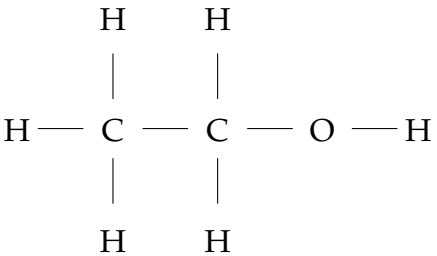
Drawing chemical structures with ppchTEX

Alan BRASLAU
Service de physique de l'état condensé, CEA/Saclay, France

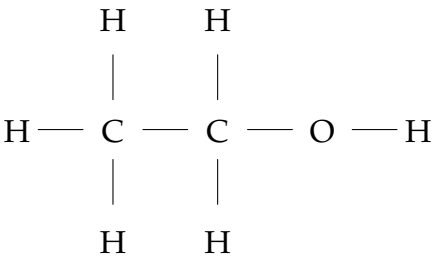
Brejlov – 15/09/2010

(The PracTEX Journal, January 2010)

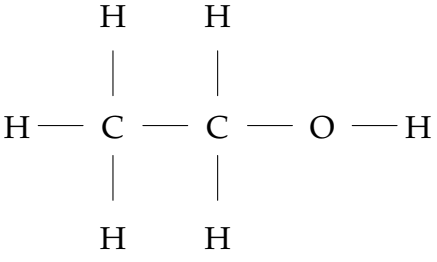
C_2H_5OH



C_2H_5OH



C_2H_5OH




```
\startchemical
    \chemical [ONE,Z0357,SB1357,MOV1,Z037,SB137,MOV1,Z01,SB1]
              [C,H,H,H,C,H,H,O,H]
\stopchemical
```

"For most people, a *solution* is the answer to a problem,
but to a **chemist**, a solution is something that is all mixed-up. . . "

"For most people, a *solution* is the answer to a problem,
but to a **chemist**, a solution is something that is all mixed-up. . . "

CTAN contains a number of macro packages aimed at writing chemical formulas, drawing reaction arrows, numbering reactions and even drawing structures (such as bpchem, chemarrow, chemcompounds, chemcono, chemsym, mhchem, . . .) The most evolved package is probably XyMTEX written by Shinsako Fujita.

"For most people, a *solution* is the answer to a problem,
but to a **chemist**, a solution is something that is all mixed-up. . . "

CTAN contains a number of macro packages aimed at writing chemical formulas, drawing reaction arrows, numbering reactions and even drawing structures (such as bpchem, chemarrow, chemcompounds, chemcono, chemsym, mhchem, . . .) The most evolved package is probably XyMTEX written by Shinsako Fujita.

With ConTEXt, we can use the ppchTEX macros.
(They can even be used with LATEX.)

Under LaTeX, positioning is performed by using PICTEX and line drawing using pstricks;

```
\documentclass{article}
\usepackage{m-ch-en} % English interface
%            m-ch-nl for a Dutch interface.
%            m-ch-de for a German interface.
```

Under ConTeXt MkII, positioning is performed by using PICTEX and line drawing using METAPOST;

```
\usemodule [chemic]
```

Under ConTeXt MkIV under LuaTeX, the internals of ppchTEX have been re-written to be included natively as core macros and no longer relies on PICTEX; both positioning and drawing are performed using METAPOST.

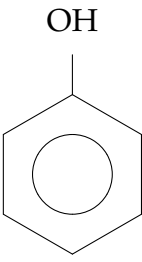
Under ConTEXt MkIV under LuaTEX, the internals of ppchTEX have been re-written to be included natively as core macros; both positioning and drawing are performed using METAPOST.

Question: Could the drawing of chemical structures be better handled entirely through METAPOST functions?

```
\usemodule [chemical]

\startMPcode
   draw chemical(...) ;
\stopMPcode
```

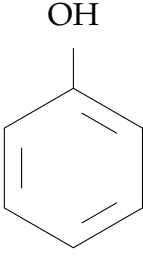
Quid alternative chemical syntax: e.g. SMILES, etc.

```
\starttext
\startchemical
      \chemical [SIX,B,C,R6,RZ6] [OH]
\stopchemical
\stoptext
```



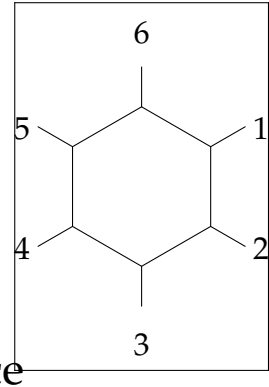
A second representation is drawn using

```
\starttext
\startchemical
      \chemical [SIX,B,EB246,R6,RZ6] [OH]
\stopchemical
\stoptext
```



The syntax of the command \chemical has two optional arguments. The first defines the structure and the second presents substituents to be placed in the structure, namely atoms. The syntax allows one to easily define a general molecular form that can be reused including different substituents to draw different molecules:

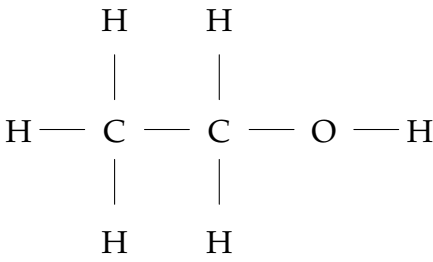
```
\definechemical [sixring]
 {\chemical [SIX,B,R,RZ]}

\startchemical [frame=on]
 \chemical [sixring] [1,2,3,4,5,6]
\stopchemical
```



The inconvenience is keeping track of the correspondence between positions and substituents for a very complicated structure. (This, in fact, can be handled by breaking down a structure into short, successive calls to \chemical, thus making the bookeeping task much easier.)

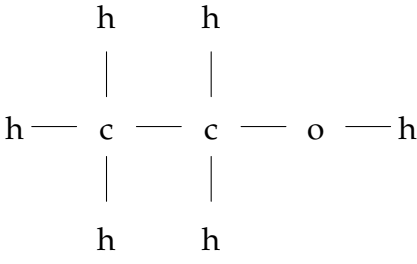
Chemical syntax (2)

```
\startchemical
  \chemical [ONE,Z0357,SB1357] [C,H,H,H]
  \chemical [MOV1,Z037,SB137] [C,H,H]
  \chemical [MOV1,Z01,SB1] [O,H]
\stopchemical
```



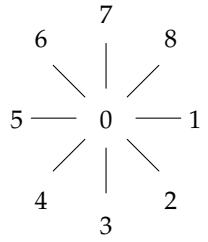
MKIV only:

```
\startchemical
  \chemical [ONE,Z0=C,Z357=H,SB1357]
  \chemical [MOV1,Z0=C,Z37=H,SB137]
  \chemical [MOV1,Z0=O,Z1=H,SB1]
\stopchemical
```

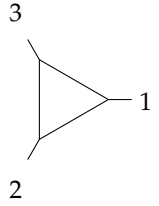


(What about not mixing tokens with parameter=value in the same argument list?)

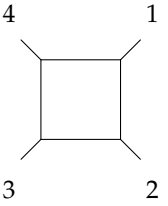
The basic molecular forms



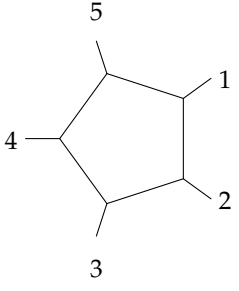

```
\chemical
[ONE,SB1..8,Z0..8]
[0,1,2,3,4,5,6,7,8]
```



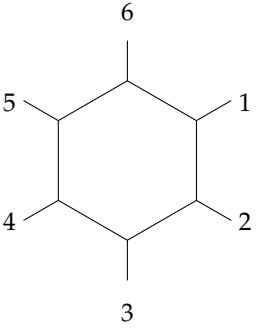

```
\chemical
[THREE,B,R,RZ1..3]
[1,2,3]
```



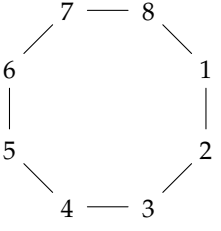

```
\chemical
[FOUR,B,R,RZ1..4]
[1,2,3,4]
```




```
\chemical
[FIVE,B,R,RZ1..5]
[1,2,3,4,5]
```

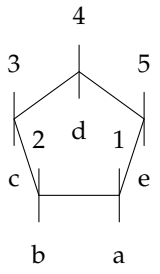



```
\chemical
[SIX,B,R,RZ1..6]
[1,2,3,4,5,6]
```

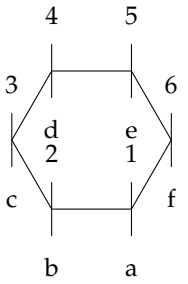



```
\chemical
[EIGHT,SB,Z1..8]
[1,2,3,4,5,6,7,8]
```

FIVE and SIX have FRONT variants




```
\chemical [FIVE,FRONT,B,R]
\chemical [+RZ1..5] [1,2,3,4,5]
\chemical [-RZ1..5] [a,b,c,d,e]
```




```
\chemical [SIX,FRONT,B,R]
\chemical [+RZ1..6] [1,2,3,4,5,6]
\chemical [-RZ1..6] [a,b,c,d,e,f]
```

Further structures

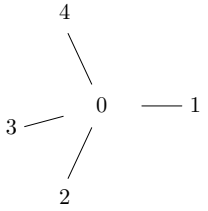
```
\chemical
[CARBON,B,Z0..4]
[0,1,2,3,4]
```

```
\chemical
[NEWMANSTAGGER,B,Z1..6]
[1,2,3,4,5,6]
```

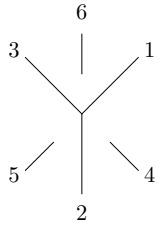
```
\chemical
[NEWMANECLIPSE,B,Z1..6]
[1,2,3,4,5,6]
```

```
\chemical [CHAIR,B]
\chemical [+R,+RZ1,+RZ2,+RZ3,+RZ4,+RZ5,+RZ6] [1,2,3,4,5,6]
\chemical [-R,-RZ1,-RZ2,-RZ3,-RZ4,-RZ5,-RZ6] [a,b,c,d,e,f]
```

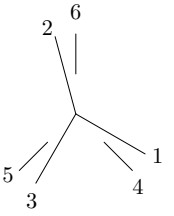
Further structures (mkii)



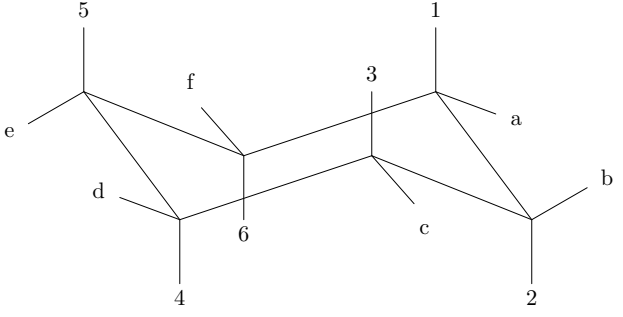

```
\chemical
[CARBON,B,Z0..4]
[0,1,2,3,4]
```




```
\chemical
[NEWMANSTAGGER,B,Z1..6]
[1,2,3,4,5,6]
```



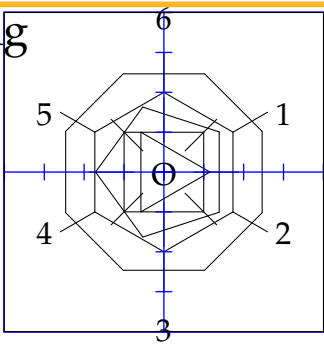

```
\chemical
[NEWMANECLIPSE,B,Z1..6]
[1,2,3,4,5,6]
```




```
\chemical [CHAIR,B]
\chemical [+R,+RZ1,+RZ2,+RZ3,+RZ4,+RZ5,+RZ6] [1,2,3,4,5,6]
\chemical [-R,-RZ1,-RZ2,-RZ3,-RZ4,-RZ5,-RZ6] [a,b,c,d,e,f]
```

Bounding box

\startchemical \stopchemical creates a TEX box having a certain bounding box. By default, this is a fixed and standard size: a square of dimensions corresponding to four bond lengths centered on the molecular “origin”.



Often, one would like this box to bound the real extension of the molecular structure, and this can be obtained by setting the following options:

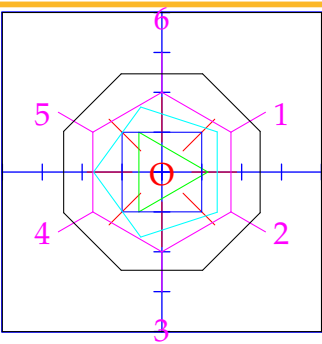
```
\setupchemical [width=fit,height=fit]
```

Alternatively, you can select options unique to each chemical structure drawn as:

```
\startchemical [width=4000,height=4000]
\stopchemical
```

Bounding box

\startchemical \stopchemical creates a TEX box having a certain bounding box. By default, this is a fixed and standard size: a square of dimensions corresponding to four bond lengths centered on the molecular "origin".



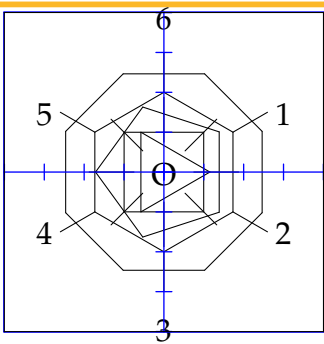
Often, one would like this box to bound the real extension of the molecular structure, and this can be obtained by setting the following options:

```
\setupchemical [width=fit,height=fit]
```

Alternatively, you can select options unique to each chemical structure drawn as:

```
\startchemical [width=4000,height=4000]
\stopchemical
```

Bounding box (2)




```
\startchemical [frame=on,axis=on,width=4000,height=4000]
    \chemical [ONE,SB,Z0] [O]
    \chemical [THREE,B]
    \chemical [FOUR,B]
    \chemical [FIVE,B]
    \chemical [SIX,B,R,RZ] [1,2,3,4,5,6]
    \chemical [EIGHT,B]
\stopchemical
```

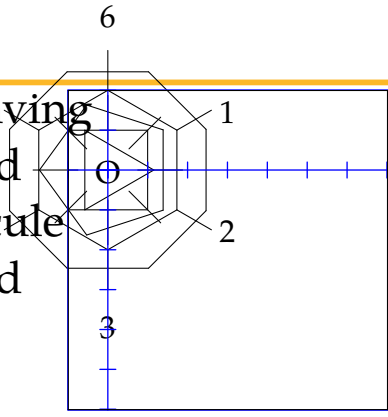
Bounding box (3)

```
\definecollector [BB]
\setupchemical [width=4000,height=4000]
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [frame=on,axis=on]
        \stopchemical
}
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [color=red,rulecolor=red]
                \chemical [ONE,SB,ZO] [O]
        \stopchemical
}
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [rulecolor=green]
                \chemical [THREE,B]
        \stopchemical
}
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [rulecolor=blue]
                \chemical [FOUR,B]
        \stopchemical
}
```

Bounding box (4)

```
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [rulecolor=cyan]
                \chemical [FIVE,B]
        \stopchemical
}
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [color=magenta,rulecolor=magenta]
                \chemical [SIX,B,R,RZ] [1,2,3,4,5,6]
        \stopchemical
}
\setcollector [BB] [corner=middle,location=middle] {
        \startchemical [rulecolor=black]
                \chemical [EIGHT,B]
        \stopchemical
}
\placefigure [right,none] {}
        {\composedcollector{BB}}
```

Bounding box (5)



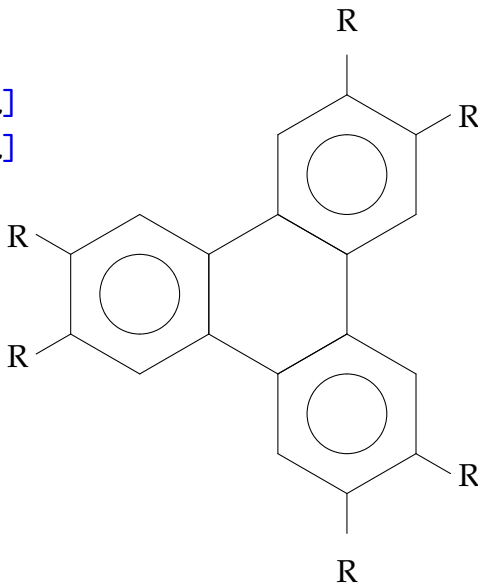
\startchemical \stopchemical creates a TEX box having a certain bounding box. The origin can be placed anywhere within this bounding box and the molecule may be drawn extending outside of this reserved space:

```
\startchemical [frame=on,axis=on,width=4000,height=4000,
               left=500,top=1000]
    \chemical [ONE,SB,Z0] [O]
    \chemical [THREE,B]
    \chemical [FOUR,B]
    \chemical [FIVE,B]
    \chemical [SIX,B,R,RZ] [1,2,3,4,5,6]
    \chemical [EIGHT,B]
\stopchemical
```

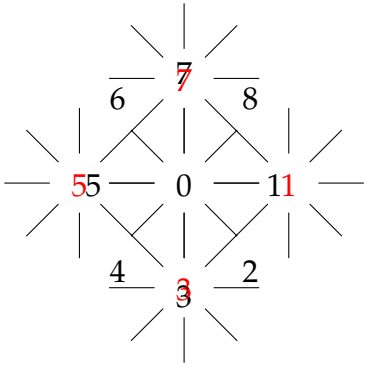
Combinations

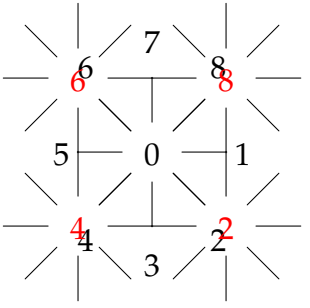
You also can combine basic forms and build complicated chemical structures, such as this disk-like molecule that forms columnar liquid-crystal mesophases.

```
\startchemical [width=5000]
        \chemical [SIX,B,MOV2]
        \chemical [B,C,R23,RZ23,MOV5,MOV4] [R,R]
        \chemical [B,C,R45,RZ45,MOV1,MOV6] [R,R]
        \chemical [B,C,R61,RZ61] [R,R]
\stopchemical
```



MOV

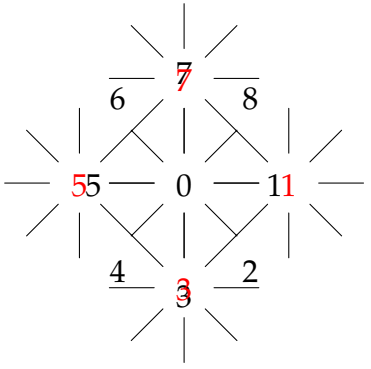


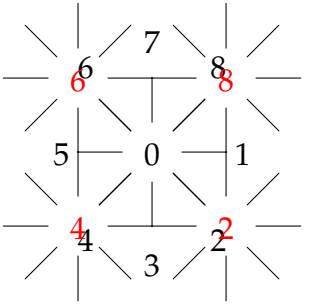



```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [MOV1,Z0,SB,MOV5]
            [{\red 1}]
  \chemical [MOV3,Z0,SB,MOV7]
            [{\red 3}]
  \chemical [MOV5,Z0,SB,MOV1]
            [{\red 5}]
  \chemical [MOV7,Z0,SB,MOV3]
            [{\red 7}]
\stopchemical
```

```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [MOV2,Z0,SB,MOV6]
            [{\red 2}]
  \chemical [MOV4,Z0,SB,MOV8]
            [{\red 4}]
  \chemical [MOV6,Z0,SB,MOV2]
            [{\red 6}]
  \chemical [MOV8,Z0,SB,MOV4]
            [{\red 8}]
\stopchemical
```

DIR

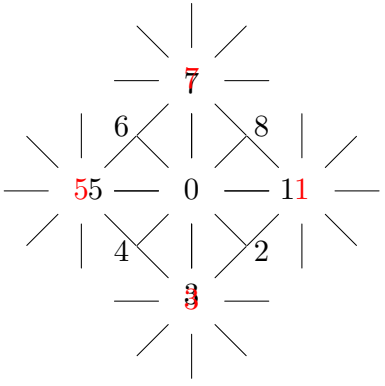


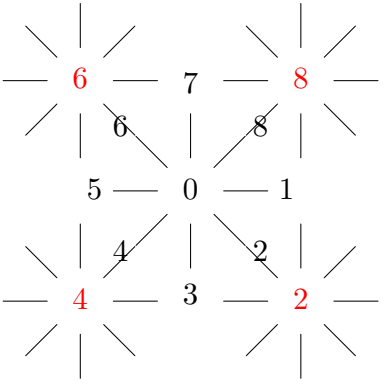



```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [DIR1,Z0,SB,DIR5]
            [{\red 1}]
  \chemical [DIR3,Z0,SB,DIR7]
            [{\red 3}]
  \chemical [DIR5,Z0,SB,DIR1]
            [{\red 5}]
  \chemical [DIR7,Z0,SB,DIR3]
            [{\red 7}]
\stopchemical
```

```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [DIR2,Z0,SB,DIR6]
            [{\red 2}]
  \chemical [DIR4,Z0,SB,DIR8]
            [{\red 4}]
  \chemical [DIR6,Z0,SB,DIR2]
            [{\red 6}]
  \chemical [DIR8,Z0,SB,DIR4]
            [{\red 8}]
\stopchemical
```

MOV (mkii)

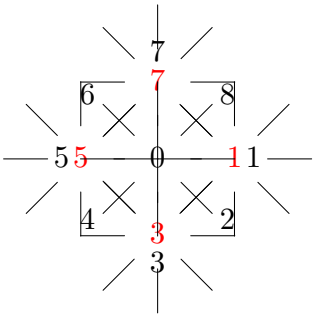


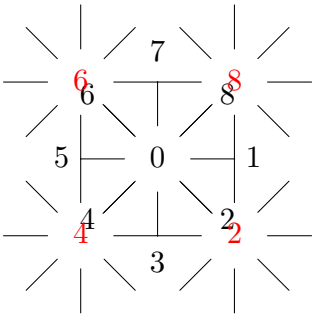



```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [MOV1,Z0,SB,MOV5]
            [{\red 1}]
  \chemical [MOV3,Z0,SB,MOV7]
            [{\red 3}]
  \chemical [MOV5,Z0,SB,MOV1]
            [{\red 5}]
  \chemical [MOV7,Z0,SB,MOV3]
            [{\red 7}]
\stopchemical
```

```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [MOV2,Z0,SB,MOV6]
            [{\red 2}]
  \chemical [MOV4,Z0,SB,MOV8]
            [{\red 4}]
  \chemical [MOV6,Z0,SB,MOV2]
            [{\red 6}]
  \chemical [MOV8,Z0,SB,MOV4]
            [{\red 8}]
\stopchemical
```

DIR (mkii)

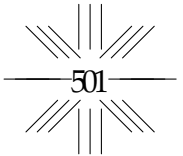


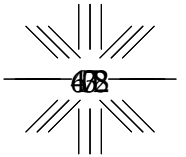



```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [DIR1,Z0,SB,DIR5]
            [{\red 1}]
  \chemical [DIR3,Z0,SB,DIR7]
            [{\red 3}]
  \chemical [DIR5,Z0,SB,DIR1]
            [{\red 5}]
  \chemical [DIR7,Z0,SB,DIR3]
            [{\red 7}]
\stopchemical
```

```
\startchemical
  \chemical [ONE,Z0..8,SB]
            [0,1,2,3,4,5,6,7,8]
  \chemical [DIR2,Z0,SB,DIR6]
            [{\red 2}]
  \chemical [DIR4,Z0,SB,DIR8]
            [{\red 4}]
  \chemical [DIR6,Z0,SB,DIR2]
            [{\red 6}]
  \chemical [DIR8,Z0,SB,DIR4]
            [{\red 8}]
\stopchemical
```

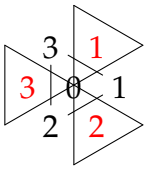
OFF

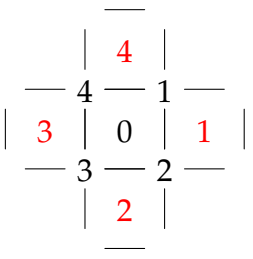


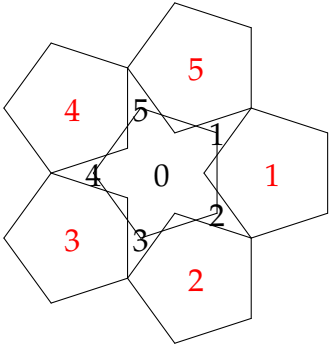


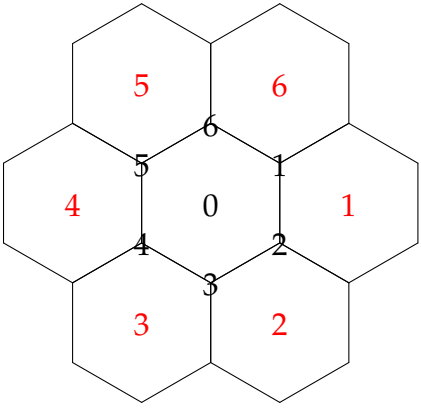
```
\startchemical
  \chemical [ONE,Z0,SB] [0]
  \chemical [OFF1,Z0,SB,OFF5] [1]
  \chemical [OFF5,Z0,SB,OFF1] [5]
\stopchemical
```

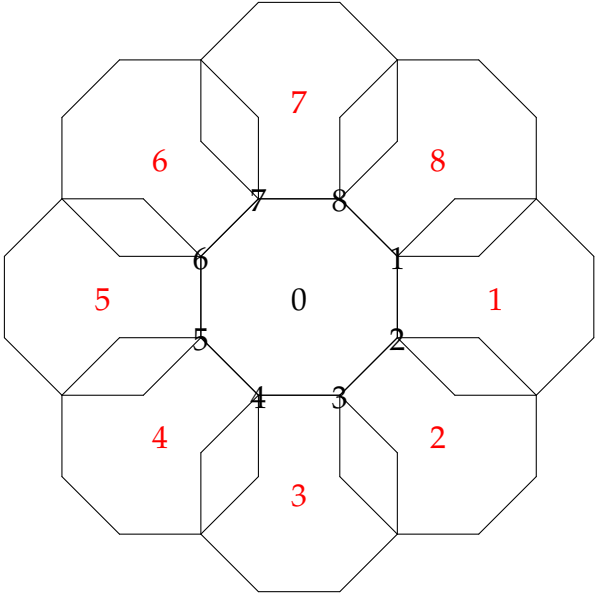
```
\startchemical
  \chemical [ONE,Z0,SB] [0]
  \chemical [OFF2,Z0,SB,OFF6] [2]
  \chemical [OFF3,Z0,SB,OFF7] [3]
  \chemical [OFF4,Z0,SB,OFF8] [4]
  \chemical [OFF6,Z0,SB,OFF2] [6]
  \chemical [OFF7,Z0,SB,OFF3] [7]
  \chemical [OFF8,Z0,SB,OFF4] [8]
\stopchemical
```

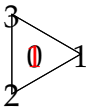

3
1
3
0
1
2
2

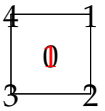

4
4
1
3
0
1
3
2
2

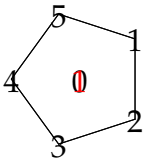

5
4
5
1
4
0
1
3
3
2
2

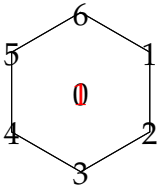

5
6
6
5
1
4
0
1
4
2
3
3
2

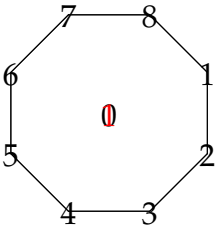

7
6
8
7
8
6
1
5
0
1
5
2
4
3
4
2
3


3
0
1
2

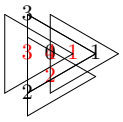

4
1
0
3
2

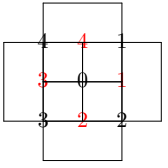

5
1
4
0
2
3

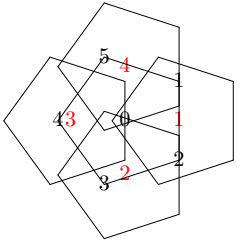

6
5
1
0
4
2
3

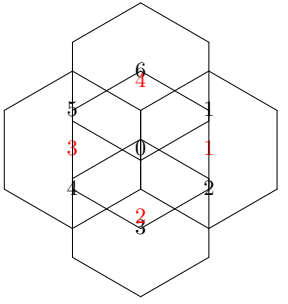

7
8
6
1
0
5
2
4
3

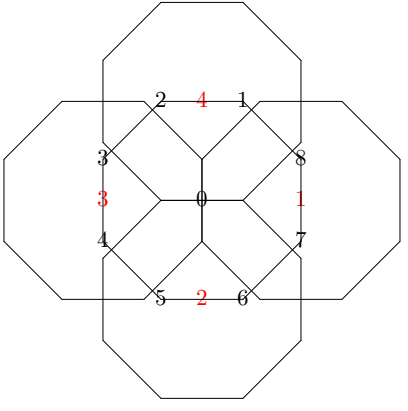
ADJ (mkii)


3
3 0 1 1
2 2

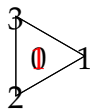

4 4 1
3 0 1
3 2 2

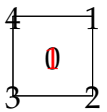

5 4
1
4 3 0 1
2
3 2

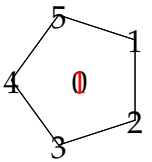

6
4
5 1
3 0 1
4 2
2
3

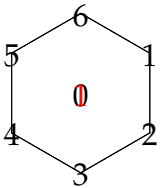

2 4 1
3 8
3 0 1
4 7
5 2 6

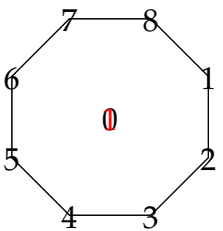
SUB



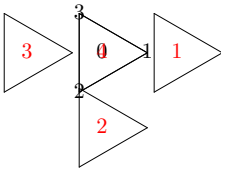


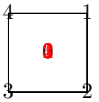


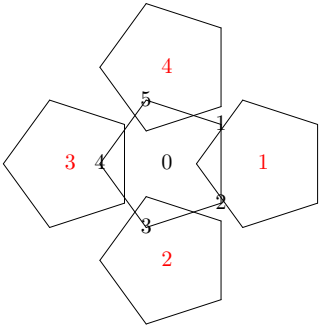


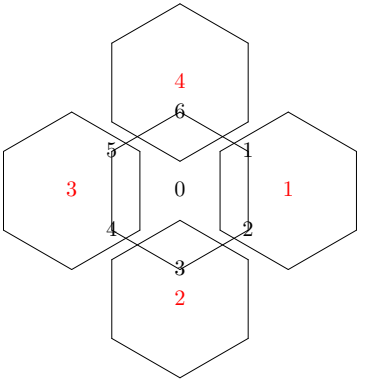


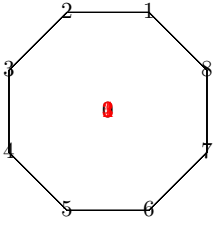
SUB (mkii)





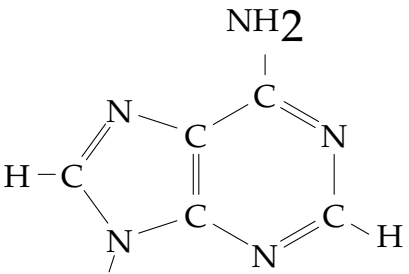




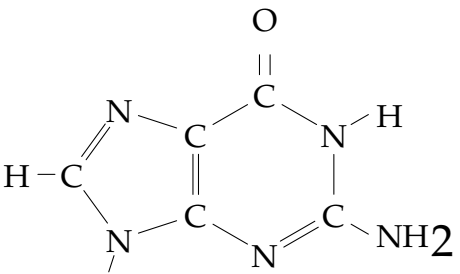


Purines

```
\startchemical
  \chemical [FIVE,Z12345,SB235,DB14,SR34,RZ4]
            [C,C,N,C,N,H]
  \chemical [ADJ1,SIX,Z1236,SB135,DB26,SR26,RZ26]
            [N,C,N,C,H,NH_2]
- or -
  \chemical [ADJ1,SIX,Z1236,SB1356,DB2,SR12,DR6,RZ126]
            [N,C,N,C,H,HN_2,O]
\stopchemical
```

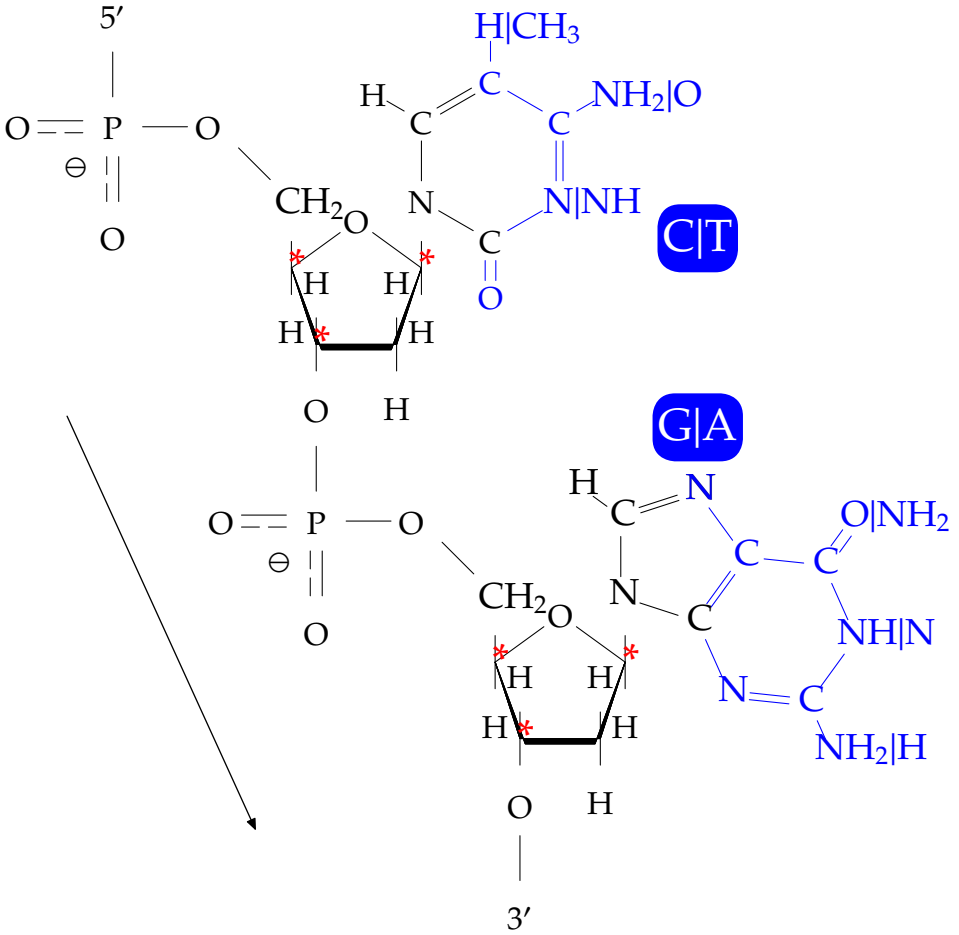


adenine

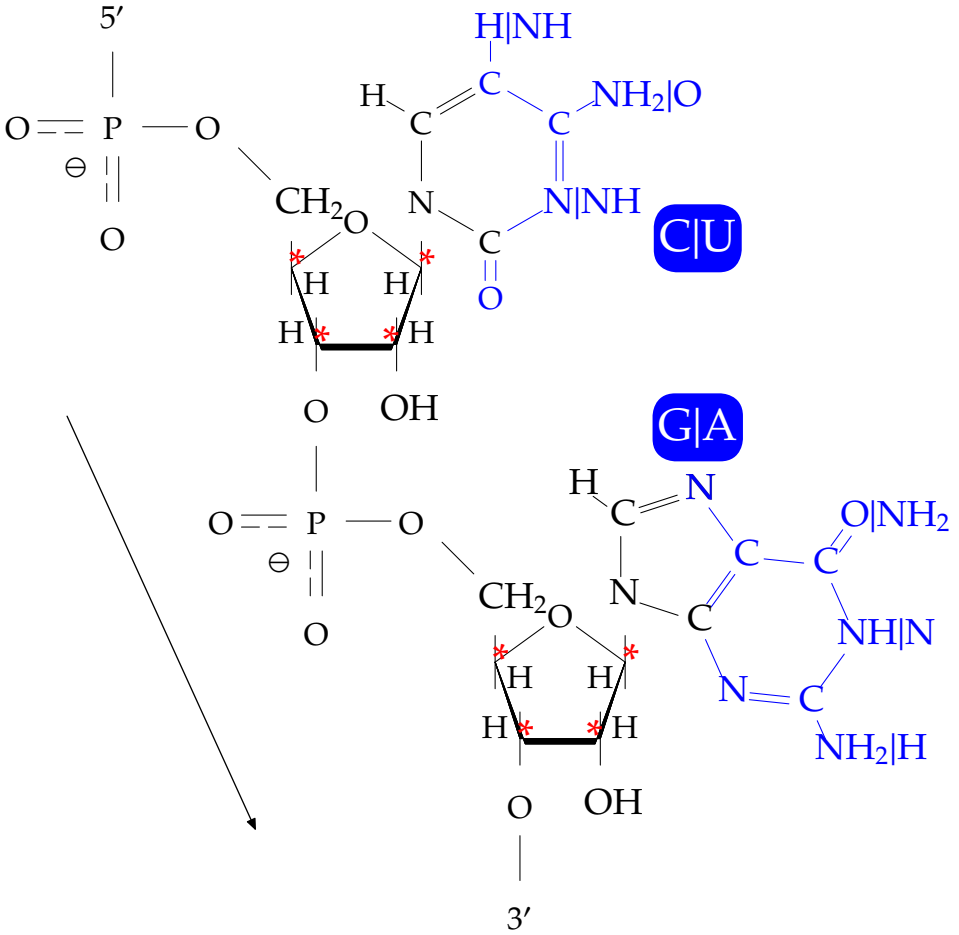


guanine

DNA


5′
O
P
O
O
CH2
O
H
H
H
H
H|CH3
C
H
C
NH2|O
C
N
N|NH
C
O
C|T
O
H
O
P
O
O
CH2
O
H
H
H
H
G|A
H
C
N
N
C
C
O|NH2
C
NH|N
N
C
NH2|H
O
H
3′

RNA


5′
O
P
O
O
CH2
O
H
H
H
H
H|NH
C
H
C
NH2|O
C
N
N|NH
C
O
C|U
O
OH
G|A
H
C
N
O|NH2
C
C
N
C
NH|N
N
C
NH2|H
O
P
O
O
CH2
O
H
H
H
H
O
OH
3′

DNA

```
%%%%%%%%%%%%%%%%%%%%
% deoxyribonucleoside
%%%%%%%%%%%%%%%%%%%%

\setupchemical [width=11800,height=11600]

\def\Rx#1{\rotate [rotation=+36] {\small #1}}%

\definecollector [DNA]
\def\firstleft{4400}
\def\firsttop{3600}
\def\RZoffset{840}
\def\secondleft{\firstleft+2545}
\def\secondtop{\firsttop+4925}

% dexoyribose
\setcollector [DNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop]
    \chemical [FIVE,FRONT,BB125,+SB3,-SB4,Z4] [O]
    \chemical [-R1235,-RZ135] [H,H,H]
    \chemical [+R1235,+RZ12] [H,H]
```

```
    \chemical [Z235] [\hbox{\space\red *},\hbox{\space\red *},
                      \hbox{\space\red *}]
  \stopchemical
}

% phosphate
\setcollector [DNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset]
    \chemical [FIVE,FRONT,PB:Z3,
               ONE,Z0,SB6,DIR6,MOV5,SB17,RDD3,LDD5,Z01357,ZT4,PE]
              [\SL{\small CH$_2$},P,O,O,O,5',\ominus]
  \stopchemical
  }

% pyrimidines
\setcollector [DNA] [corner=middle,location=middle] { % black = backbone
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset]
    \chemical [FIVE,FRONT,PB:Z5,
               SIX,PB:Z1,SIX,SB34,DB5,Z345,SR5,CRZ5,PE,PE]
              [C,N,C,H]
  \stopchemical
```

```
}
\setcollector [DNA] [corner=middle,location=middle] { % blue = bases
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset,
                  color=blue,rulecolor=blue]
    \chemical [FIVE,FRONT,PB:Z5,
               SIX,PB:Z1,SIX,SB26,DB1,Z126,SR16,DR3,CRZ136,PE,PE]
              [C,\SL{\small N$|$NH},C,\SL{\small NH$_2|$O},O,
               \SL{\small H$|$CH$_3$}]
  \stopchemical
}

% 2nd dexoyribose
\setcollector [DNA] [corner=middle,location=middle] {
  \startchemical [left=\secondleft,top=\secondtop]
    \chemical [FIVE,FRONT,BB125,+SB3,-SB4,Z4] [O]
    \chemical [-R1235,-RZ135] [H,H,H]
    \chemical [+R1235,+RZ12] [H,H]
    \chemical [Z235] [\hbox{\space\red *},\hbox{\space\red *},
                      \hbox{\space\red *}]
  \stopchemical
}
```

```
\setcollector [DNA]
  [corner=middle,location=middle,hoffset=+3cm,voffset=-3cm]
  {\framed [frame=off,corner=round,
            background=color,backgroundcolor=blue,
            style=bold,foreground=color,foregroundcolor=white] {C$|$T}}
\setcollector [DNA]
  [corner=middle,location=middle,hoffset=+3cm,voffset=-0.5cm]
  {\framed [frame=off,corner=round,
            background=color,backgroundcolor=blue,
            style=bold,foreground=color,foregroundcolor=white] {G$|$A}}

% 2nd phosphate
\setcollector [DNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop+\RZoffset+60]
    \chemical [FIVE,FRONT,PB:Z2,
               ONE,MOV3,SB17,RDD3,LDD5,Z01357,ZT4,
               MOV1,SB2,DIR2,Z0,PE]
              [P,O,O,O,O,\ominus,\SL{\small CH$_2$}]
  \stopchemical
  }
```

```
% 3'-end
\setcollector [DNA] [corner=middle,location=middle] { % +RZ3 offset =
+625
  \startchemical [left=\secondleft,top=\secondtop+\RZoffset]
    \chemical [FIVE,FRONT,PB:Z2,ONE,SB3,Z03,PE] [0,3']
  \stopchemical
}

% purines
\setcollector [DNA] [corner=middle,location=middle,rotation=-36] {
   \startchemical [height=6000,width=7000,
                   left=5355,top=2670] % ajusted empirically
    \chemical [FIVE,FRONT,PB:Z5,
               FIVE,SB23,DB4,SR4,Z2345,CRZ4,PE]
              [\Rx{C},\Rx{N},\Rx{C},\Rx{N},\Rx{H}] %common
  \stopchemical
}
\setcollector [DNA] [corner=middle,location=middle,rotation=-36] {
   \startchemical [height=6000,width=7000,
                   left=5355,top=2670,
                   color=blue,rulecolor=blue]
```

```
    \chemical [FIVE,FRONT,PB:Z5,
               FIVE,SB5,DB1,Z15,ADJ1,
               SIX,SB1356,DB2,SR2,DR6,Z1236,CRZ26,PE]
              [\Rx{C},\Rx{N},\Rx{\kern1.5em NH$|$N},\Rx{C},\Rx{N},
               \Rx{C},\Rx{\kern2em NH$_2|$H},
               \Rx{\kern2em O$|$NH$_2$}] % G&A
  \stopchemical
}

\setcollector [DNA] [corner=middle,location=middle,rotation=-65.5,
                     hoffset=-4.125cm,voffset=2cm] {
  \startMPcode
    drawarrow ((-.5,0)--(.5,0)) scaled 6cm ;
  \stopMPcode
}

\composedcollector{DNA}
```

RNA

```
%%%%%%%%%%%%%%%
% ribonucleoside
%%%%%%%%%%%%%%%

\definecollector [RNA]

% ribose
\setcollector [RNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop]
    \chemical [FIVE,FRONT,BB125,+SB3,-SB4,Z4] [O]
    \chemical [-R1235,-RZ135] [\SL{\small OH},H,H]
    \chemical [+R1235,+RZ12] [H,H]
    \chemical [Z1235] [\hbox{\red *\space},\hbox{\space\red *},
                       \hbox{\space\red *},\hbox{\space\red *}]
  \stopchemical
}

% phosphate
\setcollector [RNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset]
    \chemical [FIVE,FRONT,PB:Z3,
```

```
                ONE,Z0,SB6,DIR6,MOV5,SB17,RDD3,LDD5,Z01357,ZT4,PE]
               [\SL{\small CH$_2$},P,O,O,O,5',\ominus]
  \stopchemical
  }

% pyrimidines
\setcollector [RNA] [corner=middle,location=middle] { % black = backbone
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset]
    \chemical [FIVE,FRONT,PB:Z5,
               SIX,PB:Z1,SIX,SB34,DB5,Z345,SR5,CRZ5,PE,PE]
              [C,N,C,H]
  \stopchemical
}
\setcollector [RNA] [corner=middle,location=middle] { % blue = bases
  \startchemical [left=\firstleft,top=\firsttop-\RZoffset,
                  color=blue,rulecolor=blue]
    \chemical [FIVE,FRONT,PB:Z5,
               SIX,PB:Z1,SIX,SB26,DB1,Z126,SR16,DR3,CRZ136,PE,PE]
              [C,\SL{\small N$|$NH},C,\SL{\small NH$_2|$O},O,
               \SL{\small H$|$NH}]
  \stopchemical
```

```
}

% 2nd ribose
\setcollector [RNA] [corner=middle,location=middle] {
  \startchemical [left=\secondleft,top=\secondtop]
    \chemical [FIVE,FRONT,BB125,+SB3,-SB4,Z4] [O]
    \chemical [-R1235,-RZ135] [\SL{\small OH},H,H]
    \chemical [+R1235,+RZ12] [H,H]
    \chemical [Z1235] [\hbox{\red *\space},\hbox{\space\red *},
                       \hbox{\space\red *},\hbox{\space\red *}]
  \stopchemical
}
\setcollector [RNA]
  [corner=middle,location=middle,hoffset=+3cm,voffset=-3cm]
  {\framed [frame=off,corner=round,
            background=color,backgroundcolor=blue,
            style=bold,foreground=color,foregroundcolor=white] {C$|$U}}
\setcollector [RNA]
  [corner=middle,location=middle,hoffset=+3cm,voffset=-0.5cm]
  {\framed [frame=off,corner=round,
            background=color,backgroundcolor=blue,
```

```
            style=bold,foreground=color,foreground=white] {G$|$A}}

% 2nd phosphate
\setcollector [RNA] [corner=middle,location=middle] {
  \startchemical [left=\firstleft,top=\firsttop+\RZoffset+60]
    \chemical [FIVE,FRONT,PB:Z2,
               ONE,MOV3,SB17,RDD3,LDD5,Z01357,ZT4,
               MOV1,SB2,DIR2,Z0,PE]
              [P,O,O,O,O,\ominus,\SL{\small CH$_2$}]
  \stopchemical
  }

% 3'-end
\setcollector [RNA] [corner=middle,location=middle] { % +RZ3 offset =
+625
  \startchemical [left=\secondleft,top=\secondtop+\RZoffset]
    \chemical [FIVE,FRONT,PB:Z2,ONE,SB3,Z03,PE] [O,3']
  \stopchemical
}

% purines
```

```
\setcollector [RNA] [corner=middle,location=middle,rotation=-36] {
   \startchemical [height=6000,width=7000,
                   left=5355,top=2670] % ajusted empirically
    \chemical [FIVE,FRONT,PB:Z5,
               FIVE,SB23,DB4,SR4,Z2345,CRZ4,PE]
              [\Rx{C},\Rx{N},\Rx{C},\Rx{N},\Rx{H}] %common
  \stopchemical
}
\setcollector [RNA] [corner=middle,location=middle,rotation=-36] {
   \startchemical [height=6000,width=7000,
                   left=5355,top=2670,
                   color=blue,rulecolor=blue]
    \chemical [FIVE,FRONT,PB:Z5,
               FIVE,SB5,DB1,Z15,ADJ1,
               SIX,SB1356,DB2,SR2,DR6,Z1236,CRZ26,PE]
              [\Rx{C},\Rx{N},\Rx{\kern1.5em NH$|$N},\Rx{C},\Rx{N},
               \Rx{C},\Rx{\kern2em NH$_2|$H},
               \Rx{\kern2em O$|$NH$_2$}] % G&A
  \stopchemical
}
```

```
\setcollector [RNA] [corner=middle,location=middle,rotation=-65.5,
                     hoffset=-4.125cm,voffset=2cm] {
  \startMPcode
    drawarrow ((-.5,0)--(.5,0)) scaled 6cm ;
  \stopMPcode
}

\composedcollector{RNA}
```

Conclusions

- MKIV: some bugs need to be fixed.
  (SAVE,RESTORE currently broken, . . .)
- Stereochemistry: some new features have been added, still others are missing.
- Better handling of rotations.
- Atom and Bond colors should be selectable within \chemical.
- Now that all graphics are processed within METAPOST, should chemical become a METAPOST function?
- Would another syntax (such as SMILES) with more built-in intelligence be better?
- The manual needs to be revised!