

typesetting chemistry in ConT_EXt LMTX

work in progress

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Contents

1	Structures 5	18	Three 63
2	Bonds 9	19	Four 71
3	Frontviews 15	20	Five 81
4	Definitions 17	21	Six 93
5	Combinations 21	22	Seven 105
6	Extra text 29	23	Eight 119
7	Axis 31	24	Nine 133
8	Setups 33	25	Five Front 149
9	Symbols 37	26	Six Front 155
10	Positioning 39	27	Carbon 161
11	Reactions 45	28	Newman Stagger 167
12	Subscripts 47	29	Newman Eclipsed 169
13	Fonts 49	30	Alkyl 175
14	Color 51	31	Chair 181
15	Interaction 53	32	Boat 185
16	Summary 55	33	Symbol 189
17	One 57		

 $2 \hspace{3.5cm} ppchT_{\!\!E\!}X$

Introduction

This manual is an update of the ppchTEX manual. Being one of the first public packages in what became the ConTEXt suite, it covers a set of coherent macros that can be used to typeset chemical structure formulas. The first version of ppchTEX was ready for use in 1995 and the second release came with the previous versions of this manual. Some 15 years later, in the process of upgrading ConTEXt to suit LuaTEX, it made sense to reconsider the usage of ppchTEX. First of all, we want basic chemical support in the kernel, so it made sense to take the relevant code and turn it into a kernel module. This means that in ConTEXt MkIV one does not need to load any module. For compatibility we keep the old module around.

The old code can also be used outside ConTeXt, but the integrated code not. This permits us to get away from the old PICTeX based approach and combine the power of TeX, MetaPost and Lua. The differences for ConTeXt users are not that noticeable as we already default to MetaPost for rendering the lines and curves, but in ConTeXt MkIV users could notice that the runtime is no longer influenced by callouts to MetaPost because there we use the integrated library. We also changed a couple of aspects like dealing with fonts and provide more control over color, as we no longer need to be generic. The fact that we operate within ConTeXt also meant that we can use all its facilities (like interaction) without special precautions.

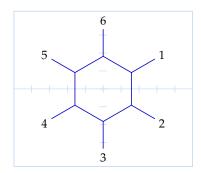
This means that this manual is just an overview as before but done a bit different. When we moved on to LuaMetaTeX and MkXL, aka LMTX, the chemical modules didn't change apart from adaptations to more efficient MetaPost integration. This manual is now targetting that version but still is mostly an overview. It is important to keep in mind that the code is not compatible with MkII, mostly because we decided to make the interface a bit more flexible for which we also needed a bit more consistency across structures, especially the usage of plus and minus signs.

As a final introductory note, chemical typesetting has its own rules and practices as well as variants. Using the chemical macros described here, it may be possible to construct structures that do not make any chemical sense, or to produce representations that are incorrect, as no chemical knowledge is built-in. Indeed, certain operations are available for completeness and by symmetry and may not have any reality in chemical practice. The user is responsible for a correct and consistant usage and should not count on the macros to ensure the construction of valid structures.

¹ The original module was written by J. Hagen and A.F. Otten (with contributions by T. Burnus and D. Kuypers) and provided a set of macros based on PCTEX or pstricks for the actual drawing of graphics. It could be used with ConTeXt as well as with LaTeX.

1 Structures

The number of commands that is used to typeset chemical structure formulas is relatively small once you see the pattern. Often most you need is the following.



Example 1

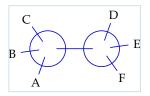
\setupchemical[axis=on,frame=on,width=5000,axis=on]

\startchemical \chemical[SIX,B,+SR,RZ][1,2,3,4,5,6] \stopchemical

Figure 1.1

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

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



Example 2

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

Figure 1.2

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

If you use(d) this module in the early days you will notice that we use +SR instead of just R here. The reason is that it is more consistent to have R for the full-length radical line in all constructs, at the TEX end as well as in MetaPost. This means that older code has to be adapted.

The carbon example looks simple but in fact is pretty complex. It actually is

\chemical[CARBON,C,SB,Z234,1.5MOV1,MIRO,C,SB,Z234][A,B,C,D,E,F]

and the simplification comes from CB1 being a shortcut definition in the CARBON namespace. This will be discussed later, so consider it a teaser.

Text is typeset in mathematical mode, this means that you may type anything that normally is allowed between \$ \$ or with \im.

We will explore the examples in more detail. The key SIX means that we want to draw a sixring. In analogy we could type ONE, THREE, FOUR and FIVE, EIGHT, CARBON, NEWMAN, CHAIR, some alternatives on these keys and some symbols.

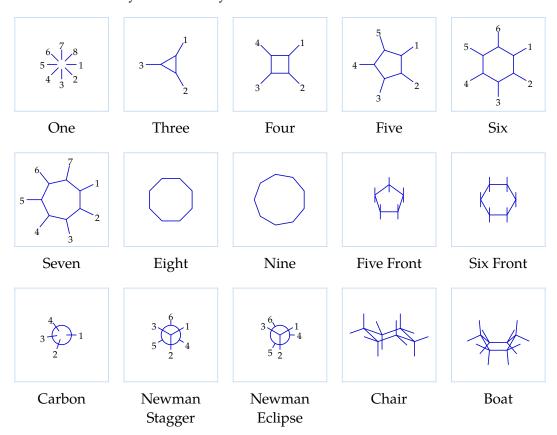


Figure 1.3 A few examples

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

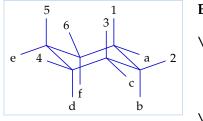


Figure 1.4

Example 3

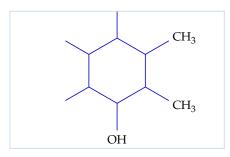
Within a structure the chemical bonds between the C-atoms are defined in the same way. In this example we use B and SR. Bonds within a structure are numbered and can be defined by:

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

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

```
\chemical[SIX,B1..6,+SR1..6]
```

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



Example 4

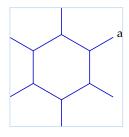
```
\startchemical[frame=on,width=6000]
\chemical
[SIX,B1..6,+SR1..6,RZ1..3]
[CH_3,CH_3,OH]
\stopchemical
```

Figure 1.5

When the second argument is left out no text (substituents) are placed on the ring and the key RZ1..3 has no effect.

Splitting the specification part from the text has the advantage that we can predefine structures (as we will see later) that we call within a structure and that pick up text from the calling structure. In such a nested case the texts are put on a sort of stack and fetching a text can involve the whole stack.

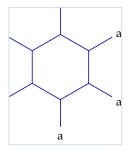
The disadvantage is that in complex structures it might be hard to see which text belongs to what specification. Therefore we provide a key/value variant as well.



Example 5

\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ1=a]
\stopchemical

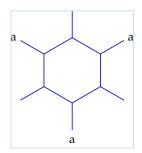
Figure 1.6



Example 6

\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ1..3=a]
\stopchemical

Figure 1.7

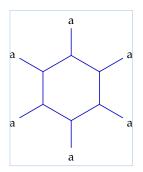


Example 7

\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ135=a]
\stopchemical

Figure 1.8

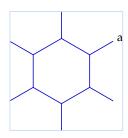
As you can see here, the text is repeated in the case of a key specification that involves more bonds. Compare this with the split definition approach:



Example 8

\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ=a]
\stopchemical

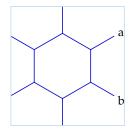
Figure 1.9



Example 9

\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ] [a]
\stopchemical

Figure 1.10



Example 10

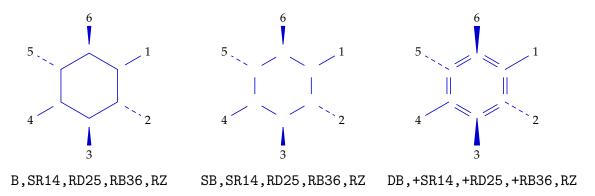
\startchemical[frame=on]
 \chemical[SIX,B,+SR,RZ] [a,b]
\stopchemical

Figure 1.11

2 Bonds

Let me know if some bolds are not mentioned here an needs to gbe discussed. As the is an update from the older syntax there might be errors, so you can also send me fixes.

This chapter gives an overview of the bonds you can use in structures. From the examples throughout this manual the use of the different keys will become more meaningful. There is a clear pattern in the specifications so we start with an example where S means single and D refers to double. The signs influence the attachment (or length for that matter).

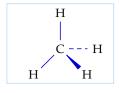


Bonds always have two alternatives: a long and a short version. The shortened bonds leave room to place atoms within a structure. A number of bonds can be shortened on both sides left (-) or right (+).

В	Bond	SB	Single Bond
ВВ	Bold Bond	-SB	Left Single Bond
НВ	Hydrogen Bond	+SB	Right Single Bond

Table 2.1 Single bonds.

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



Example 11

\startchemical[frame=on,width=3000] \chemical[ONE,SD1,SB4,BB2,SB7,Z01247][C,H,H,H,H] \stopchemical

Figure 2.1

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

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

EB	Extra Bond	DB	Double Bond
		ТВ	Triple Bond

Table 2.2Multiple bonds.

Free electrons and electron pairs can be defined in different ways. The accompanying keywords start with an E.

ES	Extra Single	ED	Extra Double
EP	Extra Pair	ET	Extra Triple

Table 2.3 Free electrons and electron pairs.

The example below shows a carbon atom with 8 outer electrons arranged in a chemically very peculiar way.



Example 12

\startchemical[frame=on,width=2000,height=2000] \chemical[ONE,Z0,ES1,ED3,ET5,EP7][C]

Figure 2.2 \stopchemical

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

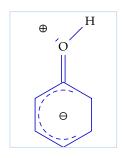
SS	Short Shortcut	S	Shortcut
-SS	Left Short Shortcut	MID	Open Mid Shortcut
+SS	Right Short Shortcut	MIDS	Closed Mid Shortcut

Table 2.4 Special bonds.

С	Circle	CD	Dashed Circle
CC	Shifted Circle	CCD	Dashed Shifted Circle

Table 2.5 Circle bonds.

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



Example 13

\startchemical[frame=on,width=3000]
 \chemical
 [SIX,B,+ER6,CCD12,Z0,SUB6,ONE,SB8,EP6,Z0,ZT6,Z8]
 [\ominus,0,\oplus,H]
\stopchemical

Figure 2.3

Substituents can be connected to all corners of a structure. A substituent can be anything you want. It depends on the presence of atoms or molecules whether the bonds are long or short. In the examples you will see a great number of the keys that are used to define substituents.

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

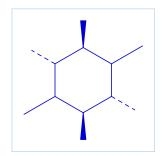
Table 2.6 Bonds to substituents.

There are a few alternatives to draw bridges.

R	.D	Radical Dashed	RB	Radical Bold
-R	.D	Left Radical Dashed	-RB	Left Radical Bold
+R	.D	Right Radical Dashed	+RB	Right Radical Bold

 Table 2.7
 Special bonds to substituents.

Radicals can be drawn in three ways.² Some alternatives are seldom used.



Example 14

\startchemical[frame=on,width=4000,height=4000] \chemical[SIX,B,R14,+RD25,+RB36] \stopchemical

Figure 2.4

SD	Single Dashed	LDD	Left Double Dashed
0E	Open Ended	RDD	Right Double Dashed

 Table 2.8
 More special bonds to substituents.

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

 $^{^{2}\,}$ The word radical schould not be interpreted chemically, but typographically.

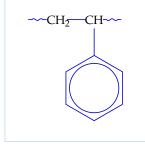


Figure 2.5

Example 15

```
\startchemical
    [width=4000,right=1500,
    top=2500,bottom=1500,
    frame=on]
    \chemical
    [SIX,
        B,C,+SR6,
        SUB6,ONE,CZ0,OE1,SB5,MOV5,CZ0,OFF5,OE5]
    [CH,CH_2]
    \stopchemical
```

It's obvious that substituents can be attached to the structure by means of double bonds.

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

Table 2.9 Double bonds to substituents.

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

Z	Atom	RZ	Radical Atom
CRZ	Center Atom	-RZ	Left Radical Atom
MIDZ	Mid Atom	+RZ	Right Radical Atom

Table 2.10 Atoms and molecules (radicals).

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



Example 16

\startchemical[frame=on,width=2500,height=2500] \chemical[SIX,B,MID,MIDZ][\SL{CH_2}] \stopchemical

Figure 2.6

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

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



Table 2.11 Labels and numbers.

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

12 ppch $T_{E}X$

RN	Radical Number	RT	Radical Text
RTN	Radical Top Number	RTT	Radical Top Text
RBN	Radical Bottom Number	RBT	Radical Bottom Text

Table 2.12 Labels and numbers.

The structure ONE has also a top and bottom alternative.

ZTN	Atom Top Number	ZTT	Atom Top Text	
ZBN	Atom Bottom Number	ZBT	Atom Bottom Text	

Table 2.13 Extra labels and numbers.

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



Example 17

\startchemical[frame=on,width=2500,height=2500] \chemical[ONE,SB,Z0,ZTT][C,a,b,c,d,e,f,g,h] \stopchemical

Figure 2.7

You can also add some symbols to the structure.

AU	Arrow Up	AD	Arrow Down	
----	----------	----	------------	--

Table 2.14 Indications.

The arrows are positioned between the atoms in a structure.



Example 18

\startchemical[frame=on,width=2500,height=2500] \chemical[SIX,B,AU] \stopchemical

Figure 2.8

We want to add that while typesetting atoms and molecules the dimensions of these atoms and molecules are taken into account. The width of C and the height of C_m^n play an important role during positioning. This mechanism may be refined in a later stage.

 $ppchT_{EX}$

Frontviews

Structures FIVE and SIX can be displayed in a frontview. However there are some limitations. Frontviews can not be rotated. Also the coupling of several structures is limited.

We illustrate the frontview keys in two examples.

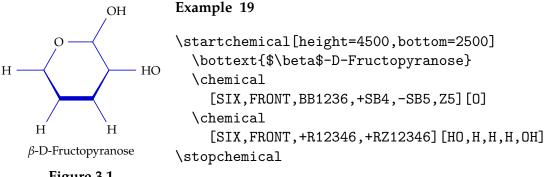


Figure 3.1

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

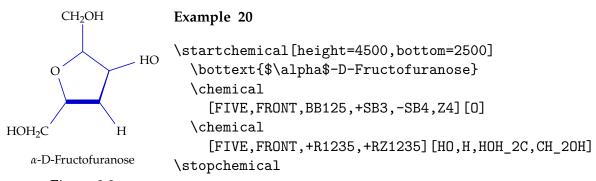


Figure 3.2

4 Definitions

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

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

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

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

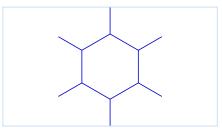


Figure 4.1

Example 21

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

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

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

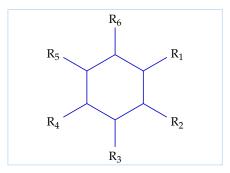


Figure 4.2

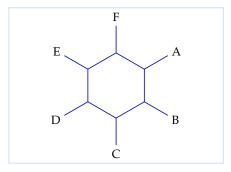
Example 22

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

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

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

 $ppchT_{E}X$



Example 23

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

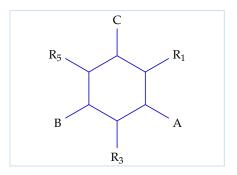
\startchemical[frame=on,width=6000] \chemical[sixring,RZ][A,B,C,D,E,F] \stopchemical

Figure 4.3

In principal the possibilities are unlimited. However, you should remember that atoms and molecules are selected from the second argument in the order of definition in the first argument.

A definition may contain atoms and molecules (texts).

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



Example 24

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

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

Figure 4.4

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

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

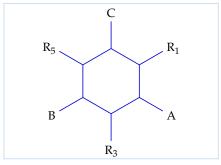


Figure 4.5

Example 25

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

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

When T_EX announces that an unknown command has occurred, you may have forgotten to type SIX, FIVE or a comparable key.

5 Combinations

Structures can be combined to more complex compounds. Moving one structure in relation to another structure is done by MOV, ROT, ADJ and SUB.

MOV	Move	moving a comparable structure structure in the direction of a bond
ADJ	Adjace	moving another structure in the direction of the x - or y -axis, adjacent to a bond
SUB	Substitute	moving one structure in relation to another in the direction of the x - or y -axis
ROT	Rotate	rotating a structure

Table 5.1 Moving and rotating.

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

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

DIR	Direction	moving a structure in a diagonal direction
OFF	Offset	moving atoms and molecules over small dis-
		tances

Table 5.2 Moving and rotating.

The structure CARBON can be mirrored with MIR.

	MIR	Mirror	mirroring a structure
--	-----	--------	-----------------------

Table 5.3 Mirroring.

We use a number to indicate the direction of a movement or the level of rotation. These keys are closely related with the structure. Therefore they have to be defined before bonds are drawn and texts are placed. So definition \chemical [FIVE,B,ROT1,R] and \chemical [FIVE,ROT1,B,R] will not have the same result. The first definition will give an undesirable result.



Figure 5.1

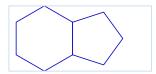
Example 26

\startchemical[frame=on,width=4000,right=3000] \chemical[SIX,B,MOV1,B] \stopchemical

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

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

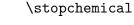
Structures can be combined. It is possible for example to combine structure FIVE with structure SIX in such a way that they have one mutual bond. Luckily the mechanism that takes care of these kinds of combinations is hidden for the user. In the next example you will see a sixring drawn by SIX, B. Then a movement in the positive *x*-direction is done by ADJ1. At last a rotated fivering is drawn: FIVE, ROT3, B.

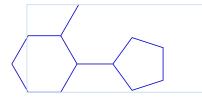


Example 27

\startchemical[frame=on,width=4000,right=3000] \chemical[SIX,B,ADJ1,FIVE,ROT3,B]

Figure 5.2





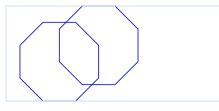
Example 28

\startchemical[frame=on,width=5000,right=4500] \chemical[SIX,ROT2,B,R6,SUB1,FIVE,B,R4] \stopchemical

Figure 5.3

To go from one structure to an adjacent one is done with ADJ. Most of the time one of these structures will have to be rotated to obtain a good attachment. This is done by ROT. Rotations are always clockwise in steps of 90.°C When a structure is attached with a bond you will have to use SUB. Movements with ADJ and SUB take place in the four directions of the x- and y-axis.

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



Example 29

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

Figure 5.4



Example 30

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

Figure 5.5

 $ppchT_{E}X$

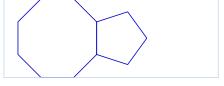


Figure 5.6

Example 31

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

It will be clear by now that the order in which the keys are defined makes a lot of difference. The order should be:

Most of the time putting structures together is done by translating and rotating. You could automate this process. In earlier versions this was done automatically, however this led to misinterpretations of users concerning the positions of bonds, atoms and substituents. A structure that consists of more than one component can best be defined per component, translations included. Rotations should wait until the last step.

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

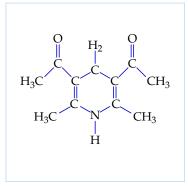


Figure 5.7

Example 32

```
\startchemical
[scale=small,width=6000,height=6000,frame=on]
\chemical[SIX,SB2356,DB14,Z2346,SR36,RZ36]
[C,N,C,C,H,H_2]
\chemical[PB:Z1,ONE,Z0,MOV8,Z0,SB24,DB7,Z27,PE]
[C,C,CH_3,0]
\chemical[PB:Z5,ONE,Z0,MOV6,Z0,SB24,DB7,Z47,PE]
[C,C,H_3C,0]
\chemical[SR24,RZ24]
[CH_3,H_3C]
\stopchemical
```

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

PB:	Picture Begin	beginning a substructure
PE	Picture End	ending a substructure

Table 5.4 Positioning.

Directly after PB you will have to define the location where the substructure is positioned. The first following atom is centered on that location. Always use a central atom on this location.

These keys were introduced after trying to obtain structures that are typeset in an acceptable quality. There are different ways to define structures. The following alternative would have resulted in:

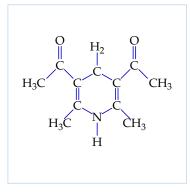


Figure 5.8

Example 33

```
\startchemical [scale=small,width=6000,height=6000,frame=on] \chemical [SIX,SB2356,DB14,Z36,SR36,RZ36][N,C,H,H_2] \chemical [PB:Z1,ONE,Z0,MOV8,Z0,SB24,DB7,Z27,PE][C,C,CH_3,0] \chemical [PB:Z5,ONE,Z0,MOV6,Z0,SB24,DB7,Z47,PE][C,C,H_3C,0] \chemical [PB:Z2,ONE,Z0,MOV2,SB6,CZ0,PE][C,CH_3] \chemical [PB:Z4,ONE,Z0,MOV4,SB8,CZ0,PE][C,H_3C] \stopchemical
```

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

The differences in outcome when using SUB in stead of PB are very small. However compare the following formulas.

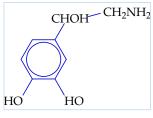


Figure 5.9

Example 34

```
\startchemical
  [width=fit,frame=on,scale=small]
  \chemical
    [SIX,ROT2,B,C,+R236,RZ23,
        SUB6,ONE,OFF1,Z0,40FF1,SB1,Z1]
    [H0,H0,CH0H,CH_2NH_2]
\stopchemical
```

Figure 5.10

Example 35

```
\startchemical
  [width=fit,frame=on,scale=small]
  \chemical
    [SIX,ROT2,B,C,R236,RZ23,
        PB:RZ6,ONE,Z0,30FF1,SB1,Z1,PE]
    [H0,H0,CH0H,CH_2NH_2]
\stopchemical
```

We try to predict rotations and shifts as good as possible but it might take some trial and error, but we assume that at some point one has (and shares) definitions.

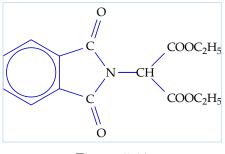


Figure 5.11

Example 36

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

Figure 5.12

Example 37

```
\startchemical
  [width=fit,height=fit,frame=on,
    scale=small]
  \chemical
    [ONE,SB15,DB7,Z057,30FF1,M0V1,Z0,30FF1,M0V1,
        Z017,SB1357,M0V3,Z0,M0V3,SB1357,Z013,30FF5,
        M0V5,Z0,30FF5,SB5,Z5]
    [C,H_2N,NH,(CH_2)_3,C,C00H,H,\SL{NH},C,C00H,H,
        (CH_2)_2,H00C]
\stopchemical
```

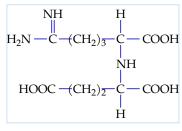


Figure 5.13

Example 38

```
\startchemical
    [width=fit,height=fit,frame=on,
        scale=small]
    \chemical [ONE,SB15,DB7,Z057,30FF1] [C,H_2N,NH]
    \chemical [MOV1,Z0,30FF1] [(CH_2)_3]
    \chemical [MOV1,Z017,SB1357] [C,C00H,H]
    \chemical [MOV3,Z0] [\SL{NH}]
    \chemical [MOV3,SB1357,Z013,30FF5] [C,C00H,H]
    \chemical [MOV5,Z0,30FF5,SB5,Z5] [(CH_2)_2,H00C]
\stopchemical
```

Figure 5.14

Example 39

```
\startchemical
  [width=fit,height=fit,frame=on,
    scale=small]
  \chemical
    [ONE,ZO,SAVE,MOV7,SB1357,Z017,30FF5,MOV5,Z0,
        30FF5,MOV5,SB15,DB7,Z057,RESTORE,
        MOV3,SB1357,Z013,MOV5,30FF5,Z0,60FF5,SB5,Z5]
    [\SL{NH},C,C00H,H,(CH_2)_3,C,H_2N,NH,C,C00H,H,
        (CH_2)_2,H00C]
\stopchemical
```

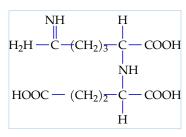
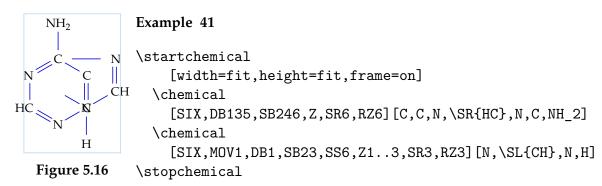


Figure 5.15

Example 40

```
\startchemical
[width=fit,height=fit,frame=on,scale=small]
\chemical
[ONE,ZO,MOV7,SB1357,ZO17,30FF5,MOV5,ZO,
30FF5,MOV5,SB15,DB7,ZO57,MOV0,MOV3,SB1357,
Z013,MOV5,30FF5,ZO,60FF5,SB5,Z5]
[\SL{NH},C,COOH,H,(CH_2)_3,C,H_2H,NH,C,COOH,H,
(CH_2)_2,HOOC]
\stopchemical
```

Notice the use of SAVE and RESTORE. These keys enable you to save a location in a structure and return to that location in another stage. As an extra we will show you a combination of SIX and FIVE.



 $ppchT_{EX}$

6 Extra text

We can add text and symbols in and around structures. For example:

Example 42

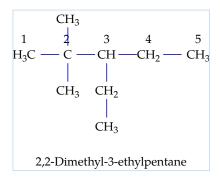


Figure 6.1

```
\startchemical
```

```
[height=4500,top=1250,width=fit,frame=on]
\bottext
    {2,2-Dimethyl-3-ethylpentane}
\chemical
    [ONE,Z3570,SB1357]
    [CH_3,\T{1}{H_3C},CH_3,\SR{\LT{2}{C}}]
\chemical
    [MOV1,0FF1,Z0,SB3]
    [\T{3}{CH}]
\chemical
    [MOV3,Z0,SB3,MOV3,Z0,MOV7,MOV7]
    [CH_2,CH_3]
\chemical
    [OFF1,SB1,MOV1,OFF1,Z0,20FF1,SB1,Z1]
    [\T{4}{CH_2},\T{5}{CH_3}]
```

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

\stopchemical

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

Table 6.1 Text: charges.

A charge is centered above the atom. For example:

```
\placeformula
  \startformula
  \chemical{S}
  \chemical{+}
  \chemical{0_2}
  \chemical{GIVES}{violent}
  \chemical{\+{4}{S}\-{2}{0_2}}
  \stopformula
```

will result in:

Compare this with:

```
\placeformula
  \startformula
  \chemical{S}
  \chemical{+}
  \chemical{0_2}
  \chemical{GIVES}{violent}
  \chemical{\+{4}{S}\-{2}{0_2}}
  \stopchemicalformula
  \stopformula
```

which gives:

7 Axis

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



Example 43

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

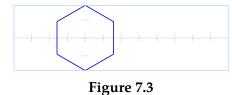
Figure 7.1



Example 44

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

Figure 7.2



Example 45

\startchemical
 [axis=on,
 frame=on,
 left=2000,right=4000]
 \chemical[SIX,B]
\stopchemical



Figure 7.4

Example 46

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

31

The dimensions of the total structure determine the dimensions of the axis. When width=fit and/or height=fit is typed the dimensions are determined by the real dimensions so there need to be content. Your choice will depend on how you want to place the structure in the text. As shown here, the axis model currently uses rather large numbers. This is an inheritance of the previous implementation and we deciced to keep it this way.

8 Setups

After \startchemical and \setupchemical you can type the setup.

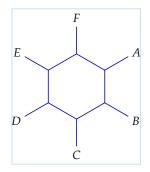
parameter	values	default
width	number	4000
height	number	4000
left	number	
right	number	
top	number	
bottom	number	
bodyfont	8pt 9pt 10pt etc.	\bodyfontsize
textstyle	\rm \bf etc.	\rm
style	\rm \bf etc.	\rm
color	colorname	
rulecolor	colorname	
scale	number	medium
size	small medium big	medium
axis	on off	off
frame	on off	off

 Table 8.1
 Setups for structures.

The axis range from -2000 upto +2000, height as well as width. The parameter Z0 is at (0,0). Other divisions can be set up with left, right, top and/or bottom in combination with width and height.

You can use the key size to setup the current text size and with scale you setup the dimensions of the structure itself. The scale is also determined by the parameter bodyfont. The values small, medium and big are proportionally related.

Contrary to the old implementation we no longer operate in math mode as it makes not much sense. The mathematical symbols are available in text mode anyway and control over super and subscripts in implemented differently. With the parameter style an alternative style can be chosen. In **example 47** the substituents are typeset *slanted*.



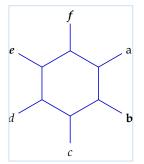
Example 47

\startchemical[frame=on,style=\sl]
 \chemical[SIX,B,+R,RZ][A,B,C,D,E,F]
\stopchemical

Figure 8.1

The style option is valid for chemical structures in a picture and in the text. The sub- and superscripts are changed accordingly. This is illustrated in CH_4 , CH_4 and CH_4 , in which the setups are \rm, \bf and \sl. Italic \it formulas lead to a bigger linewidth. The commands adjust automatically to the actual fontstyle: CH_4 , CH_4 , CH_4 etc. (\ss, \rm, \tt).

It is also possible to set the style at the instant you type them in the argument.³

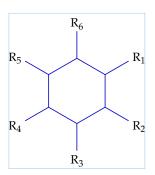


Example 48

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

Figure 8.2

The parameter frame and axis need no further explanation.



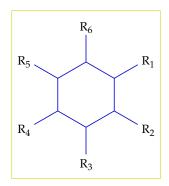
Example 49

 $\label{lem:cal} $$ \operatorname{SIX}_{R,RZ}[R_1,R_2,R_3,R_4,R_5,R_6] $$ \operatorname{SIX}_{R,RZ}[R_1,R_2,R_3,R_4,R_5,R_6] $$$

Figure 8.3

A more controlled framing is possible by setting up the encompassing frame:

Not yet documented but already available is support for the rendering prefix mystyle->a and alike. This permits a more general setup of styles.



Example 50

\setupchemicalframed[frame=on,offset=1ex] \startchemical \chemical[SIX,B,+R,RZ][R_1,R_2,R_3,R_4,R_5,R_6] \stopchemical

Figure 8.4

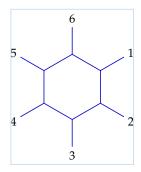
A structure can be displayed in different sizes. This is done with size and scale.



Example 51

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

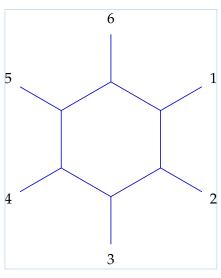
Figure 8.5



Example 52

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

Figure 8.6



Example 53

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

Figure 8.7

The values belonging to small, medium or big are proportionally related.

 $ppchT_{EX}$

9 Symbols

There are some symbols that can be used to display reactions. The reaction below is typed by:

```
\setupchemical
  [size=small,
   scale=small,
   width=fit,
   height=5500,
   bottom=1500]
\hbox
  {\startchemical
     \chemical[SIX,B,ER6,RZ6][0]
   \stopchemical
   \startchemical
     \chemical[SPACE, PLUS, SPACE]
   \stopchemical
   \startchemical
     \chemical[FIVE,ROT4,B125,+SB3,-SB4,Z4,SR4,RZ4][N,H]
   \stopchemical
   \startchemical
     \chemical[SPACE,GIVES,SPACE][?]
   \stopchemical
   \startchemical
     \chemical[SIX,B,EB6,R6,SUB4,FIVE,ROT4,B125,+SB3,-SB4,Z4][N]
   \stopchemical
   \startchemical
     \chemical[SPACE, PLUS, SPACE, CHEM][H_20]
   \stopchemical}
```

The \hbox is necessary to align the structures. The symbols GIVES and PLUS need no further explanation. With SPACE more room can be created between the structures and symbols.

Figure 9.1

An equilibrium can be displayed with EQUILIBRIUM. Over GIVES and EQUILIBRIUM you can place text. In the example the text is just a '?'. In addition MESOMERIC is also available. Braces used for displaying complexes can be created with OPENCOMPLEX and CLOSECOMPLEX.

10 Positioning

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

SAVE	Save Status	save actual status
RESTORE	Restore Status	restore actual status

Table 10.1 Positioning.

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

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

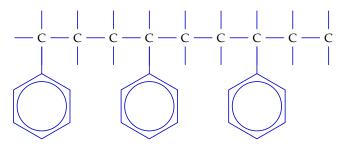


Figure 10.1

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

```
\placeformula
  \startformula
  \setupchemical
      [width=fit,top=1000,bottom=2500,]%
      scale=small,size=small]
  \startchemical
```

```
\chemical
    [ONE,
     SAVE,
        ZO,SB7,SB3,SB1,MOV1,ZO,SB1,MOV1,ZO,DB8,CZ8,SB1,Z1,
     RESTORE,
     SUB3, ONE,
     SAVE,
        ZO,SB3,SB1,MOV1,ZO,SB1,MOV1,ZO,DB8,CZ8,SB1,Z1,
     RESTORE,
     SUB3, ONE,
        ZO,SB7,SB1,MOV1,ZO,SB1,MOV1,ZO,DB8,CZ8,SB1,Z1
    [\SR{HC},0,C,0,C_{19}H_{39},
     \SR{H {2}C},0,C,0,C {17}H {29},
     \SR{H_{{2}C},0,C,0,C_{{21}H_{{41}}}
\stopchemical
\startchemical
  \chemical[SPACE, PLUS, SPACE]
\stopchemical
\startchemical[right=600]
  \chemical[ONE,CZO][3CH_{3}OH]
\stopchemical
\startchemical
  \chemical[SPACE,GIVES,SPACE,SPACE][H^+/H 20]
\stopchemical
\startchemical
  \chemical
    [ONE, ZO, SB7, SB3, SB1, Z3, OFF1,
     SUB1,
     ONE, ZO, OFF1, SAVE, -OFF1, SB3, Z3, RESTORE, SB1, OFF1,
     ONE, ZO, OFF1, SAVE, -OFF1, SB3, Z3, RESTORE, SB1, OFF1]
    [HC,OH,
     H_{2}C,OH,
     H_{2}C,OH
\stopchemical
\startchemical
  \chemical[SPACE, PLUS, SPACE]
\stopchemical
\startchemical[frame=on]
  \chemical
    [ONE,
     SAVE,
        DB8,CZ8,SB1,SB5,Z5,MOV1,Z0,SB1,Z1,
     RESTORE,
```

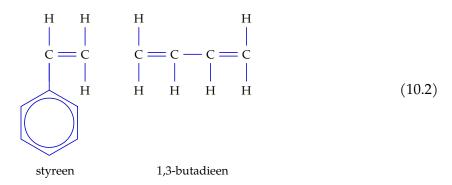
```
SUB3,ONE,
SAVE,
Z0,DB8,CZ8,SB1,SB5,Z5,MOV1,Z0,SB1,Z1,
RESTORE,
SUB3,ONE,
Z0,DB8,CZ8,SB1,SB5,Z5,MOV1,Z0,SB1,Z1
]
[C,0,C_{19}H_{39},0,CH_{3},
C,0,C_{17}H_{29},0,CH_{3},
C,0,C_{21}H_{41},0,CH_{3}]
\stopchemical
\stopformula
```

This definition might have been more compact if we would have typed SB731 in stead of SB7, SB3, SB1. But in this way the definition is readable. Complex structures can best be defined in its respective components.

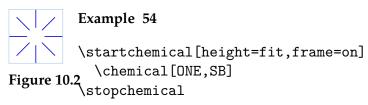
Just two more examples where we place text under a structure.

```
\placeformula
  \startformula
    \setupchemical
      [width=fit,top=1500,bottom=3500]
    \startchemical
      \chemical
        [ONE, ZO, DB1, SB3, SB7, Z7, MOV1, Z0, SB3, SB7, Z3, Z7,
         MOVO, SUB3, SIX, B, +R6, C]
        [C,H,C,H,H]
      \bottext{styreen}
    \stopchemical
    \quad\quad\quad
    \startchemical
      \chemical
        [ONE, ZO, DB1, SB3, SB7, Z3, Z7,
         MOV1,Z0,SB1,SB3,Z3,
         MOV1,Z0,DB1,SB3,Z3,
         MOV1,Z0,SB3,SB7,Z3,Z7]
        [C,H,H,C,H,C,H,C,H,H]
      \bottext{1,3-butadieen}
```

\stopchemical \stopformula



The use of OFF can be very subtle. The examples below illustrate this and show minor shifts of ONE.





Example 55

\startchemical[height=fit,frame=on]

10.3 \chemical[ONE,SB,30FF1,rulecolor,SB][red] \stopchemical

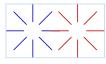


Example 56

\startchemical[height=fit,frame=on]

Figure 10.4

\chemical[ONE,SB,MOV1,rulecolor,SB][red] \stopchemical



Example 57

\startchemical[height=fit,frame=on]
 \chemical[ONE,SB,30FF1,MOV1,rulecolor,SB][red]
\stopchemical

Figure 10.5



Figure 10.6

Example 58

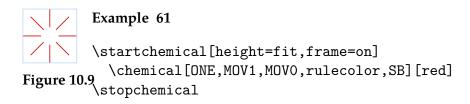
\startchemical[height=fit,frame=on] \chemical[ONE,SB,MOV1,30FF1,rulecolor,SB][red] \stopchemical

```
Example 59

| Startchemical[height=fit,frame=on] |
| Chemical[ONE,MOV1,30FF1,0FF0,rulecolor,SB][red] |
| Stopchemical |
```

```
Example 60

| Startchemical[height=fit,frame=on] |
| Chemical[ONE,MOV1,30FF1,MOV0,rulecolor,SB][red] |
| Stopchemical |
```



The next example shows the definition of complexes. Pay special attention to the use of RBT. Normally an extra spacing is not necessary but we use here —the command is not visible— a smaller bodyfont to prevent the structure to run in the margin.

```
\startformula
\setupchemical[scale=small,width=fit]
\startchemical
  \chemical[OPENCOMPLEX,SPACE]
\stopchemical
\startchemical
  \chemical[SIX,B,EB35,+R6,+LR1,+RR1]
  \chemical[SIX,ONE,SAVE,OFF1,Z0,EP57,RESTORE][\SL{OH}]
  \chemical[SIX,RZ6,LRZ1,RRZ1,RT2][H,Br,\oplus]
\stopchemical
\startchemical
  \chemical[SPACE, MESOMERIC, SPACE]
\stopchemical
\startchemical
  \chemical[SIX,B,EB25,R6,-R1,+R1]
  \chemical[SIX,PB:RZ6,ONE,OFF1,Z0,EP57,PE][\SL{OH}]
  \chemical[SIX,-RZ1,+RZ1,RT4][H,Br,\oplus]
\stopchemical
\startchemical
  \chemical[SPACE, MESOMERIC, SPACE]
\stopchemical
\startchemical
  \chemical[SIX,B,EB24,+R6,+LR1,+RR1]
```

```
\chemical[SIX,SAVE,SUB6,ONE,ZO,EP57,RESTORE][\SL{OH}]
```

\startchemical

\chemical[SPACE, MESOMERIC, SPACE]

\stopchemical

\startchemical

\chemical[SPACE, MESOMERIC, SPACE]

\chemical[SIX,B,EB24,+ER6,+LR1,+RR1]

\chemical[SIX,SAVE,SUB6,ONE,Z0,Z0,ZT7,RESTORE][\SL{OH},\T{\oplus}]

\chemical[SIX,LRZ1,RRZ1][H,Br]

\stopchemical

\startchemical

\chemical[SPACE,CLOSECOMPLEX]

\stopchemical

\stopformula

Without the use of SPACE the seperate structures would merge. Most of the time the optimization of such a reaction is an iterative proces.

$$\begin{bmatrix} & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$$

11 Reactions

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

```
\chemical{formula}
\chemical{formula}{bottom text}
\chemical{formula}{top text}{bottom text}
```

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

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

When the command is used in running text it will automatically be surrounded by $\$ Typing $\chemical{NH_4^+}$ will result in NH_4^+ .

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

The definition of the chemical part could be somewhat shorter:

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

or even:

```
\chemical{2H_2,+,0_2,->,2H_20}
```

A TEX-addict will notice from these examples that the plus sign and the arrow are on the baseline. Compare for example + and + . In the reaction you will see that the + and the \rightarrow are vertically aligned.

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

The reaction can be placed in the text. In that case a more compact display is used: $2H_2 + O_2 \rightarrow 2H_2O$. Some finetuning with \, would result in $2H_2$.

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

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

```
\placeformula
```

```
\startformula \chemical{2H_2}{hydrogen} \chemical{PLUS} \chemical{0_2}{oxygen} \chemical{GIVES}{heat} \chemical{2H_20}{water} \stopformula
```

So we can also place text over and under symbols!

$$2H_2 + O_2 oxygen \rightarrow heat 2H_2 Owater$$
 (11.2)

The last argument is placed under the compound.

liquid
$$H_2O \quad c.q.H_2O\textit{water} \tag{11.3}$$
 water

The formula above is defined with:

```
\placeformula
  \startformula
  \chemical{H_20}{liquid}{water}
  \hbox{c.q.}
  \chemical{H_20}{water}
  \stopformula
```

The size of the formulas or reactions in the running text can be set up with:

parameter	set up	default
size	small medium big	big

Table 11.1 Set up in text formulas.

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

$$H-CH=HC-H$$
 $H-CH=HC-H$ $H-CH=HC-H$

12 Subscripts

As we no longer typeset the consituents in math mode, we also no longer need to worry about the alignment of super and subscripts. We just use the same mechanism as in running text, using \low, \high and \lohi. These are applied automatically.

13 Fonts

The remarks concerning fonts in the old manual no longer apply. In principle you can use any font you want. Of course you can also use any character in the font as no encoding is involved.

14 Color

In ConTEXt you can colorize parts of a structure. In example ?? and 63 we see a directive being used for the rules but for text we just use TEX commands.



Figure 14.1

COOH Example 62

\startchemical[axis=on,frame=on,width=5000]
 \chemical[SIX,B,rulecolor,+R1,RZ1][red,COOH]
\stopchemical



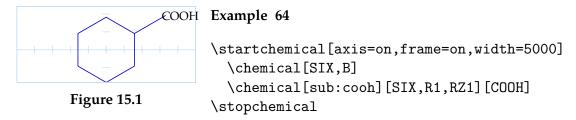
Figure 14.2

COOH Example 63

 $ppchT_{EX}$

15 Interaction

We do support interactive texts. An interactive text is a text that can be consulted on a computerscreen and contains many hyperlinked textareas. This means that clicking on such an area will result in a jump to the target area.



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

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

In this definition \goto is a ConTEXt-command. We can also refer from the structure to a particular part of the text.

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

\paragraph[txt:cooh]{Substituents}

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

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

 $ppchT_{EX}$

16 Summary

structure	#	category	keyword	arguments
alkyl	4	one	ALKYL	
boat	6	front	BOAT	
carbon	4	one	CARBON	
chair	6	front	CHAIR	
eight	8	ring	EIGHT	
five	5	ring	FIVE	
fivefront	5	front	FIVEFRONT	
four	4	ring	FOUR	
newmaneclipsed	6	one	NEWMAN, ECLIPSED	
newmanstagger	6	one	NEWMAN	
nine	9	ring	NINE	
one	8	one	ONE	
seven	7	ring	SEVEN	
six	6	ring	SIX	
sixfront	6	front	SIXFRONT	
three	3	ring	THREE	

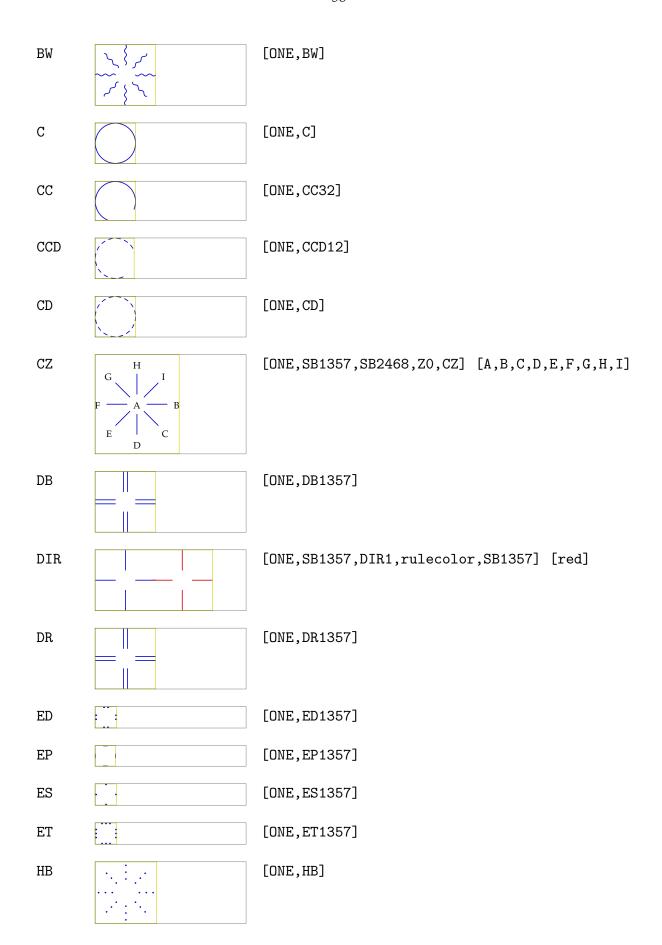
pb
pe
save
restore
reset
mp

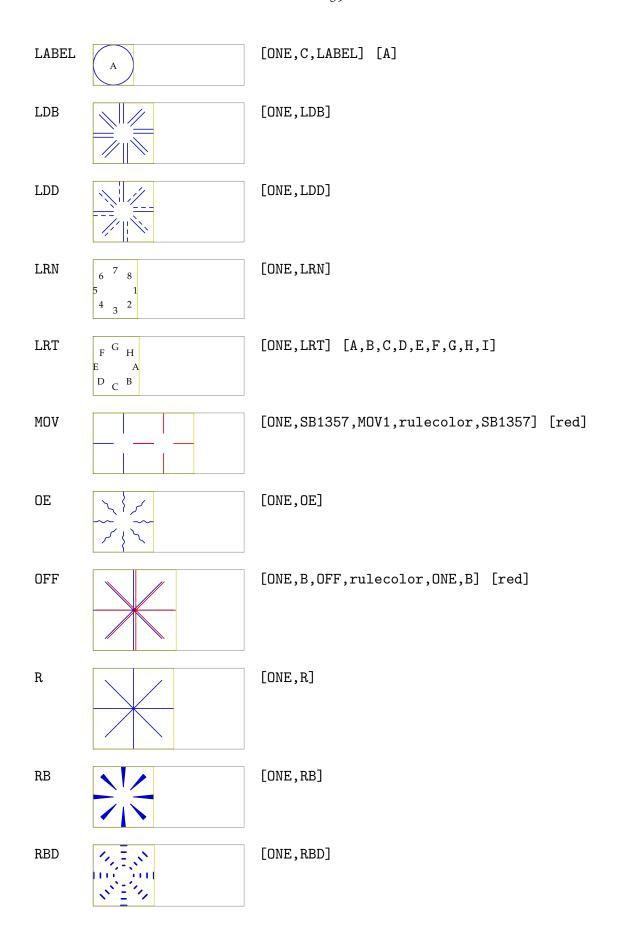
 $ppchT_{EX}$

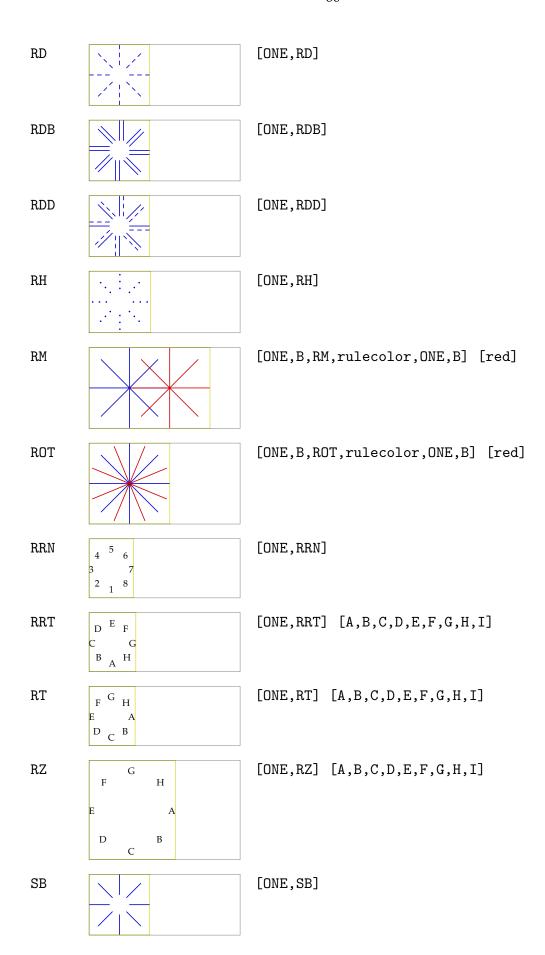
17 One

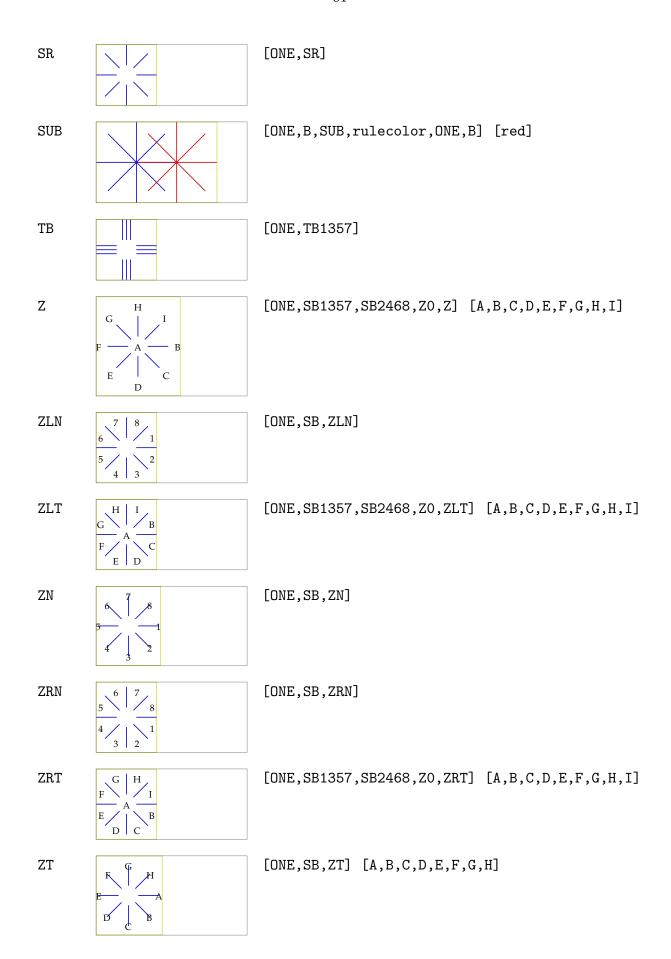
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au	line	ер	line	off	transform	sd	line
b	line	es	line	r	line	sr	line
bb	line	et	line	rb	line	sub	transform
bd	line	hb	line	rbd	line	tb	line
bw	line	label	text	rd	line	z	text
С	fixed	ldb	line	rdb	line	zln	number
СС	line	ldd	line	rdd	line	zlt	text
ccd	line	line	line	rh	line	zn	number
cd	fixed	lrn	number	rm	transform	zrn	number
cz	text	lrt	text	rn	number	zrt	text
dash	line	mark	transform	rot	transform	zt	text
db	line	mir	transform	rrn	number		
diff	transform	mov	transform	rrt	text		
AD			[ONE,AD]				
AU			[ONE,AU]				
В			[ONE,B]				
BB			[ONE,BB]				
22			[0112,22]				
BD	4, E.S.		[ONE,BD]				
	$\operatorname{In}(\mathbb{C})$ or						
	(マミケ)						

 $ppchT_{E}X$







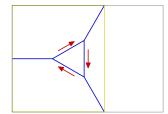


 $ppchT_{EX}$

18 Three

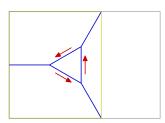
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ccd	line	lrn	number	rh	line	sr	line
cd	fixed	lrt	text	rm	transform	SS	line
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dash	line	lsr	line	rot	transform	Z	text
db	line	lsub	transform	rr	line	zln	number
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er	line	mir	transform	rrn	number	zt	text
hb	line	mov	transform	rrt	text		

AD



[THREE,B,R,rulecolor,AD] [red]

AU



[THREE,B,R,rulecolor,AU] [red]

В



[THREE,B]

С



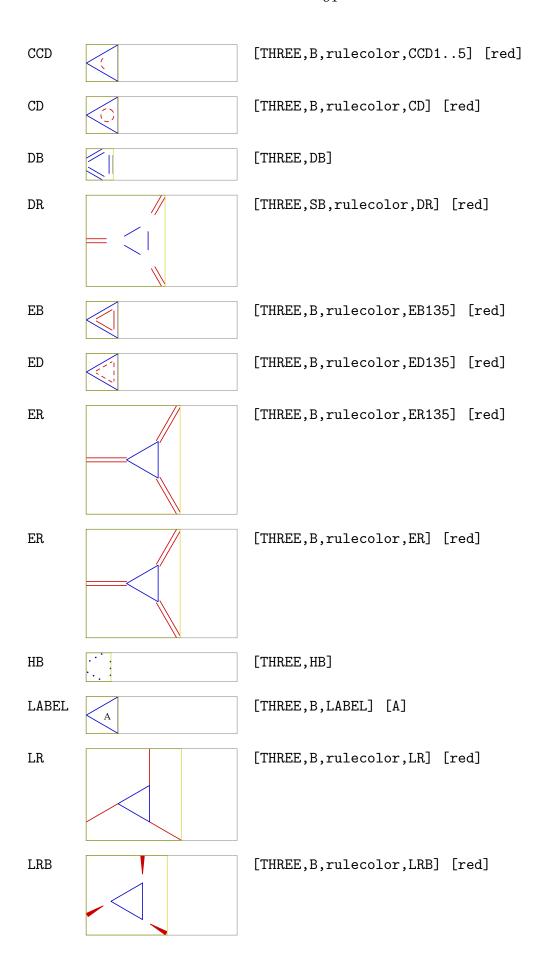
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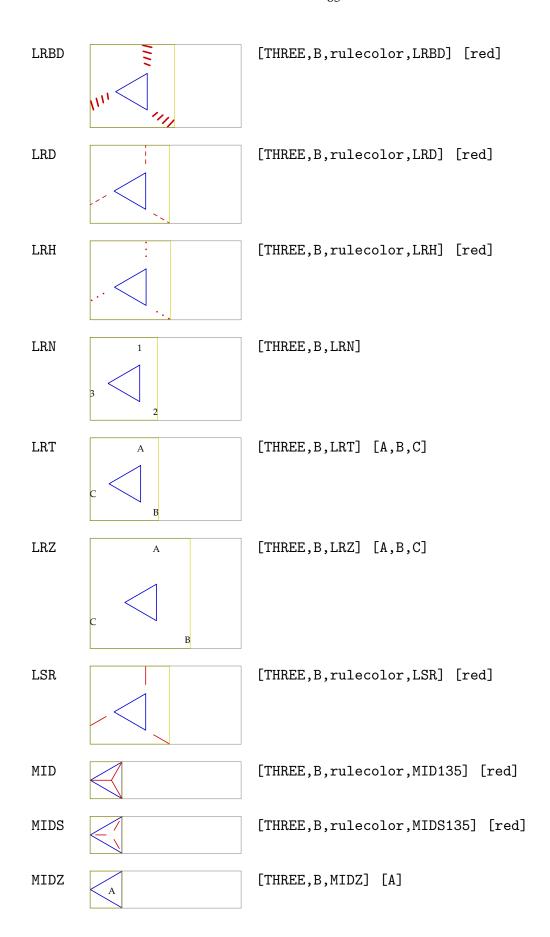
CC

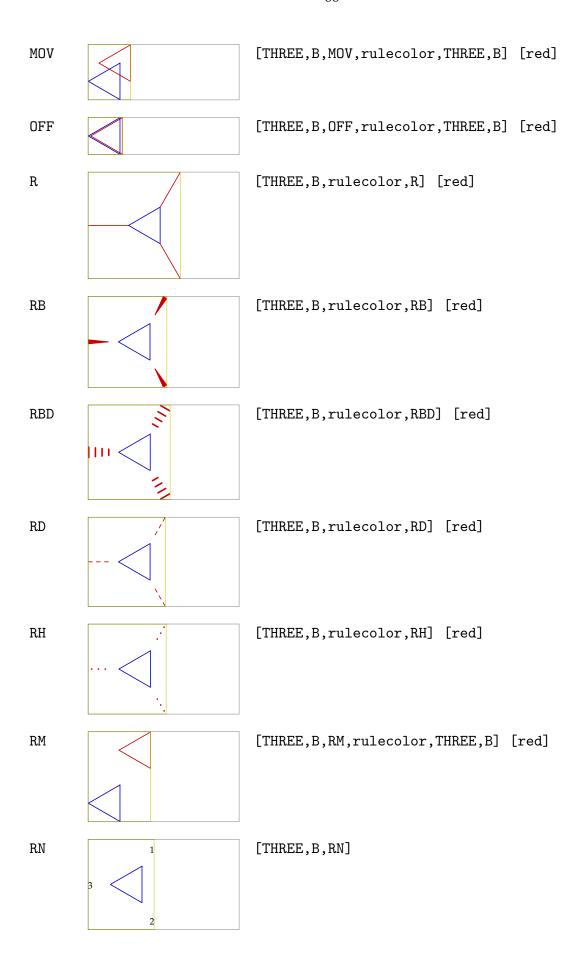


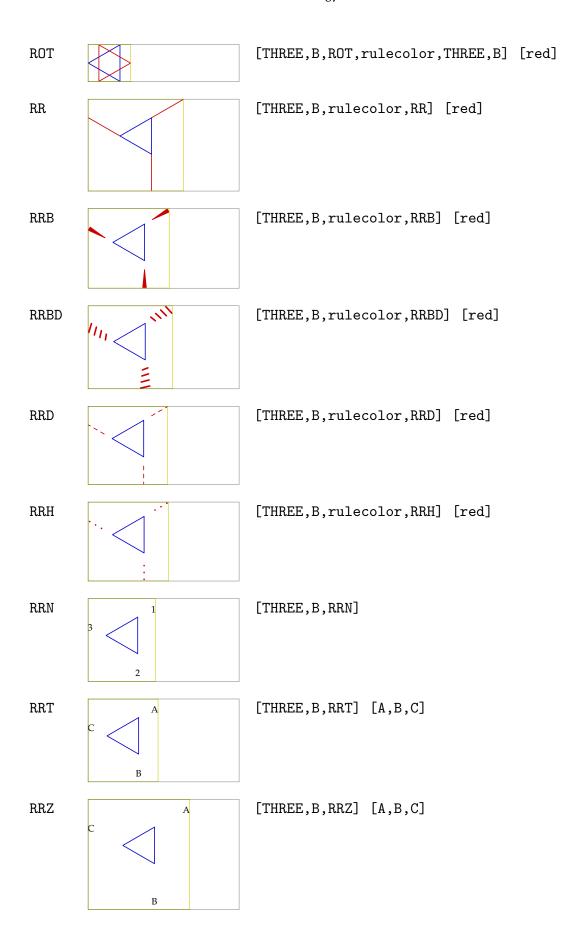
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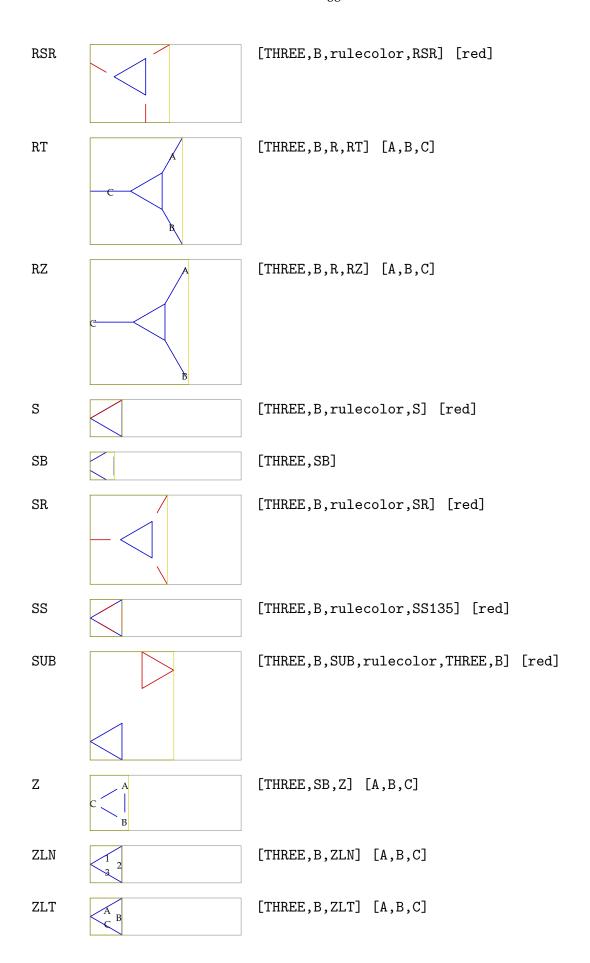
63

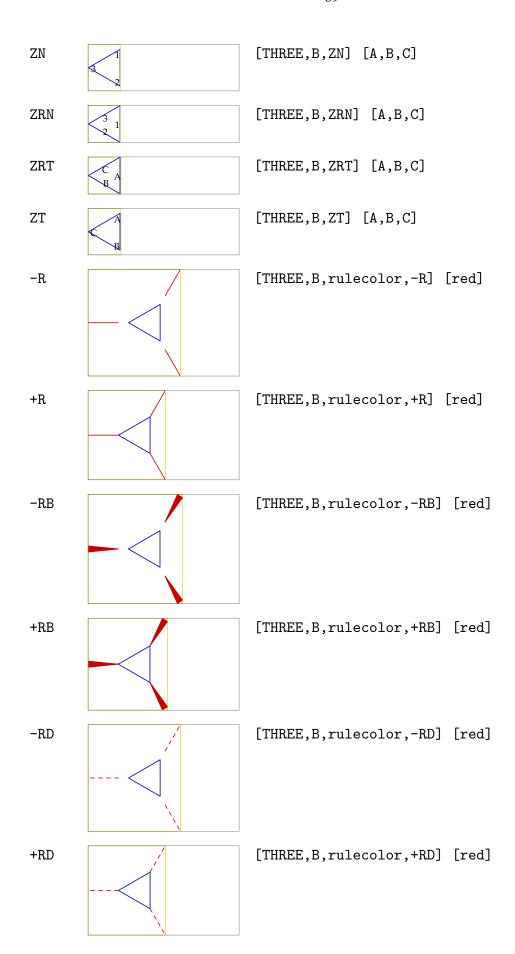


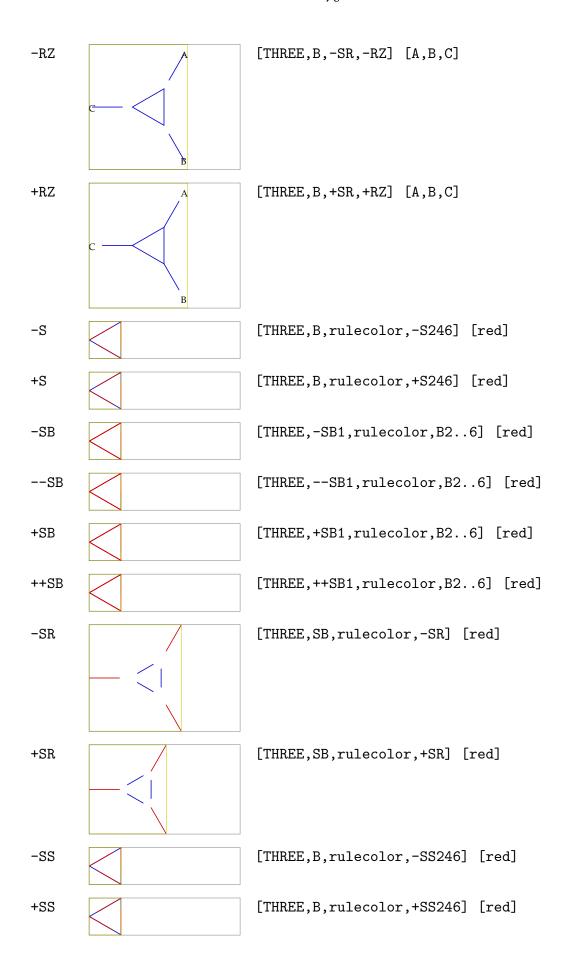








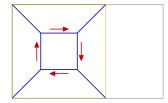




19 Four

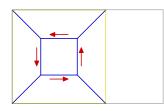
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hb	line	mov	transform	rrt	text		

AD



[FOUR,B,R,rulecolor,AD] [red]

AU



[FOUR,B,R,rulecolor,AU] [red]

В



[FOUR,B]

C

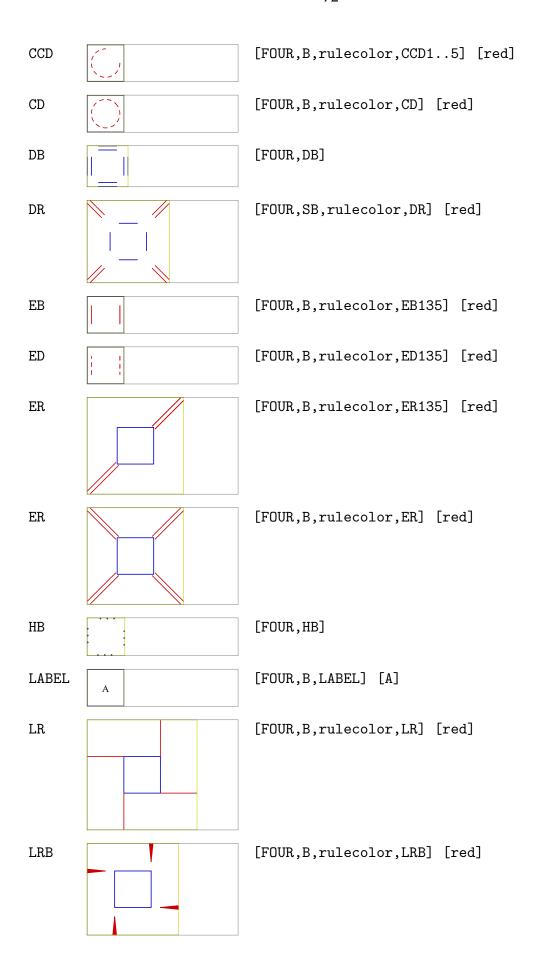


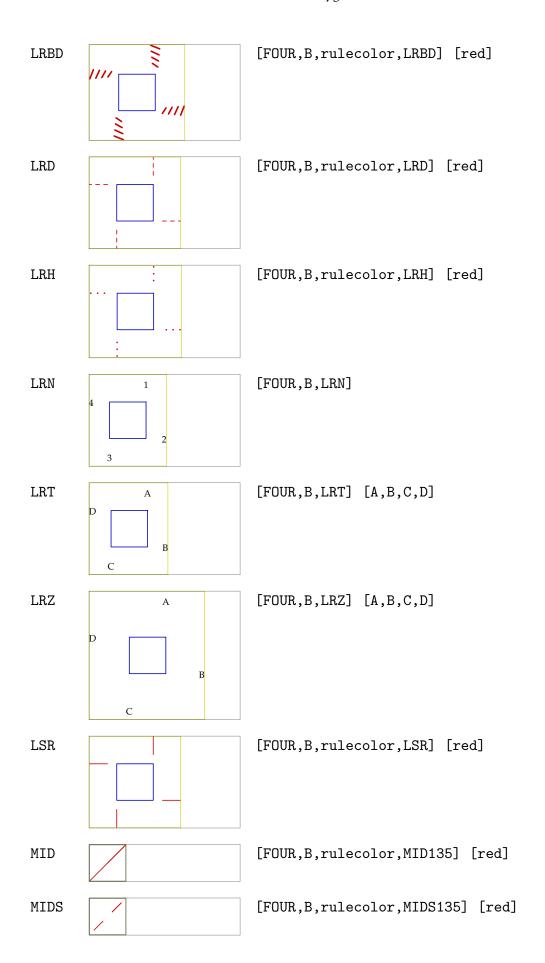
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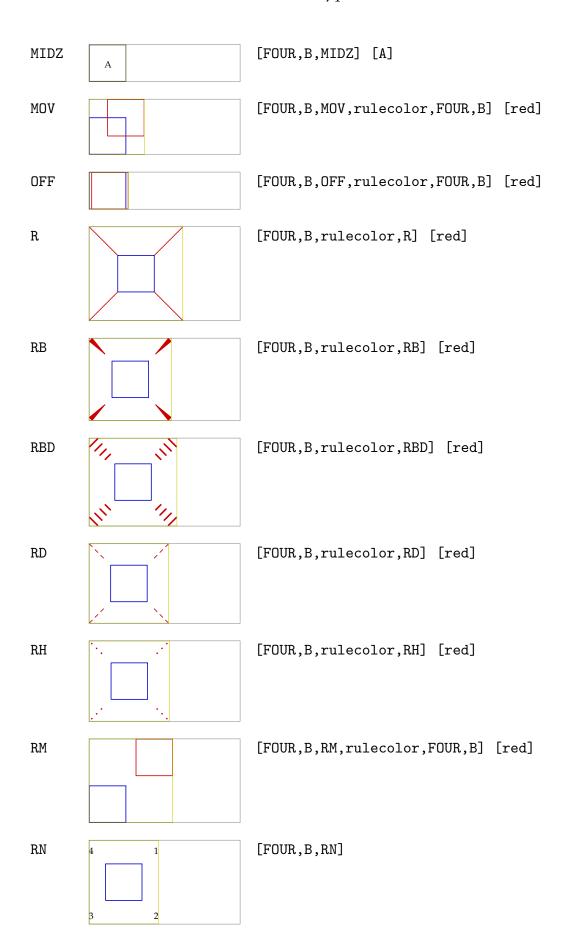
CC

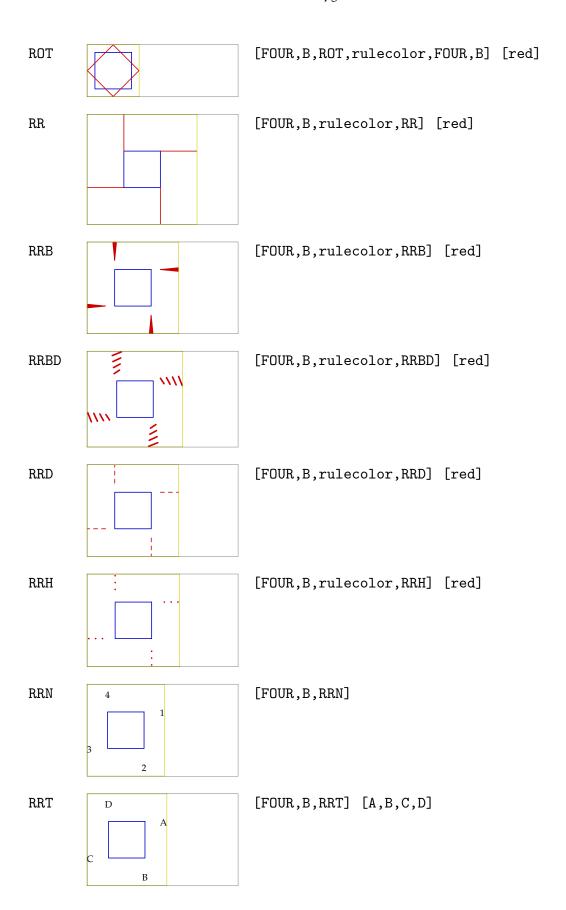


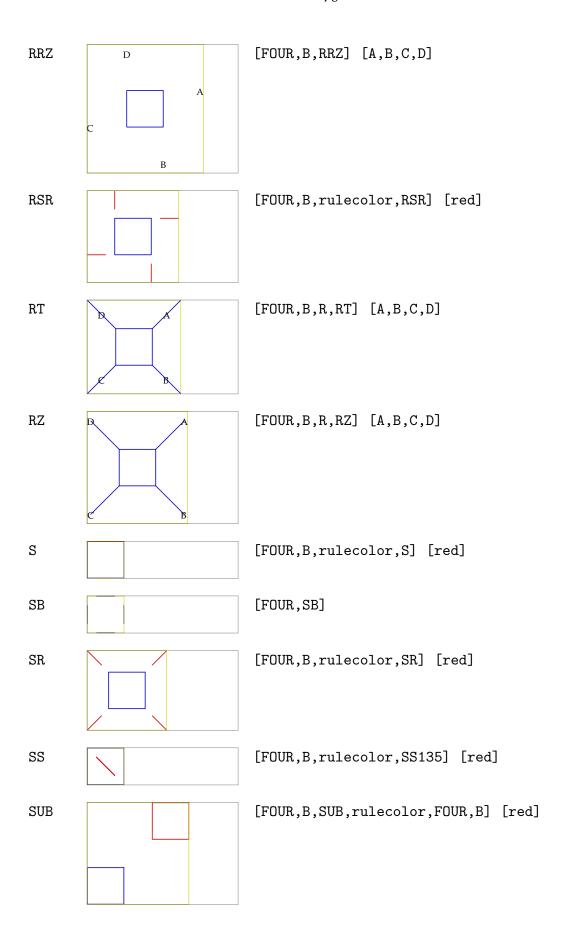
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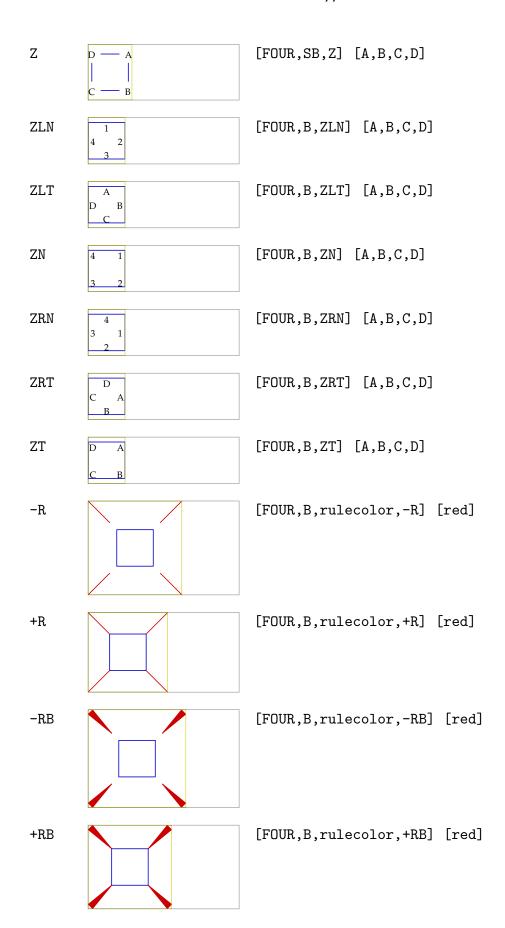


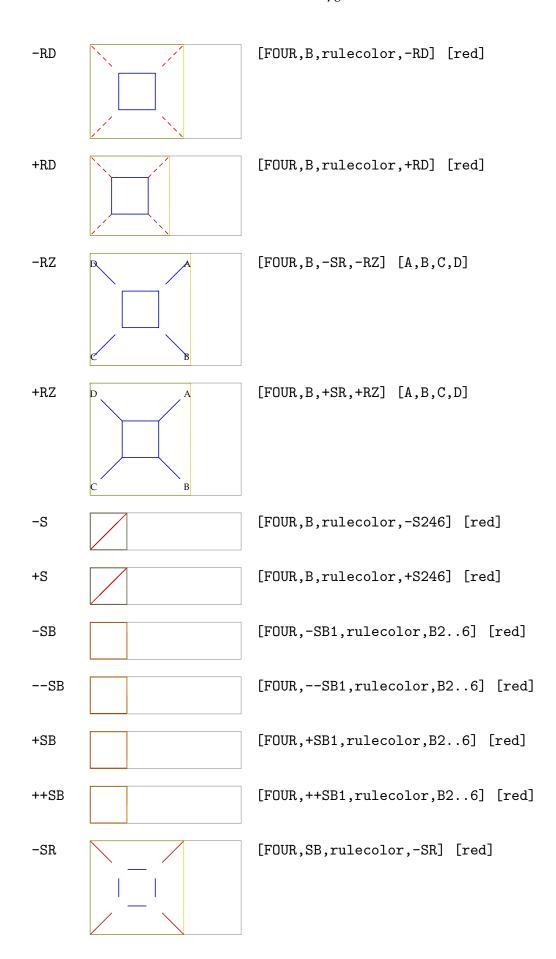


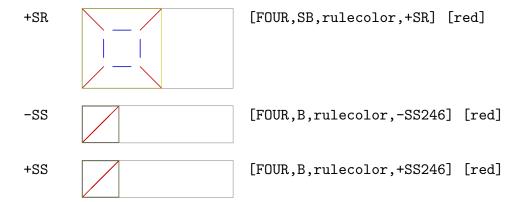










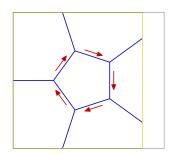


80 ppch T_{EX}

20 Five

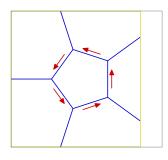
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AD



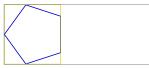
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AU

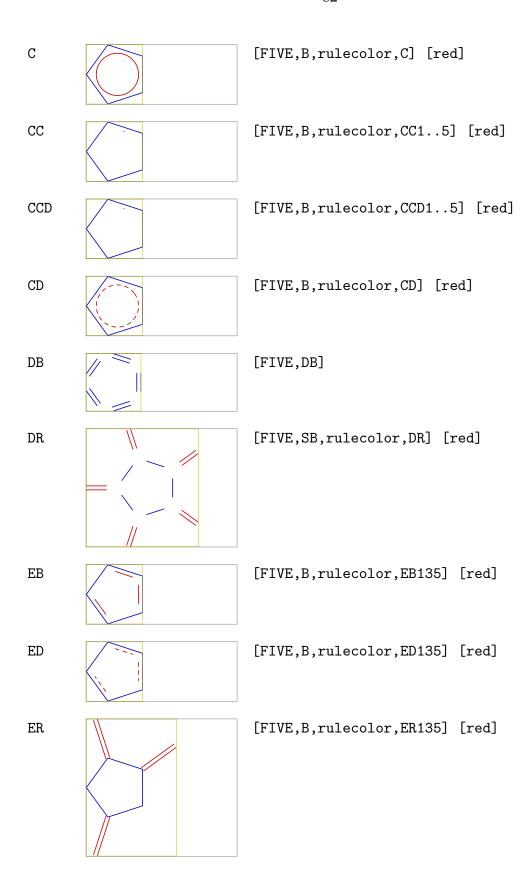


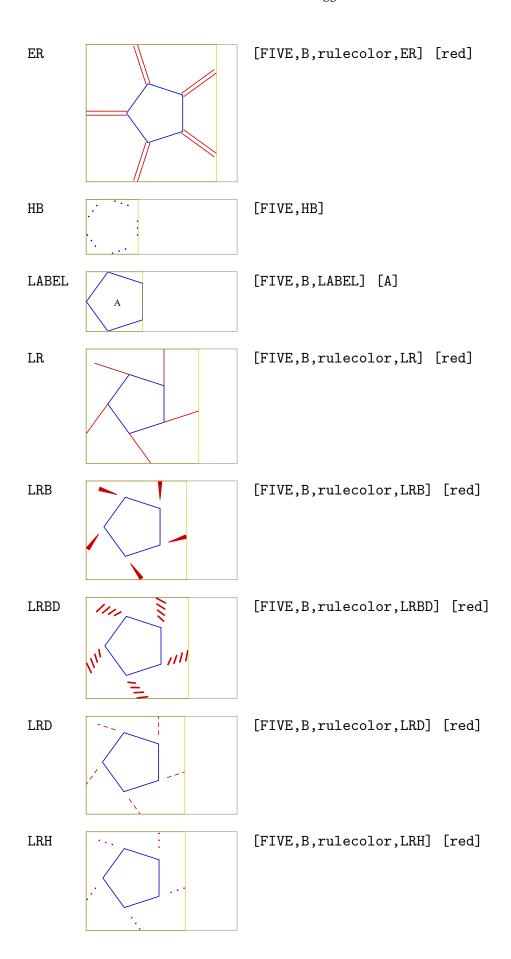
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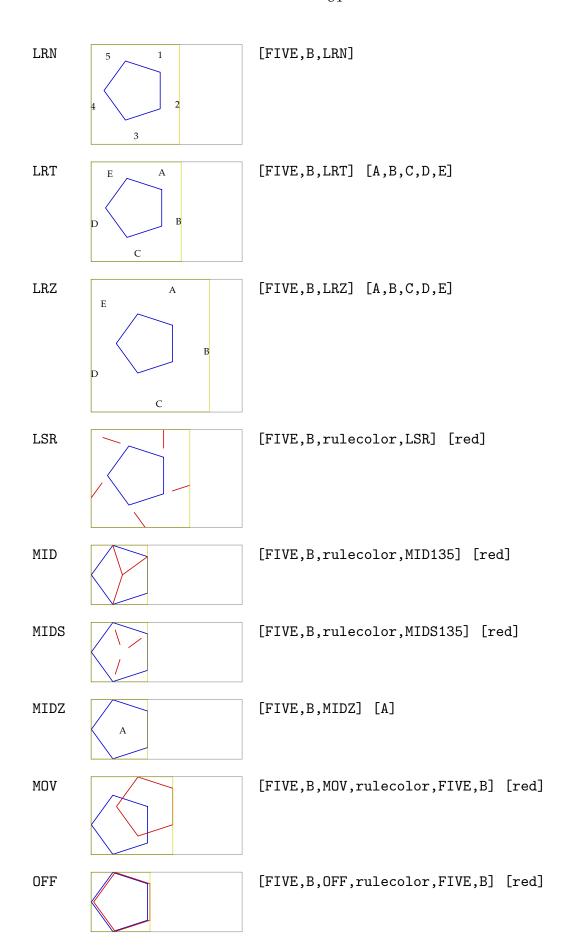
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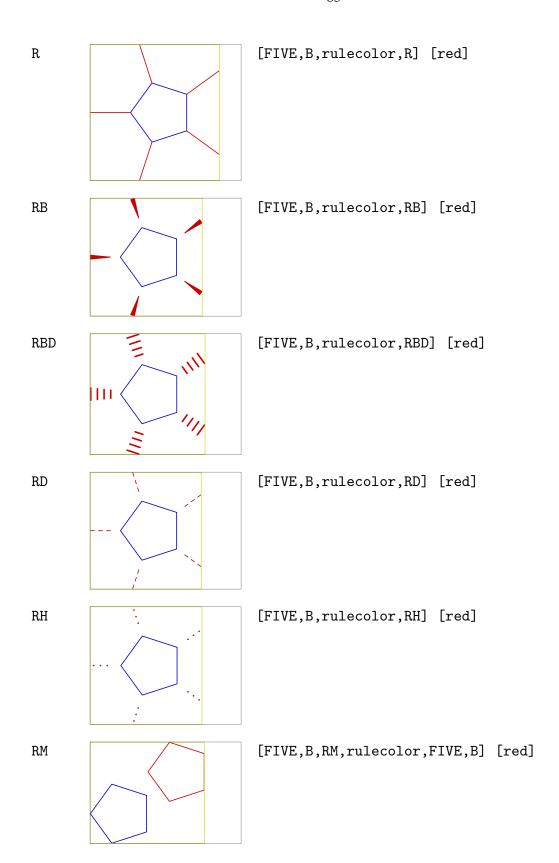


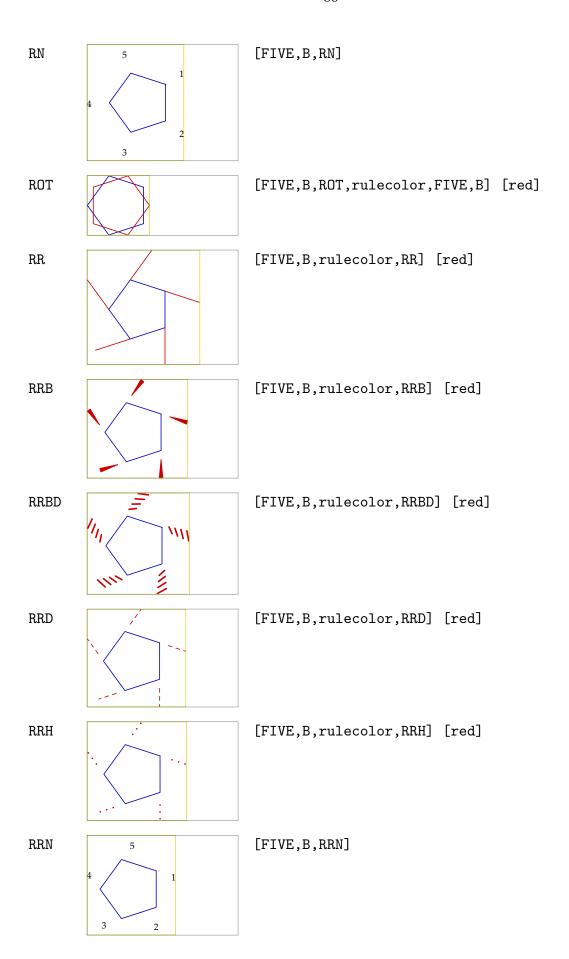
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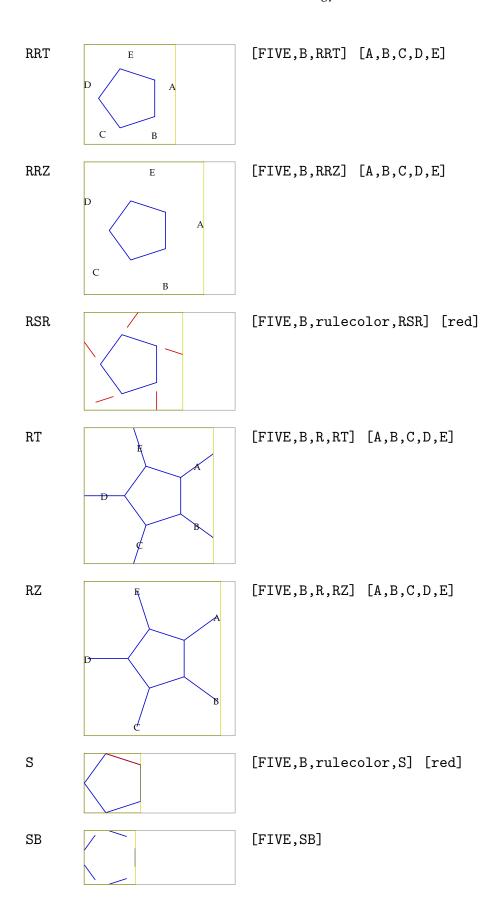


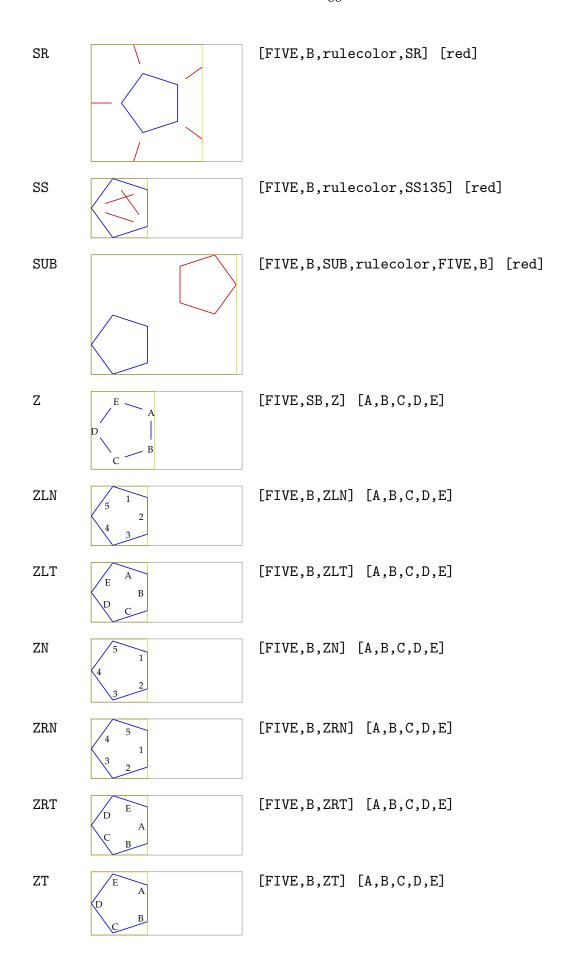


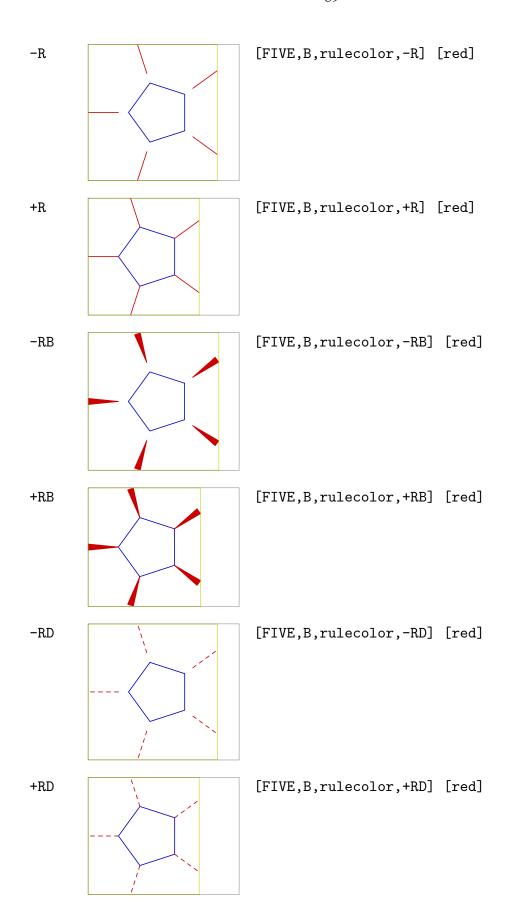


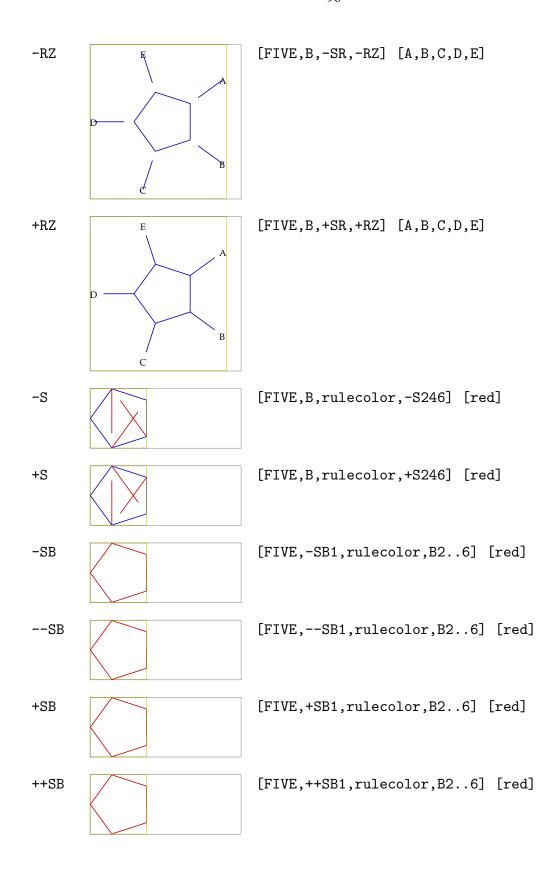


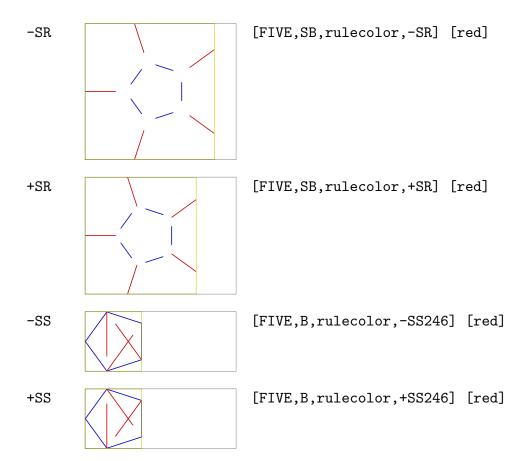










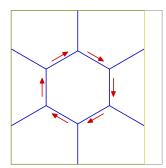


ppch T_EX

21 Six

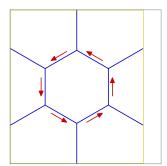
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AD

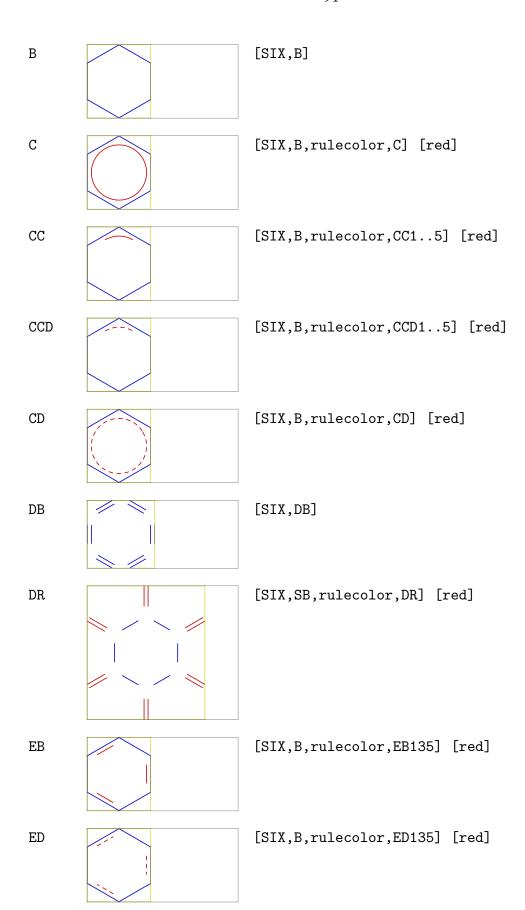


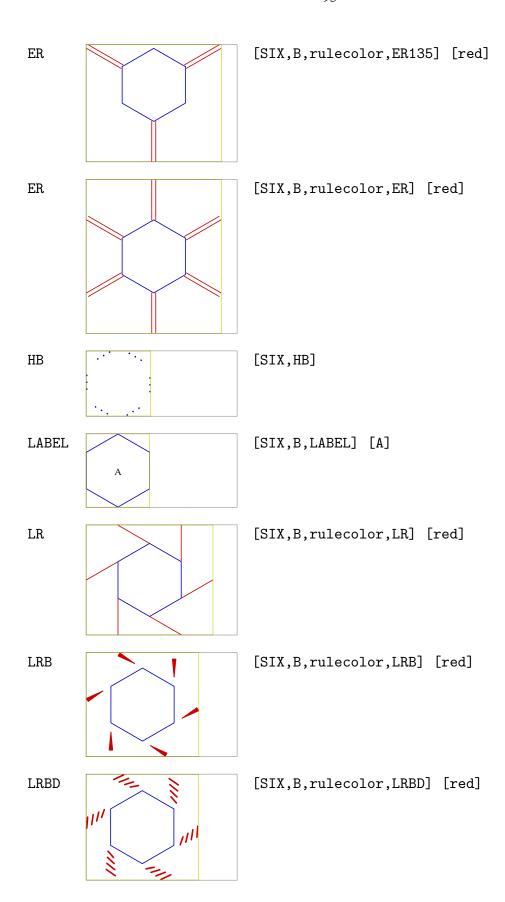
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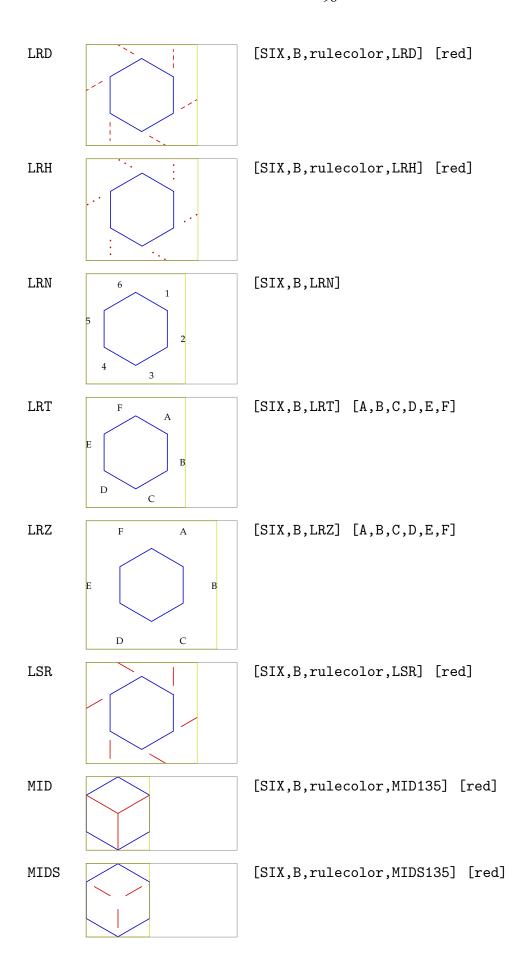
AU

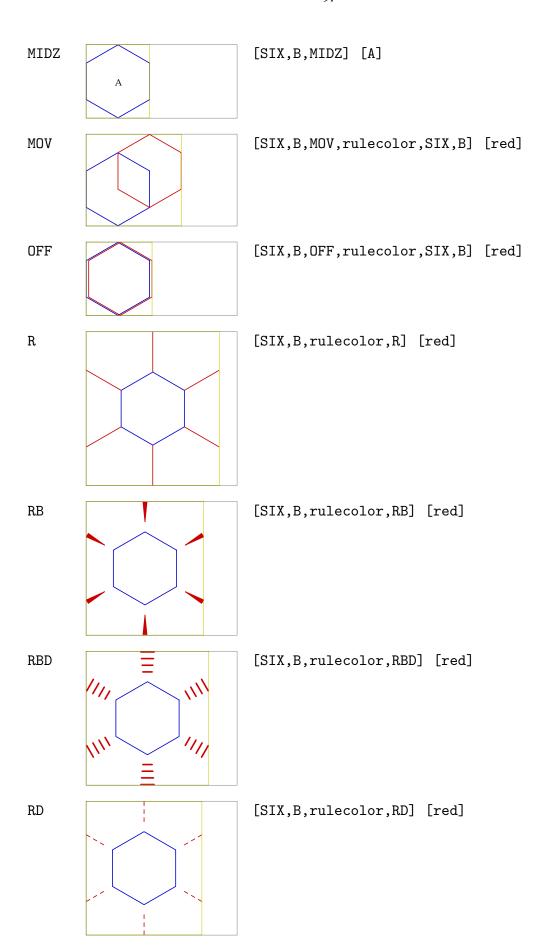


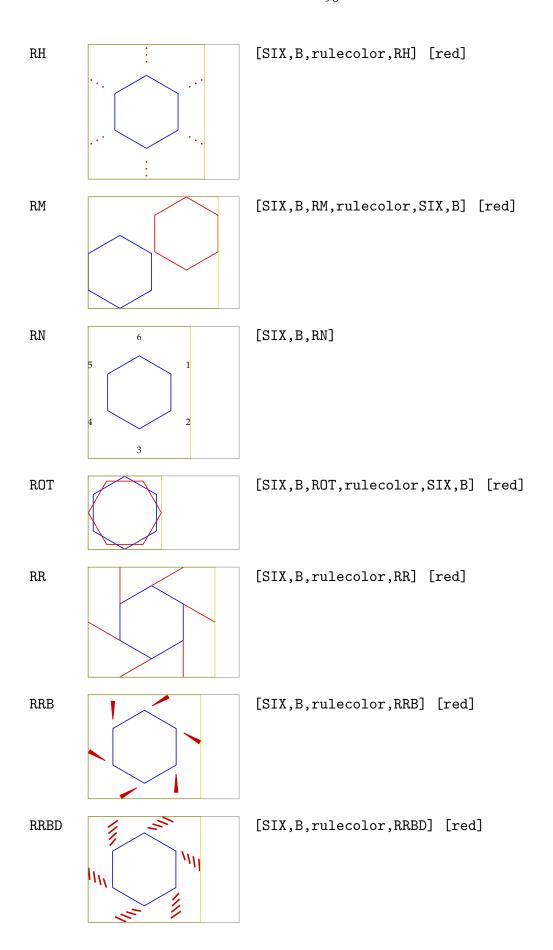
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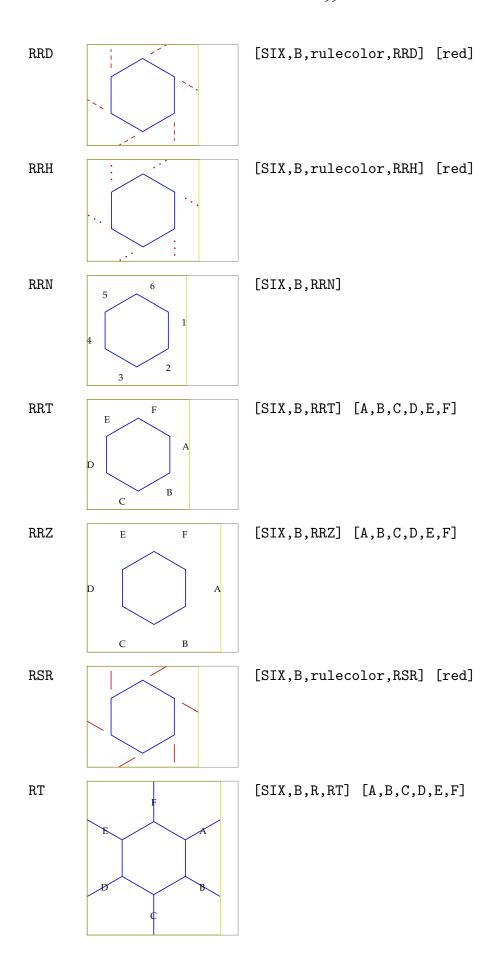


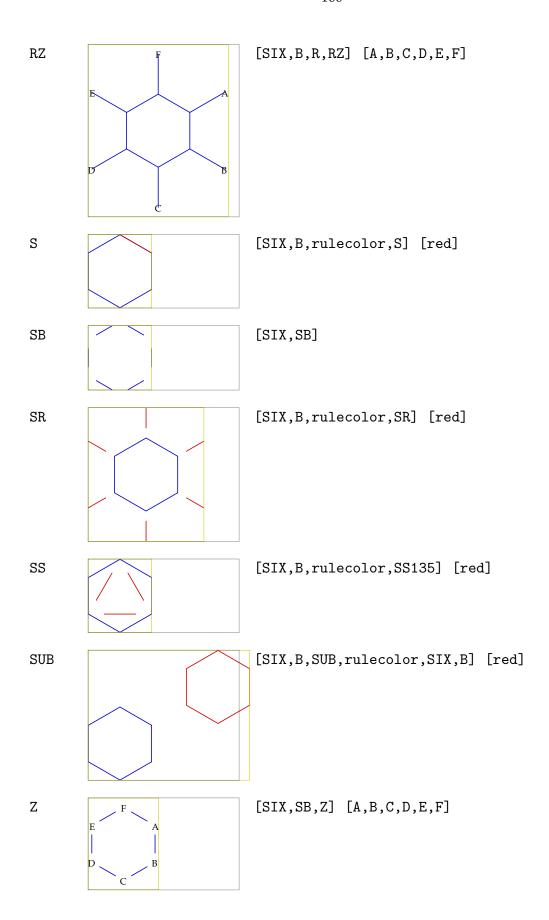


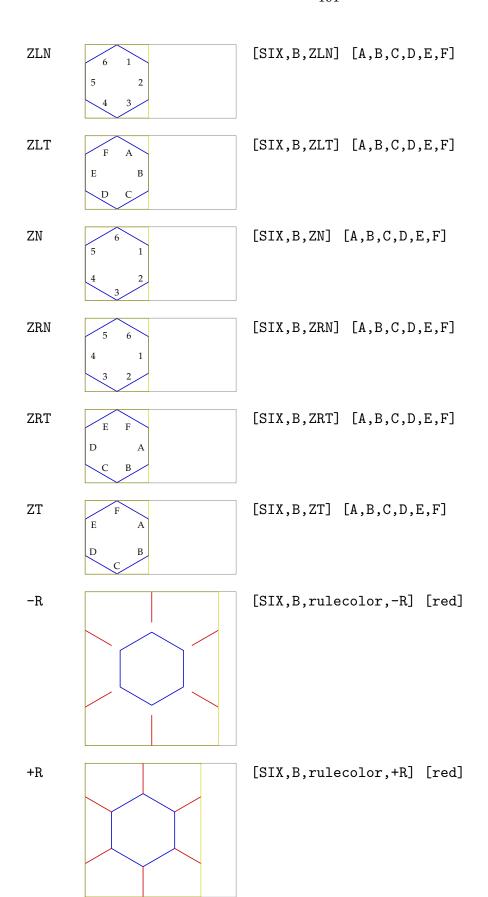


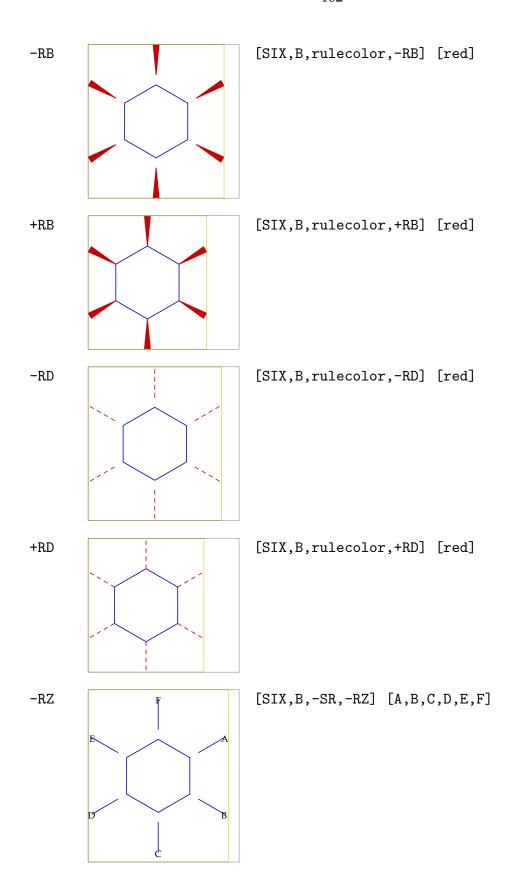


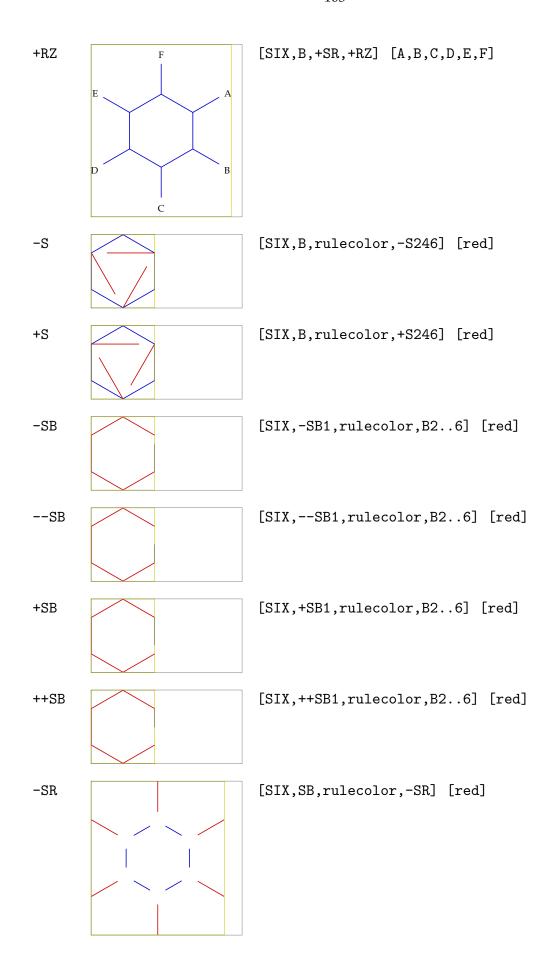


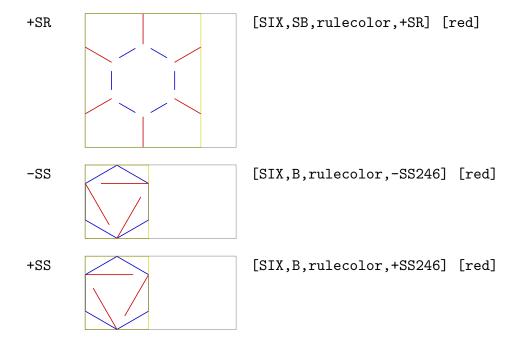








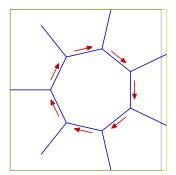




22 Seven

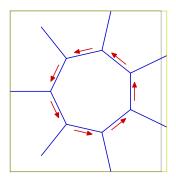
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СС	line	lrh	line	rd	line	sb	line
ccd	line	lrn	number	rh	line	sr	line
cd	fixed	lrt	text	rm	transform	ss	line
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db	line	lsub	transform	rr	line	zln	number
diff	transform	mark	transform	rrb	line	zlt	text
dr	line	mid	line	rrbd	line	zn	number
eb	line	mids	line	rrd	line	zrn	number
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er	line	mir	transform	rrn	number	zt	text
hb	line	mov	transform	rrt	text		

AD

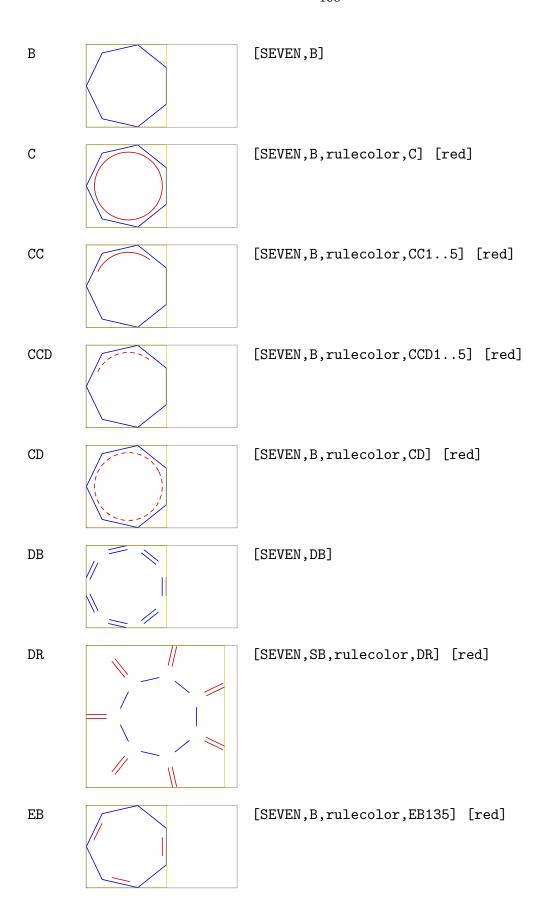


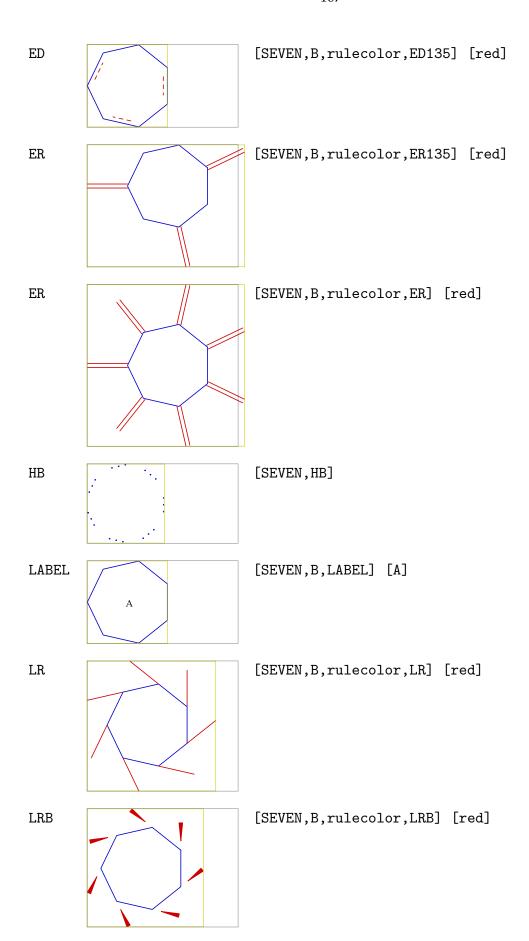
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AU

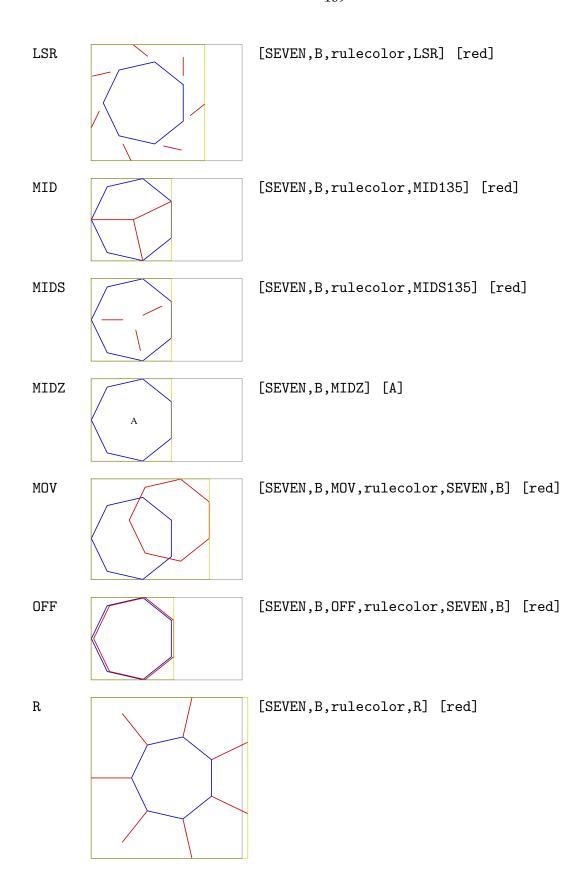


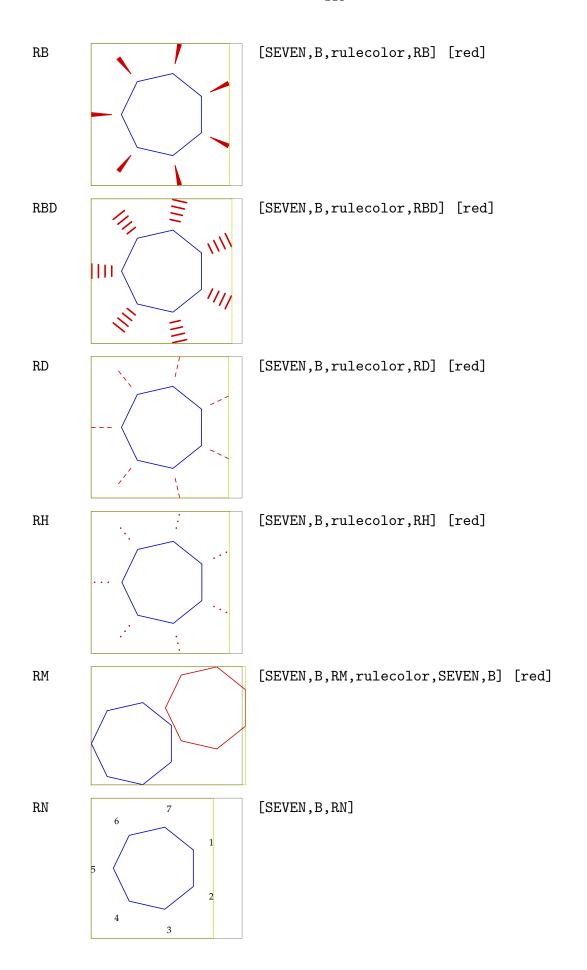
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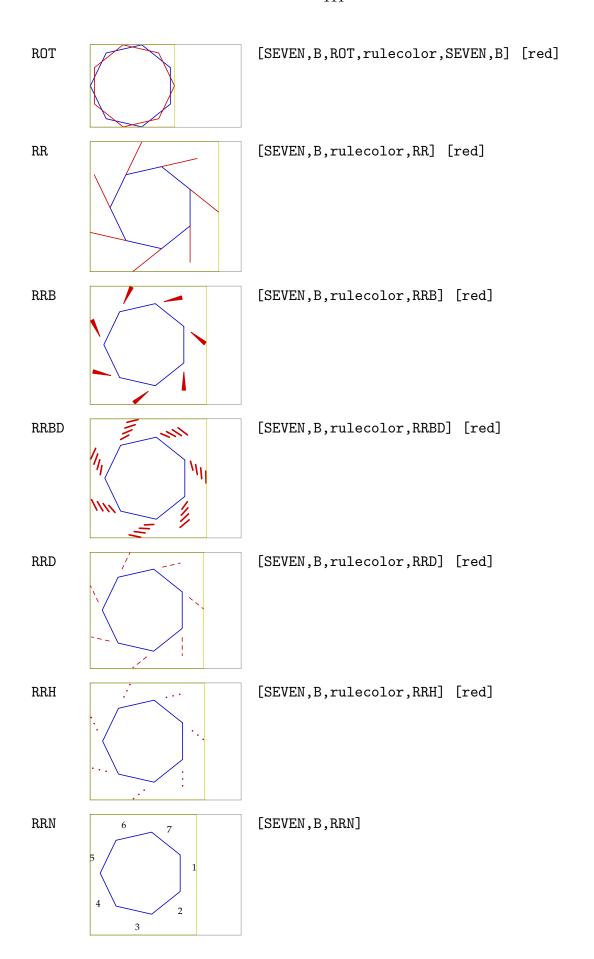




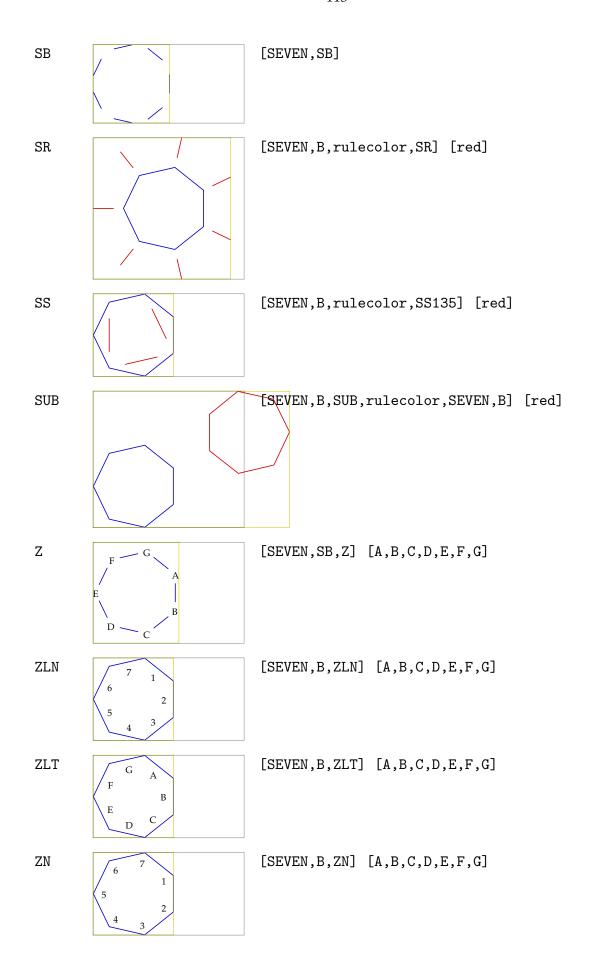
LRBD [SEVEN,B,rulecolor,LRBD] [red] /// [SEVEN,B,rulecolor,LRD] [red] LRD LRH [SEVEN,B,rulecolor,LRH] [red] LRN [SEVEN,B,LRN] 4 LRT [SEVEN,B,LRT] [A,B,C,D,E,F,G] G D LRZ [SEVEN,B,LRZ] [A,B,C,D,E,F,G] G Α В C D

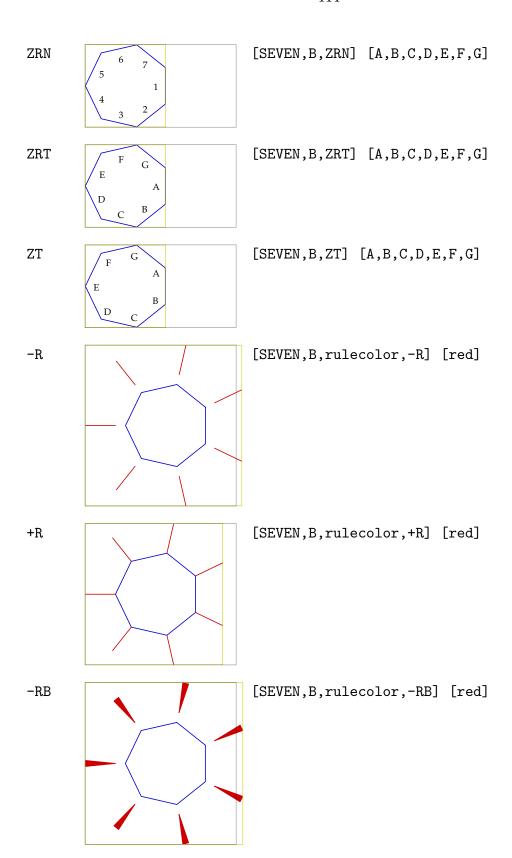




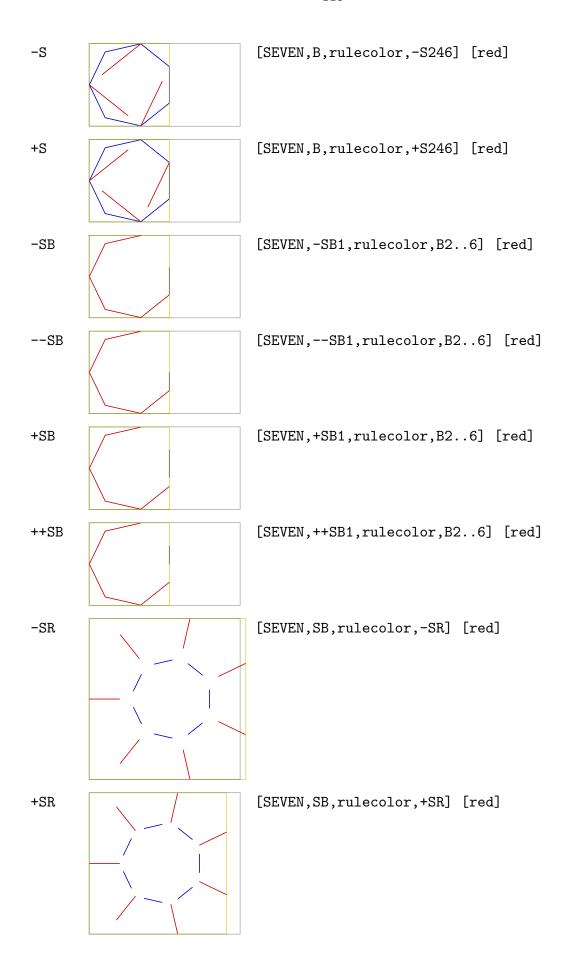


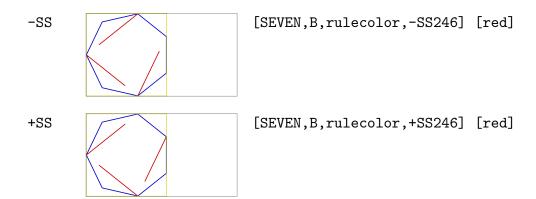
RRT[SEVEN,B,RRT] [A,B,C,D,E,F,G] F G C [SEVEN,B,RRZ] [A,B,C,D,E,F,G] RRZ F G В C [SEVEN,B,rulecolor,RSR] [red] RSR RT [SEVEN,B,R,RT] [A,B,C,D,E,F,G] RZ[SEVEN,B,R,RZ] [A,B,C,D,E,F,G] [SEVEN,B,rulecolor,S] [red] S





+RB [SEVEN,B,rulecolor,+RB] [red] -RD [SEVEN,B,rulecolor,-RD] [red] [SEVEN,B,rulecolor,+RD] [red] +RD [SEVEN,B,-SR,-RZ] [A,B,C,D,E,F,G] -RZ[SEVEN,B,+SR,+RZ] [A,B,C,D,E,F,G] +RZ



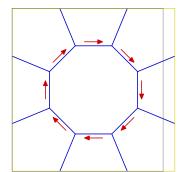


 $ppchT_{E}X$

23 Eight

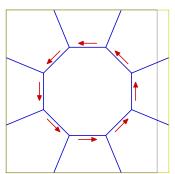
ad	line	label	text	move	transform	rrz	text
adj	transform	line	line	number	number	rsr	line
arrow	line	lr	line	off	transform	rsub	transform
au	line	lrb	line	r	line	rt	text
b	line	lrbd	line	rb	line	rz	text
С	fixed	lrd	line	rbd	line	S	line
СС	line	lrh	line	rd	line	sb	line
ccd	line	lrn	number	rh	line	sr	line
cd	fixed	lrt	text	rm	transform	SS	line
crz	text	lrz	text	rn	number	sub	transform
dash	line	lsr	line	rot	transform	z	text
db	line	lsub	transform	rr	line	zln	number
diff	transform	mark	transform	rrb	line	zlt	text
dr	line	mid	line	rrbd	line	zn	number
eb	line	mids	line	rrd	line	zrn	number
ed	line	midz	text	rrh	line	zrt	text
er	line	mir	transform	rrn	number	zt	text
hb	line	mov	transform	rrt	text		

 ${\tt AD}$

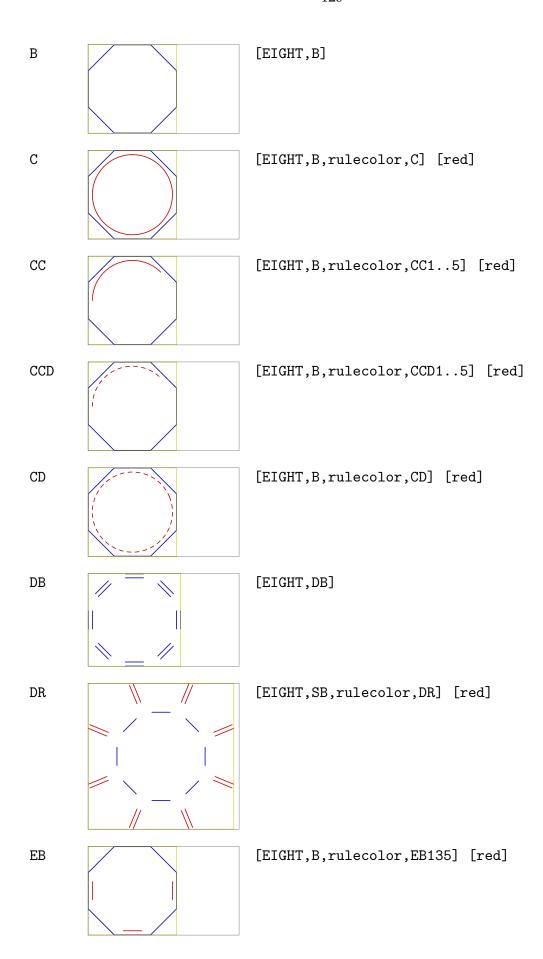


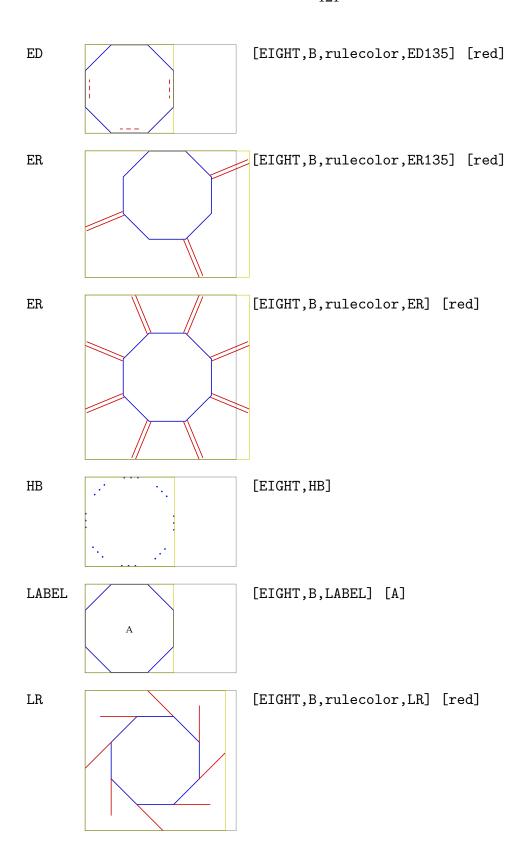
[EIGHT,B,R,rulecolor,AD] [red]

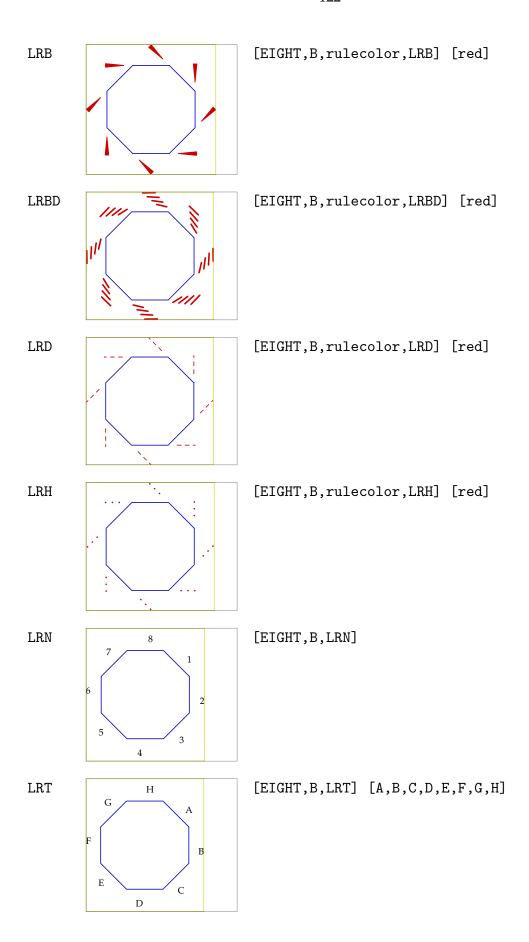
AU

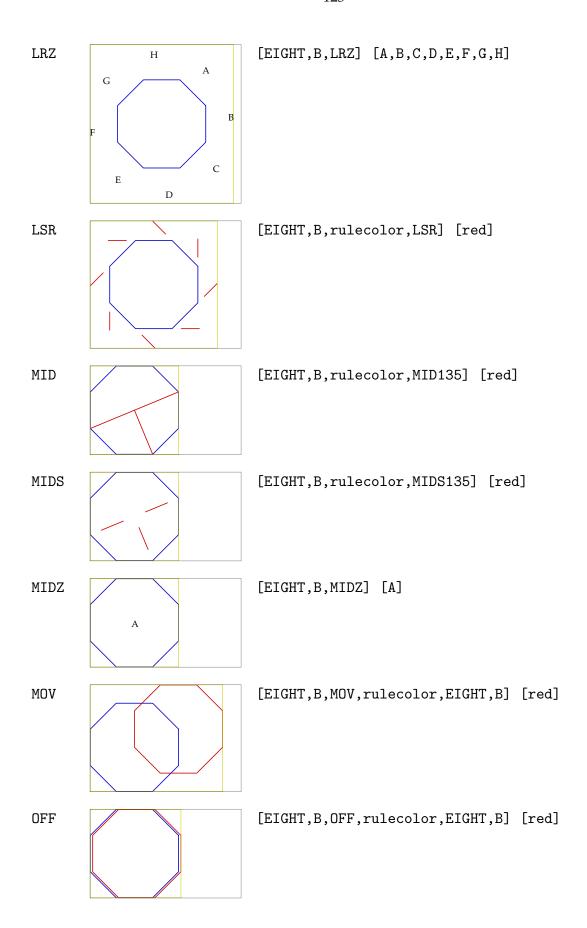


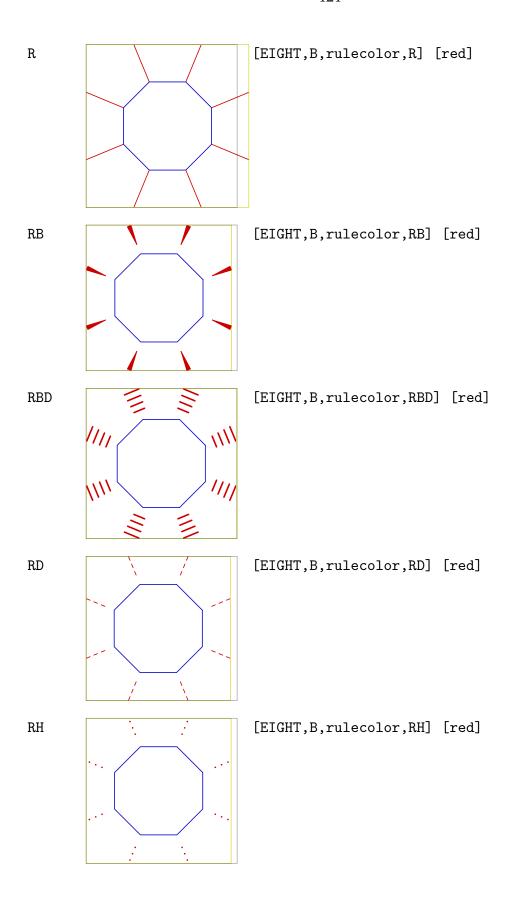
[EIGHT,B,R,rulecolor,AU] [red]

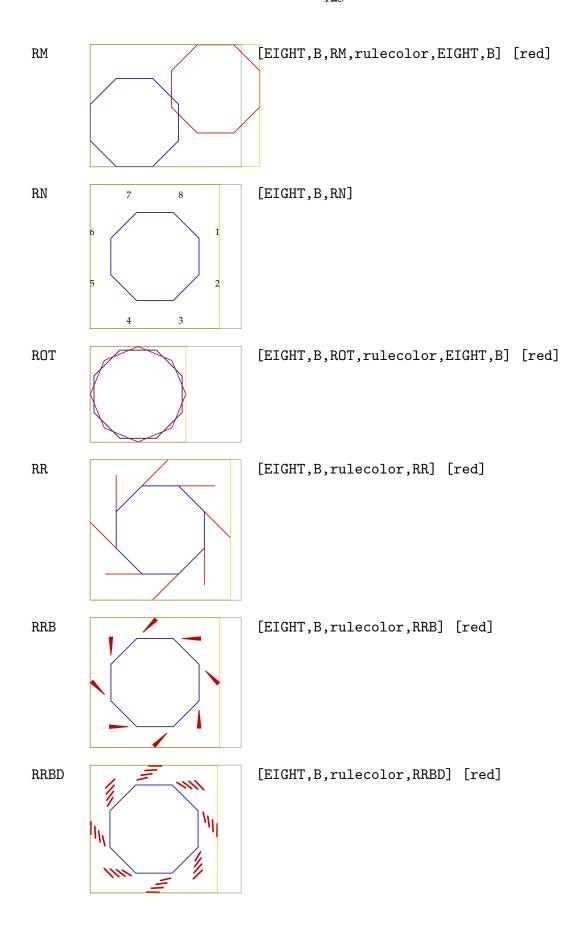


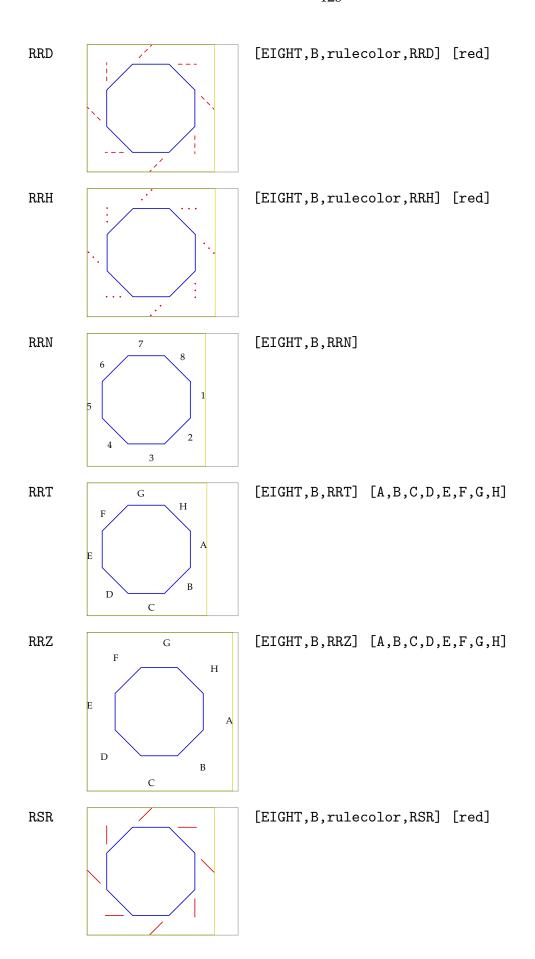


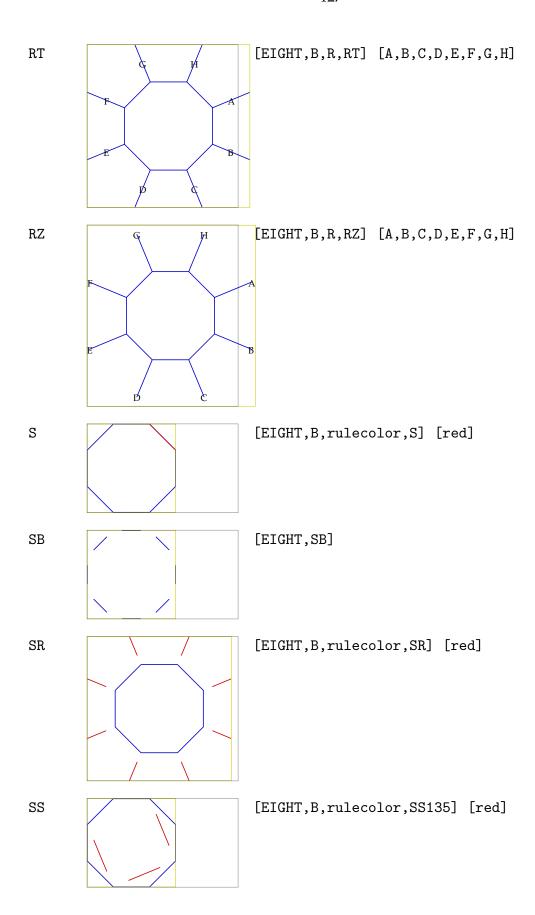


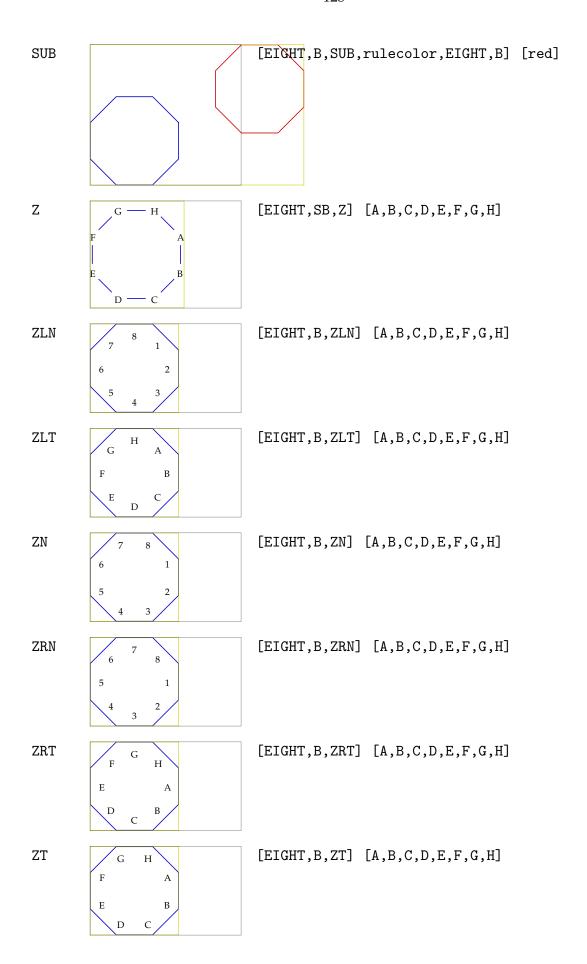


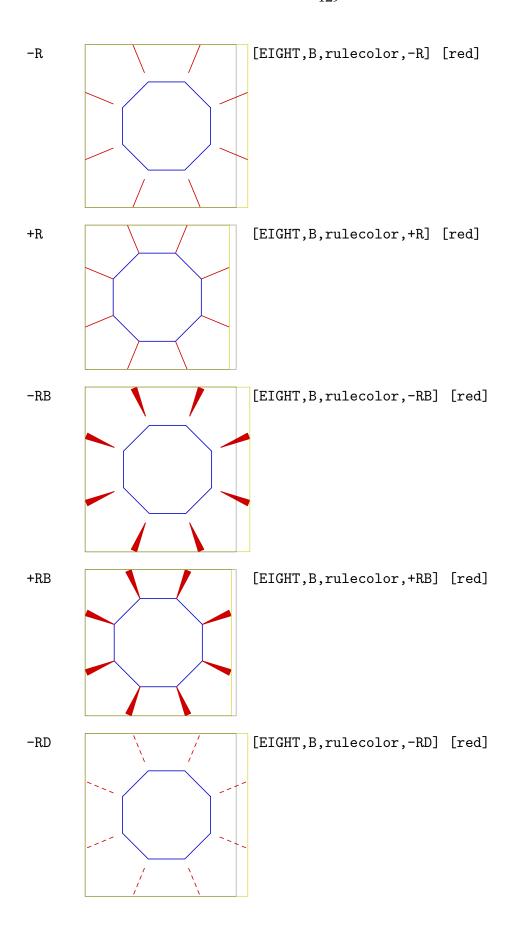


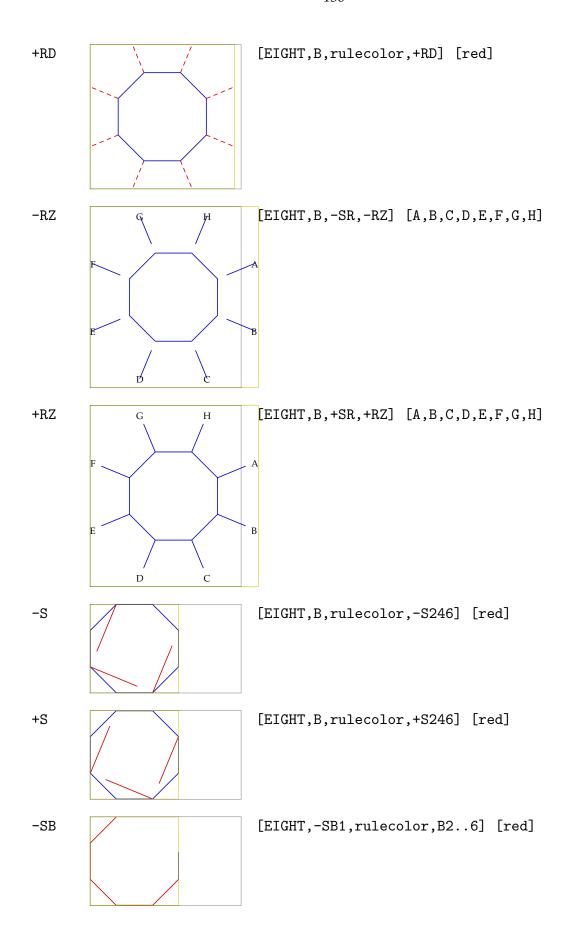


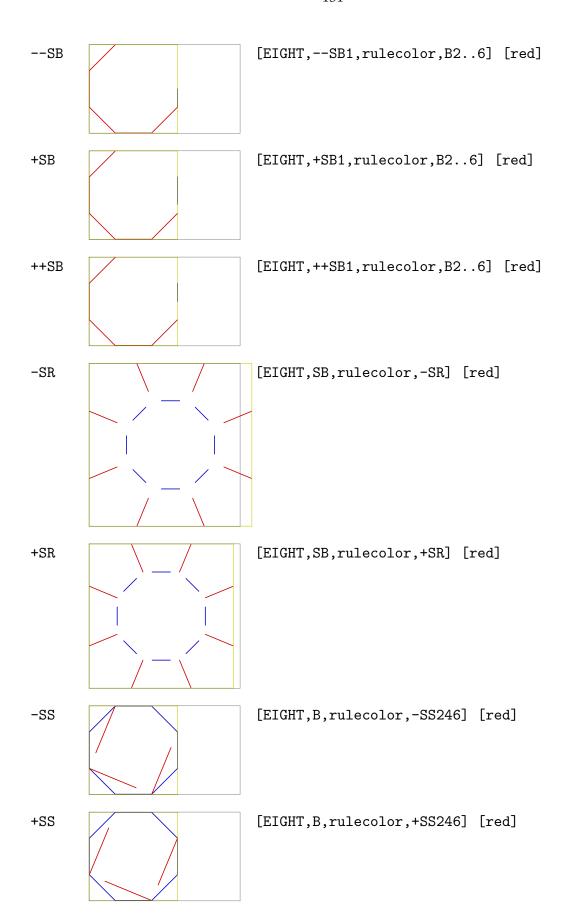










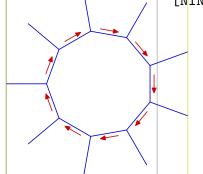


 $ppchT_{EX}$

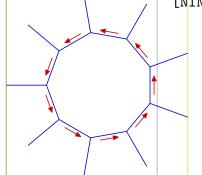
24 Nine

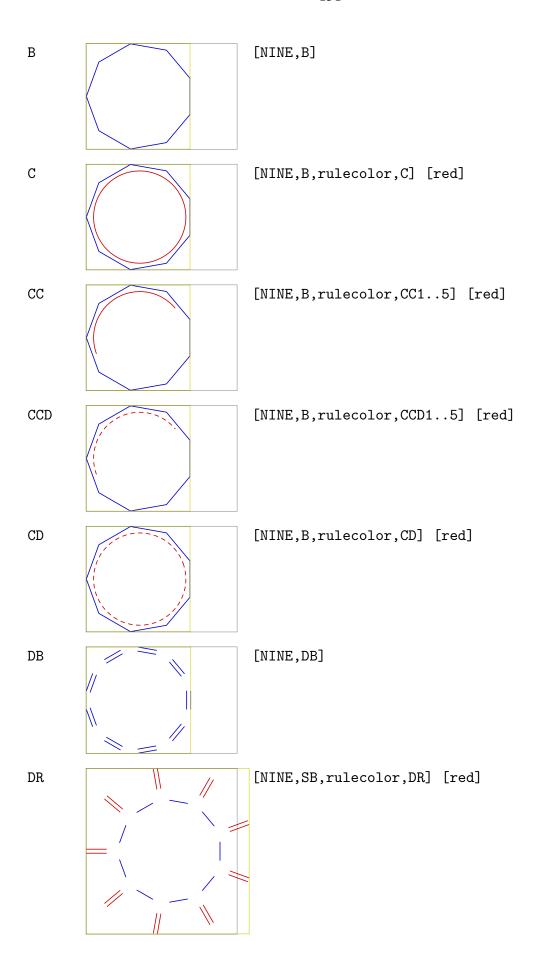
ad	line	label	text	move	transform	rrz	text
adj	transform	line	line	number	number	rsr	line
arrow	line	lr	line	off	transform	rsub	transform
au	line	lrb	line	r	line	rt	text
Ъ	line	lrbd	line	rb	line	rz	text
С	fixed	lrd	line	rbd	line	S	line
СС	line	lrh	line	rd	line	sb	line
ccd	line	lrn	number	rh	line	sr	line
cd	fixed	lrt	text	rm	transform	SS	line
crz	text	lrz	text	rn	number	sub	transform
dash	line	lsr	line	rot	transform	z	text
db	line	lsub	transform	rr	line	zln	number
diff	transform	mark	transform	rrb	line	zlt	text
dr	line	mid	line	rrbd	line	zn	number
eb	line	mids	line	rrd	line	zrn	number
ed	line	midz	text	rrh	line	zrt	text
er	line	mir	transform	rrn	number	zt	text
hb	line	mov	transform	rrt	text		

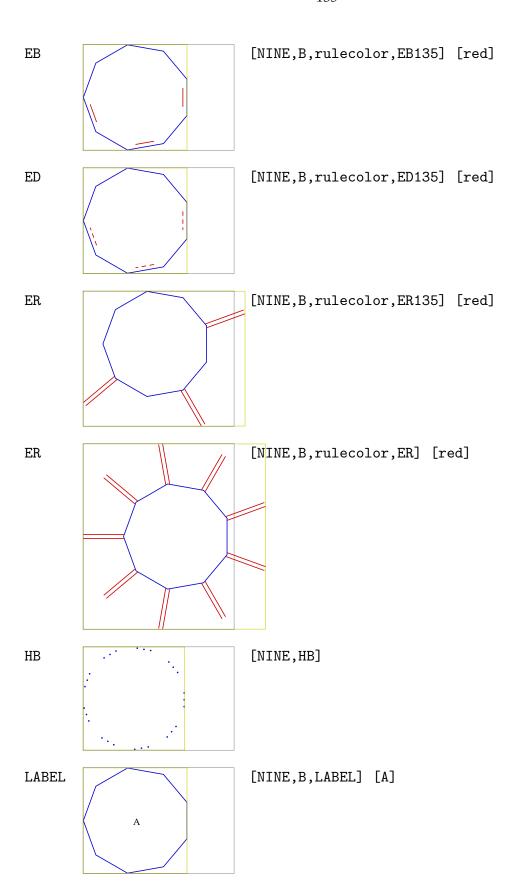
AD [NINE,B,R,rulecolor,AD] [red]

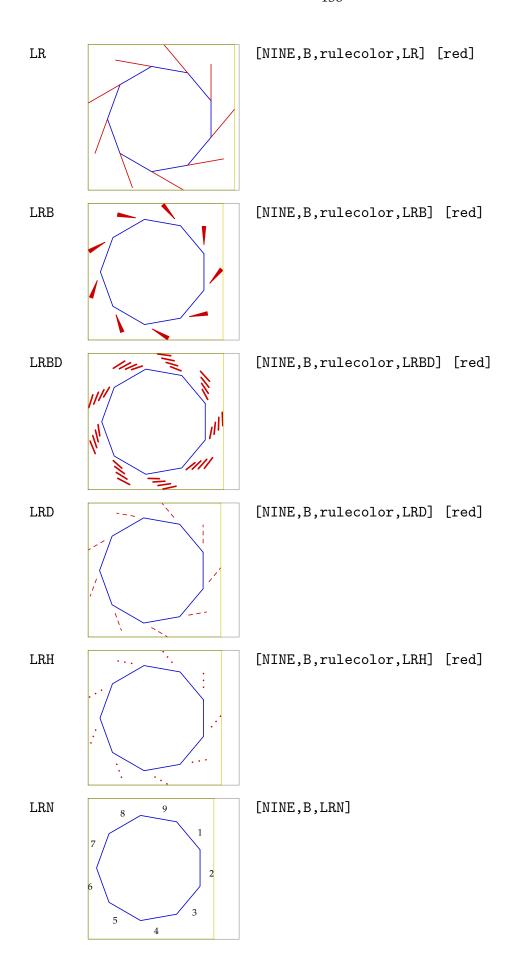


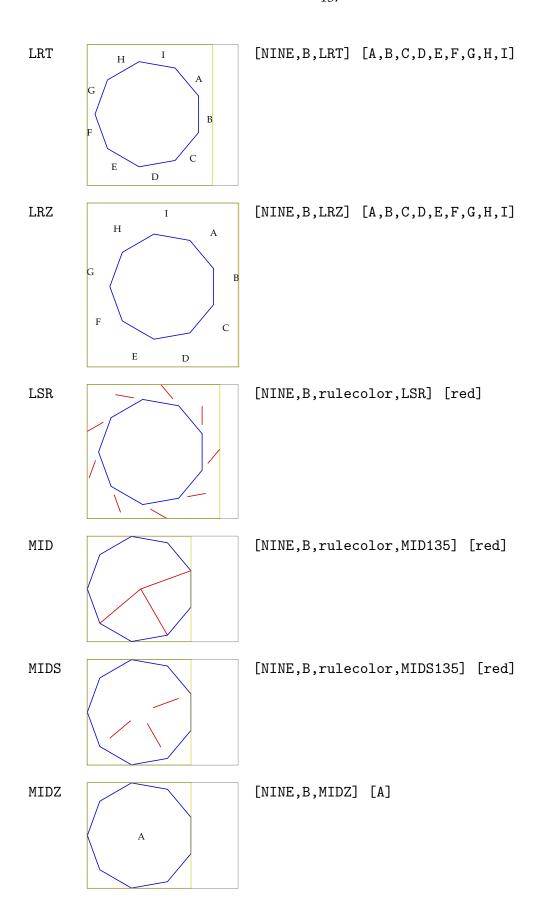
AU [NINE,B,R,rulecolor,AU] [red]

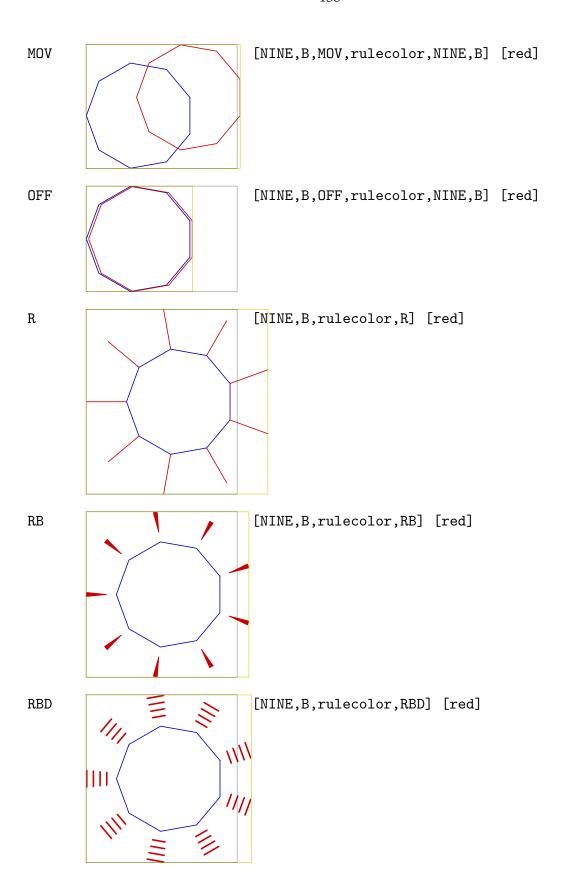


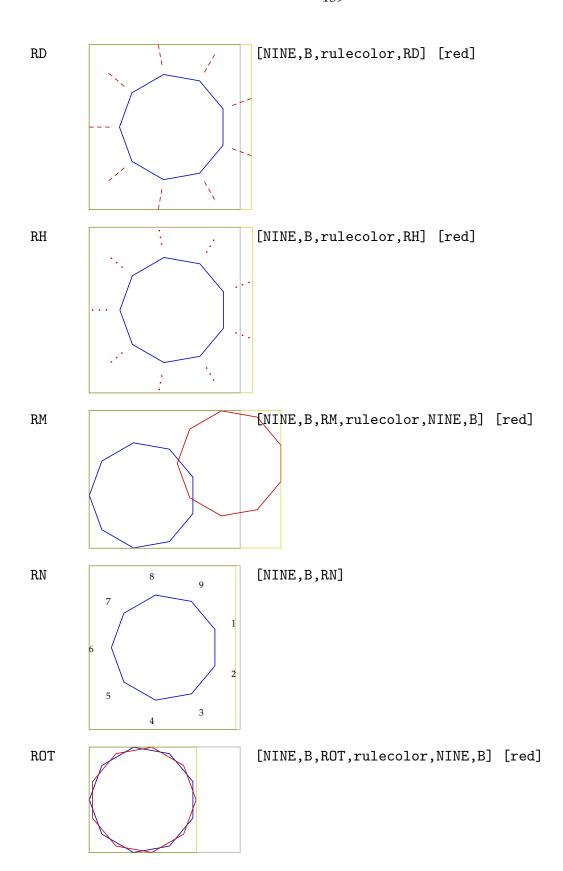


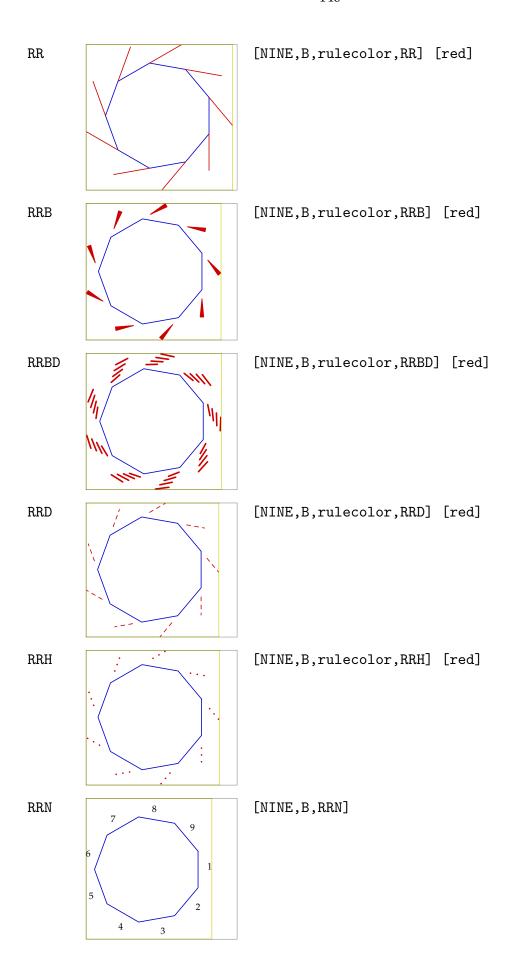




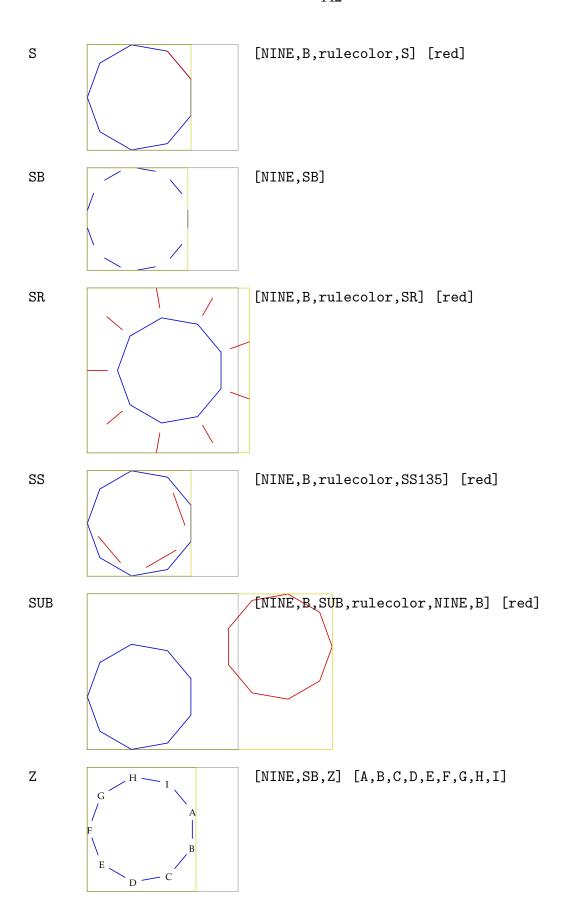


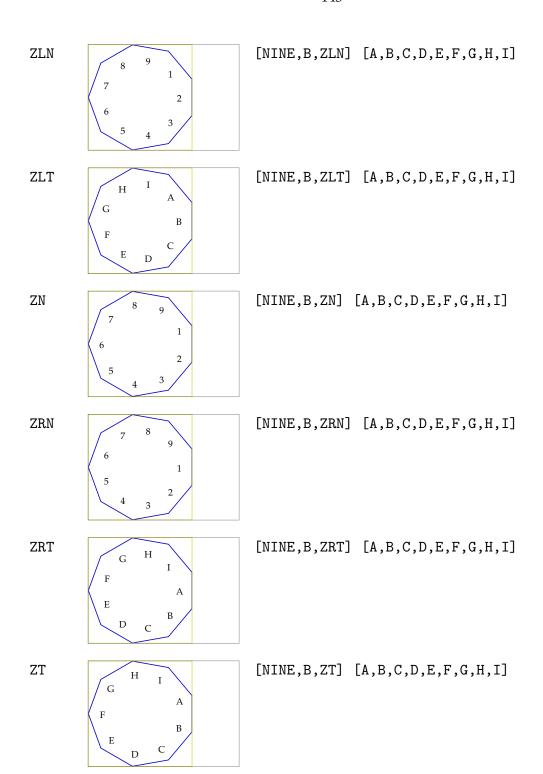


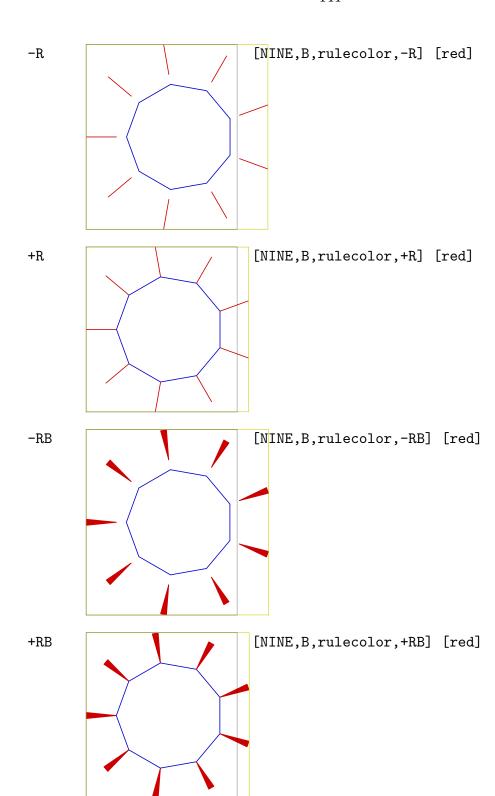




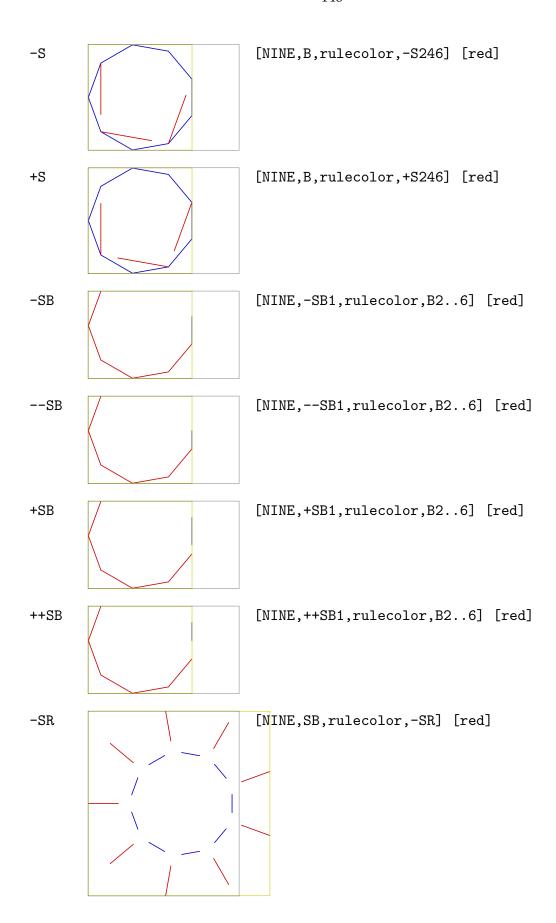
RRT[NINE,B,RRT] [A,B,C,D,E,F,G,H,I] Н G C RRZ [NINE,B,RRZ] [A,B,C,D,E,F,G,H,I] Н G I F В D C [NINE,B,rulecolor,RSR] [red] RSR [NINE,B,R,RT] [A,B,C,D,E,F,G,H,I] RT RΖ [NINE,B,R,RZ] [A,B,C,D,E,F,G,H,I]

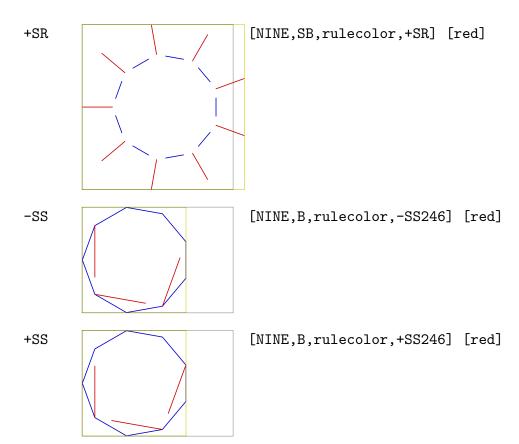






-RD [NINE,B,rulecolor,-RD] [red] [NINE,B,rulecolor,+RD] [red] +RD [NINE,B,-SR,-RZ] [A,B,C,D,E,F,G,H,I] -RZ +RZ [NINE,B,+SR,+RZ] [A,B,C,D,E,F,G,H,I] G





r

adj

transform

lrb

line

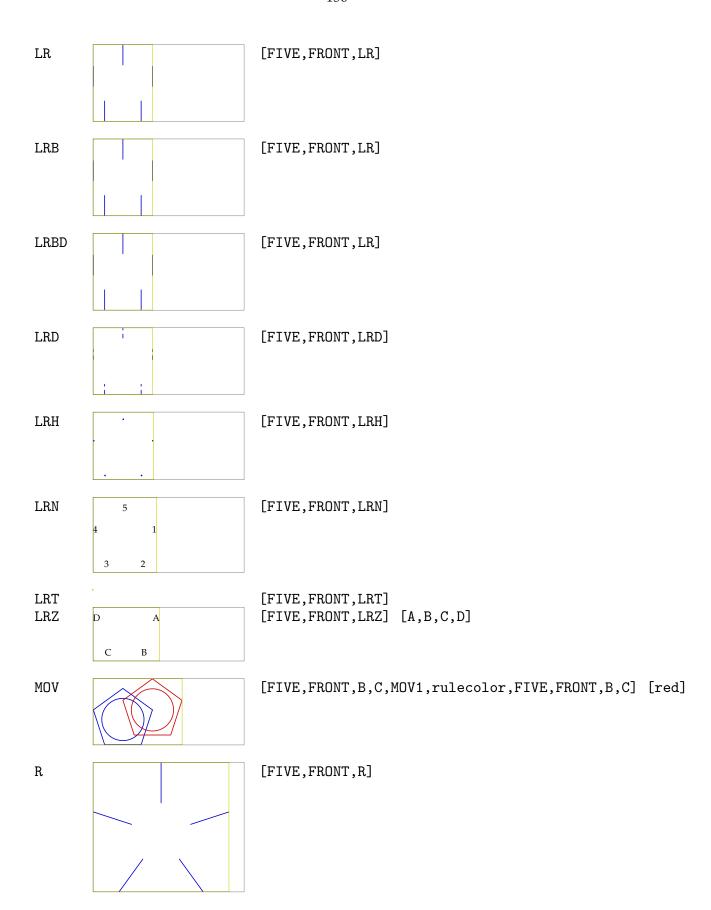
25 Five Front

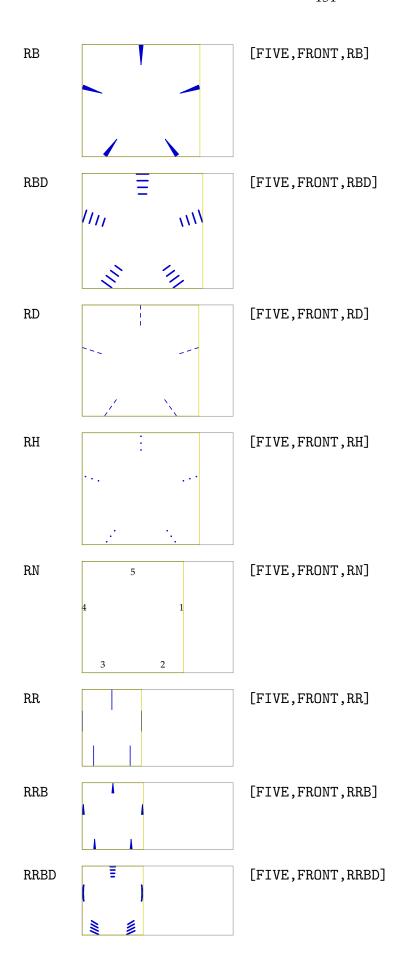
line

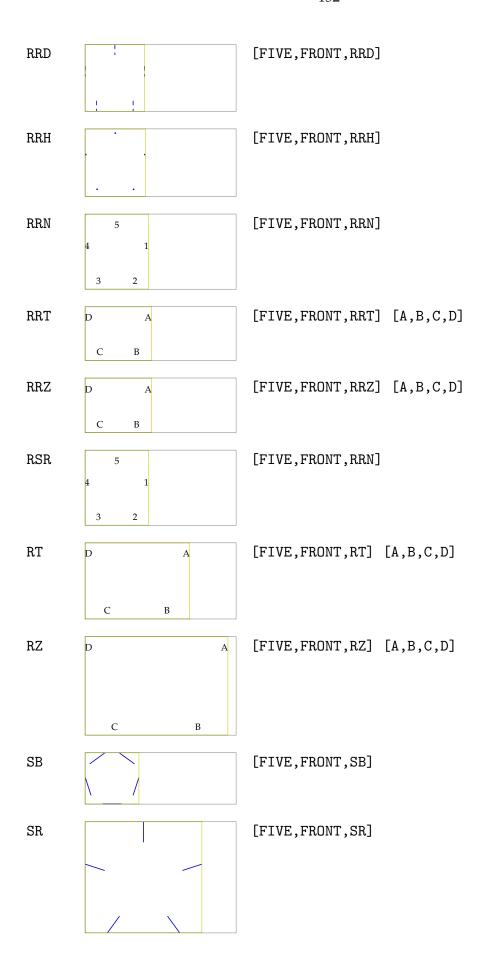
rsr

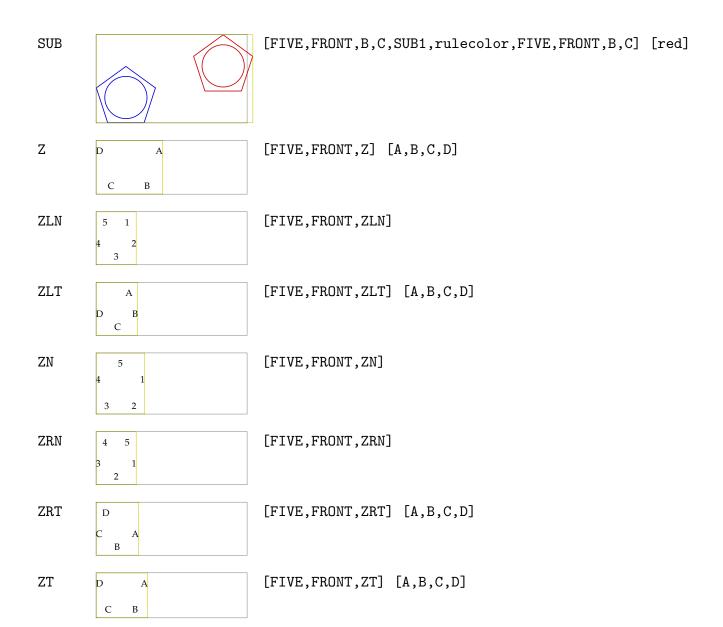
line

arrow	line	lrbd	line	rb	line	rsub	transform	
b	line	lrd	line	rbd	line	rt	text	
bb	line	lrh	line	rd	line	rz	text	
С	fixed	lrn	number	rh	line	sb	line	
СС	line	lrt	text	rn	number	sr	line	
ccd	line	lrz	text	rr	line	sub	transform	
cd	fixed	lsr	line	rrb	line	Z	text	
dash	line	lsub	transform	rrbd	line	zln	number	
diff	transform	mark	transform	rrd	line	zlt	text	
eb	line	mov	transform	rrh	line	zn	number	
label	text	move	transform	rrn	number	zrn	number	
line	line	number	number	rrt	text	zrt	text	
lr	line	off	transform	rrz	text	zt	text	
D			LETAE EDON	רמידיז				
В			[FIVE, FRON	II,D]				
BB			[FIVE,FRON	IT.BB]				
22			[1 1 1 2] 1 1 1 1 1 1 1	,223				
С			[FIVE,FRON	IT,C]				
			_ , , , , , , , , , , , , , , , , , , ,	,				
CC			[FIVE,FRON	IT CC1]				
00			[1 1 1 2] 1 1001	.,,,,,,,,				
CCD			[FIVE,FRON	וד ככוו				
ССБ			LI I VL, I ILON	11,0001]				
CD	/		[FIVE,FRON	ייי כיהן				
CD	()		LTIVE, FRUI	11,00]				
ED			CETTE EDON	נת הטן				
EB	[FIVE, FRONT, EB]							
	\/							
			F					
LINE			[FIVE, FRON	IT,LINE]				



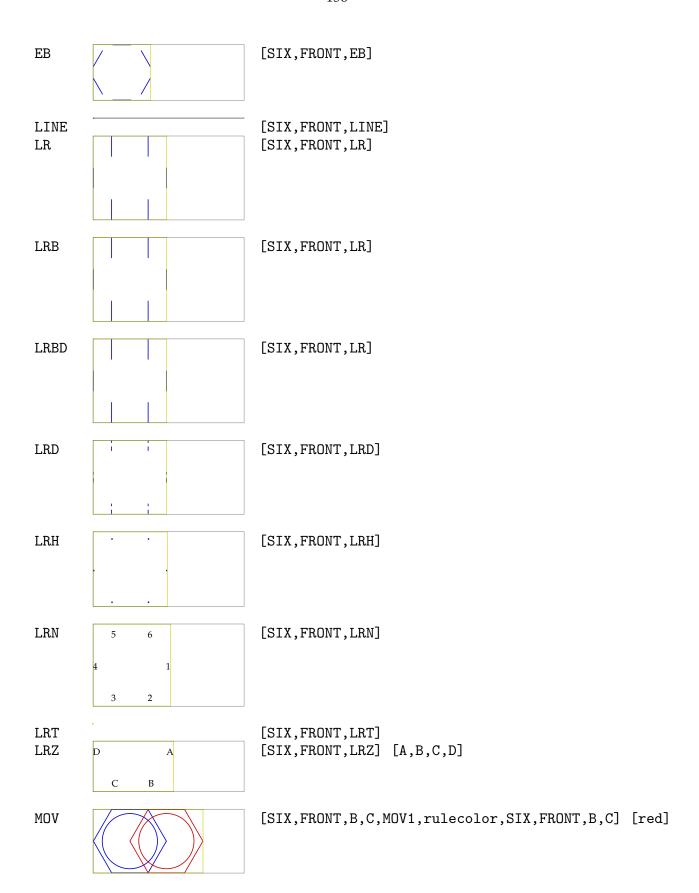


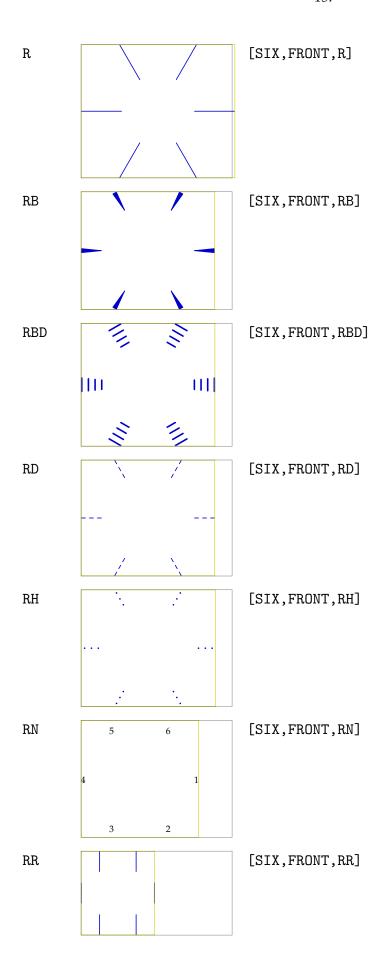


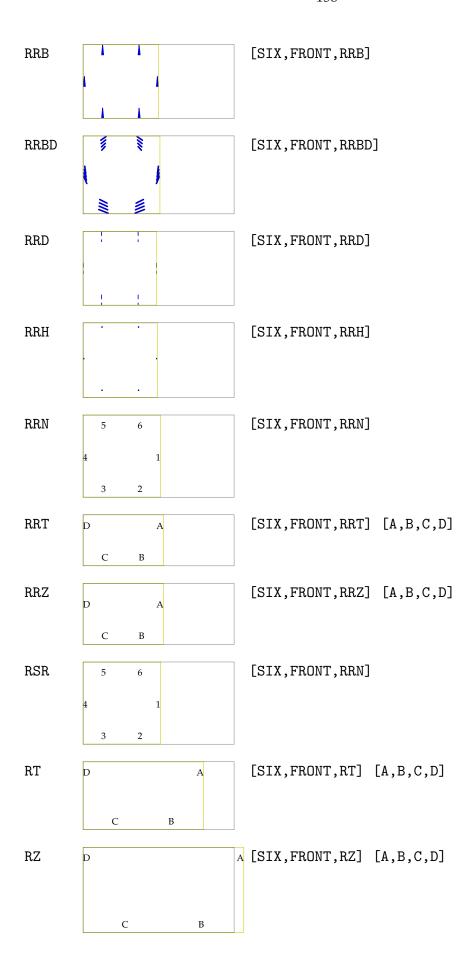


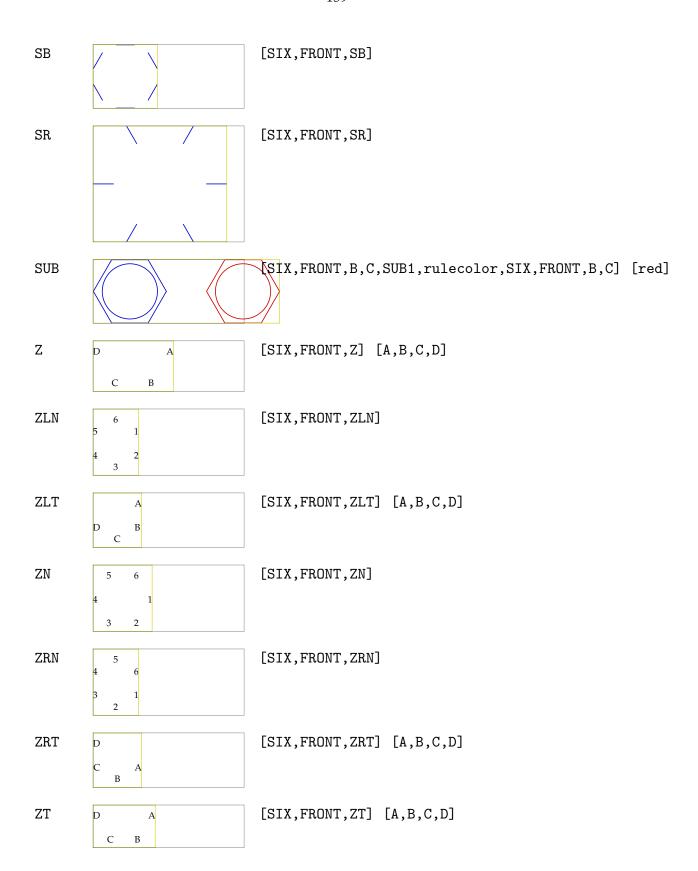
26 Six Front

adj arrow b bb c cc ccd cd dash diff eb label line lr	transform line line line fixed line fixed line transform line text line line	lrb lrbd lrd lrh lrn lrt lrz lsr lsub mark mov move number off	line line line line number text text line transform transform transform transform transform	r rb rbd rd rh rn rr rrb rrbd rrt rrt rrn	line line line line line line line line	rsr rsub rt rz sb sr sub z zln zlt zn zrn zrt zt	line transform text text line line transform text number text number number text
В			[SIX,FRONT	.,B]			
BB	[SIX,FRONT,BB]						
С			[SIX,FRONT	[,C]			
CC			[SIX,FRONT	C,CC1]			
CCD			[SIX,FRONT	C,CCD1]			
CD			[SIX,FRONT	C,CD]			





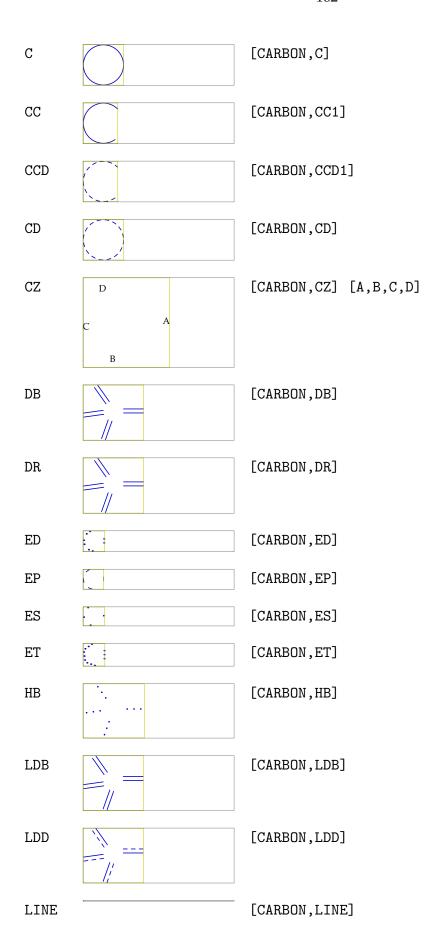


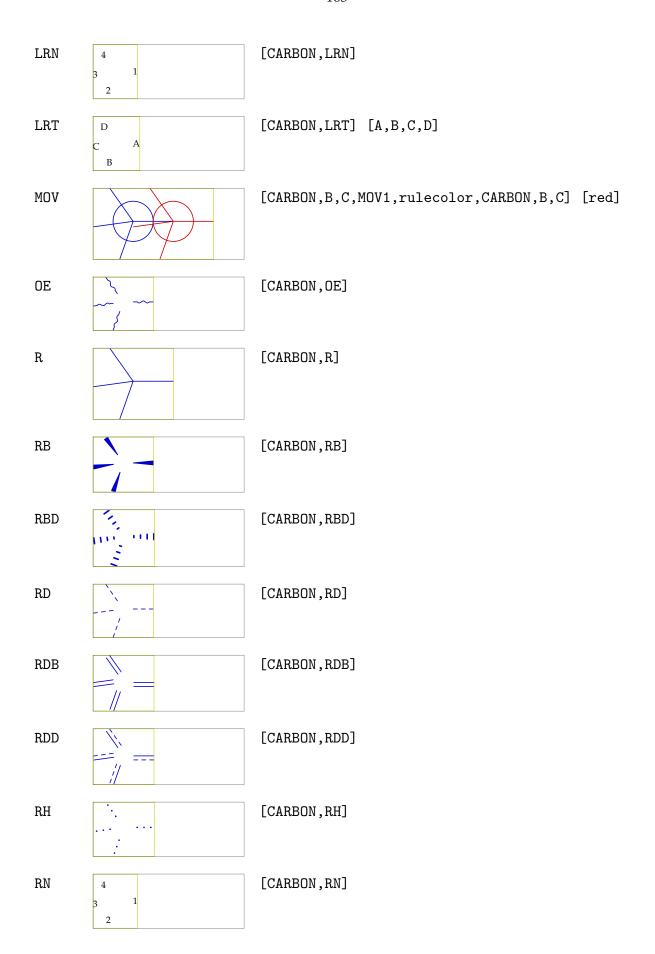


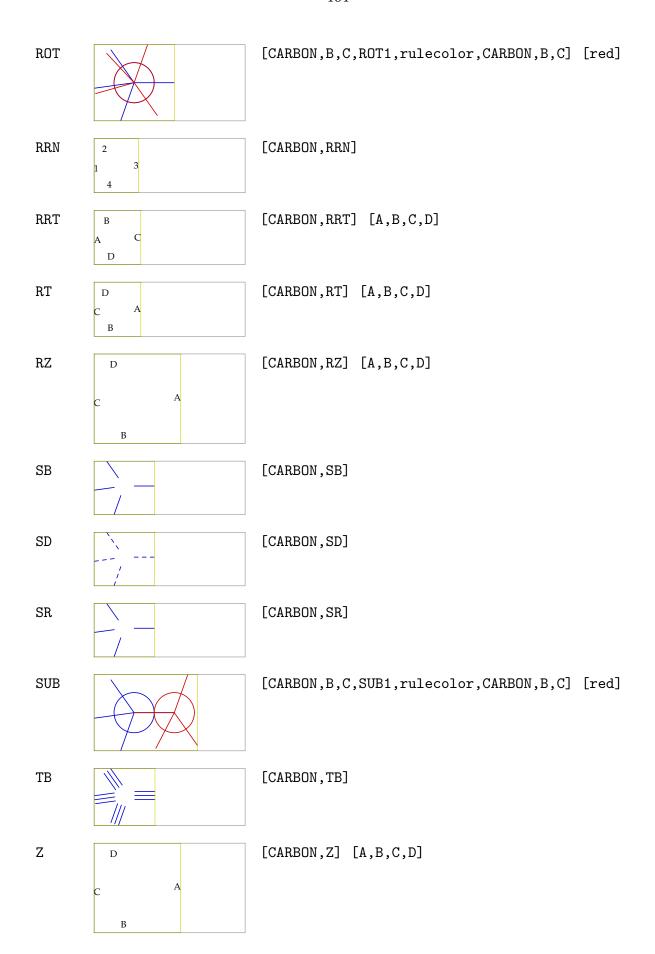
27 Carbon

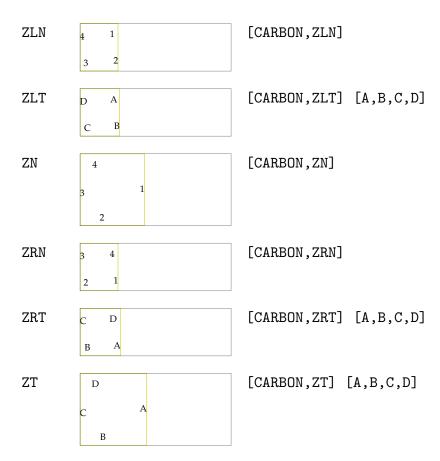
ad adj arrow au b bb bd bw c cc ccd cd dd dd diff	line transform line line line line line line line fixed line line fixed text line line line	dir dr ed ep es et hb label ldb ldd line lrn lrt mark mir mov	transform line line line line line line line line	move number oe off r rb rbd rd rdb rdd rnt rm rn rn rot rrn	transform number line transform line line line line line line transform number transform number transform number text	rt rz sb sd sr sub tb z zln zlt zn zrt zrt	text text line line line transform line text number text number number text
AD	Transform	mo v	[CARBON, AD		text		
AU	→ <u>1</u>		[CARBON, AU	7]			
В			[CARBON,B]				
BB			[CARBON, BE	3]			
BD	111111111111111111111111111111111111111		[CARBON,BD)]			
BW	~} ~~		[CARBON,BW	7]			

 $ppchT_{E}X$









move

transform

dir

28 Newman Stagger

rt

text

transform

adj	transform	dr	line	number	number	rz	text		
arrow	line	ed	line	oe	line	sb	line		
au	line	ер	line	off	transform	sd	line		
b	line	es	line	r	line	sr	line		
bb	line	et	line	rb	line	sub	transform		
bd	line	hb	line	rbd	line	tb	line		
bw	line	label	text	rd	line	z	text		
С	fixed	ldb	line	rdb	line	zln	number		
СС	line	ldd	line	rdd	line	zlt	text		
ccd	line	line	line	rh	line	zn	number		
cd	fixed	lrn	number	rm	transform	zrn	number		
CZ	text	lrt	text	rn	number	zrt	text		
dash	line	mark	transform	rot	transform	zt	text		
db	line	mir	transform	rrn	number				
diff	transform	mov	transform	rrt	text				
AD			[NEWMAN, AD]					
AU	•		[NEWMAN, AU						
В			[NEWMAN,B]						
BB			[NEWMAN,BB						
BD	[NEWMAN, BD]								
BW	[NEWMAN, BW]								
C CC	[NEWMAN, C] [NEWMAN, CC1]								
CCD	[NEWMAN, CCD1]								
CD	[NEWMAN, CD]								
CZ	[NEWMAN,CZ] [A,B,C,D]								
DB	[NEWMAN, DB]								
DR			[NEWMAN,DR	.]					
ED			[NEWMAN, ED						
EP			[NEWMAN, EP						
ES			[NEWMAN, ES						
ET HB			[NEWMAN,ET [NEWMAN,HB						
LDB	•		[NEWMAN, LD						
LDD			[NEWMAN,LD						
LINE	•		[NEWMAN,LI						
LRN			[NEWMAN, LR	N]					
LRT			[NEWMAN,LR		•				
MOV					rulecolor,NE	WMAN,B,C	[red]		
0E			[NEWMAN, OE	J					
R			[NEWMAN,R]	1					
RB			[NEWMAN, RB	7					

ppchT_EX

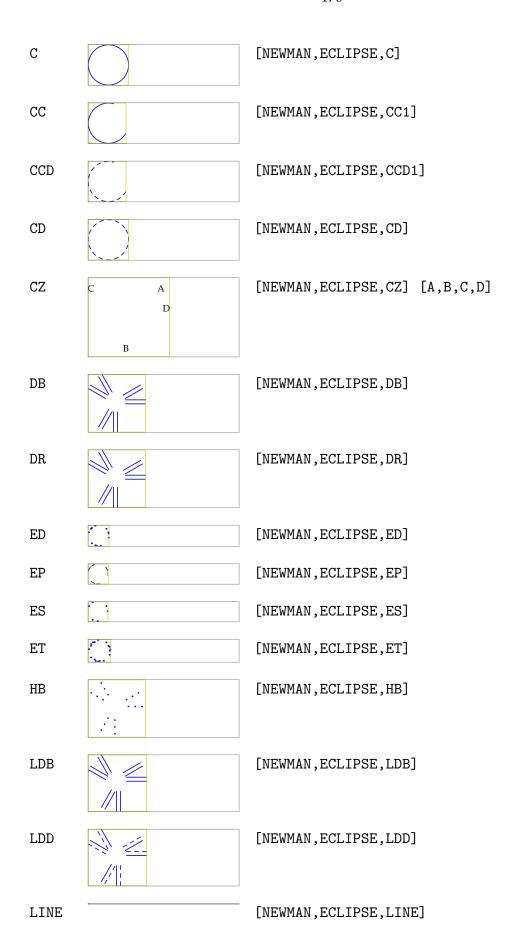
ad

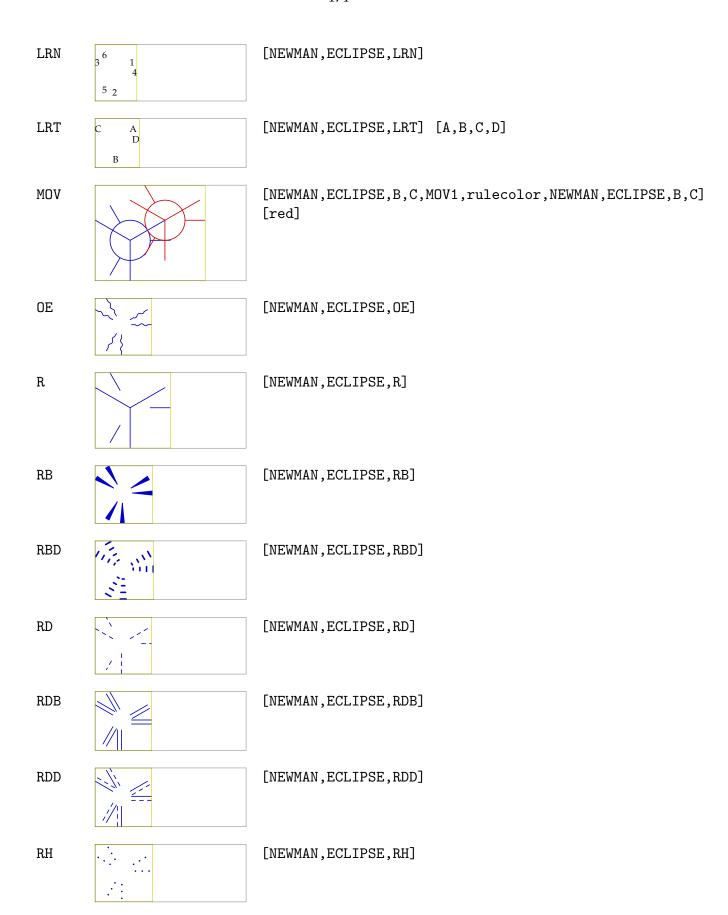
line

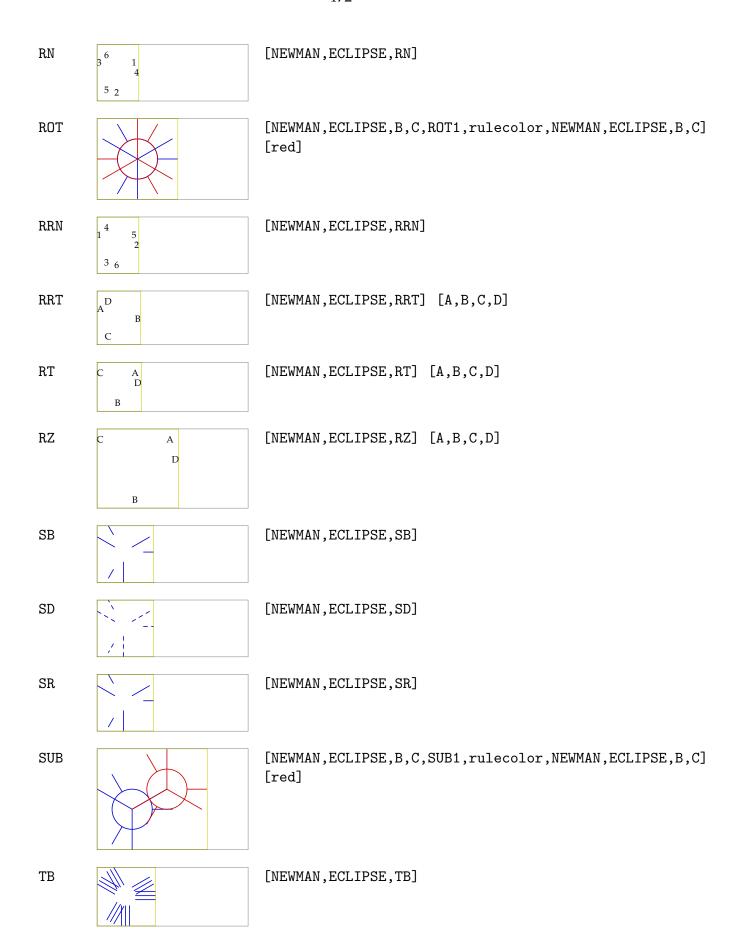
[NEWMAN, RBD]	
[NEWMAN, RD]	
[NEWMAN, RDB]	
[NEWMAN, RDD]	
·	
- , -	
•	[red]
	LICUJ
- , -	
·	
- · · -	
- , -	F -3
	[red]
- · · -	
[NEWMAN, ZLN]	
[NEWMAN, ZLT] [A, B, C, D]	
[NEWMAN, ZN]	
[NEWMAN, ZRN]	
[NEWMAN, ZRT] [A, B, C, D]	
[NEWMAN,ZT] [A,B,C,D]	
	[NEWMAN,RD] [NEWMAN,RDD] [NEWMAN,RH] [NEWMAN,RN] [NEWMAN,B,C,ROT1,rulecolor,NEWMAN,B,C] [NEWMAN,RRN] [NEWMAN,RRT] [A,B,C,D] [NEWMAN,RT] [NEWMAN,RT] [A,B,C,D] [NEWMAN,RZ] [A,B,C,D] [NEWMAN,SB] [NEWMAN,SB] [NEWMAN,SD] [NEWMAN,SR] [NEWMAN,B,C,SUB1,rulecolor,NEWMAN,B,C] [NEWMAN,TB] [NEWMAN,TB] [NEWMAN,Z] [A,B,C,D] [NEWMAN,ZLN] [NEWMAN,ZLT] [NEWMAN,ZN] [NEWMAN,ZRN] [NEWMAN,ZRN] [NEWMAN,ZRN] [NEWMAN,ZRT] [A,B,C,D]

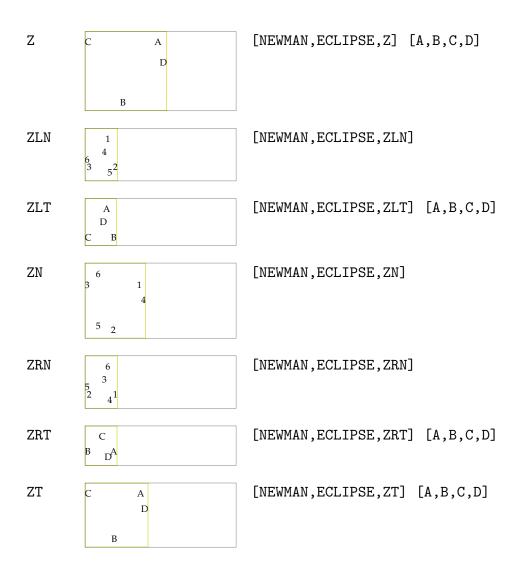
29 Newman Eclipsed

ad adj arrow au b bb bd c c cc	line transform line line line line line line line line	dir dr ed ep es et hb label ldb ldd	transform line line line line line tine line line line line text line line	move number oe off r rb rbd rd rdb rdd rdd	transform number line transform line line line line line line line line	rt rz sb sd sr sub tb z zln zlt zn	text text line line line transform line text number text number
cd	fixed	lrn	number	rm	transform	zrn	number
CZ	text	lrt	text	rn	number	zrt	text
dash	line	mark	transform	rot	transform	zt	text
db	line	mir	transform	rrn	number		
diff	transform	mov	transform	rrt	text		
AD			[NEWMAN,EC	CLIPSE,AI)]		
AU			[NEWMAN,EC	CLIPSE,AU]]		
В			[NEWMAN,EC	CLIPSE,B]	l		
ВВ			[NEWMAN,EC	CLIPSE,BE	3]		
BD			[NEWMAN,EC	CLIPSE,BI)]		
BW	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\		[NEWMAN,EC	CLIPSE,BV	v]		





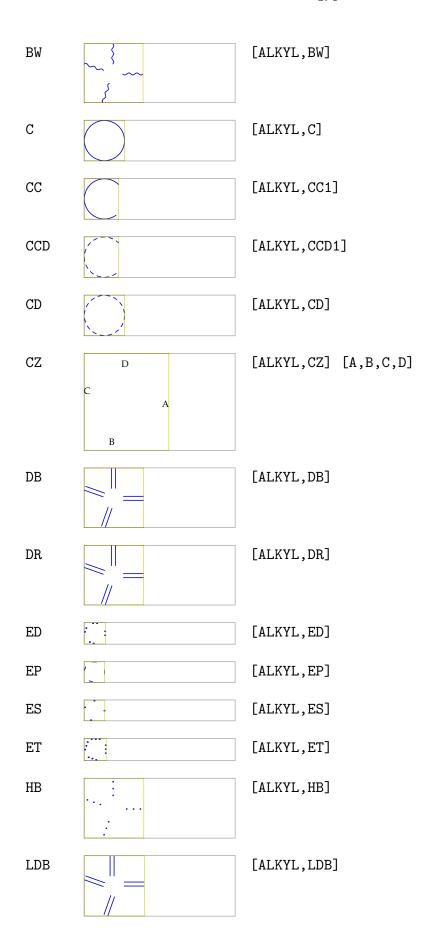


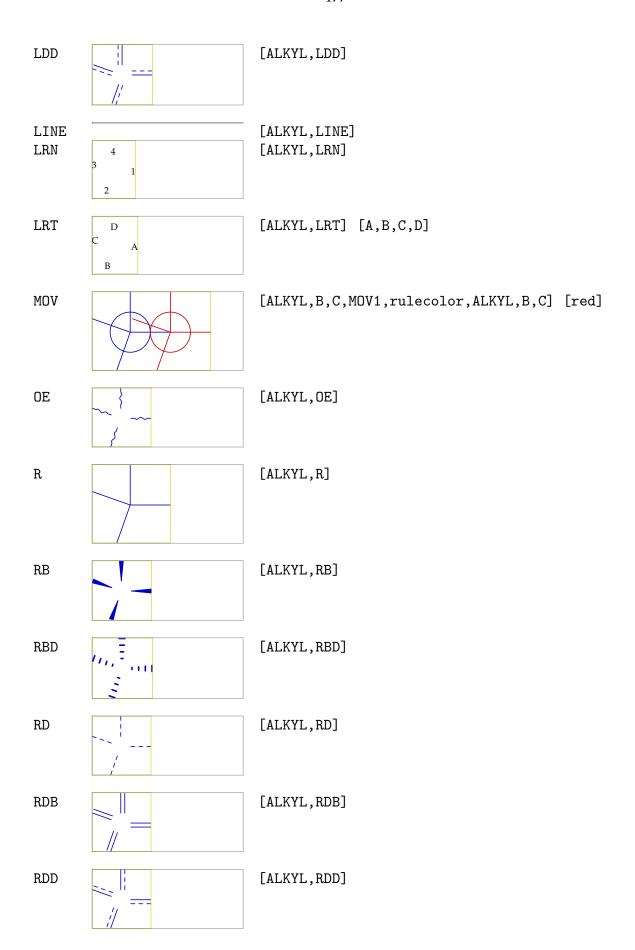


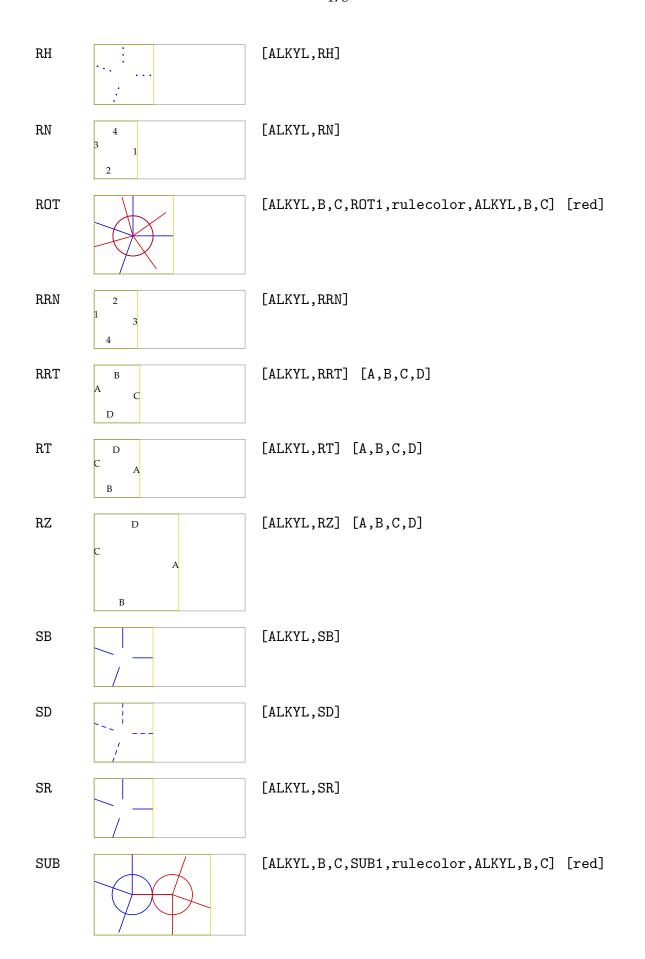
 $ppchT_{EX}$

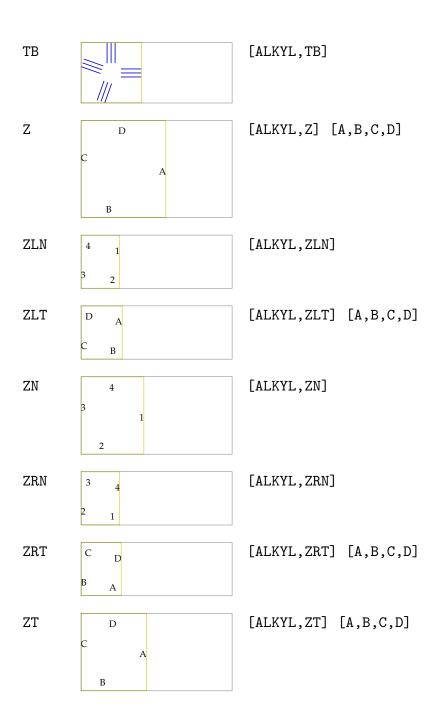
30 Alkyl

ad	line	dir	transform	move	transform	rt	text
adj	transform	dr	line	number	number	rz	text
arrow	line	ed	line	oe	line	sb	line
au	line	ер	line	off	transform	sd	line
b	line	es	line	r	line	sr	line
bb	line	et	line	rb	line	sub	transform
bd	line	hb	line	rbd	line	tb	line
bw	line	label	text	rd	line	Z	text
С	fixed	ldb	line	rdb	line	zln	number
СС	line	ldd	line	rdd	line	zlt	text
ccd	line	line	line	rh	line	zn	number
cd	fixed	lrn	number	rm	transform	zrn	number
cz	text	lrt	text	rn	number	zrt	text
dash	line	mark	transform	rot	transform	zt	text
db	line	mir	transform	rrn	number		
diff	transform	mov	transform	rrt	text		
4.5			[
AD			[ALKYL,AD]				
	1						
			.				
AU	↓ ↓		[ALKYL,AU]				
	_						
	1						
В			[ALKYL,B]				
BB			[ALKYL,BB]				
	_		_				
BD	,, -		[ALKYL,BD]				
	(1/2,000)						





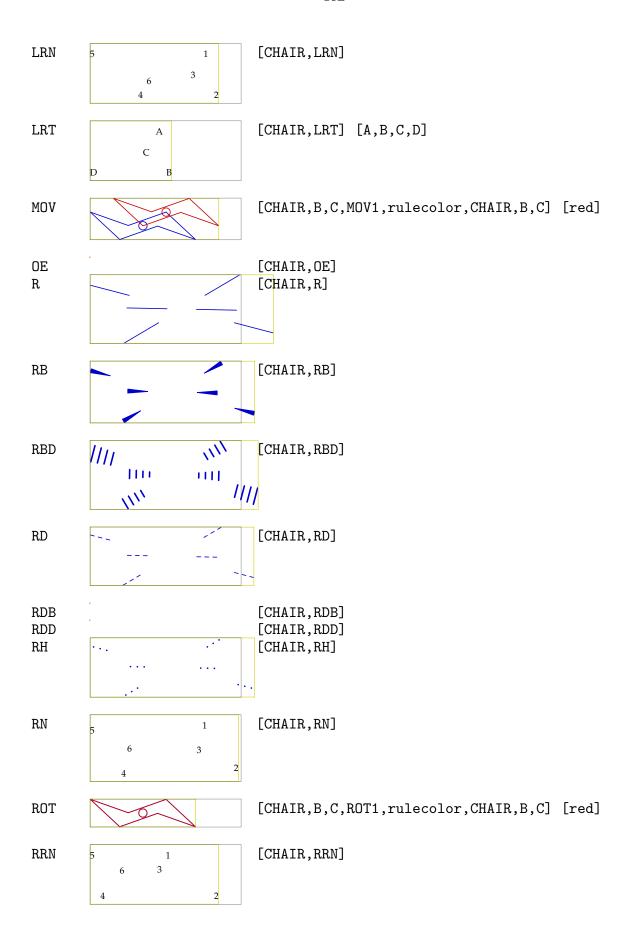


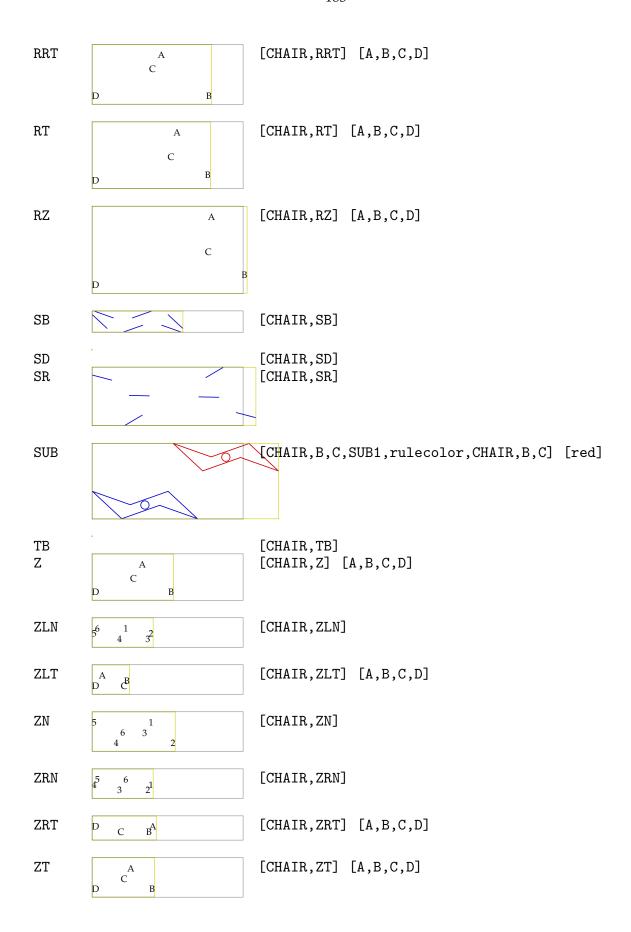


 $ppchT_EX$

31 Chair

adj	transform	lrb	line	r	line	rsr	line	
arrow	line	lrbd	line	rb	line	rsub	transform	
b	line	lrd	line	rbd	line	rt	text	
bb	line	lrh	line	rd	line	rz	text	
С	fixed	lrn	number	rh	line	sb	line	
СС	line	lrt	text	rn	number	sr	line	
ccd	line	lrz	text	rr	line	sub	transform	
cd	fixed	lsr	line	rrb	line	Z	text	
dash	line	lsub	transform	rrbd	line	zln	number	
diff	transform	mark	transform	rrd	line	zlt	text	
eb	line	mov	transform	rrh	line	zn	number	
label	text	move	transform	rrn	number	zrn	number	
line	line	number	number	rrt	text	zrt	text	
lr	line	off	transform	rrz	text	zt	text	
AD AU B			[CHAIR, AD] [CHAIR, AU] [CHAIR, B]					
ВВ			[CHAIR,BB]					
BD	•		[CHAIR, BD]					
BW	•		[CHAIR, BW]					
С			[CHAIR,C]					
CC			[CHAIR, CC1	.]				
CCD			[CHAIR, CCD1]					
CD			[CHAIR,CD]					
CZ DB DR ED EP ES ET HB LDB LDD LINE	· · · · · · · · · · · · · · · · · · ·		[CHAIR,CZ] [CHAIR,DB] [CHAIR,DR] [CHAIR,ED] [CHAIR,ES] [CHAIR,ES] [CHAIR,ET] [CHAIR,HB] [CHAIR,LDE [CHAIR,LDE	3])]	,D]			

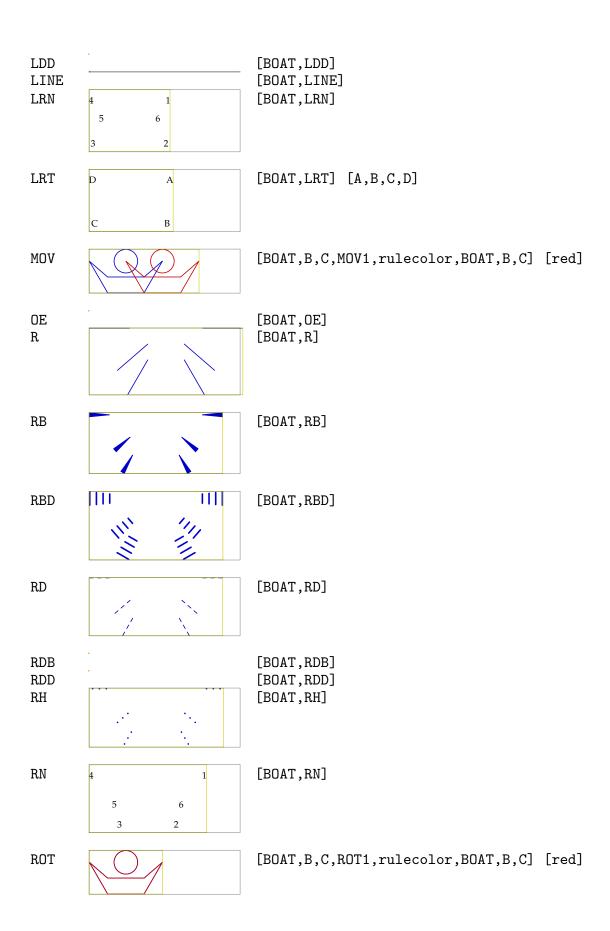


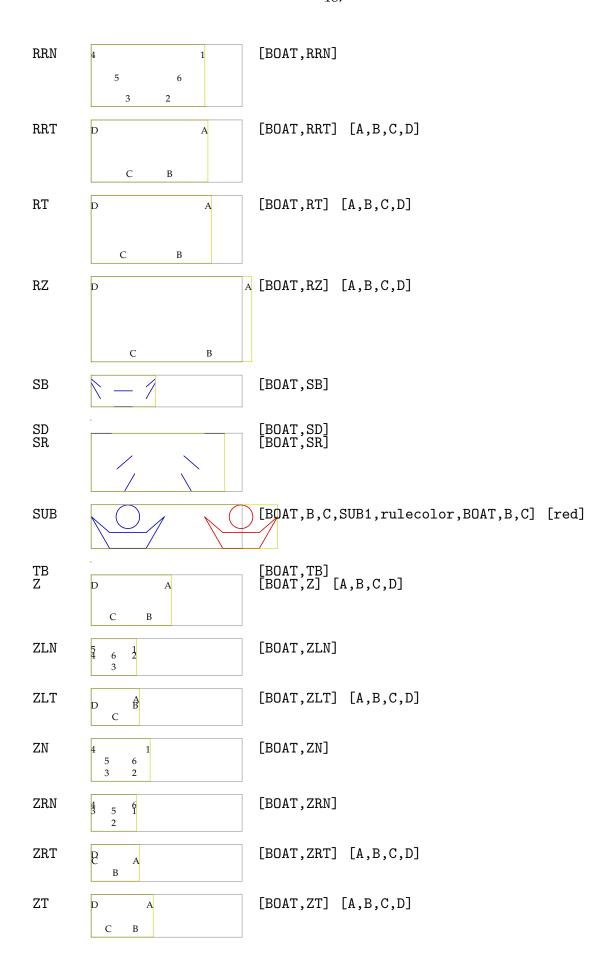


 $ppchT_EX$

32 Boat

adj arrow b bb c cc ccd cd dash diff eb label line lr	transform line line line fixed line fixed line transform line text line line	lrb lrbd lrd lrh lrn lrt lrz lsr lsub mark mov move number off	line line line line number text text line transform transform transform transform transform	r rb rbd rd rh rn rr rrb rrbd rrt rrt rrn	line line line line line line line line	rsr rsub rt rz sb sr sub z zln zlt zn zrn zrt zt	line transform text text line line transform text number text number number text	
AD AU B			[BOAT,AD] [BOAT,AU] [BOAT,B]					
BB			[BOAT,BB]					
BD BW C			[BOAT,BD] [BOAT,BW] [BOAT,C]					
CC			[BOAT,CC1]					
CCD			[BOAT,CCD1	.]				
CD			[BOAT,CD]					
CZ DB DR ED EP ES ET HB LDB			[BOAT,CZ] [BOAT,DB] [BOAT,DR] [BOAT,ED] [BOAT,EP] [BOAT,ES] [BOAT,ET] [BOAT,HB] [BOAT,LDB]	[A,B,C,1	D]			





 $ppchT_{EX}$

33 Symbol

CHEM		[CHEM]
SPACE PLUS MINUS EQUALS GIVES	. A	[SPACE] [PLUS] [MINUS] [EQUALS] [GIVES] [A]
EQUILIE RIUM	3- A ←	[EQUILIBRIUM] [A]
MESOMEF	ICA	[MESOMERIC] [A]
OPENCOM	1	[OPENCOMPLEX]
PLEX CLOSEC- OMPLEX	-	[CLOSECOMPLEX]