Molecular Coding Format manual

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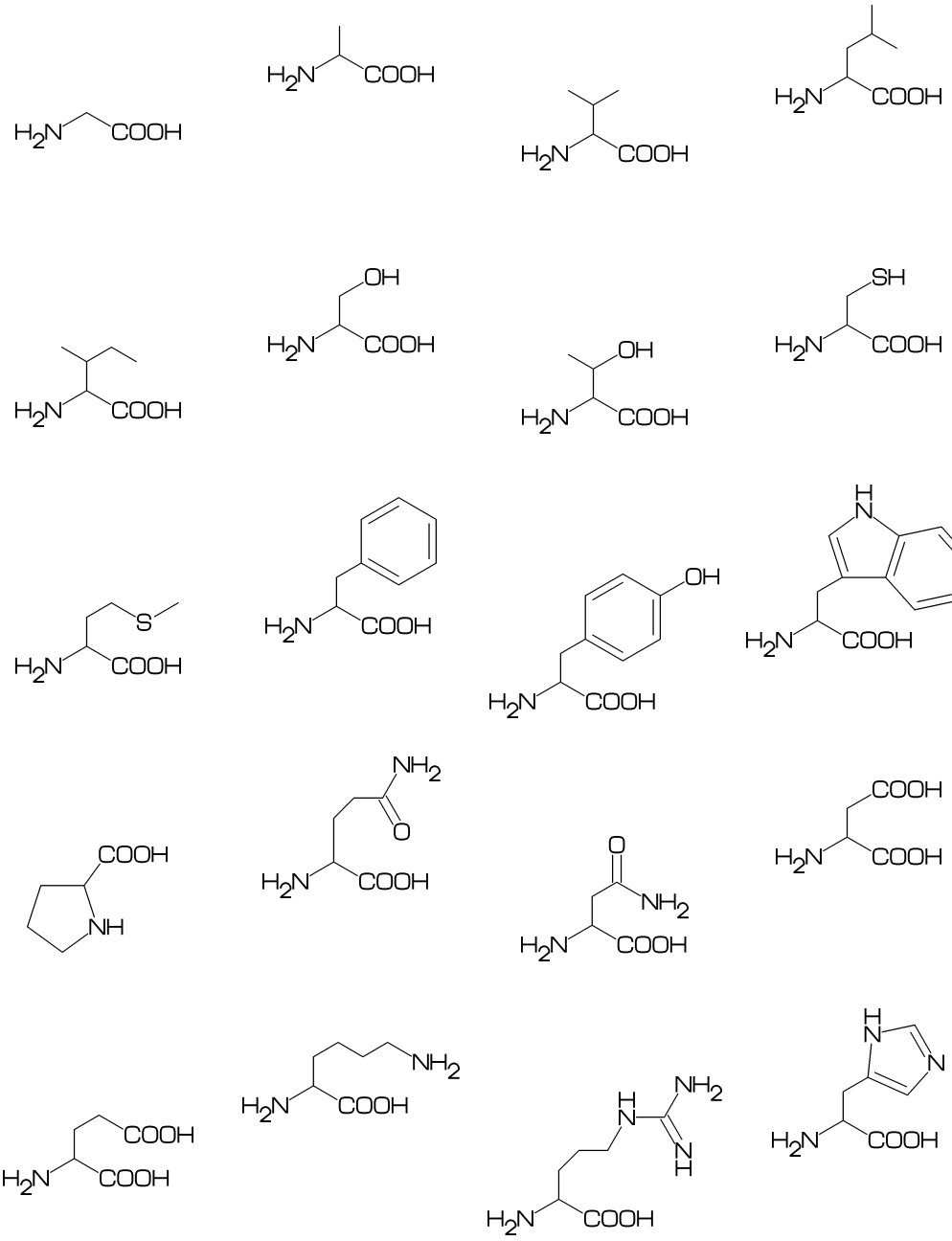
Located at http://www.ctan.org/pkg/mcf2graph



Contents

1 Introduction

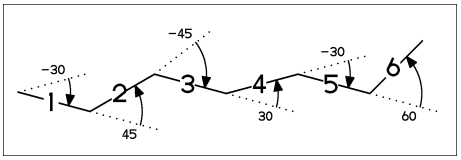
Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This 'Coding' is named from coding(programing) technique like adressing,grouping,macro,etc. There are no Meta language commands in MCF. mcf2graph.m convert MCF file to graphics file pk font,PNG,SVG,EPS or MDL MOL file(V2000).

2 MCF syntax

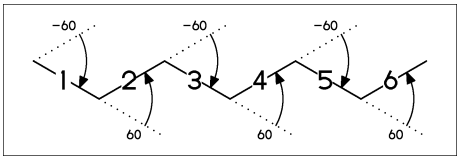
2.1 Make bond

2.1.1 Chain

```
real number plus (+): anticlockwize
real number minus(-): clockwize

<15,-30,45,-45,30,-30,60
```

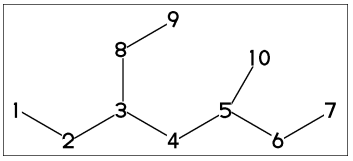



```
! : take value 60 or -60 depend on
      current angle and enviroment
!6 : !,!,!,!,!,!

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

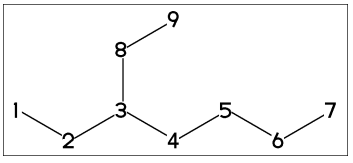


2.1.2 Jump and branch bond

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

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

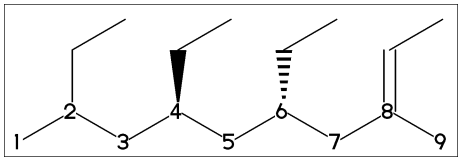



```
3:\ : 3:@,0

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

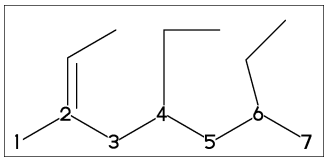


2.1.3 Branch bond

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

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

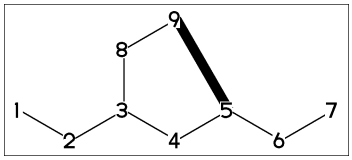



```
2:\~dr  : 2:@,0~dr
4:\‘1.5 : 4:@,0‘1.5
6:\^15  : 6:@,0^15

<-30,!6,
2:\~dr,!,
4:\‘1.5,-90,
6:\^15,-60
```



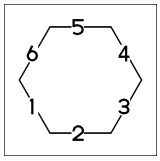
2.1.4 Connect atom

```
&n : Connect to An

<30,!6,3:\,!,&5~bd
```



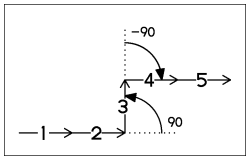
2.1.5 Ring

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



2.1.6 Rotate current angle

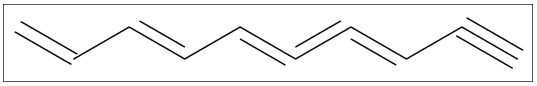
```
<angle : rotate current angle

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



2.2 Change bond type

2.2.1 Double,triple

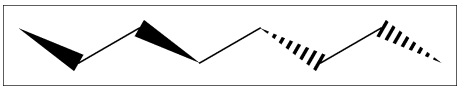
```
a~type : ~~type,a
dm  : double middle
dl  : double left side
dr  : double right side
db  : double left or right side
tm  : triple
!!  : !~db  / !!! : !~tm

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



dm dl dr db db tm

2.2.2 Wedge

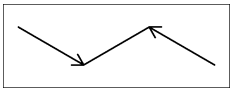
```
wf : wedge forward / wb : wedge backward
zf : wedge dotted
zb : wedge dotted backward

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



wf wb zf zb

2.2.3 Vector

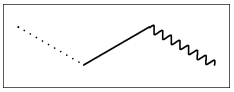
```
vf:vector forward / vb:vector backward

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



vf vb

2.2.4 Dotted,wave

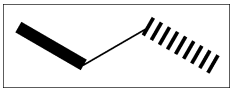
```
Bn=bond type : change bond type at Bn
dt : dotted  /  wv : wave

<30,!3,1=dt,3=wv
```



dt wv

2.2.5 Broad

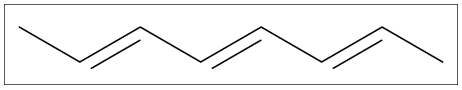
```
bd : broad  /  bz : broad dotted

<30,!3,1=bd,3=bz
```



bd bz

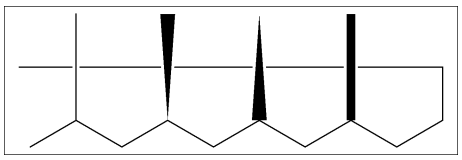
2.2.6 Change multi bond type

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

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



2.2.7 Over line

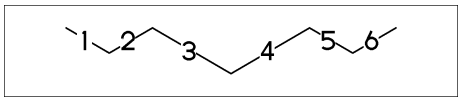
```
si_ : single over line
wf_ : wedge forward over line
wb_ : wedge backward over line
bd_ : broad over line

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



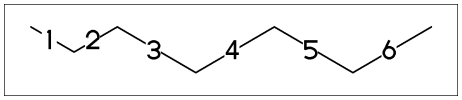
2.3 Change bond length

2.3.1 Chain length

```
(!,!n)‘length : change length of !,!n

<30,!2,!2‘1.2,!2

** !2‘1.2 : ’‘1.2,!2
```

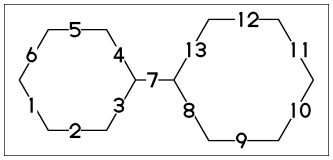



```
‘‘length : change all bond length after

<30,!2,‘‘1.2,!4
```



2.3.2 Ring length

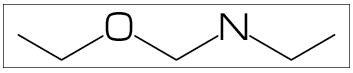
```
?n‘length : change ring length

?6,4:\,?6‘1.2
```



2.4 Change atom

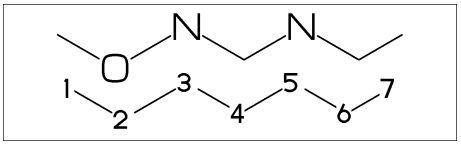
2.4.1 Insert atom

```
Insert hetero atom

<30,!2,O,!2,N,!2
```



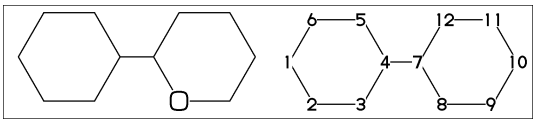
2.4.2 Addressed atom

```
2:O : change A2 C to O
{3,5}:N : change  A3,A5 C to N

<30,!6,2:O,{3,5}:N
```

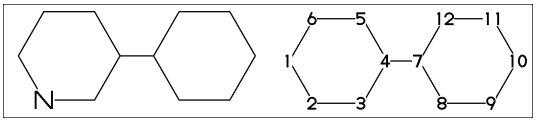


2.4.3 Brock address

```
| : divide brock

?6,4:\,|,?6,2:O
```

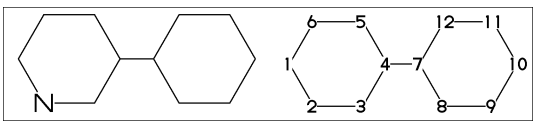



```
|| : reset brock adress

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



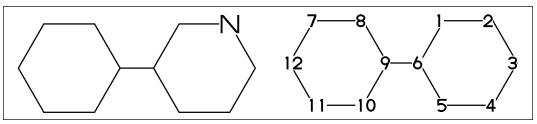
2.4.4 Absolute address

```
#2:N : change A#2 C to N
** #n : (1<=n<=3095)

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



2.4.5 Relative address

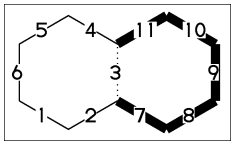
```
-2:N : change A(-2) C to N
** -n : (1<=n<=999)

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



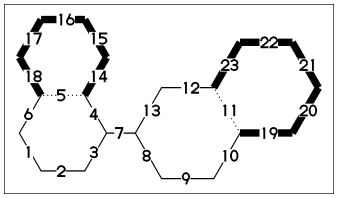
2.5 Fuse ring

2.5.1 Attached 1 bond

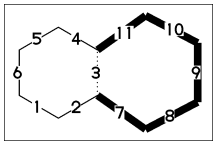
```
?6,3=?6 : fuse ?6 at B3
** Bn(n:-999<=n<=4095): bond number

?6,3=?6
```



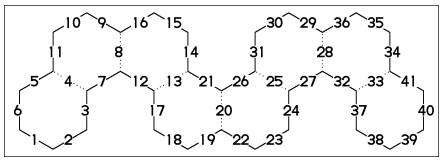

```
** fused ring size depend on
attached bond length

?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]
```

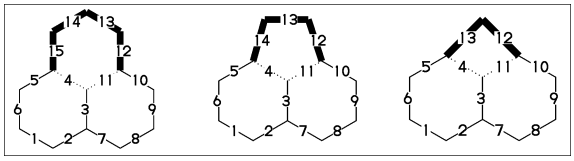



```
?6,{-3,-4,-4,-2,-2,-4,-4}=?6
?6,{4,8,13,20,25,28,33}=?6
```



2.5.2 Attached 2 bond

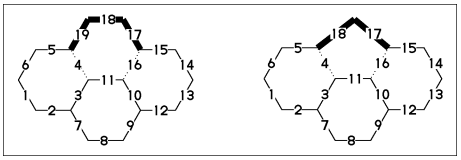
```
(4,11)=?6[4]  : fuse 4/6 ring to B11..B4
(4,11)=?5[3]  : fuse 3/5 ring to B11..B4
(4,11)=?4[2]  : fuse 2/4 ring to B11..B4
** ?m[n] (4<=m<=6,n=m-2)

1:MCd(1,.7)(  0,0)(<30,?6,3=?6,(11,4)=?6[4])
2:MCd(1,.6)(.54,1)(<30,?6,3=?6,(11,4)=?5[3])
3:MCd(1,.6)(  1,0)(<30,?6,3=?6,(11,4)=?4[2])
```



1 2 3

2.5.3 Attached 3 bond

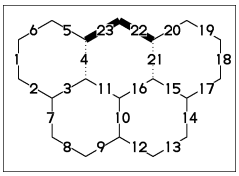
```
(16,4)=?6[3] : fuse 3/6 ring to B16..B4
(16,4)=?5[2] : fuse 2/5 ring to B16..B4
** ?m[n] (5<=m<=6,n=m-3)

1:MCd(1,.55)(0,0)(?6,{3,10}=?6,(16,4)=?6[3])
2:MCd(1,.55)(1,0)(?6,{3,10}=?6,(16,4)=?5[2])
```



1 2

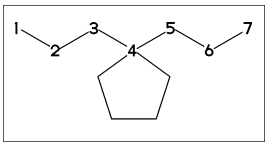
2.5.4 Attached 4 bond

```
(21,4)=?6[2] : fuse 2/6 ring to B21..B4

MCf(<-30,?6,{3,10,15}=?6,(21,4)=?6[2])

** ?m[n] (m=6,n=2)
```



2.5.5 Spiro ring

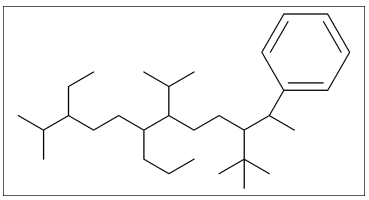
```
4:@,?5 : add ?5 at A4

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

An:@ : jump to An
```



2.6 Substituent

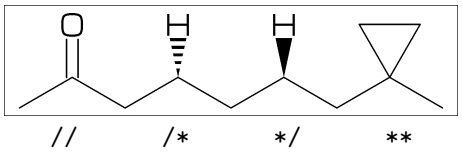
2.6.1 Insert substituent

```
/  : 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
```



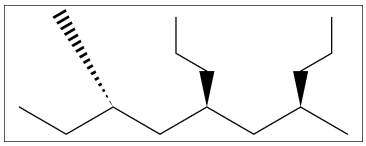
2.6.2 Insert modified substituent

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

<30,!,//O,!,/*H,!,*/H,!,/?3,!,**?3,!
```



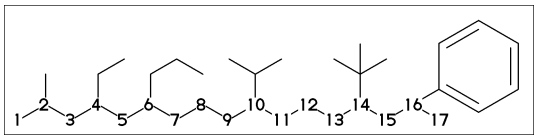
// /* */ **

```
~ : change type
^ : change angle
‘ : change length
> : change enviroment

<30,‘‘1,!,/_~zf‘2^30,
 !2,*/!2>lr,!2,*/!2>rl,!)
```



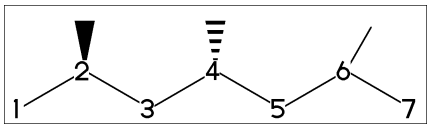
2.6.3 Add substituent

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

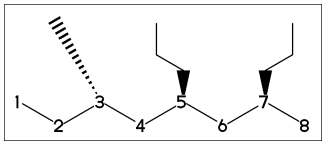


2.6.4 Add modified substituent

```
~,^,‘ : change type,angle,length

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



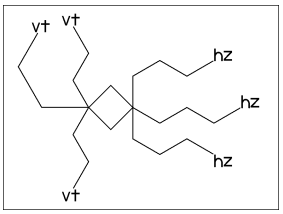
```
^,‘,> : change angle,length,environment

<30,!7‘1,
3:/*_‘2^30,5:*/!2>lr,7:*/!2>rl
```



2.7 Chain environment

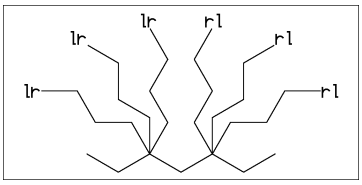
2.7.1 Horizontal,vertical

```
>hz : horizontal enviroment (default)
>vt : vertical enviroment

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



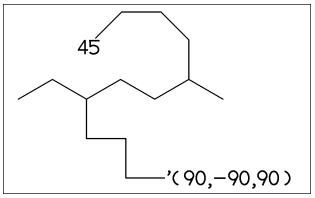
2.7.2 Left-right,right-left

```
>lr : left-right enviroment
>rl : right-left enviroment

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



2.7.3 Fixed angle,multi angle

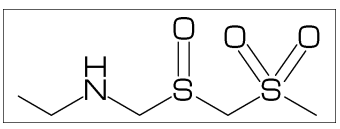
```
>45 : fixed angle enviroment
>'(-90,90,-90) : multi angle enviroment

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



2.8 Miscellaneous

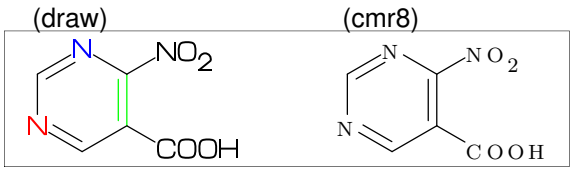
2.8.1 Change atom and Substituent

```
NH,SO,SOO :
 inset hetero atom and substituent
 simultaneously

<30,!2,NH,!,SO,!,SOO,!
```



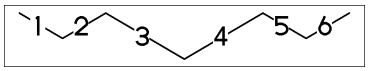
2.8.2 Change color, atom font

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

defaultfont:="uhvr8r";
defaultsize:=8bp;
MCa(0,0.5)(<30,Ph,{1,5}:N,3:/COOH,4:/NO2,
            1:red,5:blue,3=green)
ext(label.urt("(draw)",p0+(0,ht));)
atomfont:="cmr8";   % default:"draw"
atomfontsize:=8bp;  % default:8bp
MCa(1,0.5)(<30,Ph,{1,5}:N,3:/COOH,4:/NO2)
ext(label.urt("(cmr8)",p0+(0,ht));)
```



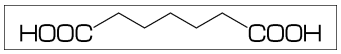
2.8.3 Make block

```
|< : start brock
>| : end brock

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

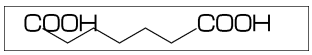


2.8.4 Chain start multiple characters

```
if chain start multi charactor string,
use !0 instead of !

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

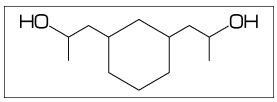



```
MCf(<30,COOH,!4,COOH)
```

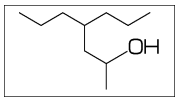


2.8.5 User definition

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




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

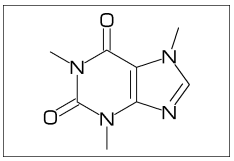


3 Option parameter

3.1 Size parameter

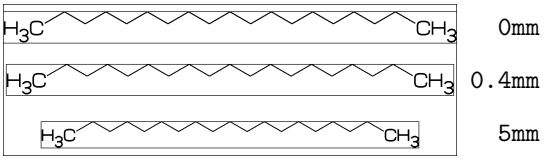
3.1.1 Font size

```
beginfont("EN:Caffeine")
  font_wd:=30mm;  %<==font width
  font_ht:=20mm;  %<==font height
  MCf(<30,?6,-4=?5,{3,8}=dl,{2,6,7,9}:N,
     {2,6,9}:/_,{1,5}://O)  endfont
```



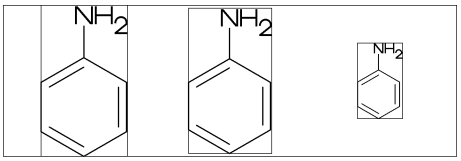
3.1.2 Margin left and right

default: margin_left_right=0.4mm



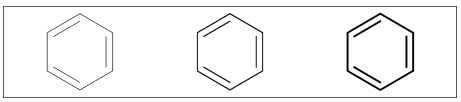
3.1.3 Margin top and bottom

default: margin_top_bottom=0.4mm



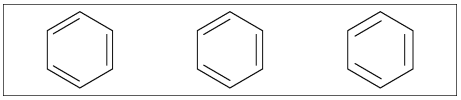
3.1.4 Offset thickness of bond

default: offset_thickness=0.2pt



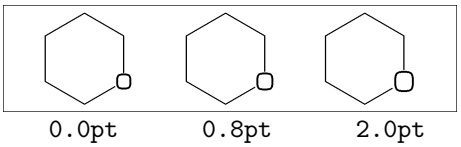
3.1.5 Offset of doublebond gap

default: offset_bond_gap=0.3pt



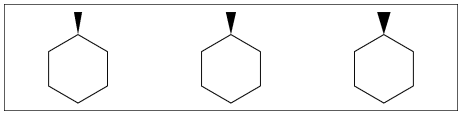
3.1.6 Offset of atom width

default: offset_atom=0.8pt



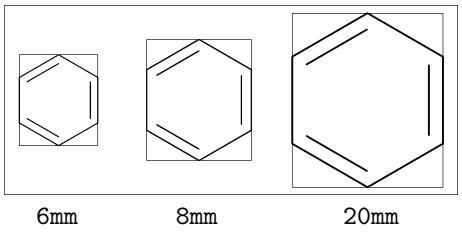
3.1.7 Offset of wedge width

default: offset_wedge=0.4pt



3.1.8 Max bond length

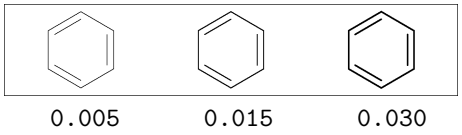
default: max_bond_length=10mm



3.2 Ratio parameter

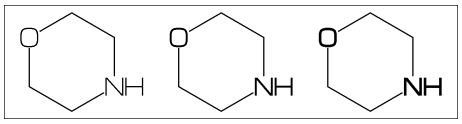
3.2.1 Thickness/bond length

default: ratio_thickness_bond=0.015



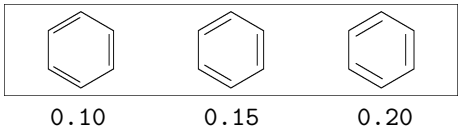
3.2.2 Char/bond thickness

default: ratio_char_bond=1.5



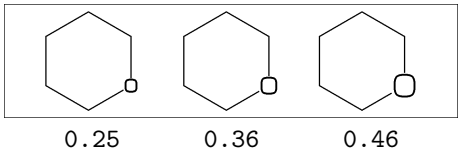
3.2.3 Bondgap/bond length

default: ratio_bondgap_bond= 0.15



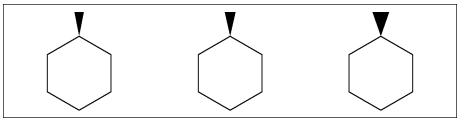
3.2.4 Atom/bond length

default: ratio_atom_bond= 0.36



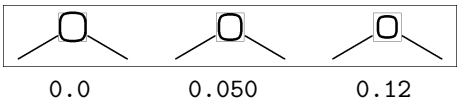
3.2.5 Wedge/bond length

default: ratio_wedge_bond=0.12



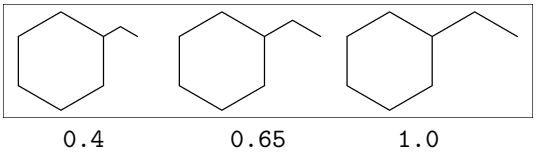
3.2.6 Font atom gap/atom length

default: ratio_atomgap_atom= 0.050



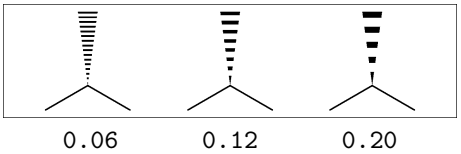
3.2.7 Chain/ring length

default: ratio_chain_ring= 0.66



3.2.8 Zebra gap/bond length

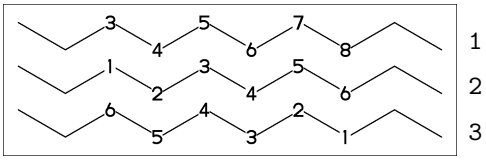
default: ratio_zebragap_bond=0.12



3.3 Drawing mode

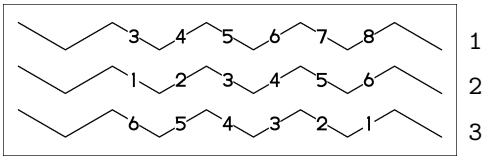
3.3.1 Numbering atom

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



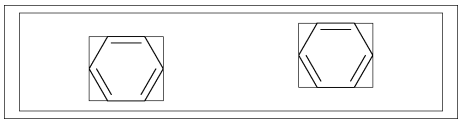
3.3.2 Numbering bond

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

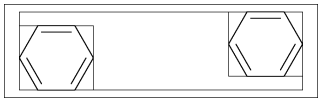


3.3.3 Clipping mode

sw_clip:=0;
MCd(1,0.7)(0.2,0.3)(Ph)
MCd(1,0.7)(0.8,0.7)(Ph)
** default: sw_clip=0

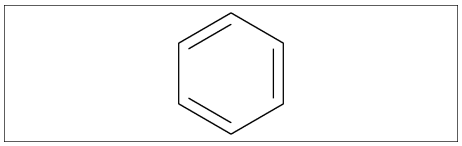


sw_clip:=1;
MCd(1,0.7)(0.2,0.3)(Ph)
MCd(1,0.7)(0.8,0.7)(Ph)

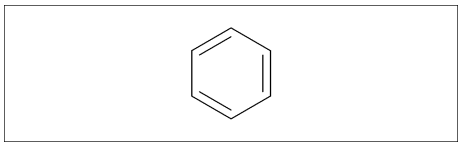


3.3.4 Solid mode

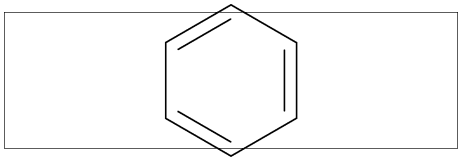
(fit to font size)
sw_solid=0 ** default



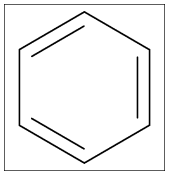
(solid ratio bond/font width)
sw_solid:=1;
ratio_bond_width=0.1
font_width=60mm
(bond_len=60mm*0.1=6mm)
** ignore bond_len



(solid bond length)
sw_solid:=2;
bond_len=10mm
** ignore ratio_bond_width

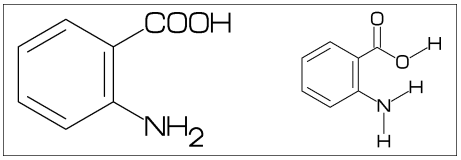


(solid bond length and clip)
sw_solid:=2;
sw_clip:=1;
bond_len=10mm



3.3.5 Expand mode

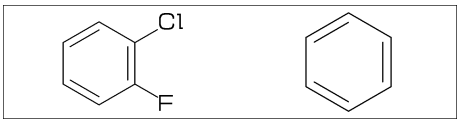
default: sw_expand=0



0 :default 1

3.3.6 Substituent off mode

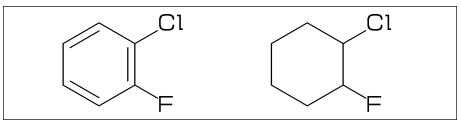
default: sw_subst_off=0



0 :default 1

3.3.7 Single bond mode

default: sw_bond_single=0

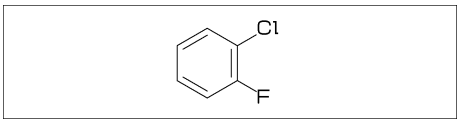


0 :default 1

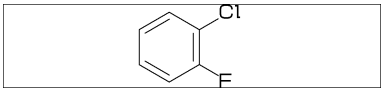
3.4 Frame

3.4.1 Font frame

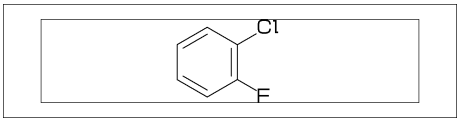
```
(Draw font frame)
margin_left_right:=5mm;
margin_top_bottom:=2mm;
sw_font_frame:=1;
MCf(<30,Ph,4:/Cl,3:/F)
```




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

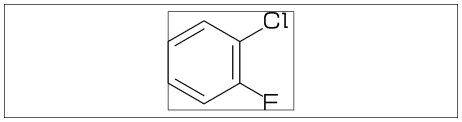



```
(Draw both frame)
sw_font_frame=3
```



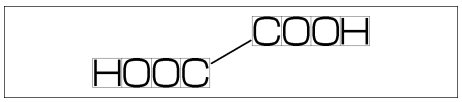
3.4.2 Molecular frame

```
sw_mol_frame:=1;
MCd(1,.5)(1,0.5)(<30,Ph,4:/Cl,3:/F)
** default: sw_mol_frame=0
```



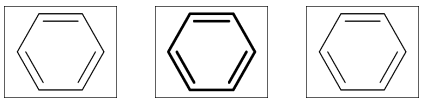
3.4.3 Atom frame

```
sw_atom_frame:=1;
MCf(<30,COOH,!0,COOH)
** default: sw_atom_frame=0
```



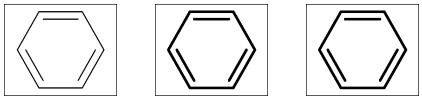
3.5 Local parameter setting

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



3.6 Global parameter setting

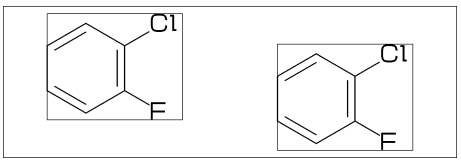
```
beginfont()
  MCf(Ph)
endfont
%--------------------------
ratio_thickness_bond:=0.05;
%--------------------------
beginfont()
  MCf(Ph)
endfont
beginfont()
  MCf(Ph)
endfont
```



4 Function

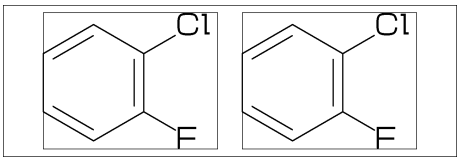
4.1 Function MCd()

```
(Draw molecule)

MCd(a,b)(c,d)(...)
  a: ratio molecular width/font width
  b: ratio molecular hight/font hight
  c: x axis position
  d: y axis position

beginfont()
  MCd(1,0.8)(0.2,0.9)(<30,Ph,3:/F,4:/Cl)
  MCd(1,0.8)(0.8,0.1)(<30,Ph,3:/F,4:/Cl)
endfont
```



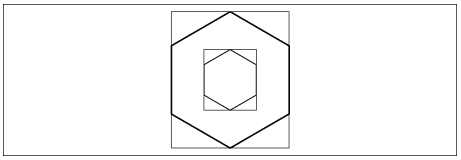
4.2 Function MCa()

```
(Draw molecule at (x,y))

MCa(a,b)(...) : MCd(1,1)(a,b)(...)
  a: x axis position
  b: y axis position

beginfont()
  MCa(0.2,0.5)(<30,Ph,3:/F,4:/Cl)
  MCa(0.8,0.5)(<30,Ph,3:/F,4:/Cl)
endfont
```



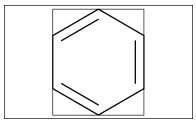
4.3 Function MCc()

```
(Draw molecule to center of font)

MCc(a,b)(...) : MCd(a,b)(0.5,0.5)(...)
  a: ratio molecular width/font width
  b: ratio molecular hight/font hight

beginfont()
  MCc(1,1)(<30,?6)
  MCc(0.5,0.5)(<30,?6)
endfont
```

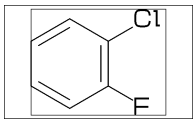


4.4 Function MCf()

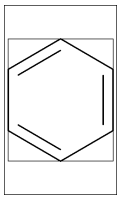
```
(Draw molecule fit to font size)

MCf(...) : MCd(1,1)(0.5,0.5)(...)

(Draw molecule fit to font height)

beginfont()
  font_wd:=25mm;
  font_ht:=15mm;
  MCf(<30,Ph)
endfont
```



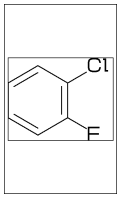
```
beginfont()
  font_wd:=25mm;
  font_ht:=15mm;
  MCf(<90,Ph,3:/F,4:/Cl)
endfont
```




```
(Draw molecule fit to font width)

beginfont()
  font_wd:=15mm;
  font_ht:=25mm;
  MCf(<30,Ph)
endfont
```

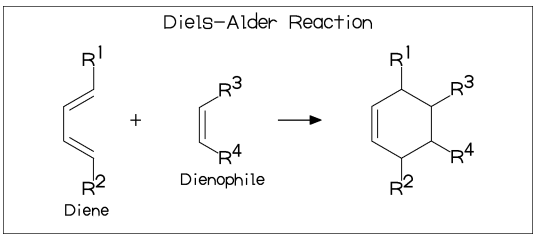


```
beginfont()
  font_wd:=15mm;
  font_ht:=25mm;
  MCf(<30,Ph,3:/F,4:/Cl)
endfont
```



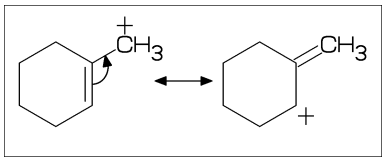
4.5 Function EXT()

```
(Add extra graphic to font)

 w:  font width
 h:  font height
 wd: font width-margin_left_right*2
 ht: font height-margin_top_bottom*2
 aw: atom font size
 em: label font size
 p0: x=margin_left_right
     y=margin_top_bottom
 n:  molecular number
 p[m]: molecular origin position

%---------------------------------------
beginfont()
 font_wd:=70mm;
 font_ht:=30mm;
 ratio_bond_width:=0.065;
 sw_solid:=1;
 %---------------------------------------
 MCd(1,1)(0.1,0.5)
  (<-210,60‘1,60‘1,60‘1,{1,3}=dl,
   1:/R1,4:/R2^-60)
 ext(
   defaultscale:=0.6;
   label.bot("Diene",p0+(0.5wd,0));
 )
 %---------------------------------------
 MCd(1,1)(0.4,0.5)
  (<-30,-60‘1,1=dl,1:/R3,2:/R4^60)
 ext(
   defaultscale:=0.6;
   label.bot("Dienophile",p0+(0.5wd,0));
 )
 %---------------------------------------
 MCd(1,1)(0.9,0.5)
  (<30,?6,6=dl,2:/R2,3:/R4,4:/R3,5:/R1)
 %---------------------------------------
 EXT(
   drawarrow (0.52w,0.5h)..(0.6w,0.5h);
   defaultscale:=0.7;
   label("+",(0.25w,0.5h));
   label.bot("Diels-Alder Reaction",
            (0.5w,h));
 )
 %---------------------------------------
endfont
```



4.6 Function ext()

```
(Add extra graphic to molecule)

 wd:      molecular width
 ht:      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]dir: branch direction of A[m]
 Bn:      bond number
 B[m]s:   bond start position
 B[m]e:   bond end position
 B[m]:    bond position(0.5[B[m]s,B[m]e])
 B[m]dir: bond direction

%---------------------------------------
beginfont()
  font_wd:=50mm;
  font_ht:=20mm;
 %---------------------------------------
  MCd(1,0.7)(0,0.5)(<30,?6,3=dl,4:/CH3)
  ext(
    label.top("+",A7);
    drawarrow B3{dir(B3dir-90)}..
              {dir(B7dir+90)}0.4[B7s,B7e];
    )
 %---------------------------------------
  MCd(1,0.7)(1,0.5)(<30,?6,4://CH3)
  ext(
    labeloffset:=0bp;
    label.lrt("+",A3);
  )
 %---------------------------------------
  EXT(
    drawdblarrow (0.4w,0.5h)..(0.55w,0.5h);
  )
 %---------------------------------------
endfont
```

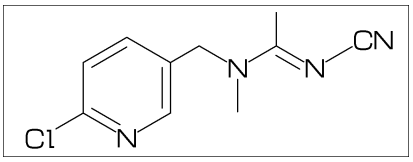



```
label:
 defaultfont: label font
 defaultfont="draw": draw font
 **default defaultfont="draw"

drawarrow & drawdblarrow:
 sw_arrow=0: emulation mode
 sw_arrow=1: plain.mp mode
 **default sw_arrow=0
```

5 MCF example

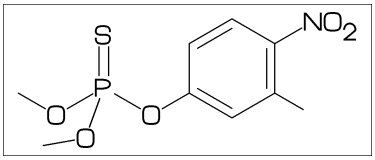
5.1 Acetamiprid

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



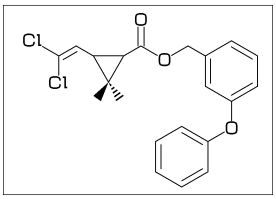
5.2 Fenitrothion

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



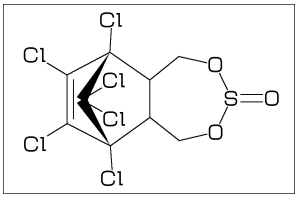
5.3 Permethrin

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



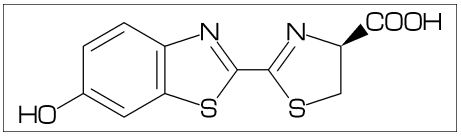
5.4 Endosulfan

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



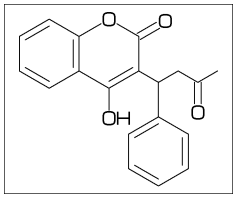
5.5 Luciferin

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



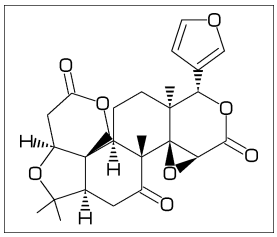
5.6 Warfarin

```
<30,Ph,3=?6,8=dl,
10:O,7:/OH,9://O,
8:\,/Ph‘1,60,!,//O,!
```



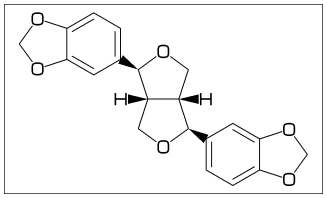
5.7 Limonin

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



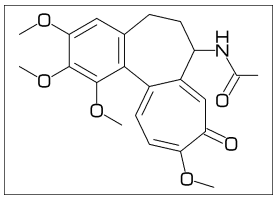
5.8 Sesamine

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



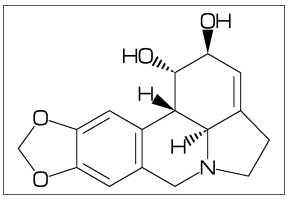
5.9 Colchicine

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



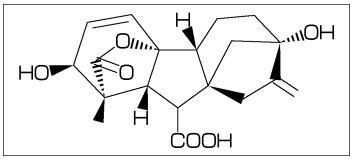
5.10 Lycorine

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



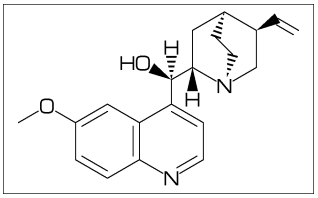
5.11 Gibberellin

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



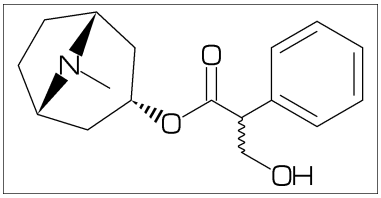
5.12 Quinine

```
<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
```



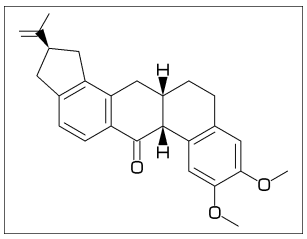
5.13 Atoropin

```
<-30,O,!,//O,!,!,Ph,
#1:@,-120~zb,
|,?7,6:*\^190‘1.02,N,/_,&3~wb,
#3:\~wv,!,OH
```



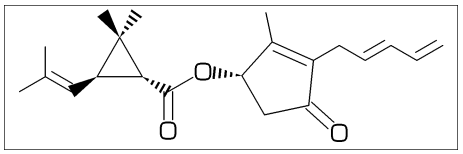
5.14 Rotenone

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



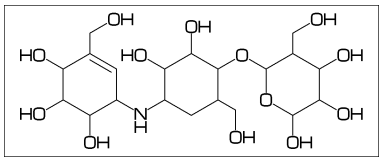
5.15 Pyrethrin I

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



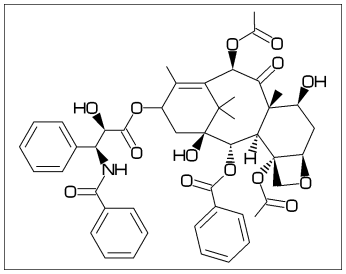
5.16 Validamycin

```
<30,?6,{5,6}:/OH,3:/!OH>rl,
#4:\,O,-60,|,?6,2:O,{3,4,5}:/OH,6:/!OH,
#1:\,NH,!,|,?6,2=dl,{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:O,||,
{4^35,4^-35,6}:/_,{3^-60,15}:*/OH,
8:/*H^-60,9:*/_^60,10://O,
1:\,O,!,//O,!,*/OH,!,/Ph,
60~wf,NH,-60,//O,60,Ph,
7:\*,O,-45,//O,60,Ph,11:*\,O,-60,//O,60,
12:\*^-15,O,60,//O,-60
```



6 Example to use mcf2graph

6.1 Molecular definition file

```
%-------------------------------------------------------------------------
input mcf2graph.mf;                                  % input macro
%-------------------------------------------------------------------------
sw_auxout:=1;          % aux(information) file output on > Gloval setting
font_wd:=60mm;         % font width                      >
font_ht:=40mm;         % font height                     >
var3:="cal_MW"; tag3:="cMW";                             > AUX file table
var4:="cal_FM"; tag4:="cFM";                             >
%%%% sw_report:=1;                                      > Report output
%%%% sw_MOLout:=1;                                      > MOL file output
outputformat:="png"; hppp:=vppp:=0.1;                    > PNG output
outputtemplate:="%j-%3c.png";                            >
%-------------------------------------------------------------------------
beginfont("NO:1","EN:Ampicillin")                  > begin font(information)
  MCf(<45,?4,2:N,2=?5,-1:S,                              > begin MCF (1)
     {3^45,4^-45}:/*H,1://O^15,5:/*COOH^-18,             >
     {6^35,6^-35}:/_,                                    >
     4:@,75,NH,!,//O,!,/*NH,!,Ph)                        > end MCF
endfont                                                  > end font
%-------------------------------------------------------------------------
beginfont("NO:2","EN:Cholesterol")                 > begin font(information)
  MCf(<30,?6,{-4,-2}=?6,-4=?5,7=dl,                      > 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)
  MCf(<30,?6,{-3,-4}=?6,                                 > begin MCF (3)
      -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,                >
      {13,15,17,20}:O,{3,12,21}://O,                     >
      {4~wf^60,8~zf^60,18^35,18^-35}:/_,                 >
      {1^60,5^180,16^60}:/*H,                            >
      14:\*,|,?5,{1,4}=dl,3:O)                           > end MCF
endfont                                                  > end font
%-------------------------------------------------------------------------
beginfont("NO:4","EN:beta-carotene)                > begin font(information)
  MCf(<30,?6,3=dl,{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=dl,{6,2^35,2^-35}:/_)                       > end MCF
endfont                                                  > end font
%-------------------------------------------------------------------------
beginfont("NO:5","EN:Gibberellin A3");             > begin font(information)
  MCf(<18,?5,3=?7,5=?6[12],                              > begin MCF (5)
     8:@,160‘1.3,&3,13=dl,6=wf,8=wb,                     >
     5:@,40~zf‘1,O,60,//O^180,&14~zb,                    >
     2:/COOH,7://_,13:*/OH,8:/*OH,                       >
     14:*/_,{1^60,4^60}:*/H)                             > end MCF
endfont;                                                 > end font
%-------------------------------------------------------------------------
bye
```

6.2 Information auxfile output

(Insert option parameter setting)

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

(Command line)

```
  >mpost -s ahangle=0 FILENAME (molecular definition file)
```

(Sourse)

```
beginfont("EN:Ampicillin")(....)
beginfont("EN:Cholesterol")(....)
beginfont("EN:Limonin")(....)
beginfont("EN:beta-Carotene")(....)
beginfont("EN:Gibberellin A3")(....)
```

(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_auxfix=0)
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
F:mcf_exa_soc;C:5;cMW:346.3742;cFM:C19H22O6;EN:Gibberellin A3

(sw_auxfix=1)
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
mcf_exa_soc;5;346.3742;C19H22O6;Gibberellin A3

(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
F:mcf_exa_soc/C:5/cMW:346.3742/cFM:C19H22O6/EN:Gibberellin A3
```

(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_report:=1;
  ** default : sw_report=0
```

(Command line)

```
  >mpost -s ahangle=0 -s ahlength=2 FILENAME (molecular definition file)
```

(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
 Fomula  Calc: C10H14N2 / Input:
===================================================================
```

6.4 Molfile output

(Insert option parameter setting)

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

(Command line)

```
  >mpost -s ahangle=3  FILENAME (molecular definition file)
```

(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

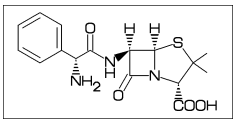
```
%-----------------------------------------------------------------------
\documentclass{article}
\usepackage{luamplib}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\everymplib{if unknown Ph1:
              input mcf2graph.mf;
              mp_log_name:="temp-info.aux";
              sw_auxout:=1;
            fi}%
%-----------------------------------------------------------------------
\begin{document}
\noindent%
%-----------------------------------------------------------------------
\begin{mplibcode}
  font_wd:=50mm; font_ht:=50mm;
  beginfont("NO:2","EN:Limonin","MW:470.51")
  MCf(<30,
    ?6,{-3,-4}=?6,
      -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
      {13,15,17,20}:O,{3,12,21}://O,
      {4~wf^60,8~zf^60,18^35,18^-35}:/_,
      {1^60,5^180,16^60}:/*H,
      14:\*,|,?5,{1,4}=dl,3:O
  )
  endfont
\end{mplibcode}\\
%-----------------------------------------------------------------------
\begin{mplibcode}
  font_wd:=80mm; font_ht:=50mm;
  beginfont("NO:3","EN:beta-carotene","MW:536.87")
    MCf(<30,
      ?6,3=dl,{3,5^35,5^-35}:/_,
      4:\,|,!18,{1,3,5,7,9,11,13,15,17}=dr,
      {3,7,12,16}:/_,
      |,?6,6=dl,{6,2^35,2^-35}:/_
    )
  endfont
\end{mplibcode}\\
%-----------------------------------------------------------------------
\begin{mplibcode}
  font_wd:=50mm; font_ht:=50mm;
  beginfont("NO:4","EN:Gibberellin A3","MW:346.37");
  MCf(<18,?5,3=?7,5=?6[12],
     8:@,160‘1.3,&3,13=dl,6=wf,8=wb,
     5:@,40~zf‘1,O,60,//O^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#1\empty\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