm`, `\tt`): CH_4 , CH_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`. Standardly, `PfCTEX` uses a 5 point period to draw the lines. As one chooses alternative 2 smaller points are used. Therefore thinner lines are drawn.



Example 6.2

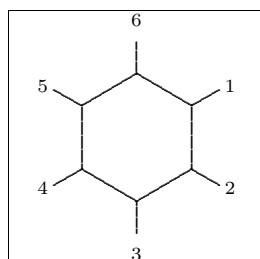
```
\startchemical [border=on, option=test, alternative=2]
\chemical [SIX,B,R,RZ] [R_1,R_2,R_3,R_4,R_5,R_6]
\stopchemical
```

³ In `CONTEXT` the mechanism is a little more complex than is stated here. Actually the coupling is achieved by another variable: `\fontpoints`.

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

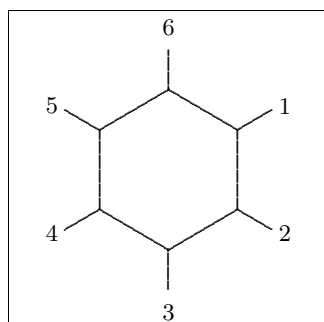
7 | Dimensions

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



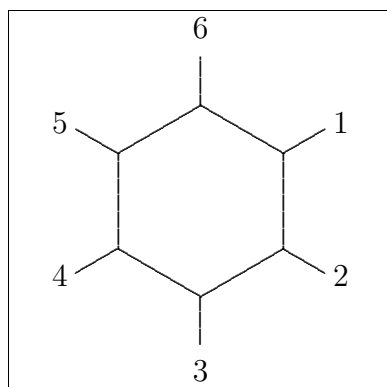
Example 7.1

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



Example 7.2

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



Example 7.3

```
\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.

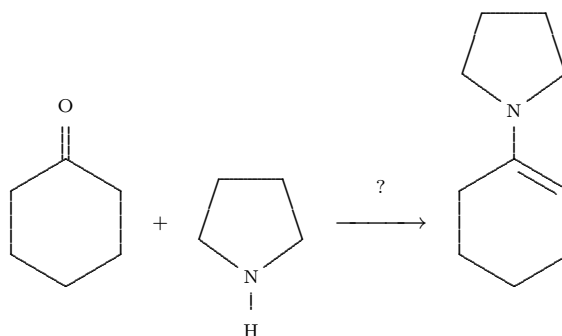
8 | Symbols

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] [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}
```

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 is a question mark is typeset.

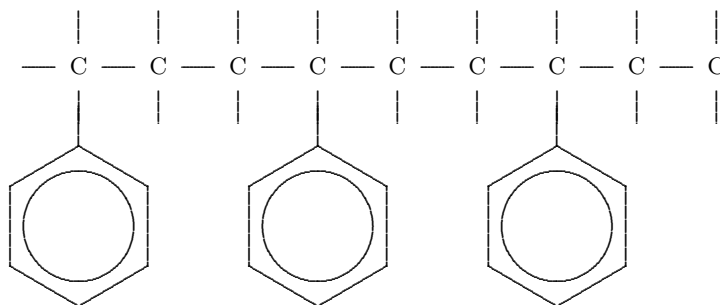
9 | Positioning

When we are combining molecules, for instance using `SUB`, some characteristics like dimensions and positions change, for instance the origin. Therefore it is possible to save and restore the characteristics at hand.

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

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

This example also shows in which way molecules can be combined to bigger ones.



The next example is a bit more advanced and shows a way to typeset reaction formulas. In situations like this, we have to take care of the proper heights.

```
$$
\setupchemical
  [width=fit,
   top=2000,
   bottom=2000,
   %axis=on,
   scale=small,
```



```

    size=small]
\startchemical
  \chemical
    [ONE,
    SAVE,
      Z0,2OFF1,SB7,SB3,SB1,
      MOV1,Z0,SB1,
      MOV1,Z0,DB8,CZ8,SB1,Z1,
    RESTORE,
    SAVE,
      SUB4,ONE,Z0,2OFF1,SB3,SB1,
      MOV1,Z0,SB1,
      MOV1,Z0,DB8,CZ8,SB1,Z1,
    RESTORE,
    SUB2,ONE,Z0,2OFF1,SB7,SB1,
    MOV1,Z0,SB1,
    MOV1,Z0,DB8,CZ8,SB1,Z1]
    [HC,0,C,0,C_{19}H_{39},
    H_{2}C,0,C,0,C_{17}H_{29},
    H_{2}C,0,C,0,C_{21}H_{41}]
\stopchemical
\startchemical
  \chemical [SPACE,PLUS,SPACE]
\stopchemical
\startchemical [right=1000]
  \chemical [ONE,CZ0] [3CH_{3}OH]
\stopchemical
\startchemical
  \chemical [SPACE,GIVES,SPACE]
\stopchemical
\startchemical
  \chemical
    [ONE,
    SAVE,
      Z0,2OFF1,SB7,SB3,SB1,Z1,
    RESTORE,
    SAVE,
      SUB4,ONE,Z0,2OFF1,SB3,SB1,Z1,
    RESTORE,
    SUB2,ONE,Z0,2OFF1,SB7,SB1,Z1]
    [HC,OH,
    H_{2}C,OH,

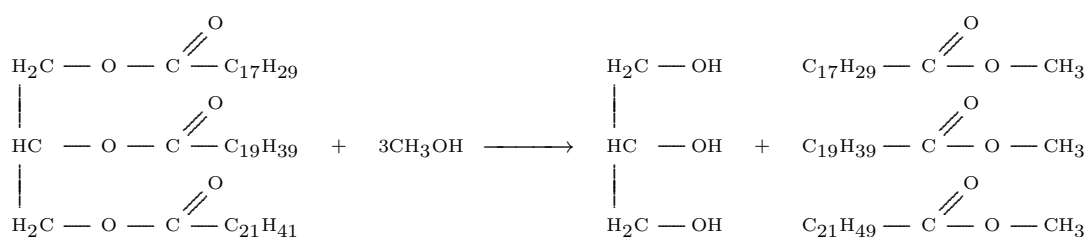
```

```

      H_{2}C,OH]
\stopchemical
\startchemical
  \chemie[SPACE,PLUS,SPACE]
\stopchemical
\startchemical
  \chemie
    [ONE,
     SAVE,
     Z0,DB8,CZ8,SB1,SB5,Z5,
     MOV1,Z0,SB1,Z1,
     RESTORE,
     SAVE,
     SUB4,ONE,Z0,DB8,CZ8,SB1,SB5,Z5,
     MOV1,Z0,SB1,Z1,
     RESTORE,
     SUB2,ONE,Z0,DB8,CZ8,SB1,SB5,Z5,MOV1,Z0,SB1,Z1]
    [C,O,C_{19}H_{39},O,CH_{3},
     C,O,C_{17}H_{29},O,CH_{3},
     C,O,C_{21}H_{49},O,CH_{3}]
\stopchemical
$$

```

We could have made this definition a bit more compact (`SB731` instead of `SB7,SB3,SB1`) at the cost of readability. Huge definitions like this one can best be build stepwise in a separate file (maybe in Plain `TEX`).



Next we show some examples of formulas combined with text. We have not yet implemented a centering mechanism.

```

$$
\setupchemical
  [width=fit,
   top=1500,
   bottom=3000]

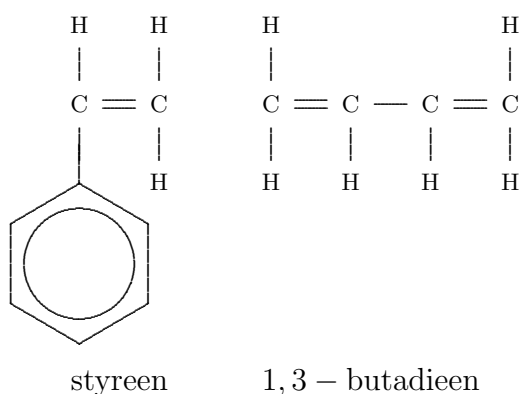
```

```

\eqalign
{
  \startchemical
  \chemical
  [ONE,ZO,DB1,SB3,SB7,Z7,MOV1,ZO,SB3,SB7,Z3,Z7,
  MOV0,SUB2,SIX,B,R6,C]
  [C,H,C,H,H]
  \stopchemical
  \quad\quad\quad
&
  \startchemical
  \chemical
  [ONE,ZO,DB1,SB3,SB7,Z3,Z7,
  MOV1,ZO,SB1,SB3,Z3,
  MOV1,ZO,DB1,SB3,Z3,
  MOV1,ZO,SB3,SB7,Z3,Z7]
  [C,H,H,C,H,C,H,C,H,H]
  \stopchemical
\cr
  \rm styreen
  \quad\quad\quad
&
  \rm 1,3-butadien
}
$$

```

Here we let `\eqalign` take care of the alignment and use `\quad`'s to improve the spacing.

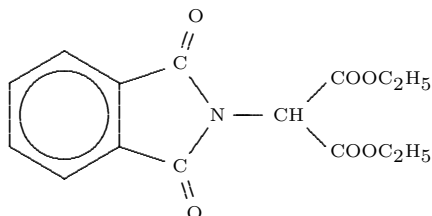


10 | Special features

By using `ONE`, `Z0` can consist of more than one atom. In this case, the reserved space is insufficient. If more space is needed for the command `Z0`, 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,Z0,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, but more is possible, e.g. `3OFF1`. Similar, at first sight quite complicated, definitions 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}`.

<code>OFF</code>	Offset	<code>CRZ</code>	Centered Radical Atom
------------------	--------	------------------	-----------------------

Table 10.1 Special commands.

11 | Textformulas

Along with the typesetting of structure formulas, the typesetting of reaction equations is supported too. Therefore, the former 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:

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

or even:

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

The more experienced $\text{T}_\text{E}\text{X}$ -user will notice that the plus-sign as well as the arrow are located at the base-line. If you just compare `+` and `+`. Independent of the size of reflection, the `+` and the `→` are in aligned.

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

This formula can also be typeset in the current text. In this case a smaller layout is chosen: $2\text{H}_2 + \text{O}_2 \longrightarrow 2\text{H}_2\text{O}$. It is also possible to show bonds. For example, the rather long sequence `\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}` gives $\text{H}-\text{CH}=\text{HC}-\text{H}$. This can also be achieved in a shorter way: `\chemical{H,-,CH,--,HC,-,H}`. A triple bond can be called with TRIPLE or ---: $\text{HC}\equiv\text{CH}$.

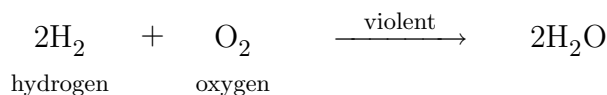
Now we just return to the display-mode. The second argument can be used to give an explanation of the formula:

```


$$\begin{array}{c}
 \text{\textbackslash chemical\{2H\_2\}\{hydrogen\} \text{\textbackslash chemical\{PLUS\}\{ } \text{\textbackslash chemical\{0\_2\}\{oxygen\}} \\
 \text{\textbackslash chemical\{GIVES\}\{violent\} \text{\textbackslash chemical\{2H\_2O\}\{ } \\
 \text{\textbackslash chemical\{EQUILIBRIUM\}\{ }
 \end{array}$$


```

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 11.1 Setups for textformulas.

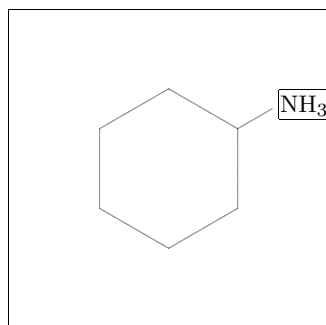
When `big`, `medium` or `small` is used, `\chemical{H,SINGLE,CH,DOUBLE,HC,SINGLE,H}` gives the successive formulas:

$$\begin{array}{l}
 \text{H}-\text{CH}=\text{HC}-\text{H} \\
 \text{H}-\text{CH}=\text{HC}-\text{H} \\
 \text{H}-\text{CH}=\text{HC}-\text{H}
 \end{array}$$

12 | Subscripts

Sub- and superscripts are placed a little lower, as is recommended by Knuth in the $\text{T}_{\text{E}}\text{X}$ book. Like this, the example on page 179 in the $\text{T}_{\text{E}}\text{X}$ book, that is chemically a bit strange, can be typeset by typing `\chemical{Fe_2^{+2}Cr_2O_4}`. This command gives $\text{Fe}_2^{+2}\text{Cr}_2\text{O}_4$. Without a correction the command would have given the result: $\text{Fe}_2^{+2}\text{Cr}_2\text{O}_4$.

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



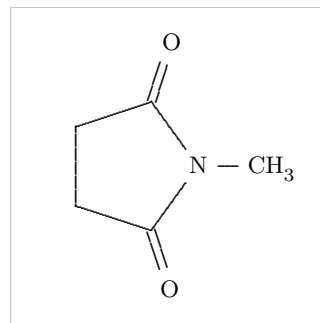
Example 12.1

```
\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 `\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}` in H_2O .

Part 2 Backgrounds



1 | Installation

The package `PPCHTEX` is developed as an extension to `CONTEXT`. Within this macropack-
age `PPCHTEX` can be activated with the command:¹

```
\usemodules[chemic]
```

The macros can be found in the file `m-chemie.tex`, with the `m` standing for module.
Therefore the macros are not standard available.

Furthermore, the package can be used in combination with `LATEX`. In this case the file
`m-chemie.sty` is used too.² `PPCHTEX` can be activated by means of `\documentstyle`:

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

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

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

The undermentioned commands can be found in the file `m-chemie.sty`. The english and
dutch equivalents can be deduced from the following list:

```
\defineinterface [english]

\redefinecommand {chemie}          {chemical}
\redefinecommand {definieerchemie} {definechemical}
\redefinecommand {naarchemie}      {tochemical}
\redefinecommand {startchemie}     {startchemical}
\redefinecommand {stelchemiein}    {setupchemical}
\redefinecommand {stopchemie}      {stopchemical}

\redefineconstant {aan}             {on}
\redefineconstant {assenstelsel}   {axis}
\redefineconstant {boven}           {top}
\redefineconstant {breedte}        {width}
\redefineconstant {file}            {file}
\redefineconstant {formaat}        {size}
```

¹ At the moment, only dutch commands are available in `CONTEXT`, so actual this command is named:
`\gebruikmodules`.

² The dutch word `chemie` stands for `chemics` in english.

```

\redefineconstant {getal}           {number}
\redefineconstant {groot}           {big}
\redefineconstant {hoogte}          {height}
\redefineconstant {intekst}         {intext}
\redefineconstant {kader}           {border}
\redefineconstant {klein}           {small}
\redefineconstant {korps}           {corps}
\redefineconstant {letter}          {style}
\redefineconstant {links}           {left}
\redefineconstant {middel}          {medium}
\redefineconstant {onder}           {bottom}
\redefineconstant {optie}           {option}
\redefineconstant {passend}         {fit}
\redefineconstant {plaats}          {location}
\redefineconstant {rechts}          {right}
\redefineconstant {resolutie}       {resolution}
\redefineconstant {schaal}          {scale}
\redefineconstant {start}           {start}
\redefineconstant {status}          {status}
\redefineconstant {stop}            {stop}
\redefineconstant {tekstformaat}    {textsize}
\redefineconstant {test}            {test}
\redefineconstant {uit}             {off}
\redefineconstant {variant}         {alternative}

```

After these commands the `corpssize` and `systemresolution` are set up. The variables used are dutch named `CONTEXT`-variables. The corps can also be set up with `\setupchemical`.

```

\def\systemeresolutie {300}
\def\systemekorps    {12pt}

```

Within the new font-selection-scheme of \LaTeX the command `\rm` cannot be used anymore in the mathematical mode. This command has been replaced by `\mathrm`. Depending on the availability of this command the following setup is executed:

```

\setupchemical [style=\mathrm]

```

2 | Some dutch

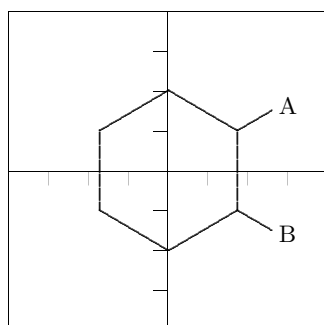
The original interface of PPCH_{TEX} is dutch. One can switch back to dutch with:

```
\resetinterface
```

Switching back to english can be done with:

```
\setinterface[english]
```

Although more interfaces are possible, only the dutch and english are implemented. The file `m-chemie.sty` shows how an interface is defined.



Voorbeeld 2.1

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

3 | Extensions

Of course, T_EX–users are allowed to use the PPCH_{TEX}–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. One of the (hidden) macros that is responsible for all this, is `\getparameters`. In turn, `\getparameters` uses the macros `\processcommalist` and `\doassign`.

A look at the file `m-chemie.tex` shows that use is made of the `\processaction`–macros, while interpreting the commands that are given in `\chemical` between []. These macros are relative slow, since also in this case nesting and a well–ordered layout must be possible. On the other hand, PPCH_{TEX}–macros have to be as intuitive as possible. In the mean time, the macros as well as the use of the macros within PPCH_{TEX} are quite optimized. Tests with a stopwatch have shown that a further optimisation hardly produces a gain of time. However, it is at the expense of the flexibility.

While developing PPCH_{TEX}, the way commands are shown within the production–environment T_EXEDIT was taken into account. In this program the T_EX–commands and –symbols with a special function are shown in color.

4 | Fonts

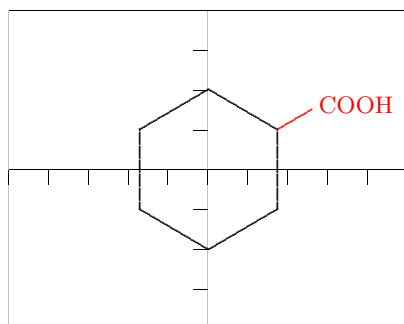
The macros make use of the mathematical mode and therefore of `\textfont`, `\scriptfont` and `\scriptscriptfont`. If necessary, the `\fontdimen`'s 14, 16 and 17 of `\font2` will be adjusted. By doing so the actual corpsize is taken into account, which is gathered from the *x*-height (`\fontdimen5`).

Changes in the `\fontdimen`'s have a global character, so grouping makes no sense. That's why the dimensions are always set and reset. The present solution may not be the best, but the other solutions bring about problems with scaled fonts.

The placement of the atoms and the molecules (text) can take a bit of of processing-time. In `CONTEXT` this is also dependent on the complexity of the called macro `\rm`. A more efficient implementation is possible.

5 | Color

Within `CONTEXT` it is possible to color parts of a structure. In example 5.1 both the substituent and the bond to the substituent are colored red.

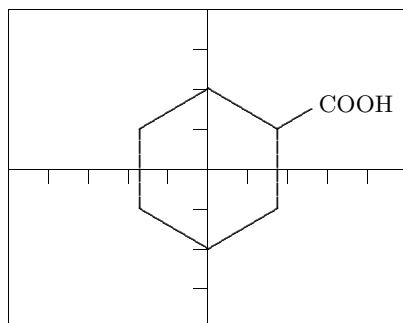
**Example 5.1**

```
\startchemical[axis=on,border=on,width=5000]
\chemical[SIX,B]
\kleur[rood]{\chemical[SIX,R1,RZ1][COOH]}
\stopchemical
```

Of course the color-mechanism has to be activated with the (dutch) `CONTEXT`-command `\stelkleurenin[status=start]`.

6 | Interaction

At least when `CONTEXT` is used, `PPCHTEX` supports the make-up of interactive texts. We understand by an interactive text a text that can be consulted on a computer, while parts of this text can be active. This means that clicking a word results in a jump to the explanation belonging to this word. Clicking in the text on `COOH` for instance can result in a displacement of the cursor to the position of this substituent in the structure. The other way round, clicking the substituent in the structure can bring on a jump to the explanation of this substituent.



Example 6.1

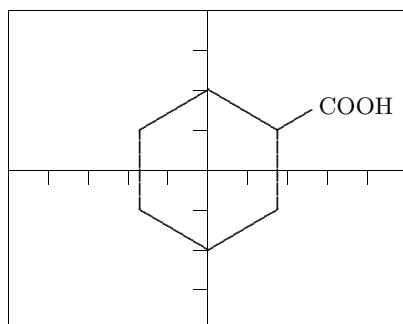
```
\startchemical[axis=on,border=on,width=5000]
\chemical[SIX,B]
\chemical[sub:cooh][SIX,R1,RZ1][COOH]
\stopchemical
```

As we can see a third argument is given: a reference `[sub:cooh]`. This means that we can refer from the text to the substituent `COOH`:

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

In this example `\to` (dutch: `\naar`) is a `CONTEXT`-command. Clicking on text that is marked in this way results in the positioning of the cursor to the substituent in the figure.

The other way round is also possible. We can refer from a structure to a text. Of course, the reference must exist.



Example 6.2

```
\startchemical[axis=on,border=on,width=5000]
\chemical[SIX,B]
\tochemical[txt:cooh][SIX,R1,RZ1][COOH]
\stopchemical
```

Clicking COOH in the figure results in a jump to the text belonging to it, for example marked with:

```
\section[txt:cooh]{Substituents}

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

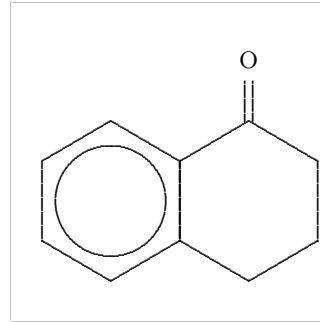
It is also possible to make a combination. In this case it is wise to mark first with `\chemical` and next to refer with `\tochemical`.

A coupling with the interaction mechanism is made with the following macros:

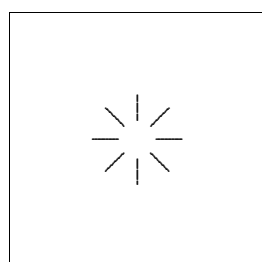
```
\gotochemical {reference} {text}
\thisischemical {reference}
```

A further explanation is given in the source. This coupling can also be used for other purposes. By doing so, some experience is recommended.

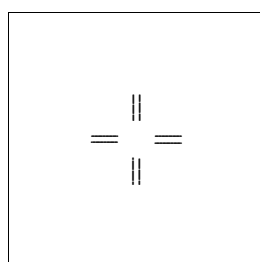
Part 3 Overview



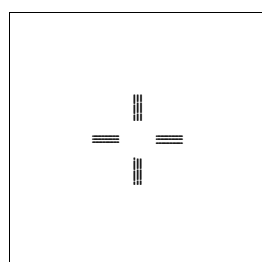
1 | One



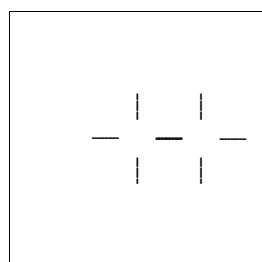
SB



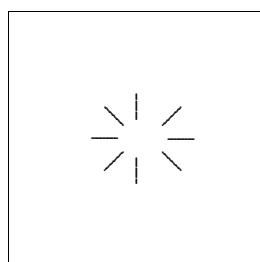
DB



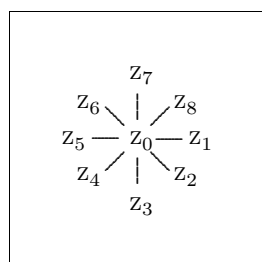
TB



MOV

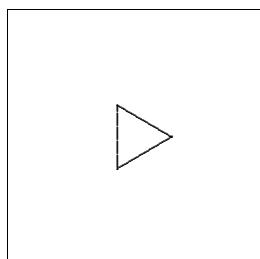


OFF

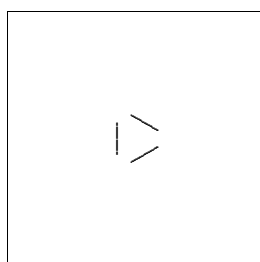


Z

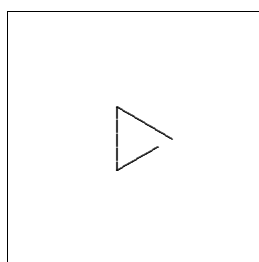
2 | Three



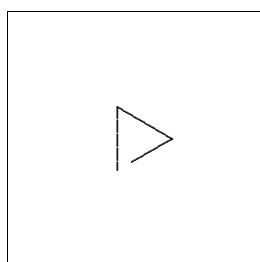
B



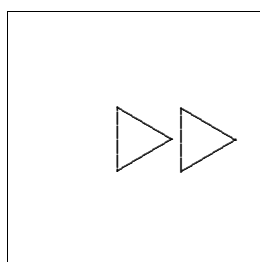
SB



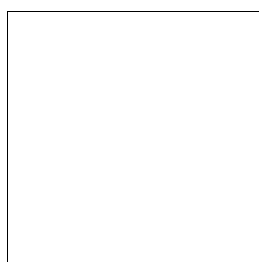
-SB



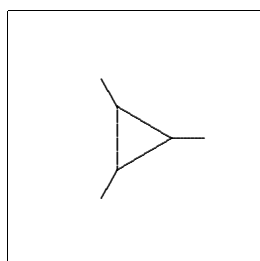
+SB



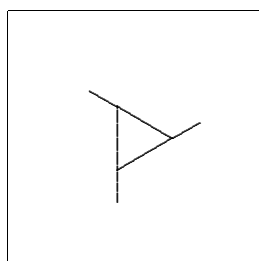
MOV



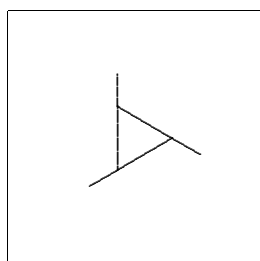
ROT



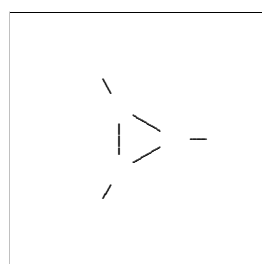
R



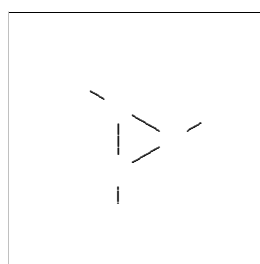
-R



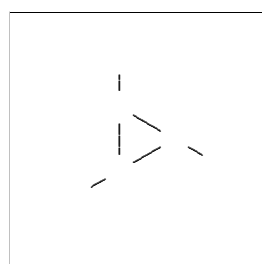
+R



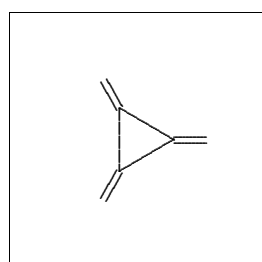
SR



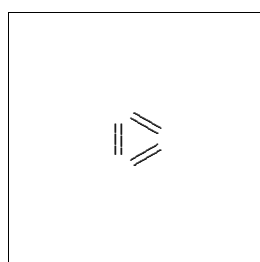
-SR



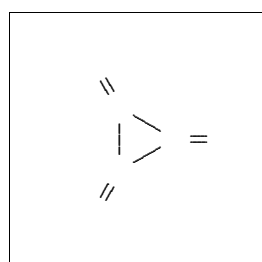
+SR



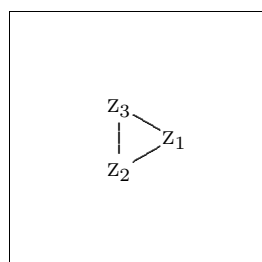
ER



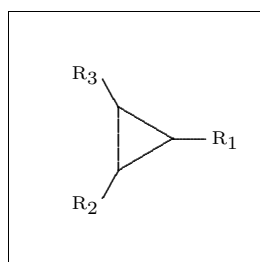
DB



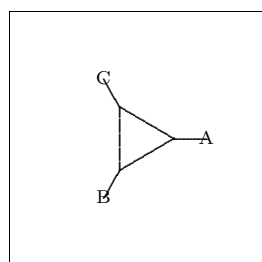
DR



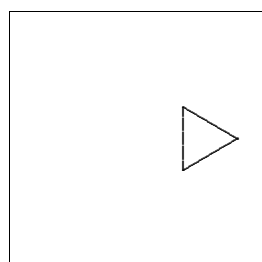
Z



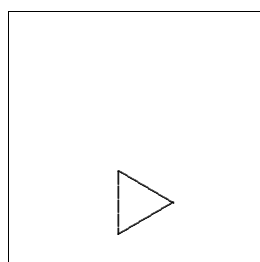
RZ



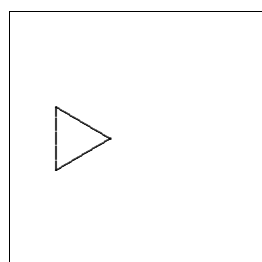
CRZ



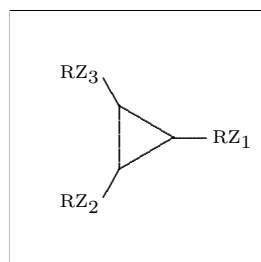
MOV1



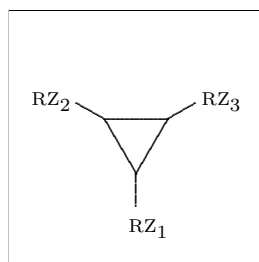
MOV2



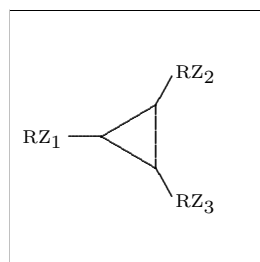
MOV3



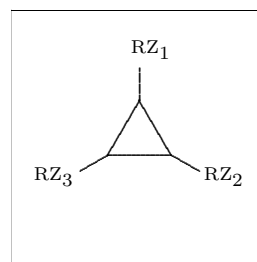
ROT1



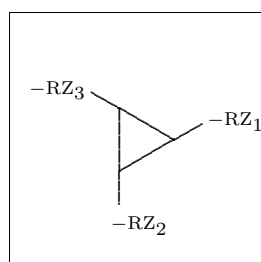
ROT2



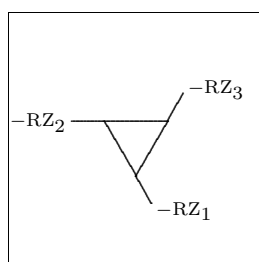
ROT3



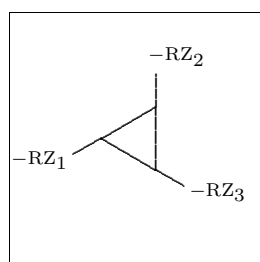
ROT4



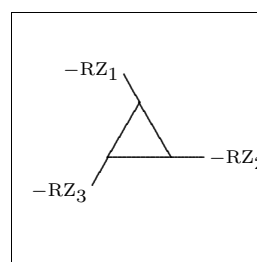
ROT1



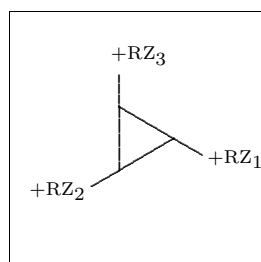
ROT2



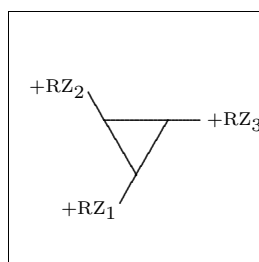
ROT3



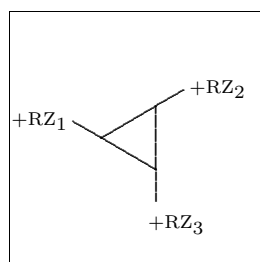
ROT4



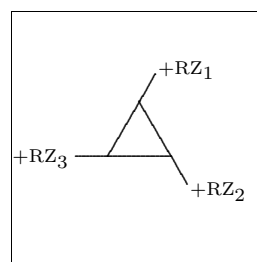
ROT1



ROT2

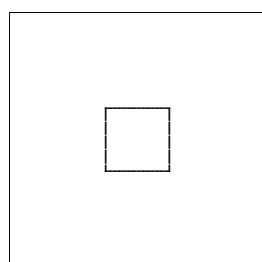


ROT3

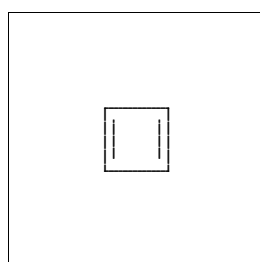


ROT4

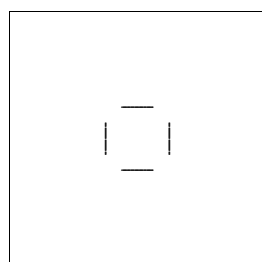
3 | Four



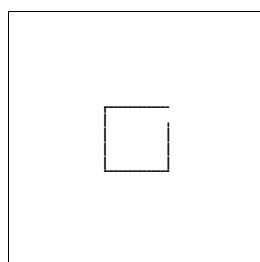
B



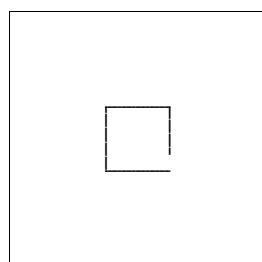
EB



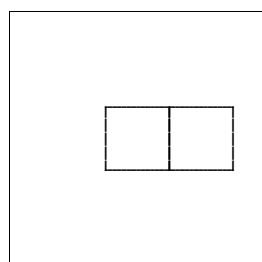
SB



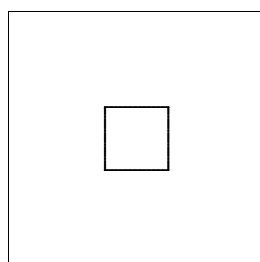
-SB



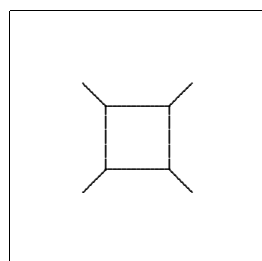
+SB



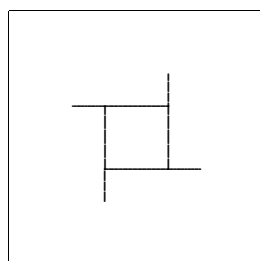
MOV



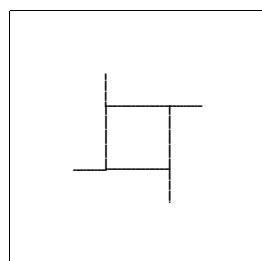
ROT



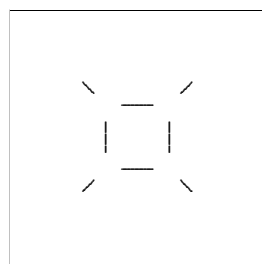
R



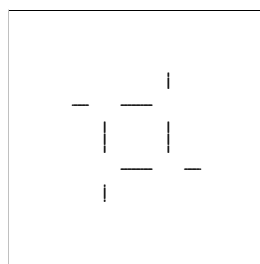
-R



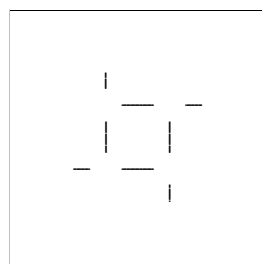
+R



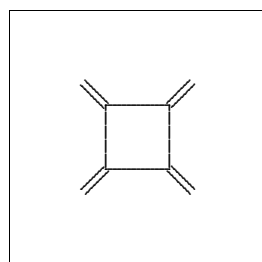
SR



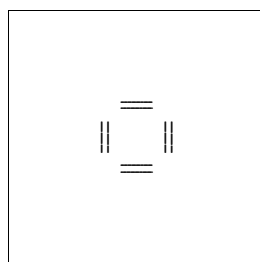
-SR



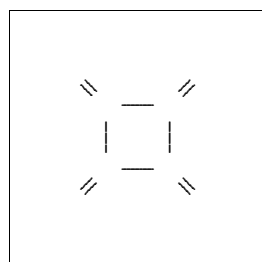
+SR



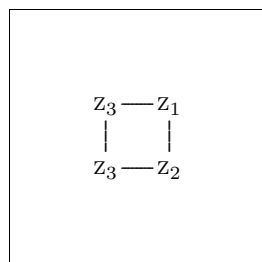
ER



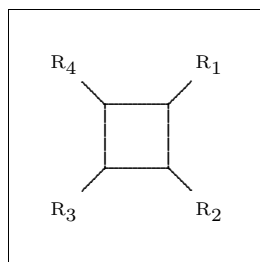
DB



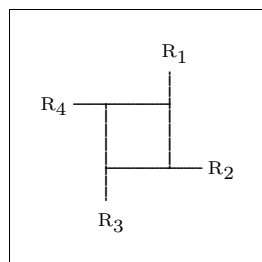
DR



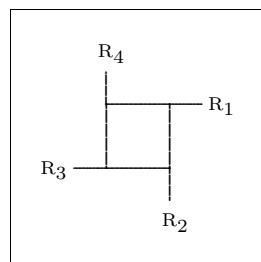
Z



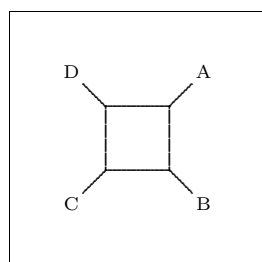
RZ



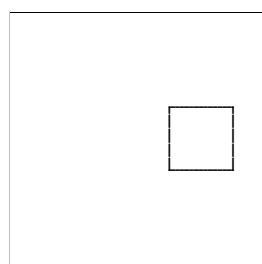
-RZ



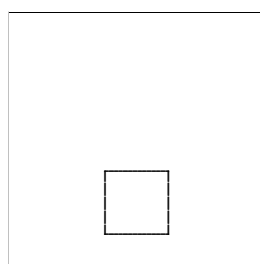
+RZ



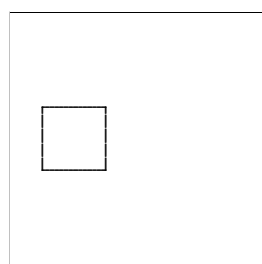
CRZ



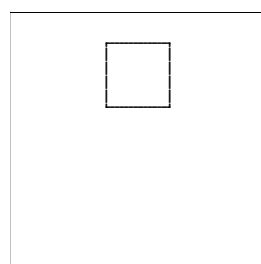
MOV1



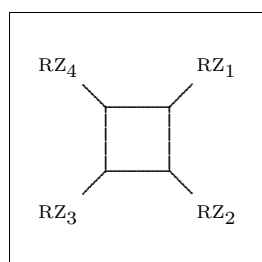
MOV2



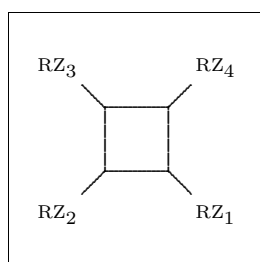
MOV3



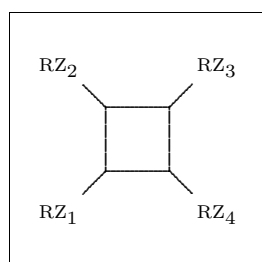
MOV4



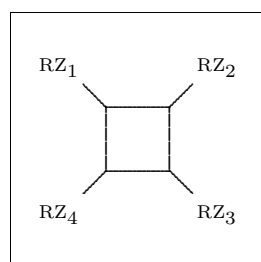
ROT1



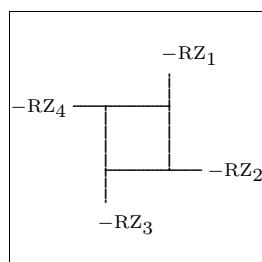
ROT2



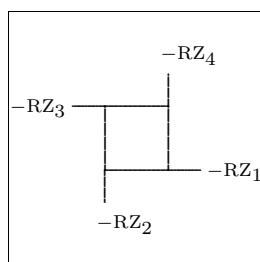
ROT3



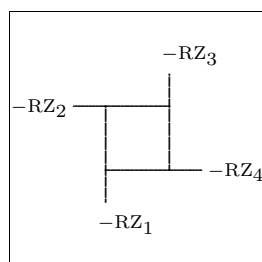
ROT4



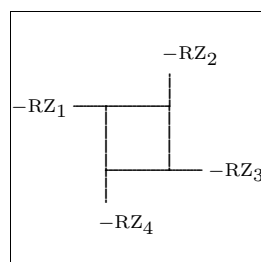
ROT1



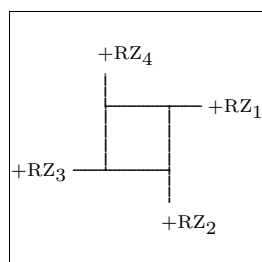
ROT2



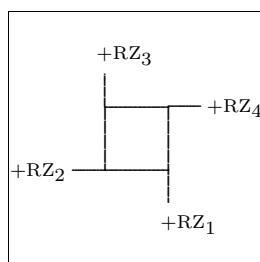
ROT3



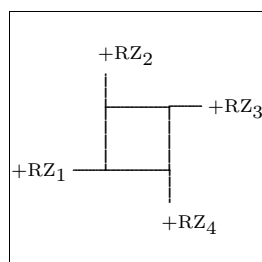
ROT4



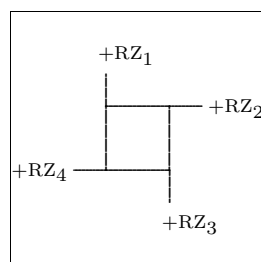
ROT1



ROT2

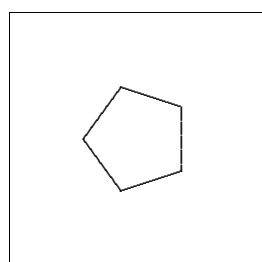


ROT3

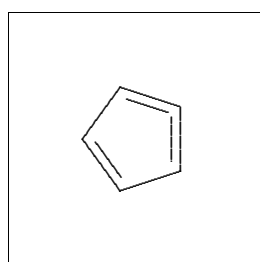


ROT4

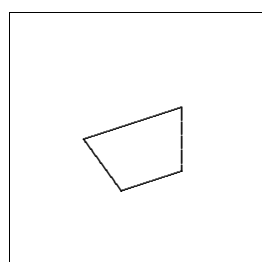
4 | Five



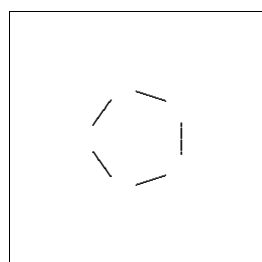
B



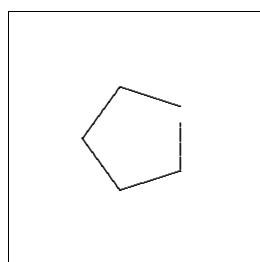
EB



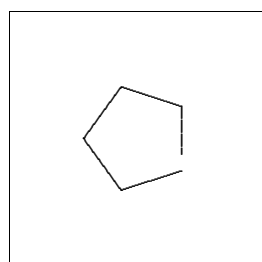
S



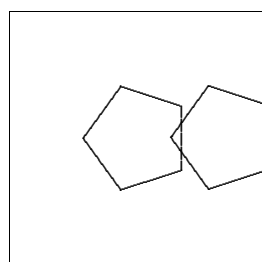
SB



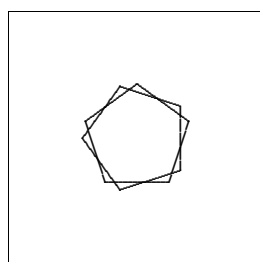
-SB



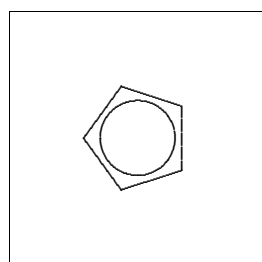
+SB



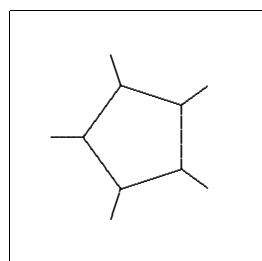
MOV



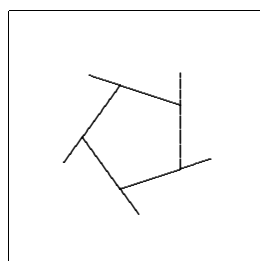
ROT



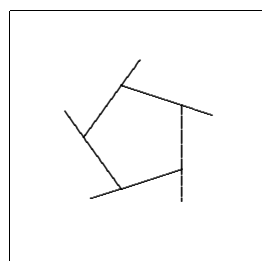
C



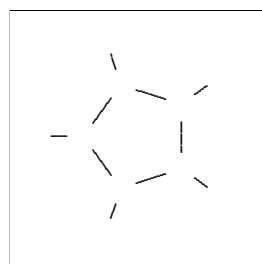
R



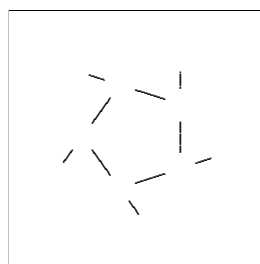
-R



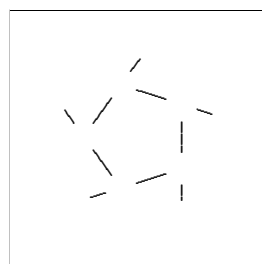
+R



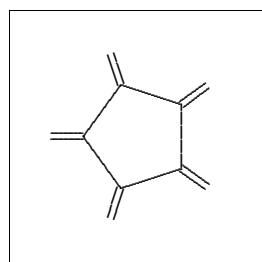
SR



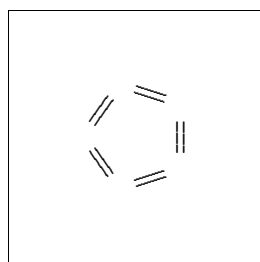
-SR



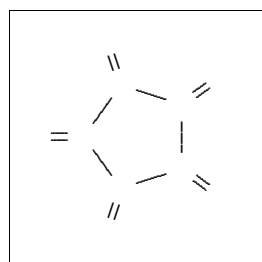
+SR



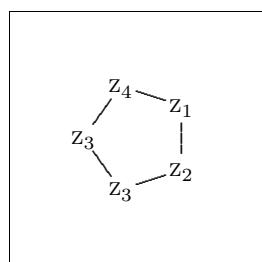
ER



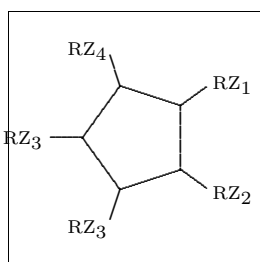
DB



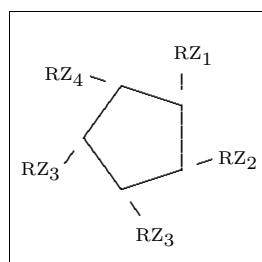
DR



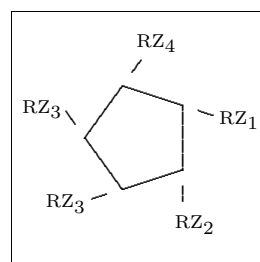
Z



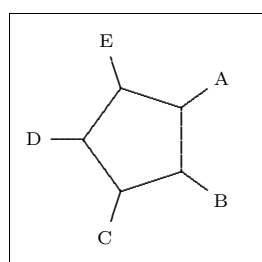
RZ



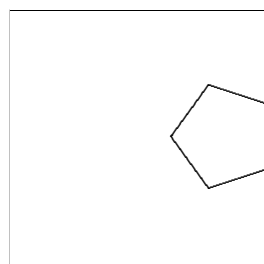
-RZ



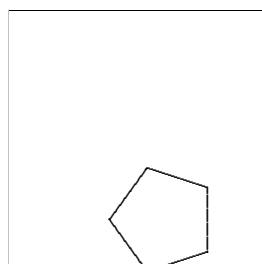
+RZ



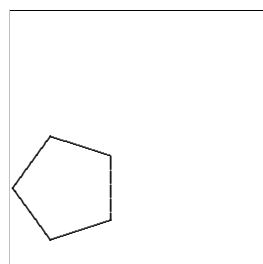
CRZ



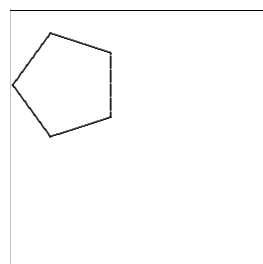
MOV1



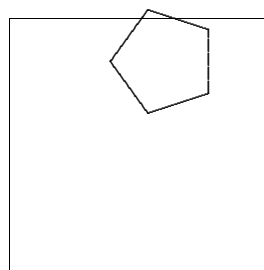
MOV2



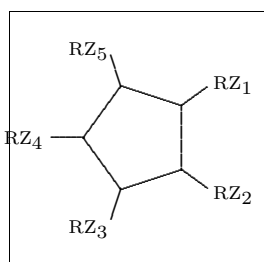
MOV3



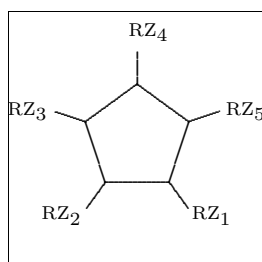
MOV4



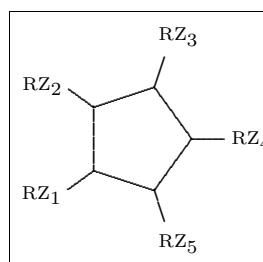
MOV5



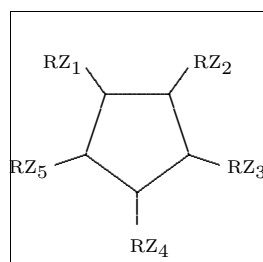
ROT1



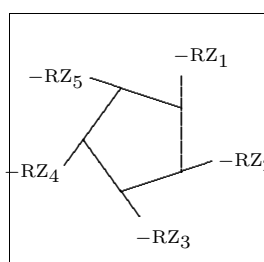
ROT2



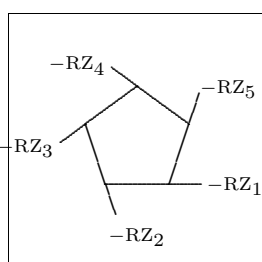
ROT3



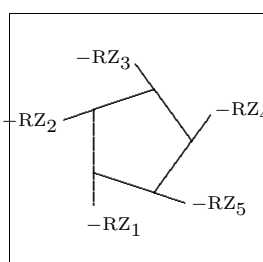
ROT4



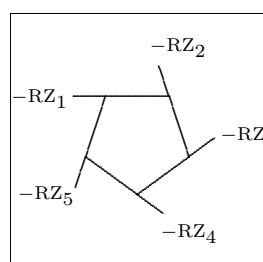
ROT1



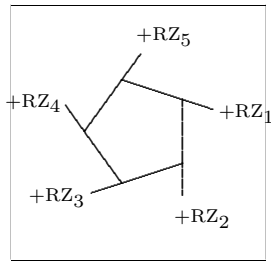
ROT2



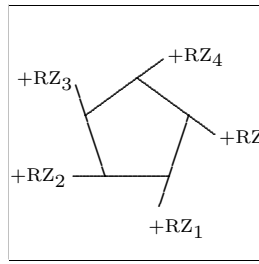
ROT3



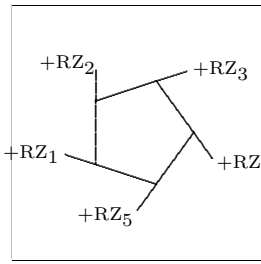
ROT4



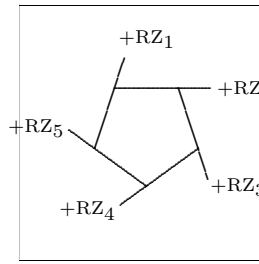
ROT1



ROT2

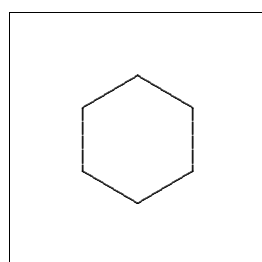


ROT3

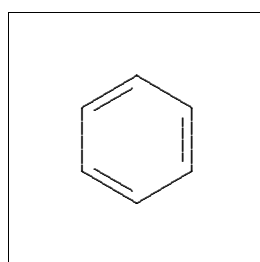


ROT4

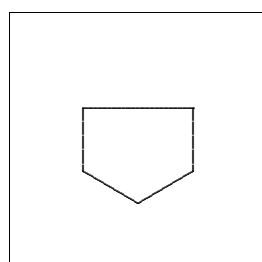
5 | Six



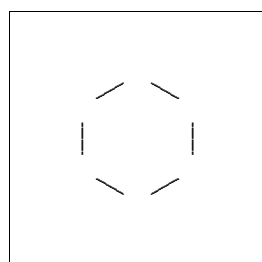
B



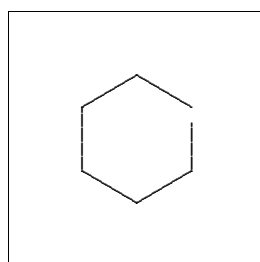
EB



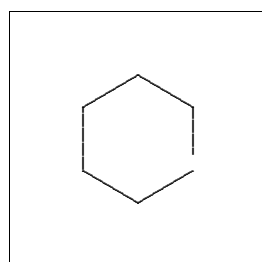
S



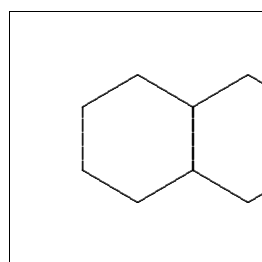
SB



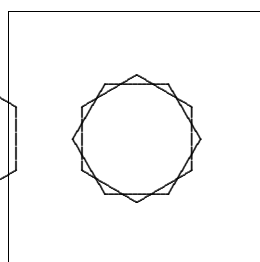
-SB



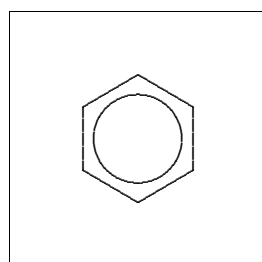
+SB



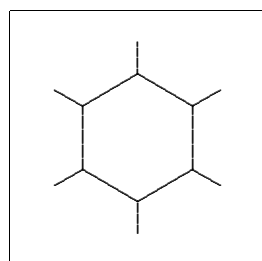
MOV



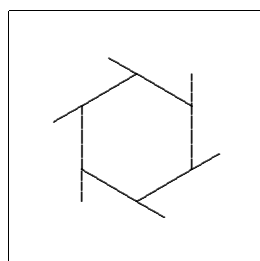
ROT



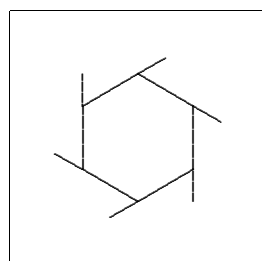
C



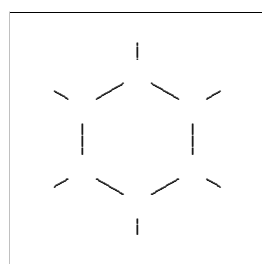
R



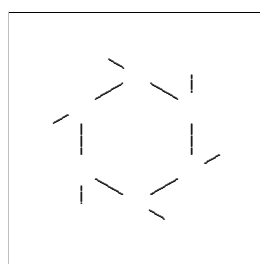
-R



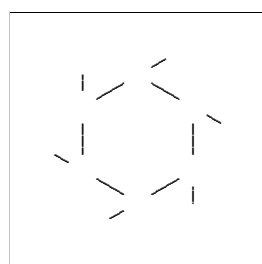
+R



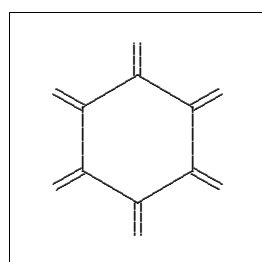
SR



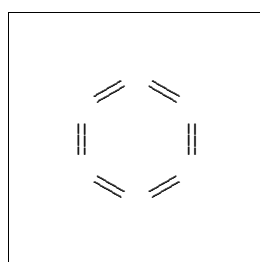
-SR



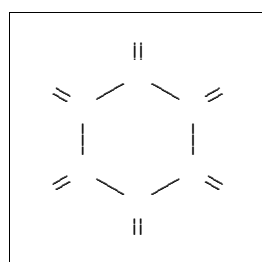
+SR



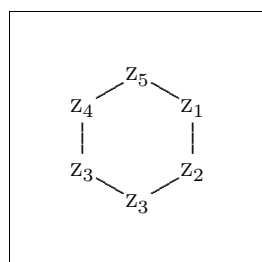
ER



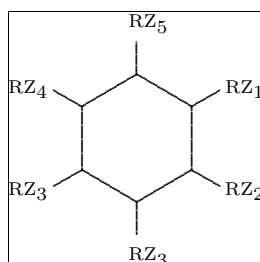
DB



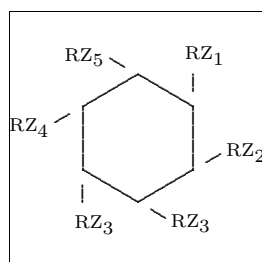
DR



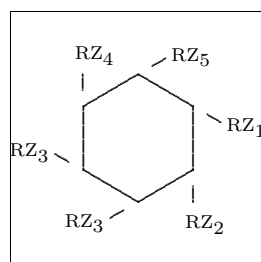
Z



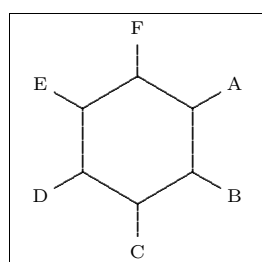
RZ



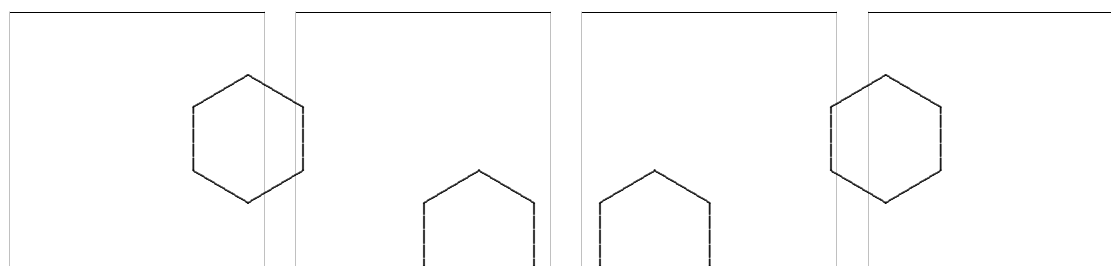
-RZ



+RZ

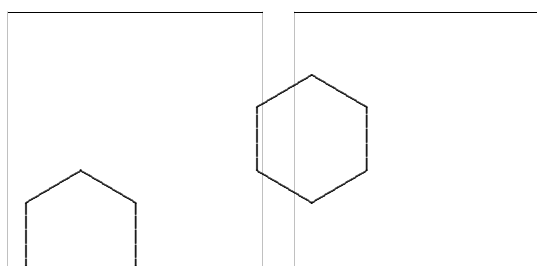


CRZ



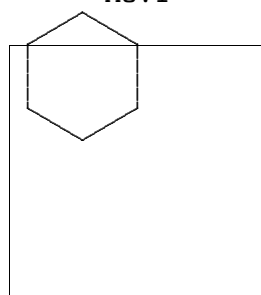
MOV1

MOV2

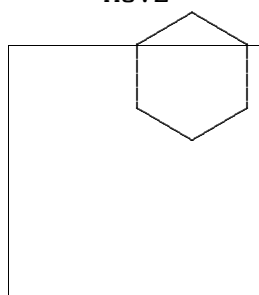


MOV3

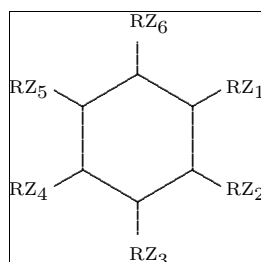
MOV4



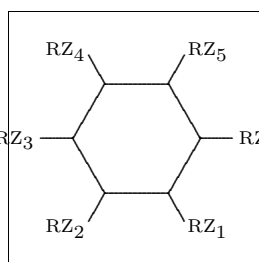
MOV5



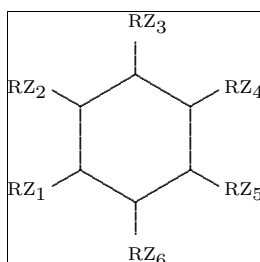
MOV6



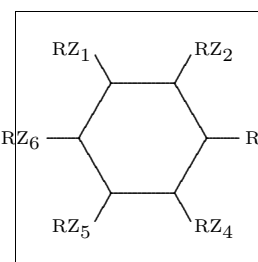
ROT1



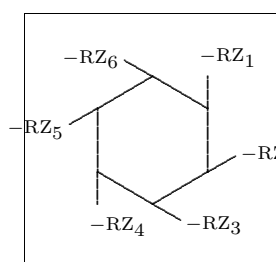
ROT2



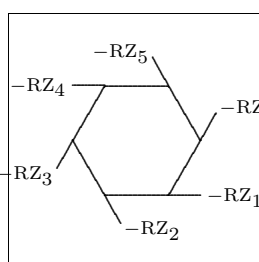
ROT3



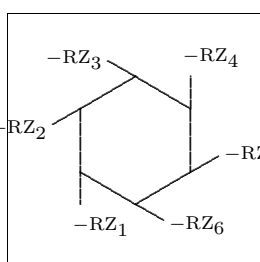
ROT4



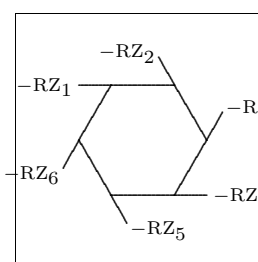
ROT1



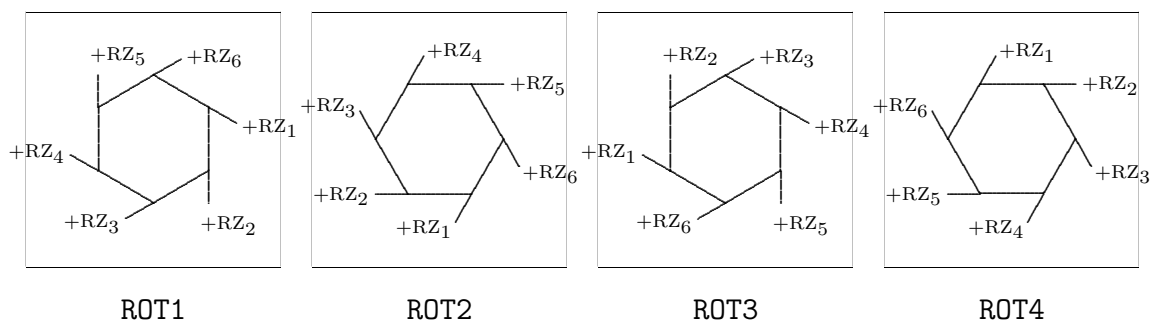
ROT2



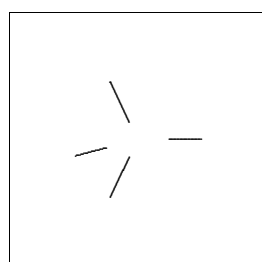
ROT3



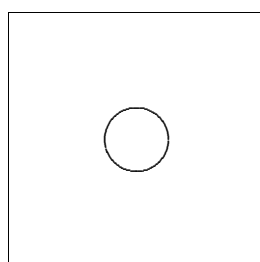
ROT4



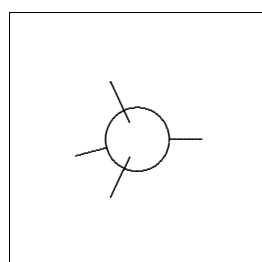
6 | Carbon



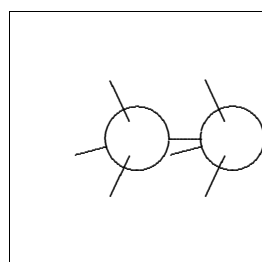
B



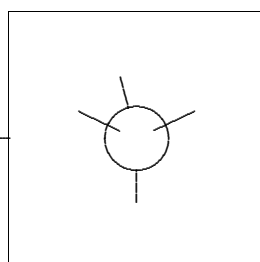
C



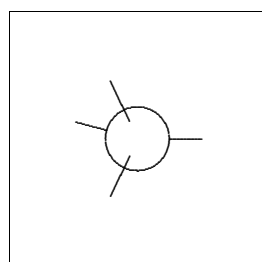
CB



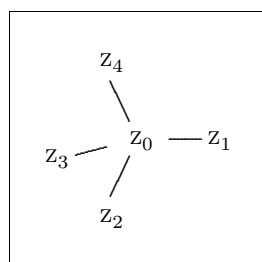
MOV



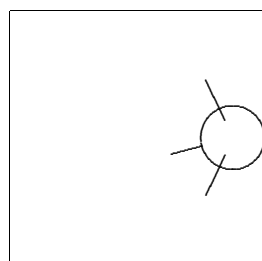
ROT



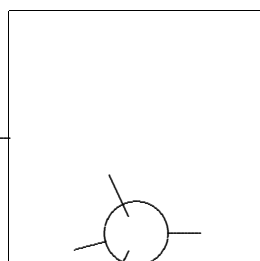
MIR



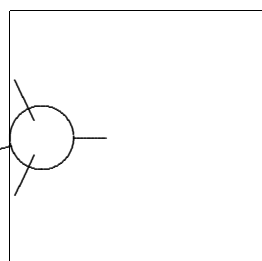
Z



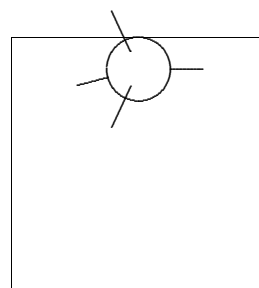
MOV1



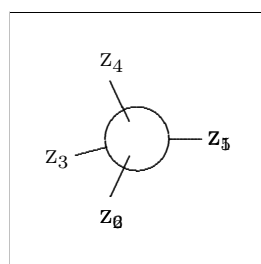
MOV2



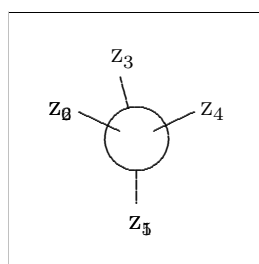
MOV3



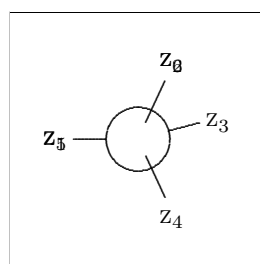
MOV4



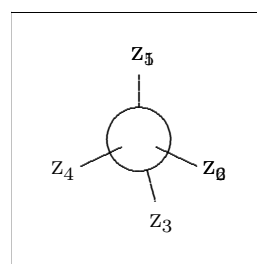
ROT1



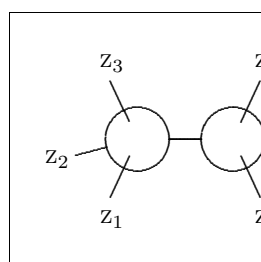
ROT2



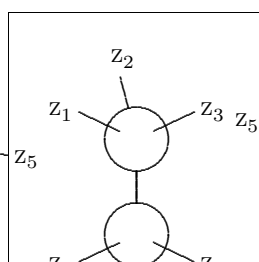
ROT3



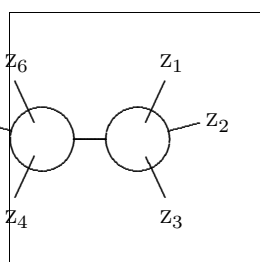
ROT4



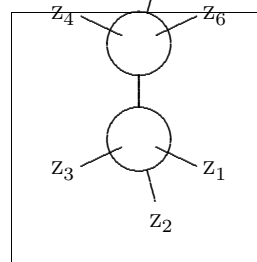
CB1



CB2

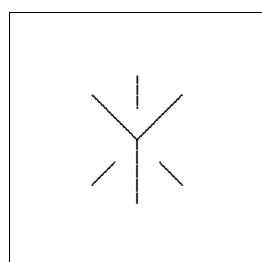


CB3

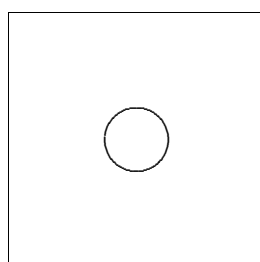


CB4

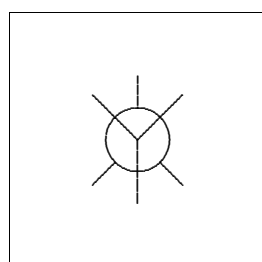
7 | Newman



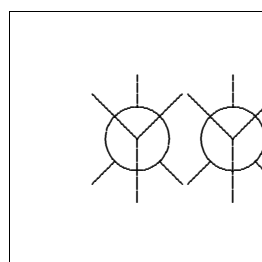
B



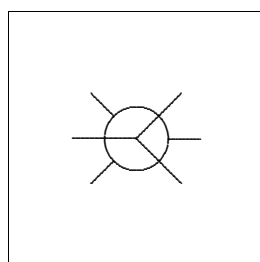
C



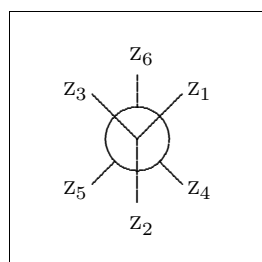
CB



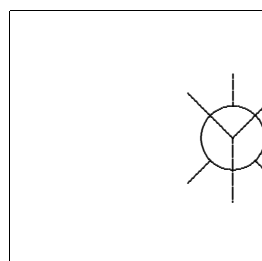
MOV



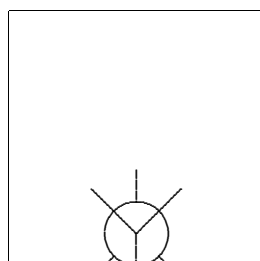
ROT



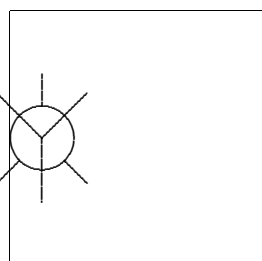
Z



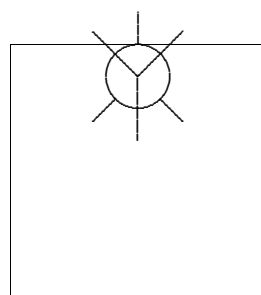
MOV1



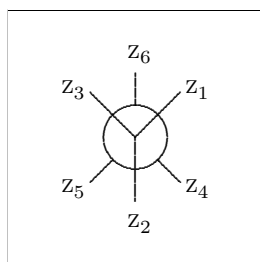
MOV2



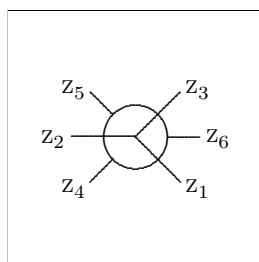
MOV3



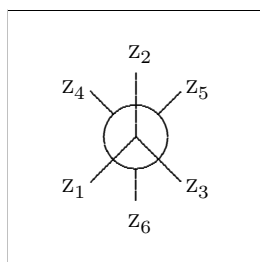
MOV4



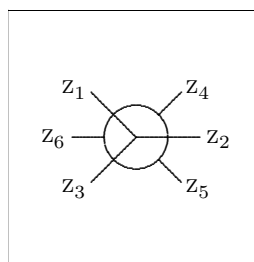
ROT1



ROT2



ROT3



ROT4

8 | Symbol

