

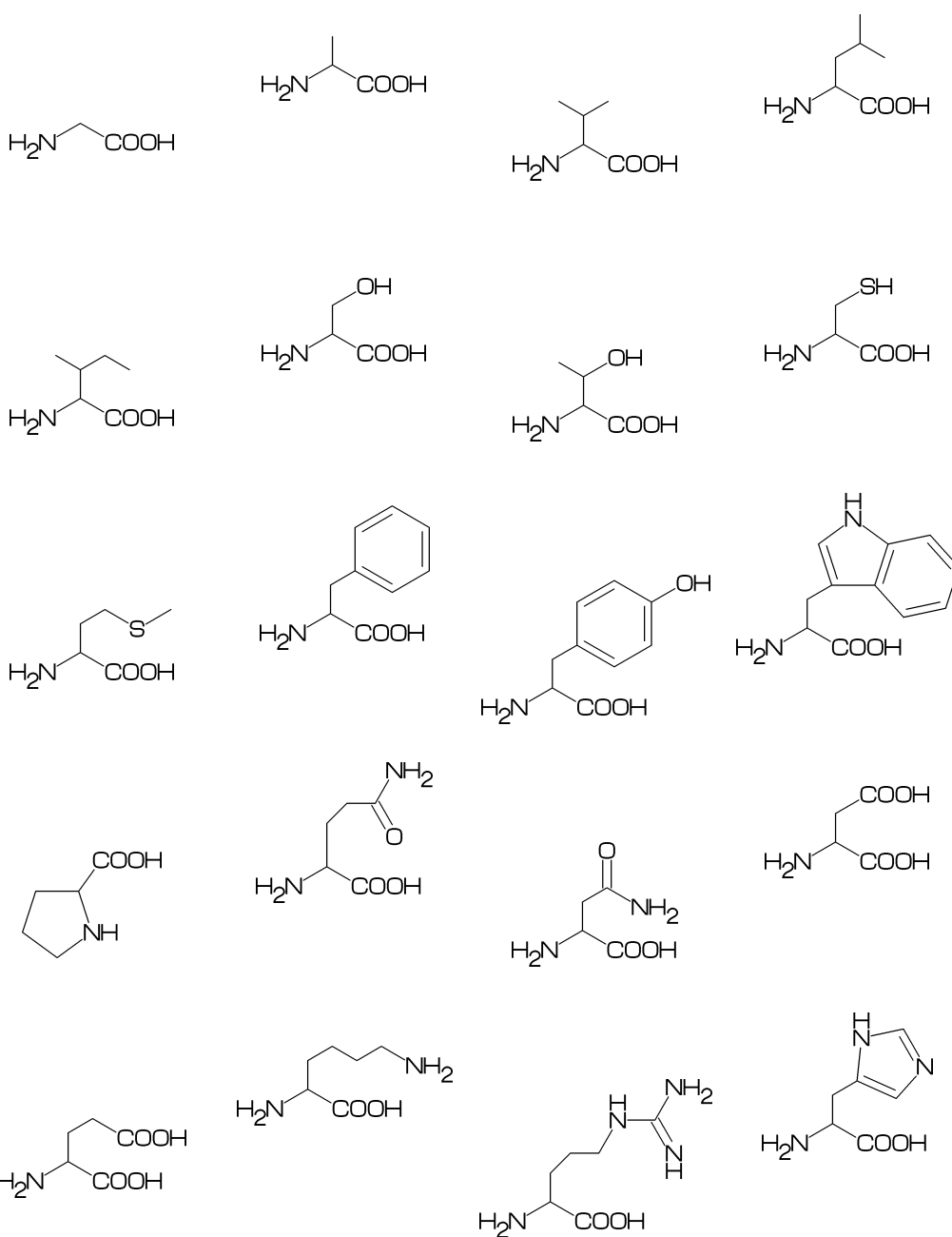
Molecular Coding Format manual

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December 8, 2019

Located at <http://www.ctan.org/pkg/mcf2graph>

Suggestion or request mail to: mcf2graph@gmail.com



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1 Introduction

Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This 'Coding' is named from coding(programing) technique like addressing,grouping,macro,etc. There are no Meta language commands in MCF. mcf2graph convert MCF file to graphics file pk font,PNG,SVG,EPS or MDL MOL file.

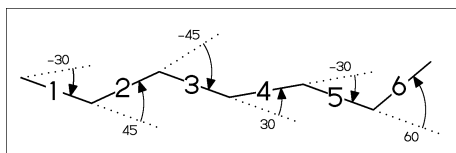
2 MCF syntax

2.1 Make bond

2.1.1 Chain

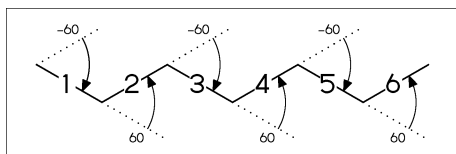
real number plus (+): Counterclockwise
real number minus(-): Clockwise

<10,-30,45,-45,30,-30,60



! : take value 60 or -60 depend on current angle and enviroment
!6 : !,!,!,!,!,!

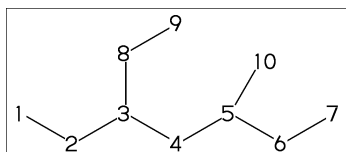
<30,! ,! ,! ,! ,! ,!
<30,!6



2.1.2 Jump and branch bond

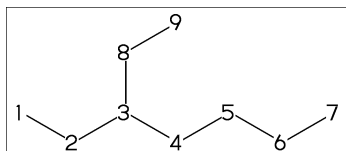
n:@ : Jump to An
** An: atom number(-999<=n<=4095)

<30,!6,3:@,0,! ,5:@,-30



3:\ : 3:@,0

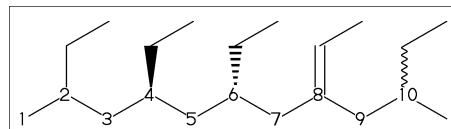
<30,!6,3:\,! ,



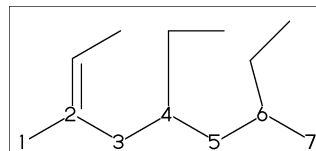
2.1.3 Branch bond

2:\ : 2:@,0
4:* \ : 4:@,0~wf
6:* : 6:@,0~zf
8:\\ : 8:@,0~dm
10:* * : 10:@,0~wv

<30,!8,
2:\,! ,4:* \,! ,6:* \,! ,8:\\,! ,10:* * \,! ,



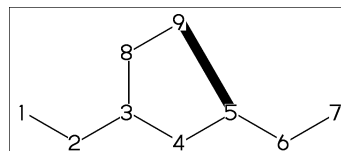
<-30,!6,
2:\~dr,! , : 2:@,0~dr,!
4:\'1.5,-90, : 4:@,0'1.5,-90
6:\^15,-60 : 6:@,0^15,-60



2.1.4 Connect atom

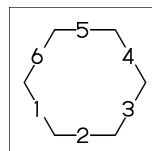
n:# : Connect to An

<30,!6,3:\,! ,5~bd:#



2.1.5 Ring

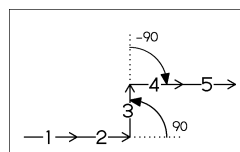
?n : n membered ring(3<=n<=20)
?6 : <-120,60,60,60,60,60,1:#
?6



2.1.6 Rotate current angle

<angle : rotate current angle

0,0,<90,0,<-90,0,0,{1,2,3,4,5}=vf

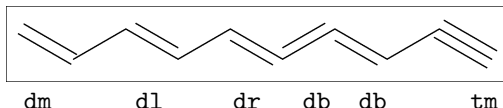


2.2 Change bond type

2.2.1 Double, triple

a~type : ~type,a
dm : double middle
dl : double left side
dr : double right side
db : double left or right side
tm : triple
!! : !~db / !!! : !~tm

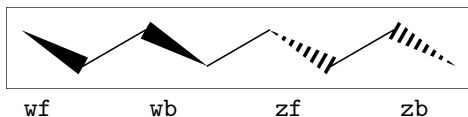
```
<30,!~dm,!~dl,!~dr,!~db,!~db,!~tm
<30,!~dm,!~dl,!~dr,!! ,!! ,!!!
```



2.2.2 Wedge

wf : wedge forward / wb : wedge backward
zf : wedge dotted
zb : wedge dotted backward

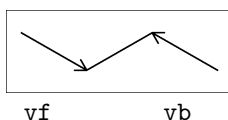
```
<30,!~wf,!~wb,!~zf,!~zb
```



2.2.3 Vector

vf:vector forward / vb:vector backward

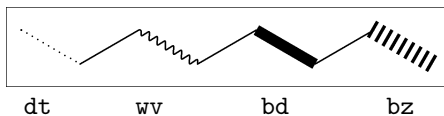
```
<30,!~vf,!~vb
```



2.2.4 Dotted, wave

Bn=bond type : change bond type at Bn
dt : dotted / wv : wave
bd : broad / bz : broad dotted

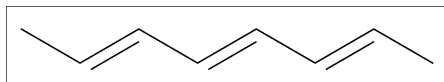
```
<30,!7,1=dt,3=wv,5=bd,7=bz
```



2.2.5 Change multiple bond type

```
{2,4,6}=dr : 2=dr,4=dr,6=dr
```

```
<30,!7,{2,4,6}=dr
```



2.2.6 Over line

si_ : single over line
wf_ : wedge forward over line
wb_ : wedge backward over line
bd_ : broad over line

```
<-30,!8,!60,90'8,
{2~si_,4~wf_,6~wb_,8~bd_}:/_'2
```



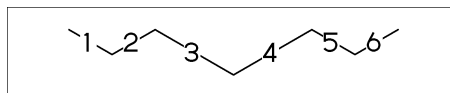
2.3 Change bond length

2.3.1 Chain length

(!,!n)'length : change length of !,!n

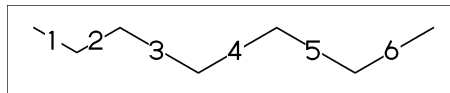
```
<30,!2,!2'1.2,!2
```

```
** !2'1.2 : ''1.2,!2
```



''length : change all bond length after

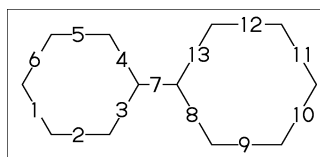
```
<30,!2, ''1.2,!4
```



2.3.2 Ring length

?n'length : change ring length

```
?6,4:\,?6'1.2
```

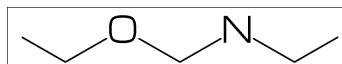


2.4 Change atom

2.4.1 Insert atom

Insert hetero atom

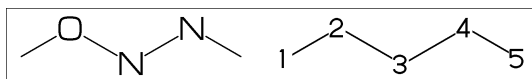
```
<30,!2,0,!2,N,!2
```



2.4.2 Addressed atom

2:0 : change A2 C to O
 {3,4}:N : change A3,A4 C to N

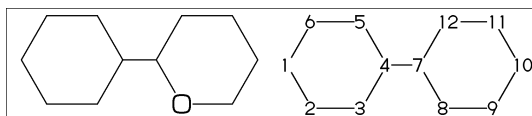
<30,!4,2:0,{3,4}:N



2.4.3 Brock address

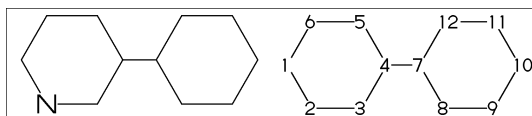
| : divide brock

?6,4:\,|,?6,2:0



|| : reset brock address

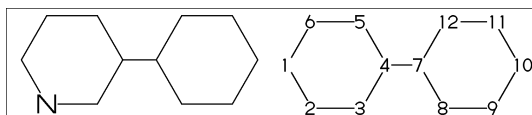
?6,4:\,|,?6,||,2:N



2.4.4 Absolute address

\$2:N : change A\$2 C to N
 ** \$n : (1<=n<=3095)

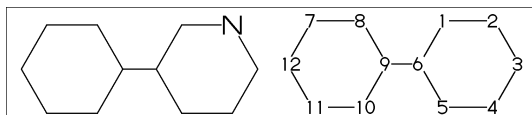
?6,4:\,|,?6,\$2:N



2.4.5 Relative address

-2:N : change A(-2) C to N
 ** -n : (1<=n<=999)

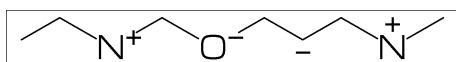
?6,4:\,?6,-2:N



2.4.6 Charged atom

N[1]:N+ / O[-1]:O- / A,&"c":A+c

<-30,!2,N[1],!2,O[-1],
 !2,&"-" ,!2,N,&"+"^180,!



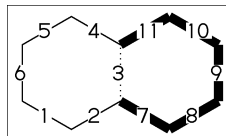
2.5 Fuse ring

(Attached 1 bond)

?6,3=?6 : fuse ?6 at B3

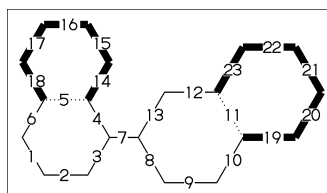
** Bn(n:-999<=n<=4095): bond number

?6,3=?6



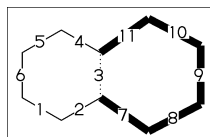
** fused ring size depend on
 attached bond length

?6,4:\,?6'1.2,5=?6,11=?6

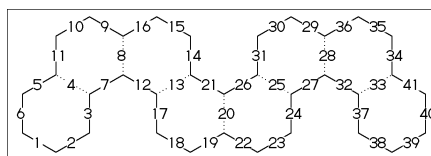


?6,3=?6[13] : fuse ?6[13] at B3
 ?6[13]: 6 membered ring scaled 13/10
 ** ?m[n] (5<=m<=8,11<=n<=15)

?6,3=?6[13]



?6,{-3,-4,-4,-2,-2,-4,-4}=?6
 ?6,{4,8,13,20,25,28,33}=?6



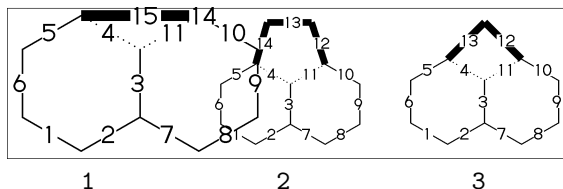
(Attached 2 bond)

(4,11)=?6[4] : fuse 4/6 ring to B11..B4
 (4,11)=?5[3] : fuse 3/5 ring to B11..B4
 (4,11)=?4[2] : fuse 2/4 ring to B11..B4
 ** ?m[n] (4<=m<=6,n=m-2)

1:<30,?6,3=?6,(11,4)=?6[4]

2:<30,?6,3=?6,(11,4)=?5[3]

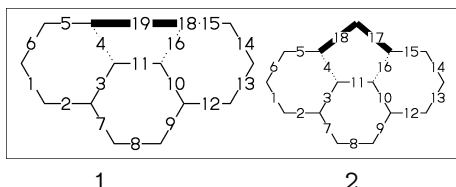
3:<30,?6,3=?6,(11,4)=?4[2]



(Attached 3 bond)

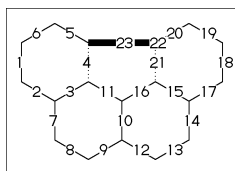
(16,4)=?6[3] : fuse 3/6 ring to B16..B4
 (16,4)=?5[2] : fuse 2/5 ring to B16..B4
 ** ?m[n] (5<=m<=6,n=m-3)

1:?6,{3,10}=?6,(16,4)=?6[3]
 2:?6,{3,10}=?6,(16,4)=?5[2]



(Attached 4 bond)

(21,4)=?6[2] : fuse 2/6 ring to B21..B4
 MC(<-30,?6,{3,10,15}=?6,(21,4)=?6[2])
 ** ?m[n] (m=6,n=2)

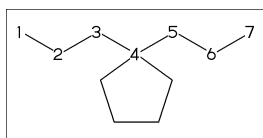


2.6 Spiro ring

4:@,?5 : add ?5 at A4

<30,!6,4:@,?5

An:@ : jump to An

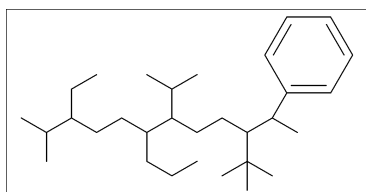


2.7 Substituent

2.7.1 Insert substituent

/ : single
 <30,!/,Me,!/,Et,!3,/Pr,!/,iPr,
 !3,/tBu,!/,Ph^-30,!)

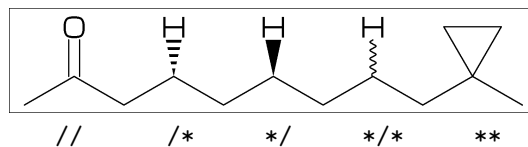
** Me:methyl(/_) Et:ethyl(!)
 Pr:propyl(!2) iPr:isopropyl
 tBu:tertial buthyl Ph:phenyl



2.7.2 Insert modified substituent

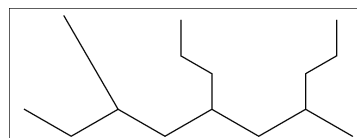
// : double (double middle)
 */ : wedge forward
 /* : wedge dotted forward
 / : wave
 ** : direct

<30,!/,/0,!2,/*H,!2,*/H,!2,*/H,!2,**?3,!)



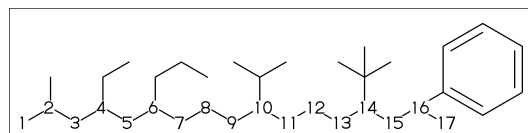
~ : change type
 ^ : change angle
 ' : change length
 > : change enviroment

<30,'^1,!/
 /_'^2^30,!2,/!2>lr,!2,/!2>r1,!)



2.7.3 Add substituent

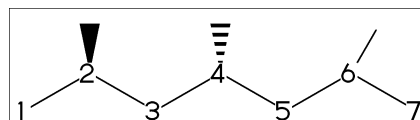
<-30,!17,2:/_,4:/!,6:/!2,
 10:/iPr,14:/tBu,16:/Ph^-60



2.7.4 Add modified substituent

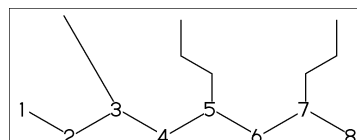
~,^,' : change type,angle,length

<-30,!6,
 {2~wf,4~zf,6^-30}:/_



~,^,> : change angle,length,environment

<30,!7^1,
 3:/_'^2^30,5:/!2>lr,7:/!2>r1

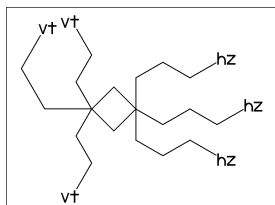


2.8 Chain environment

2.8.1 Horizontal,vertical

>hz : horizontal environment (default)
>vt : vertical environment

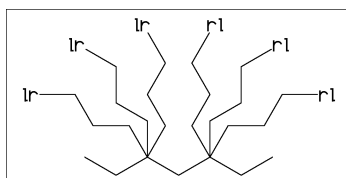
```
?4,{3^-90,3^-30,3^90}:/'(!3,"{hz}")>hz,  
{1^-60,1'^2,1^60}:/'(!2,"{vt}")>vt
```



2.8.2 Left-right,right-left

>lr : left-right environment
>rl : right-left environment

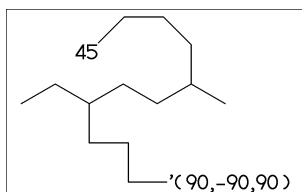
```
<30,!6,  
{3^-30,3,3^30}:/'(!3,"{lr}")>lr,  
{5^-30,5,5^30}:/'(!3,"{rl}")>rl
```



2.8.3 Fixed angle,multi angle

>45 : fixed angle environment
>'(-90,90,-90) : multi angle environment

```
<-30,!6,2>45:/'(!3,"{45}"),  
{6>'(-90,90,-90)}:/'(!3,"{(-90,90,-90)}")
```

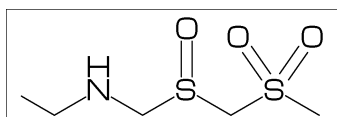


2.9 Miscellaneous

2.9.1 Change atom and Substituent

NH,S0,S00 :
inset hetero atom and substituent
simultaneously

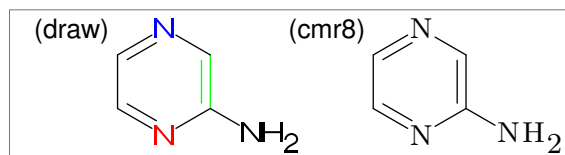
```
<30,!2,NH,! ,S0,! ,S00,!
```



2.9.2 Change color, atom font

1=green : change color of B1 green
3:red : change color of A3 red
atomfont:="cmr8" : use cmr8 for atom font

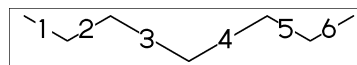
```
defaultfont:="cmr8";  
defaultsize:=8bp;  
MCat(0.25,0)(<30,Ph,{2,5}:N,3:/NH2,  
2:red,5:blue,3=green)  
add(label.lft("(draw)",p0+(0,0.9h));)  
atomfont:="cmr8"; % default:"draw"  
MCat(1,0)(<30,Ph,{2,5}:N,3:/NH2)  
add(label.lft("(cmr8)",p0+(0,0.9h));)
```



2.9.3 Make block

|< : start block
>| : end block
|=n, bond length=n, =|

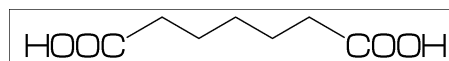
```
<30,!2,|<,'1.2,!2,>|,!2  
<30,!2,|=1.2,!2,=|,!2
```



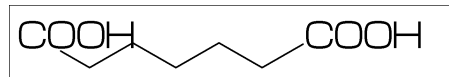
2.9.4 Chain start multiple characters

if chain start multi character string,
use !0 instead of !

```
MC(<30,COOH,!0,!3,COOH)
```

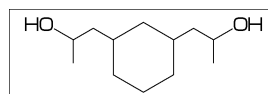


```
MC(<30,COOH,!4,COOH)
```

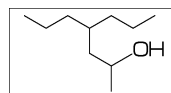


2.9.5 User definition

user defined substructure
iBuOH:='(!,/_,!,OH)
<30,?6,{4,6}:/iBuOH



Insert user defined substructure
<30,!3,/ '(!,/_,!,OH),!3



3 Option parameter

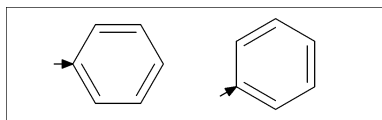
3.1 Angle parameter

mangle=0 ** default

MCat(0.2,0.5)(Ph)

mangle:=30;

MCat(0.8,0.5)(Ph)

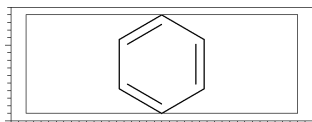


3.2 Size/Ratio parameter

3.2.1 Bond length

(fit to font size)

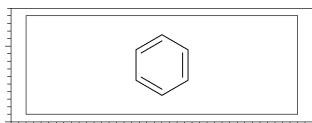
blength=0 ** default



(ratio bond/font width)

blength=0.1 ** (0<blength<=1)

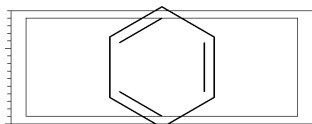
blength=60mm(width)*0.1=6mm



(bond length)

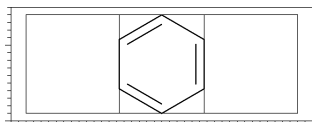
blength=9mm

** (blength>1) ignore msize(w,h)



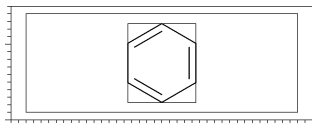
3.2.2 Molecular size

msize=(1,1) ** default

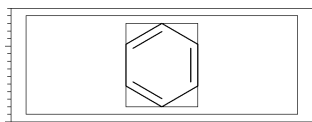


msize=(0.25,1)

msize=40mm-4mm*0.25=9mm

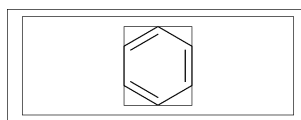


msize=(11mm,11mm)



3.2.3 Molecular position

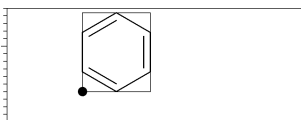
mposition=(0.5,0.5) ** default



mposition=(1,0)



mposition=(10mm,4mm)



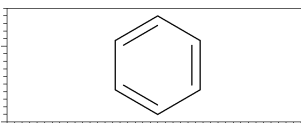
3.3 Size parameter

3.3.1 Font size

fsize=(font width,font height)

** default: (30mm,20mm)

fsize=(40mm,15mm)

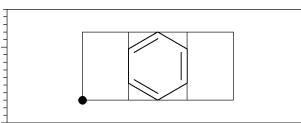


3.3.2 Font margin

fmarg=(margin left right,top bottom)

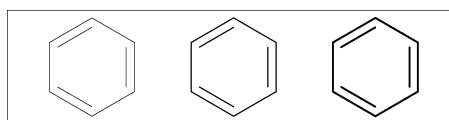
** default: (0.4mm,0.4mm)

fmarg=(10mm,2mm)



3.3.3 Offset thickness of bond

default: offset_thickness=0.2pt



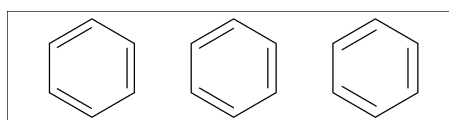
0pt

0.2pt

0.5pt

3.3.4 Offset of doublebond gap

default: offset_bond_gap=0.3pt



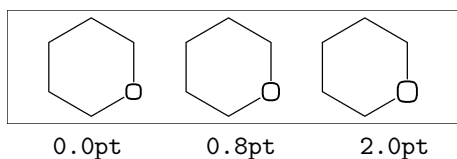
0.0pt

0.3pt

1.0pt

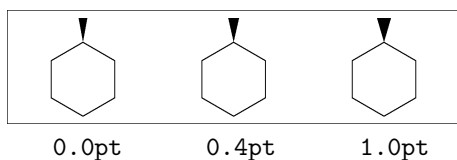
3.3.5 Offset of atom width

default: `offset_atom=0.8pt`



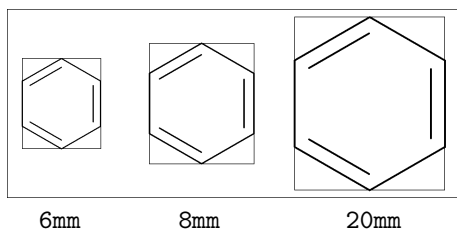
3.3.6 Offset of wedge width

default: `offset_wedge=0.4pt`



3.3.7 Max bond length

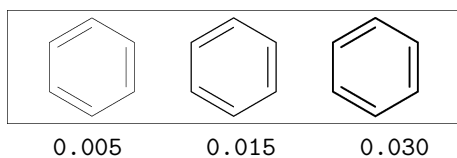
default: `max_blength=10mm`



3.4 Ratio parameter

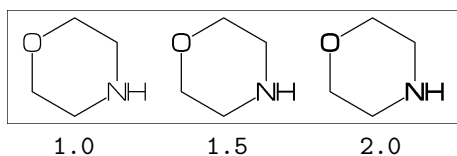
3.4.1 Thickness/bond length

default: `ratio_thickness_bond=0.015`



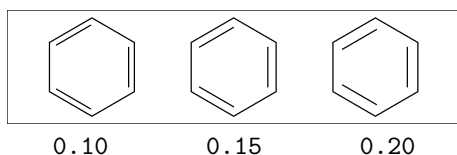
3.4.2 Char/bond thickness

default: `ratio_char_bond=1.5`



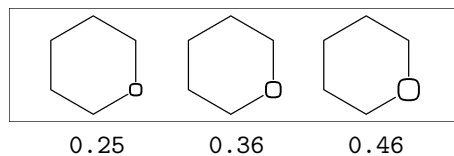
3.4.3 Bondgap/bond length

default: `ratio_bondgap_bond= 0.15`



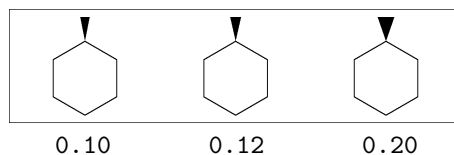
3.4.4 Atom/bond length

default: `ratio_atom_bond= 0.36`



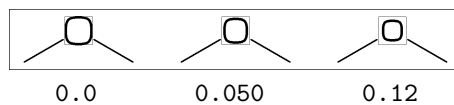
3.4.5 Wedge/bond length

default: `ratio_wedge_bond=0.12`



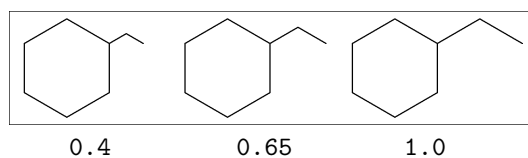
3.4.6 Font atom gap/atom length

default: `ratio_atomgap_atom= 0.050`



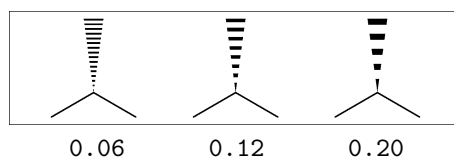
3.4.7 Chain/ring length

default: `ratio_chain_ring= 0.66`



3.4.8 Zebra gap/bond length

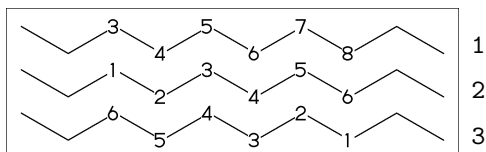
default: `ratio_zebragap_bond=0.12`



3.5 Drawing mode

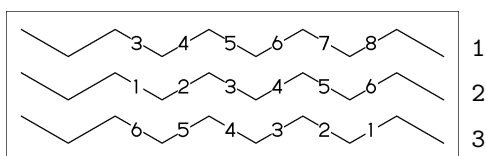
3.5.1 Numbering atom

```
numberA_start:=3; numberA_end:=8;
default: sw_numberA=0 :
  numberA_start=1 numberA_end=4095
```



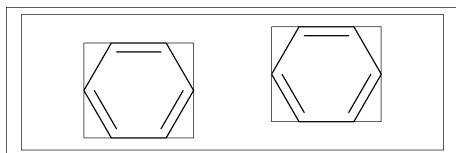
3.5.2 Numbering bond

```
numberB_start:=3; numberB_end:=8;
default: sw_numberB=0 :
  numberB_start=1 numberB_end=4095
```

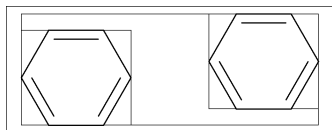


3.5.3 Trimming mode

```
sw_trimming:=0; ** default
msize:=(1,0.7);
MCat(0.2,0.3)(Ph)
MCat(0.8,0.7)(Ph)
```

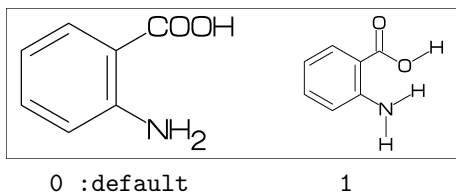


```
sw_trimming:=1;
MCat(0.2,0.3)(Ph)
MCat(0.8,0.7)(Ph)
```



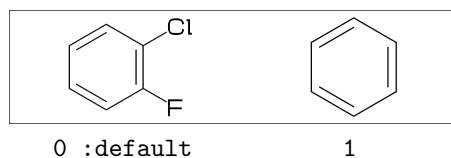
3.5.4 Expand mode

```
MCat(0, .5)(<30,Ph,4:/COOH,3:/NH2)
sw_expand:=1;
MCat(1, .5)(<30,Ph,4:/COOH,3:/NH2)
** default: sw_expand=0
```



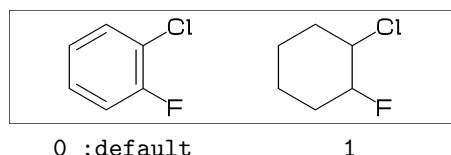
3.5.5 Substituent off mode

```
** default: sw_subst_off=0
```



3.5.6 Single bond mode

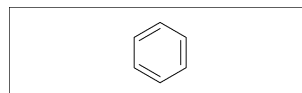
```
** default: sw_single=0
```



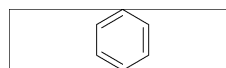
3.6 Frame

3.6.1 Font frame

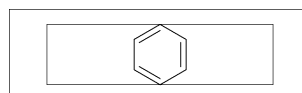
```
(Draw font frame)
fmargin:=(5mm,2mm);
sw_fframe=1
```



```
(Draw frame inside margin)
sw_fframe=2
```

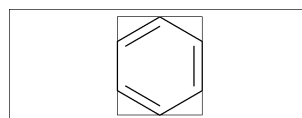


```
(Draw both frame)
sw_fframe=3
```



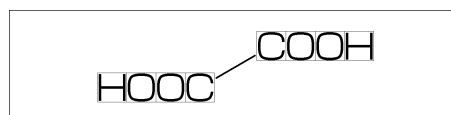
3.6.2 Molecular frame

```
sw_mframe=1 ** default:sw_mframe=0
```



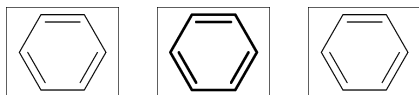
3.6.3 Atom frame

```
sw_aframe=1 ** default: sw_aframe=0
MC(<30,COOH,!0,COOH)
```



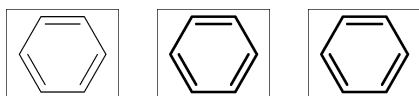
3.7 Local parameter setting

```
beginfont()
  MC(Ph)
endfont
beginfont()
  %-----
  ratio_thickness_bond:=0.05;
  %-----
  MC(Ph)
endfont
beginfont()
  MC(Ph)
endfont
```



3.8 Global parameter setting

```
beginfont()
  MC(Ph)
endfont
%-----
ratio_thickness_bond:=0.05;
%-----
beginfont()
  MC(Ph)
endfont
beginfont()
  MC(Ph)
endfont
```



4 Function

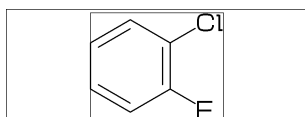
4.1 Function MC()

(Draw molecule)

```
msize=(a,b)      **default (1,1)
mposition=(c,d)  **default (0.5,0.5)
```

a: ratio molecular width/font width
b: ratio molecular height/font height
c: x axis position
d: y axis position

```
beginfont()
  MC(<30,Ph,3:/F,4:/Cl)
endfont
```



4.2 Function MCat()

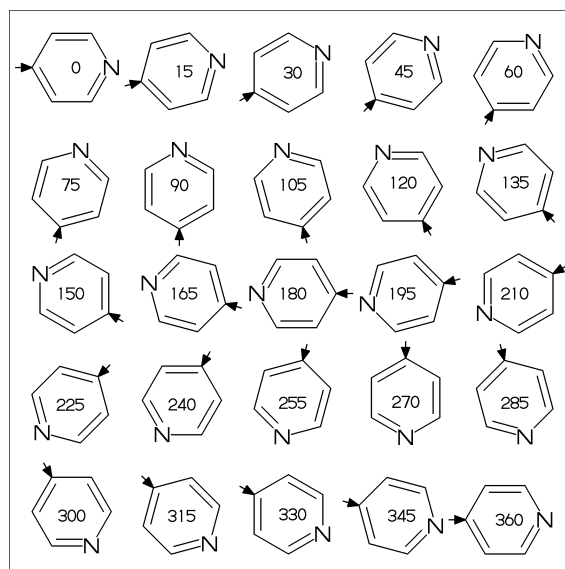
(Draw molecule at mposition)

MCat(c,d)(...) :

mposition:=(c,d);
MC(...)

c: x axis position
d: y axis position

```
beginfont()
defaultsize:=5bp;
fsize:=(75mm,75mm);
fmargin:=(3mm,3mm);
blength:=0.07;
sw_fframe:=1;
mangle:=0;
for i=1 step -0.25 until 0:
  for j=0 step 0.25 until 1:
    MCat(j,i)(Ph,4:N)
    add(
      drawarrow((A1+A1up**aw)..A1);
      label(decimal(mangle),
        p0+(0.5w,0.5h));
    )
    mangle:=mangle+15;
  endfor
endfor
endfont
```



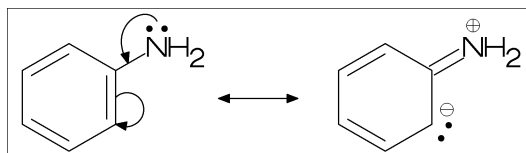
4.3 Function add()

(Add graphic to molecule)

```

w:      molecular width
h:      molecular height
aw:     atom font size
em:     label font size
p0:     origin of molecular structure
l:      bond length
An:     atom number
A[m]:   atom position
A[m]ang: branch angle of A[m]
A[m]up:  dir A[m]ang
A[m]left: dir A[m]ang+90
A[m]right: dir A[m]ang-90
A[m]down: dir A[m]ang+180
Bn:     bond number
B[m]:   bond(path)
B[m]s:  bond start position
B[m]m:  bond middle position
B[m]e:  bond end position
B[m]ang: bond angle
B[m]up:  dir B[m]ang
B[m]left: dir B[m]ang+90
B[m]right: dir B[m]ang-90
B[m]down: dir B[m]ang+180
plus : '+' circled
minus : '-' circled
        circlediam = 0.6aw (default)
        circlepen = 0.2bp (default)
lonpair r: ':' rotated r
        lonpairdiam = 0.3aw (default)
        lonpairspace = 0.7aw (default)
** : scaled
<< : rotated
a /* b : point b of a
%-----
beginfont()
  fsize:=(60mm,20mm);
  msize:=(1,0.85);
  MCat(0,0)(<30,Ph,3=d1,4://NH2)
  add(
    labeloffset:=.7aw;
    label.top(lonpair 90,A7);
    drawarrow (A7+up**1.2aw){A7left}
      ..{B7right}B7/*0.3;
    drawarrow B3m..A3+B2up**1.5aw
      ..{A3down}A3;
  )
  MCat(1,0)(<30,?6,{1,5}=d1,4://NH2)
  add(
    labeloffset:=.7aw;
    label.top(plus,A7);
    label.urt(minus,A3);
    label(lonpair A3ang,A3+A3up**1.7aw);
  )
  ext(drawdblarrow (.4w,.4h)..(.55w,.4h));
endfont

```



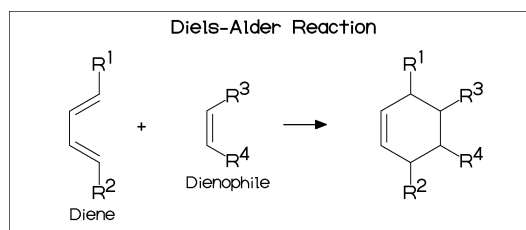
4.4 Function ext()

(Extra graphic to font)

```

w:      font width
h:      font height
w0:     font width-2xpart(fmargint)
h0:     font height-2ypart(fmargint)
aw:     atom font size
em:     label font size
p0:     fmargint
n:      molecular number
p[m]:   molecular origin position
w[m]:   molecular width
h[m]:   molecular height
ratio_thickness_char:
        pen thickness / char width
%=====
ext(label(inf_EN,(.5w,0));) => all font
%=====
beginfont()
  fsize:=(70mm,30mm); blength:=0.065;
  MCat(0.1,0.5)
    (<-210,60'1,60'1,{1,3}=d1,
     1:/R1,4:/R2~60)
    add(defaultscale:=0.6;
        label.bot("Diene",p0+(0.5w,0));)
  MCat(0.4,0.5)
    (<-30,-60'1,1=d1,1:/R3,2:/R4~60)
    add(defaultscale:=0.6;
        label.bot("Dienophile",p0+(.5w,0));)
  MCat(0.9,0.5)
    (<30,?6,6=d1,2:/R2,3:/R4,4:/R3,5:/R1)
  ext(
    drawarrow (.52w,.5h)..(.6w,.5h);
    defaultscale:=0.7;
    label("+",(0.25w,0.5h));
    ratio_thickness_char:=0.125;
    label.bot("Diels-Alder Reaction",
              (.5w,h));
  )
%-----
endfont

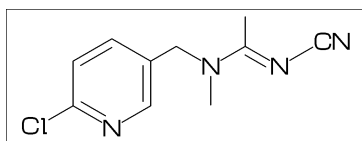
```



5 MCF example

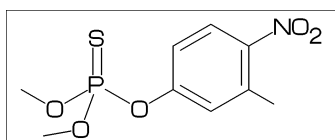
5.1 Acetamidrid

<30,Ph,2:N,1:/Cl,
4:\,!,N,/_,!/_,!N,!,CN



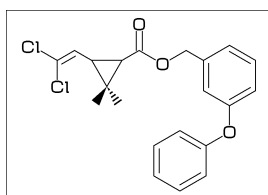
5.2 Fenitrothion

<30,!,0,!,P,//S,/O!^160,!,0,!,
|,Ph,3:/_,4:/NO2



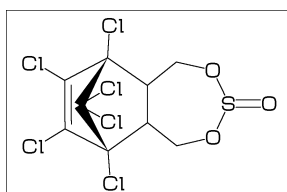
5.3 Permethrin

<-30,?3,2^-35:*/_ ,2^35:*/_ ,
1:\,!!,/Cl,!,Cl,
3:\,//0,!,0,!2,Ph,
-4:\,0,-60,Ph



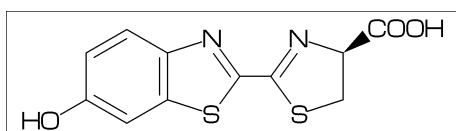
5.4 Endosulfan

<26,?7,7=?6[13],11:0,208~wf'1.45,8~wb:#,
10=d,{3,5}:0,4:S,4://0,
{8,9,10,11,12^-210,12^-150}:/Cl



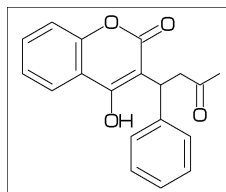
5.5 Luciferin

<30,Ph,3=?5,8:\,?5,{9,16}=d1,
{9,14}:N,{7,11}:S,
1:/OH,-2:*/COOH



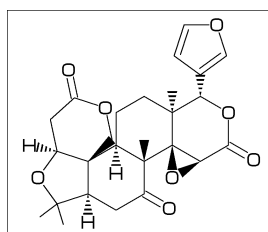
5.6 Warfarin

<30,Ph,3=?6,8=d1,
10:0,7:/OH,9://0,
8:\,/Ph'1,60,!,//0,!



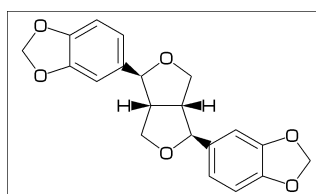
5.7 Limonin

<30,?6,{-3,-4}=?6,-5=?3,
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
{13,15,17,20}:0,{3,12,21}://0,
{4~wf^60,8~zf^60,18^35,18^-35}:/_ ,
{1^60,5^180,16^60}:/*H,
14:*,|,?5,{1,4}=d1,3:0



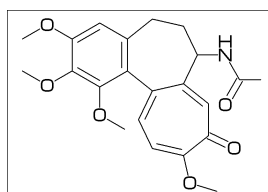
5.8 Sesamine

<54,?5,1=?5,
{4,7}:0,{1^-54,2^54}:*/H,
5:*^-12,Ph,-3=?5,{-1,-3}:0,
8:*^-12,Ph,-3=?5,{-1,-3}:0



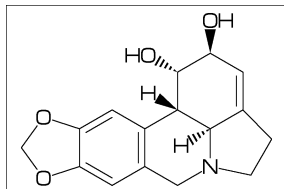
5.9 Colchicine

<30,Ph,{1,2,6}:/O!,
-4=?7,-5=?7,
{-1,-4,-6}=d1,-2://0,-3:/O!,
9:\,NH,!,//0,!



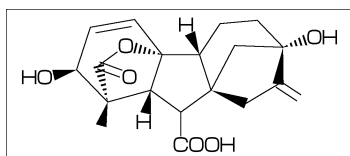
5.10 Lycorine

<30,Ph,
-4=?6,-2=?6,6=?5,(9,12)=?5[3],
13=d1,
8:N,{15,17}:0,
9:/*H^180,10:/*H^60,
13:*/OH,14:/*OMe



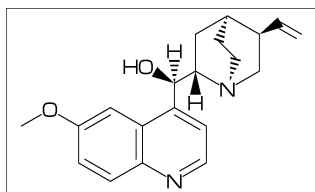
5.11 Gibberellin

<18,?5,3=?7,5=?6[12],
8:@,160'1.3,3:#,
13=d1,6=wf,8=wb,
5:@,40~zf'1,0,60,//0^180,14~zb:#,
2:/COOH,7://_,13:*/OH,8:*/OH,
14:*/_,{1,4}:*/H^60



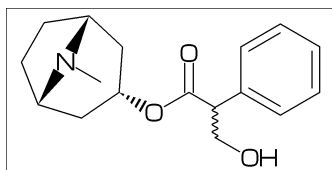
5.12 Quinine

<30,Ph,3=Ph,7:N,6:/O!,
10:\,*/OH,/H~zf^-60,!,
|,?6,2:N,1:*/H^60,
4:*!,!!,
2:@,165~zf,60,5~zb:#



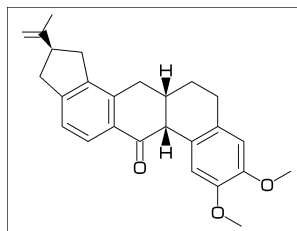
5.13 Atoropin

<-30,0,!,//0,!,!,Ph,
\$1:@,-120~zb,
|,?7,6:*^190'1.02,N/_ ,3~wb:#,
\$3:*!,!,OH



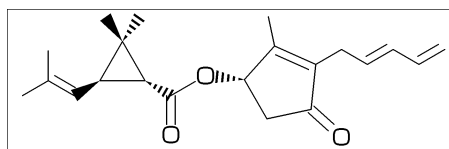
5.14 Rotenone

<-60,?5,{-3,-2,-3,-4}=?6,
{7,9,-2,-4}=d1,{3,17}=dr,
{2,13,16}:0,10://0,{11^-60,12^60}:*/H,
{-2,-3}:/O!,1:*!,/_ ,!!



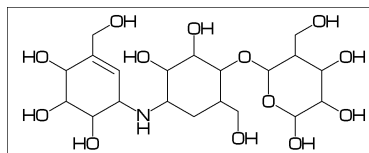
5.15 Pyrethrin I

<30,?3,{3^35~wf,3^-35~zf}:/_ ,
1:*!,!! ,iPr,2:*,//0,!,0,-36~zb,|,
?5,-2=d,-1:/_, -3://0,-2\,!4,{-1,-3}=d1



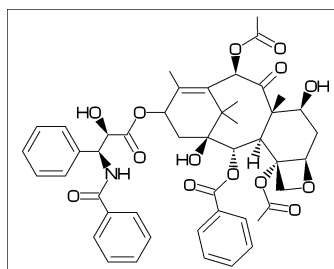
5.16 Validamycin

<30,?6,{5,6}:/OH,3:/!OH>r1,
\$4:\,0,-60,|,?6,2:0,{3,4,5}:/OH,6:/!OH,
\$1:\,NH,!,|,?6,2=d1,{4,5,6}:/OH,3:/!OH



5.17 Paclitaxel

?6,5=d,3:@,|=1,36,45,45,45,45,=|,\$5:#,
-4=?6,-4=?4,-1=wb,-3=wf,-1:0,||,
{4^35,4^-35,6}:/_ ,{3^-60,15}:*/OH,
8:/*H^-60,9:*/_ ^60,10://0,
1:\,0,!,//0,!,*/OH,!,/Ph,
60~wf,NH,-60,//0,60,Ph,
7:*,0,-45,//0,60,Ph,11:*!,0,-60,//0,60,
12:*^-15,0,60,//0,-60



6 Example to use mcf2graph

6.1 Molecular definition file

```
%-----
input mcf2graph.mf;                                % input macro
%-----
sw_aux_out:=1;          % aux(information) file output on > Gloval setting
fsize:=(60mm,40mm);    % (font width,font height)      >
var3:="cal_MW"; tag3:="cMW";                               > AUX file table
var4:="cal_FM"; tag4:="cFM";                               >
%%% sw_rep_out:=1;    > Report output
%%% sw_mol_out:=1;    > MOL file output
outputformat:="png"; hppp:=vppp:=0.1;                     > PNG output
outputtemplate:="%j-%3c.png";                             >
%-----
beginfont("NO:1","EN:Ampicillin")                    > begin font(information)
  MC(<45,?4,2:N,2=?5,-1:S,                               > begin MCF (1)
    {3^45,4^-45}:/*H,1://0^15,5:/*COOH^-18,              >
    {6^35,6^-35}:/_ ,                                    >
    4:@,75,NH,! ,//0,! ,/*NH,! ,Ph)                     > end MCF
endfont                                                  > end font
%-----
beginfont("NO:2","EN:Cholesterol")                    > begin font(information)
  MC(<30,?6,{-4,-2}=?6,-4=?5,7=d1,                       > begin MCF (2)
    1:*/OH,{4,12}:*/_ ^60,9:*/H^60,                      >
    10:/*H^180,{11,-1}:/*H^-60,                          >
    -1:@,17,/*_ ,!4,/_ ,!)                               > end MCF
endfont                                                  > end font
%-----
beginfont("NO:3","EN:Limonin")                        > begin font(information)
  MC(<30,?6,{-3,-4}=?6,                                   > begin MCF (3)
    -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,                 >
    {13,15,17,20}:0,{3,12,21}://0,                      >
    {4~wf^60,8~zf^60,18^35,18^-35}:/_ ,                 >
    {1^60,5^180,16^60}:/*H,                             >
    14:\*,| ,?5,{1,4}=d1,3:0)                            > end MCF
endfont                                                  > end font
%-----
beginfont("NO:4","EN:beta-carotene")                  > begin font(information)
  MC(<30,?6,3=d1,{3,5^35,5^-35}:/_ ,                     > begin MCF (4)
    4:\ ,| ,!18,{1,3,5,7,9,11,13,15,17}=dr,              >
    {3,7,12,16}:/_ ,                                     >
    | ,?6,6=d1,{6,2^35,2^-35}:/_ )                      > end MCF
endfont                                                  > end font
%-----
bye
```

6.2 Information auxfile output

(Insert option parameter setting)

```
sw_aux_out=1 : tag1:var1;tag2:var2
sw_aux_out=2 : tag1;tag2 var1;var2
** default : sw_aux_out=0
```

(Command line)

```
>mpost -s ahlength=1 FILENAME (sw_aux_out=1)
>mpost -s ahlength=2 FILENAME (sw_aux_out=2)
```

(Source)

```
beginfont("EN:Ampicillin")(...)
beginfont("EN:Cholesterol")(...)
beginfont("EN:Limonin")(...)
beginfont("EN:beta-Carotene")(...)
```

(Setting)

```
tag1:="F";   var1:="jobname";      * default output
tag2:="C";   var2:="char_num";     * default output
tag3:="cMW"; var3:="calc_weight";
tag4:="cFM"; var4:="calc_formula";
```

(Output)

```
(sw_aux_out=1)
F:mcf_man_soc;C:1;cMW:349.40462;cFM:C16H19N3O4S;EN:Ampicillin
F:mcf_man_soc;C:2;cMW:386.6532;cFM:C27H46O;EN:Cholesterol
F:mcf_exa_soc;C:3;cMW:470.5113;cFM:C26H30O8;EN:Limonin
F:mcf_exa_soc;C:4;cMW:536.8722;cFM:C40H56;EN:beta-Carotene
```

```
(sw_aux_out=2)
F;C;cMW;cFM;EN
mcf_man_soc;1;349.40462;C16H19N3O4S;Ampicillin
mcf_man_soc;2;386.6532;C27H46O;Cholesterol
mcf_exa_soc;3;470.5113;C26H30O8;Limonin
mcf_exa_soc;4;536.8722;C40H56;beta-Carotene

(aux_delimiter:="/");
F:mcf_man_soc/C:1/cMW:349.40462/cFM:C16H19N3O4S/EN:Ampicillin
F:mcf_man_soc/C:2/cMW:386.6532/cFM:C27H46O/EN:Cholesterol
F:mcf_exa_soc/C:3/cMW:470.5113/cFM:C26H30O8/EN:Limonin
F:mcf_exa_soc/C:4/cMW:536.8722/cFM:C40H56/EN:beta-Carotene
```

(Tag)

```
F : filename
C : char number
NO : serial number
EN : english name
JN : japanese name
FM : formula from literature data
MW : molecular weight from literature data
USE : the use
cMW : molecular weight calculated
cMI : monoisotopic mass calculated
cFM : molecular formula calculated
```


6.3 Report output

(Insert option parameter setting)

```
sw_rep_out:=1;  
** default : sw_rep_out=0
```

(Command line)

```
>mpost -s ahlenth=3 FILENAME
```

(Output)

```
-----  
Molecular name = Nicotine  
Warnings = 0 / Expanded command = 40  
Width * Height = 49.57332 * 41.37605  
Shift width * height = 0 * -9.07253  
Bond length = 12.75589 Atom size = 5.38914  
Atom count= 12 Bond count= 13 Ring count= 2 Hide H count= 14  
-----  
< NO. >( x axis , y axis )< atom >< bond >< hide_H >  
A1 ( 0 , 0 ) C 3 1  
A2 ( 0.866 , -0.5 ) N 3  
A3 ( 1.732 , 0 ) C 3 1  
A4 ( 1.732 , 1 ) C 4  
A5 ( 0.866 , 1.5 ) C 3 1  
A6 ( 0 , 1 ) C 3 1  
A7 ( 2.304 , 1.33 ) C 3 1  
A8 ( 3.217 , 0.923 ) N 3  
A9 ( 3.886 , 1.666 ) C 2 2  
A10 ( 3.386 , 2.532 ) C 2 2  
A11 ( 2.408 , 2.325 ) C 2 2  
A12 ( 3.399 , 0.067 ) C 1 3  
-----  
< NO. >< bond (sdt)><angle + ( +- )><length ( pt )>  
B1 1 -> 2 ( 2) 330 ( -30) 1 ( 12.76)  
B2 2 -> 3 ( 1) 30 ( 30) 1 ( 12.76)  
B3 3 -> 4 ( 2) 90 ( 90) 1 ( 12.76)  
B4 4 -> 5 ( 1) 150 ( 150) 1 ( 12.76)  
B5 5 -> 6 ( 2) 210 ( -150) 1 ( 12.76)  
B6 6 -> 1 ( 1) 270 ( -90) 1 ( 12.76)  
B7 4 -> 7 ( 1) 30 ( 30) 0.66 ( 8.42)  
B8 7 -> 8 ( 1) 336 ( -24) 1 ( 12.76)  
B9 8 -> 9 ( 1) 48 ( 48) 1 ( 12.76)  
B10 9 -> 10 ( 1) 120 ( 120) 1 ( 12.76)  
B11 10 -> 11 ( 1) 192 ( -168) 1 ( 12.76)  
B12 11 -> 7 ( 1) 264 ( -96) 1 ( 12.76)  
B13 8 -> 12 ( 1) 282 ( -78) 0.66 ( 8.42)  
-----  
<atom>( atom wt ) [ mi wt ] < cnt > < sum wt > [ sum mi wt ]  
C ( 12.0107 ) [ 12 ] * 10 = 120.10696 [ 120 ]  
H ( 1.00793 ) [ 1.00783 ] * 14 = 14.11108 [ 14.10959 ]  
N ( 14.0067 ) [ 14.00307 ] * 2 = 28.0134 [ 28.00613 ]  
Molecular Weight [Mono Isotopic] = 162.2314 [ 162.11572 ]  
-----  
Weight Calc: 162.2314 / Input: 162.23 / weight gap= 0.00145  
Formula Calc: C10H14N2 / Input:  
=====
```

6.4 MOL file output

(Insert option parameter setting)

```
sw_mol_out:=1;      % MOL(V2000)
sw_mol_out:=2;      % MOL(V3000)
** default : sw_mol_out=0
```

(Command line)

```
>mpost -s ahlength=5 -s FILENAME      % MOL(V2000)
>mpost -s ahlength=6 -s FILENAME      % MOL(V3000)
```

(Output)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
-MCFtoMOL- EN:Caffeine
```

```
14 15  0  0  0  0  0  0  0  0999 V2000
      0      0      0 C  0  0  0  0
  0.86603    -0.5      0 N  0  0  0  0
  1.73206      0      0 C  0  0  0  0
  1.73206      1      0 C  0  0  0  0
  0.86603     1.5      0 C  0  0  0  0
      0      1      0 N  0  0  0  0
  2.6831   -0.30902      0 N  0  0  0  0
  3.27089      0.5      0 C  0  0  0  0
  2.6831    1.30902      0 N  0  0  0  0
  0.86603   -1.36383      0 C  0  0  0  0
 -0.76894    1.44394      0 C  0  0  0  0
 -0.76894   -0.44394      0 O  0  0  0  0
  0.86603    2.36383      0 O  0  0  0  0
  2.95299    2.1396      0 C  0  0  0  0
```

```
 1  2  1  0      0  0
 2  3  1  0      0  0
 3  4  2  0      0  0
 4  5  1  0      0  0
 5  6  1  0      0  0
 6  1  1  0      0  0
 3  7  1  0      0  0
 7  8  2  0      0  0
 8  9  1  0      0  0
 9  4  1  0      0  0
 2 10  1  0      0  0
 6 11  1  0      0  0
 1 12  2  0      0  0
 5 13  2  0      0  0
 9 14  1  0      0  0
```

M END

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

6.5 LuaTeX file example

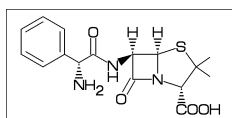
```
%-----
\documentclass{article}
\usepackage{luamplib}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\everymplib{if unknown Ph1:
    input mcf2graph.mf;
    mp_log_name:="temp-info.aux";
    sw_aux_out:=1;
fi}%
%-----
\begin{document}
\noindent%
%-----
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfont("N0:2","EN:Limonin","MW:470.51")
  MC(<30,
    ?6,{-3,-4}=?6,
    -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
    {13,15,17,20}:0,{3,12,21}://0,
    {4~wf^60,8~zf^60,18^35,18^-35}:/_ ,
    {1^60,5^180,16^60}:/*H,
    14:\*,|,?5,{1,4}=d1,3:0
  )
  endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
  fsize:=(80mm,50mm);
  beginfont("N0:3","EN:beta-carotene","MW:536.87")
  MC(<30,
    ?6,3=d1,{3,5^35,5^-35}:/_ ,
    4:\,|,!18,{1,3,5,7,9,11,13,15,17}=dr,
    {3,7,12,16}:/_ ,
    |,?6,6=d1,{6,2^35,2^-35}:/_
  )
  endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfont("N0:4","EN:Gibberellin A3","MW:346.37");
  MC(<18,?5,3=?7,5=?6[12],
    8:@,160'1.3,3:#,13=d1,6=wf,8=wb,
    5:@,40~zf'1,0,60,//0^180,14~zb:#,
    2:/COOH,7://_,13:*/OH,8:/*OH,
    14:*/_,{1^60,4^60}:*/H
  )
endfont;
\end{mplibcode}\\
%-----
\end{document}
%-----
```

6.6 LaTeX file example

```
%-----
\documentclass[a4paper]{article}
\usepackage{graphicx}
\pagestyle{empty}
\makeatletter%
%-----
\def\@F{F}\def\@C{C}\def\@EN{EN}\def\@NO{NO}\def\@MW{MW}\def\@FMc{FMc}%
\def\@fst@param#1:#2;{#1}\def\@sec@param#1:#2;{#2}%
\def\mol@sel#1{%
\if#1empty\relax\else%
\edef\@tag{\expandafter\@fst@param#1;}%
\edef\@var{\expandafter\@sec@param#1;}%
\ifx\@tag\@F\edef\MOLfile{\@var}\fi%
\ifx\@tag\@C\edef\MOLchar{\@var}\fi%
\ifx\@tag\@EN\edef\MOLnameE{\@var}\fi%
\ifx\@tag\@NO\edef\MOLnum{\@var}\fi%
\ifx\@tag\@MW\edef\CALmw{\@var}\fi%
\ifx\@tag\@FMc\edef\CALfm{\@var}\fi%
\fi}%
\def\put@char{%
\begin{picture}(84,42)%
\put(0,38){\bf [MOLnum]\MOLnameE{ }\small\tt/FM:\CALfm/MW:\CALmw}%
\put(10,0){\font\@strufont=\MOLfile\relax%
\hbox{\@strufont\char\MOLchar}}%
\end{picture}%
\def\INFO#1{\@for\@temp:=#1\do{\mol@sel\@temp}\put@char}%
\makeatother
%-----
\begin{document}
\unitlength=1mm%
\INFO{F:mcf_man_soc,C:134,NO:1,cMW:349.40462,cFM:C16H19N3O4S,EN:Ampicillin}%
\INFO{F:mcf_man_soc,C:135,NO:2,cMW:386.6532,cFM:C27H46O,EN:Cholesterol}%
\end{document}
%-----
```

[1]Ampicillin

FM:C16H19N3O4S MW:349.40462



[2]Cholesterol

FM:C27H46O MW:386.6532

