

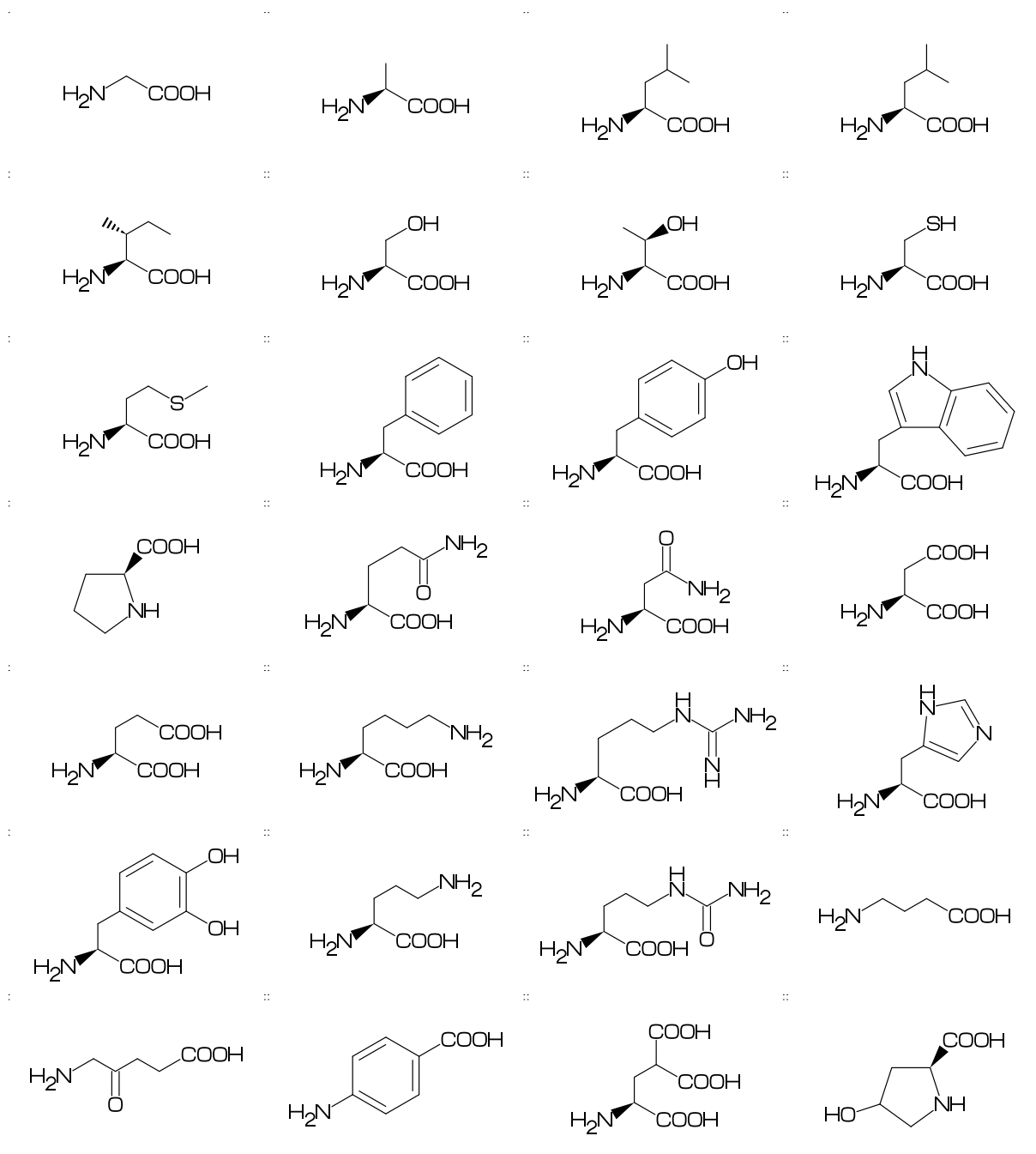
# Molecular Coding Format manual

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

Suggestion or request mail to: [mcf2graph@gmail.com](mailto: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 programming technique such as operator, array, scope, macro, addressing, etc. mcf2graph convert from MCF to pk font, PNG, SVG, EPS, MOL file. It is also able to calculate molecular weight, exact mass, molecular formula.

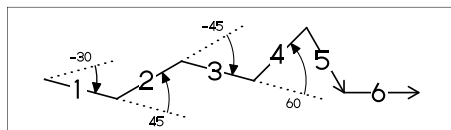
## 2 MCF syntax

### 2.1 Make bond

#### 2.1.1 Chain

real number plus (+): counterclockwise  
real number minus(-): clockwise  
\$n (0<=n<360): absolute angle

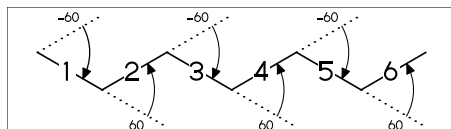
<10,-30,45,-45,60,\$300,\$0



#### 2.1.2 Chain use !,!n

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

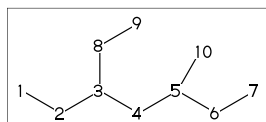
<-30,!6



#### 2.1.3 Jump to atom

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

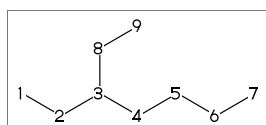
<-30,!6,@3,0,!,@5,-30



#### 2.1.4 Branch bond

\ : 0

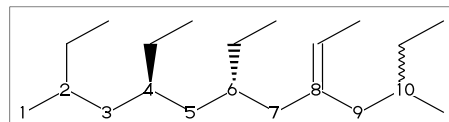
<-30,!6,@3,\,!



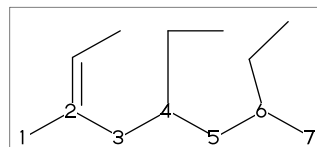
#### 2.1.5 Branch modified bond

\ : 0  
\*\ : 0~wf  
\\* : 0~zf  
\ \ : 0~dm  
\*\\* : 0~wv

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



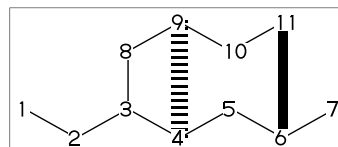
<30,!6,  
\~dr,! : 0~dr,!  
\'1.5,-90 : 0'1.5,-90  
\^15,-60 : 0^15,-60



#### 2.1.6 Connect atom

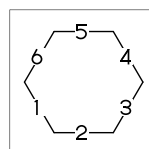
&n : Connect to An

<-30,!6,@3,\,!3,&6~bd,@9,&4~bz



#### 2.1.7 Ring

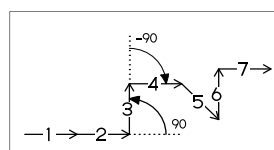
?n : n membered ring(3<=n<=20)  
?6 : <-120,60,60,60,60,60,&1  
?6



#### 2.1.8 Rotate current angle

<angle : rotate current angle

0,0,<90,0,<-90,0,<\$315,0,<\$90,0,<\$0,0

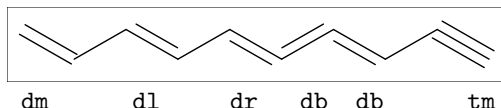


## 2.2 Change bond type

### 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

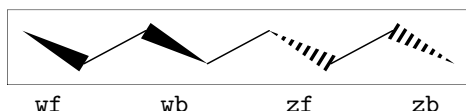
```
<-30,!~dm,!~dl,!~dr,!~db,!~db,!~tm  
<-30,!~dm,!~dl,!~dr,!! ,!! ,!! ,!!!
```



### 2.2.2 Wedge

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

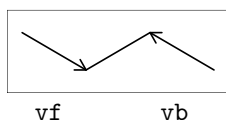
```
<-30,!~wf,!~wb,!~zf,!~zb
```



### 2.2.3 Vector

vf:vector forward / vb:vector backward

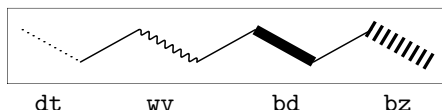
```
<-30,!~vf,!~vb
```



### 2.2.4 Dotted, wave

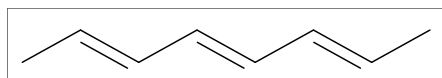
Bn=bond type : change bond type at Bn  
dt : dotted / wv : wave  
bd : broad / bz : broad dotted

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



### 2.2.5 Change multiple bond type

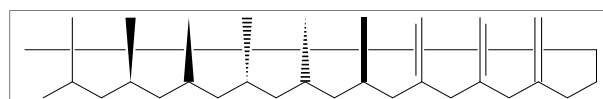
```
{2,4,6}=dr : 2=dr,4=dr,6=dr  
<30,!7,{2,4,6}=dr
```



### 2.2.6 Over line

si\_ : single over line  
wf\_ : wedge forward over line  
wb\_ : wedge backward over line  
zf\_ : hashed wedge forward over line  
zb\_ : hashed wedge backward over line  
bd\_ : broad over line  
dl\_ : duple left over line  
dr\_ : duple right over line  
dm\_ : duple over line

```
<30,!8,!60,90'18,  
{2~si_,4~wf_,6~wb_,8~zf_,10~zb_,  
12~bd_,14~dl_,16~dr_,18~dm_}:/_ '2
```

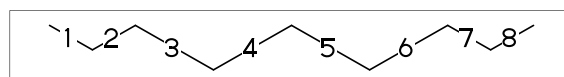


## 2.3 Change bond length

### 2.3.1 Chain length

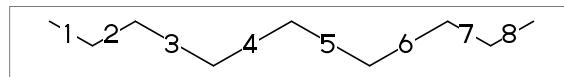
(!,!n)'length : change length of !,!n

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



#n : bond length=n  
## : reset bond length

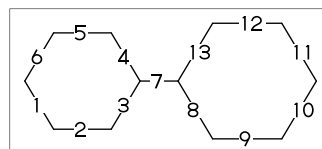
```
<-30,!2,#1.2,!4,##,!2
```



### 2.3.2 Ring length

?n'length : change ring length

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

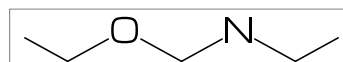


## 2.4 Change atom

### 2.4.1 Insert atom

Insert hetero atom

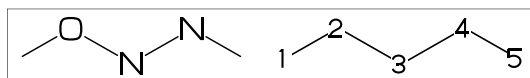
```
<-30,!2,0,!2,N,!2
```



## 2.4.2 Addressed atom

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

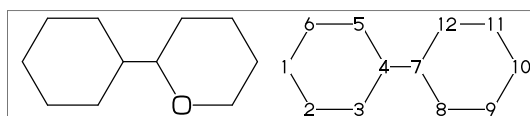
<30,!4,2:0,{3,4}:N



## 2.4.3 Brock address

| : divide brock

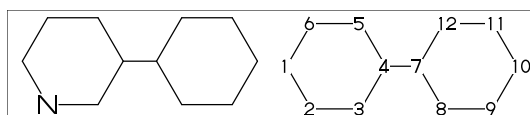
?6,@4,\,|,?6,2:0



## 2.4.4 Reset brock address

|| : reset brock address

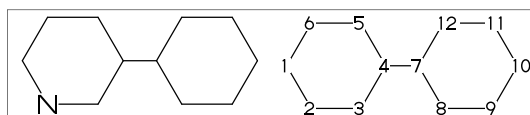
?6,@4,\,|,?6,||,2:N



## 2.4.5 Absolute address

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

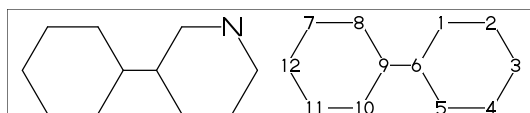
?6,@4,\,|,?6,\$2:N



## 2.4.6 Relative address

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

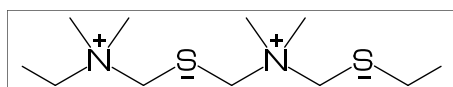
?6,@4,\,?6,-2:N



## 2.4.7 Charged atom

p\_ : positive / n\_ : negative

<-30,!2,N,??,p\_,!2,S,n\_~180,  
!6,7:N,7:??,9:S,7:n\_,9:n\_~180



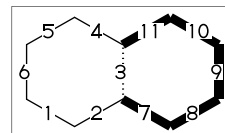
## 2.5 Fuse ring

### 2.5.1 Attached 1 bond

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

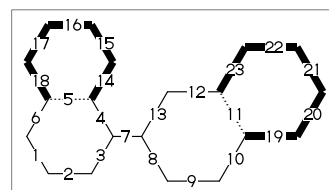
\*\* Bn(n:-999<=n<=4095): bond number

?6,3=?6



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

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

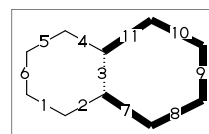


?6,3=?6[13] : fuse ?6[13] at B3

?6[13]: 6 membered ring scaled 13/10

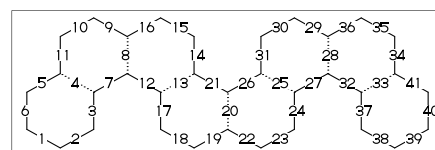
\*\* ?m[n] (5<=m<=8,11<=n<=15)

?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

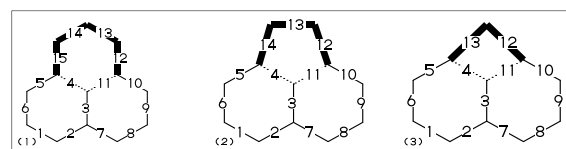
(4,11)=?4[2] : fuse 2/4 ring to B11..B4

\*\* ?m[n] (4<=m<=6,n=m-2)

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

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

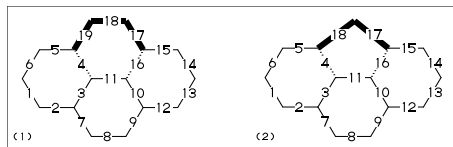
3:<30,?6,3=?6,(11,4)=?4[2]



### 2.5.3 Attached 2 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]

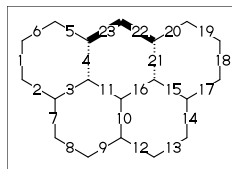


### 2.5.4 Attached 4 bond

(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)

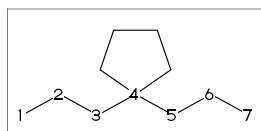


### 2.5.5 Spiro ring

@4,?5 : add ?5 at A4

<30,!6,@4,?5

@An : jump to An



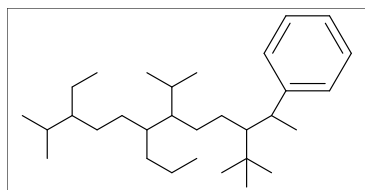
## 2.6 Group

### 2.6.1 Insert group

/ : single

<-30,!/\_,!/,!/,!3,!2,!/,?!  
!3,/??!,!/,/Ph^-30,!

\*\* /\_ : methyl      /! : ethyl  
/!2 : propyl      /?! : isopropyl  
/??? : tert-butyl    /Ph : phenyl



### 2.6.2 Insert modified group

// : double (double middle)

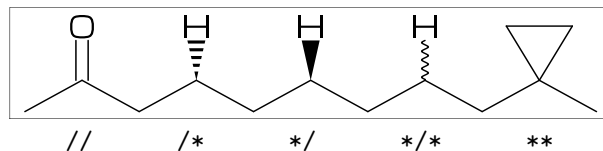
\*/ : wedge forward

/\* : hashed wedge forward

\*/ : wave

\*\* : direct

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



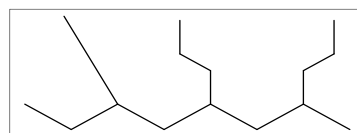
~ : change type

^ : change angle

` : change length

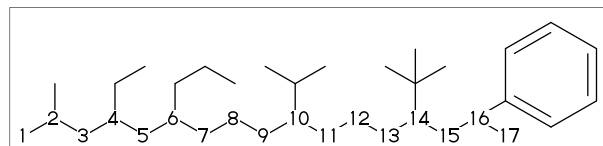
> : change environment

<-30,`1,!,  
/\_`2^30,!2,/!2>lr,!2,/!2>r1,!)



### 2.6.3 Add group

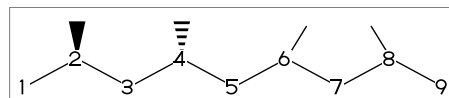
<30,!17,2:/\_,4:!/!,6:/!2,  
10:/?!,14:/??!,16:/Ph^-60



### 2.6.4 Add modified group

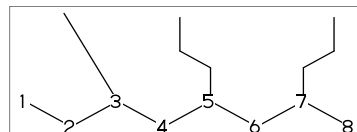
~,^,` : change type,angle,length

<30,!6,{2~wf,4~zf,6^-30,8^\$120}:/\_



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

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

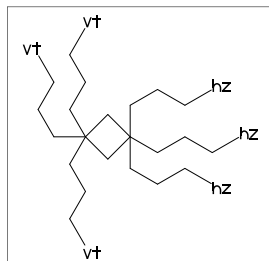


## 2.7 Chain environment

### 2.7.1 Horizontal,vertical

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

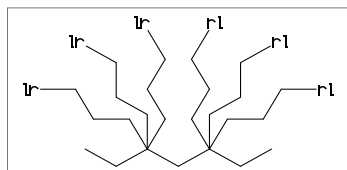
```
?4,  
{3~-90,3~-30,3^90}:/'(!3,"{hz}")>hz,  
{1~-60,1,1^60}:/'(!3,"{vt}")>vt
```



### 2.7.2 Left-right,right-left

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

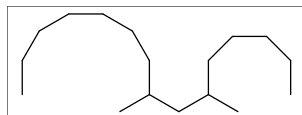
```
<-30,!6,  
{3~-30,3,3^30}:/'(!3,"{lr}")>lr,  
{5~-30,5,5^30}:/'(!3,"{rl}")>rl
```



### 2.7.3 Fixed rotate angle

>n : rotate n

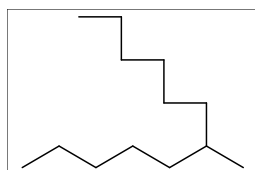
```
<30,!4,  
2:/!6>30, % 2:\,30,30,30,30,30,30  
4:/!4>-45 % 4:\,-45,-45,-45,-45
```



### 2.7.4 Multi rotate angle

>'(90,-90,...) : rotate 90,-90,...

```
<30,!6,6>'(90,-90,90,-90,90):/!5
```

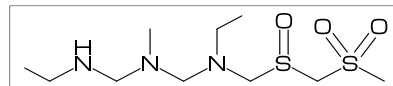


## 2.8 Miscellaneous

### 2.8.1 Abbreviated parts

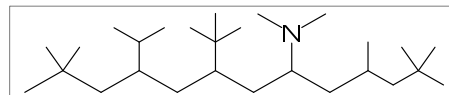
```
NH : N,/H~n1  
N! : N,/_  
N!2 : N,/!  
S0 : S,//0  
S00 : S,//0^35,/^~-35
```

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



```
?! : /_,!  
?? : /_~35,/_-35  
/?! : isopropyl  
/??? : tert-butyl  
/N?! : dimethylamino
```

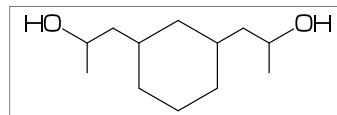
```
<30,!9'1,?!,! ,??,! ,  
2:??,4:/??,6:/??!,8:/N?!
```



### 2.8.2 Parts definition

'(..) : user defined parts

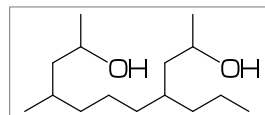
```
iBuOH:= '(!,/_,! ,OH);  
MC(<30,?6,{4,6}:/iBuOH)
```



### 2.8.3 Parts inline definition

```
<30,! , /'(!,/_,! ,OH),!
```

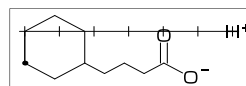
```
<30,!8,{2,6}:/'(!,/_,! ,OH)
```



### 2.8.4 Move position

@(x,y) : Move to (l\*x,l\*y) from origin  
\*\* l=bond length of ring

```
<30,?6,@3,!4,//0,! ,0,n_~60,@(6,1),H,p_~15
```



## 3 Option parameter

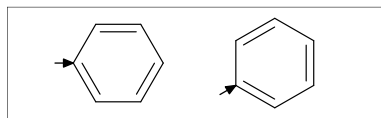
### 3.1 Angle parameter

mangle=0 \*\* default

MCat(0.2,0.5)(Ph)

mangle:=30;

MCat(0.8,0.5)(Ph)

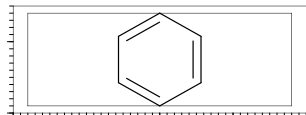


### 3.2 Size/Ratio parameter

#### 3.2.1 Bond length

(fit to font size)

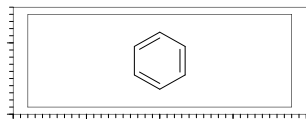
blength=0 \*\* default



(ratio bond/font width)

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

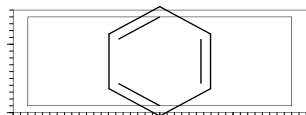
blength=60mm(width)\*0.1=6mm



(bond length)

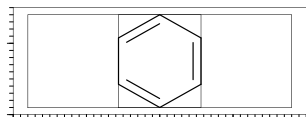
blength=9mm

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



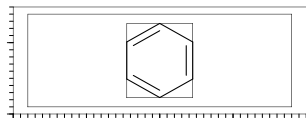
#### 3.2.2 Molecular size

msize=(1,1) \*\* default

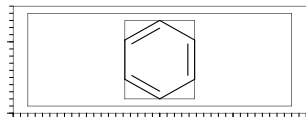


msize=(0.25,1)

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

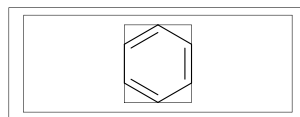


msize=(11mm,11mm)



#### 3.2.3 Molecular position

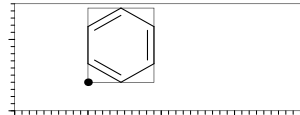
mposition=(0.5,0.5) \*\* default



mposition=(1,0)



mposition=(10mm,4mm)



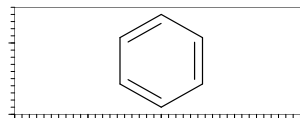
## 3.3 Size parameter

#### 3.3.1 Font size

fsize=(font width,font height)

\*\* default: (30mm,20mm)

fsize=(40mm,15mm)

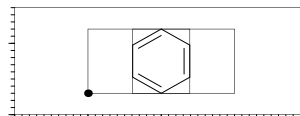


#### 3.3.2 Font margin

fmargin=(margin left right,top bottom)

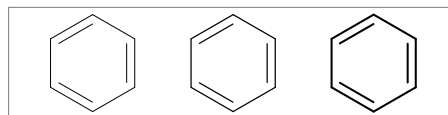
\*\* default: (0.4mm,0.4mm)

fmargin=(10mm,2mm)



#### 3.3.3 Offset thickness of bond

default: offset\_thickness=0.2pt



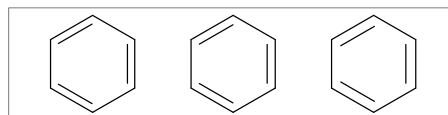
0pt

0.2pt

0.5pt

#### 3.3.4 Offset of double bond gap

default: offset\_bond\_gap=0.3pt



0.0pt

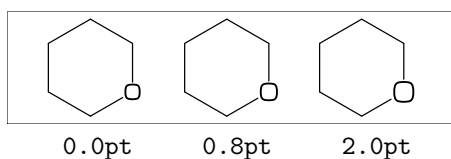
0.3pt

1.0pt



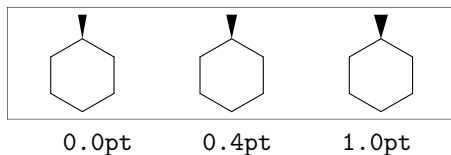
### 3.3.5 Offset of atom width

default: `offset_atom=0.8pt`



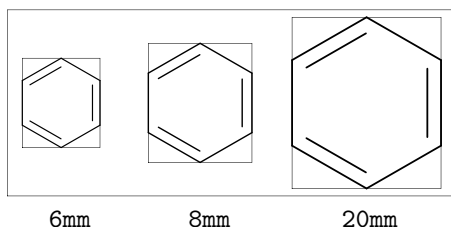
### 3.3.6 Offset of wedge width

default: `offset_wedge=0.4pt`



### 3.3.7 Max bond length

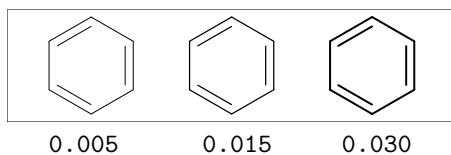
default: `max_blength=10mm`



## 3.4 Ratio parameter

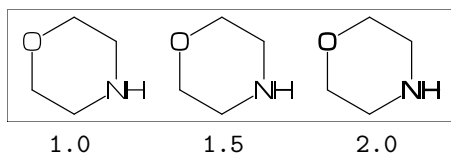
### 3.4.1 Thickness/bond length

default: `ratio_thickness_bond=0.015`



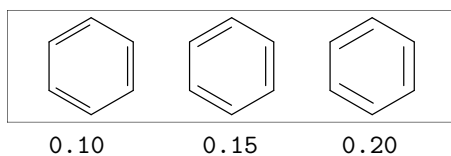
### 3.4.2 Char/bond thickness

default: `ratio_char_bond=1.5`



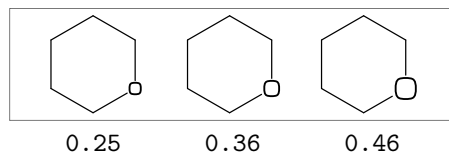
### 3.4.3 Bond gap/bond length

default: `ratio_bondgap_bond= 0.15`



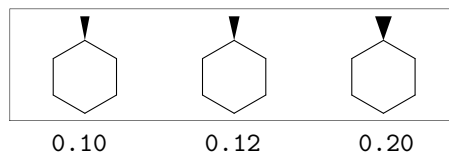
### 3.4.4 Atom/bond length

default: `ratio_atom_bond= 0.36`



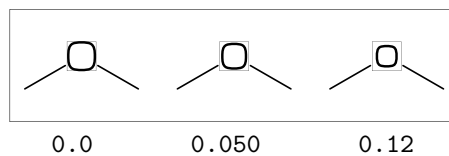
### 3.4.5 Wedge/bond length

default: `ratio_wedge_bond=0.12`



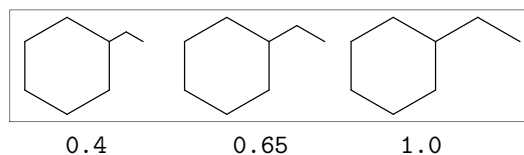
### 3.4.6 Font atom gap/atom length

default: `ratio_atomgap_atom= 0.050`



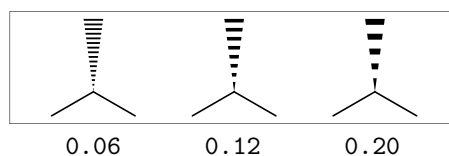
### 3.4.7 Chain/ring length

default: `ratio_chain_ring= 0.66`



### 3.4.8 Hash gap/bond length

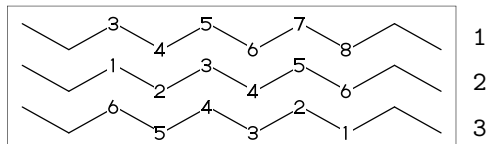
default: `ratio_hashgap_bond=0.12`



## 3.5 Drawing mode

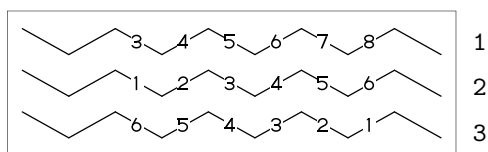
### 3.5.1 Numbering atom

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



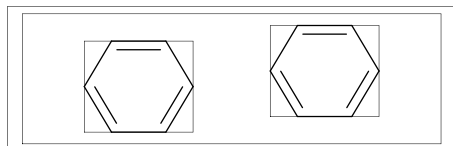
### 3.5.2 Numbering bond

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

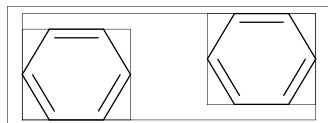


### 3.5.3 Trimming mode

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

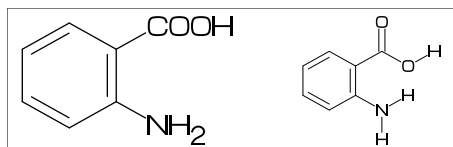


```
sw_trimming:=1;  
MCat(0.2,0.3)(Ph)  
MCat(0.8,0.7)(Ph)
```



### 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 Group off mode

```
** default: sw_group_off=0
```



### 3.5.6 Single bond mode

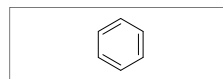
```
** default: sw_single=0
```



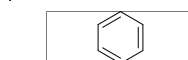
## 3.6 Frame

### 3.6.1 Font frame

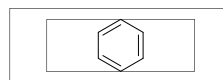
```
** default:sw_fframe=0  
(Draw font frame)  
fmargin:=(5mm,2mm);  
sw_fframe=1
```



(Frame inside margin)  
sw\_fframe=2

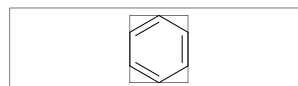


(Draw both frame)  
sw\_fframe=3



### 3.6.2 Molecular frame

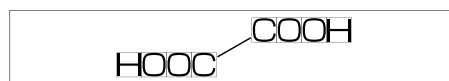
```
sw_mframe=1  
** default:sw_mframe=0
```



### 3.6.3 Atom frame

```
sw_aframe=1  
** default: sw_aframe=0
```

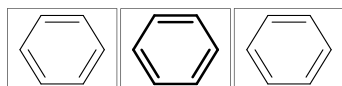
```
MC(<30,COOH,! ,COOH)
```



## 3.7 Parameter setting

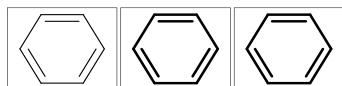
### 3.7.1 Local parameter setting

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



### 3.7.2 Global parameter setting

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



## 4 Function

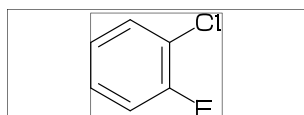
### 4.1 Function MC()

(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()

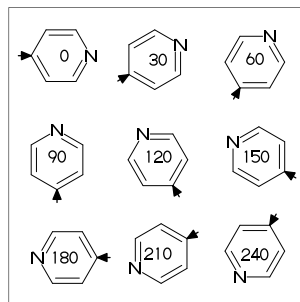
(Draw molecule at mposition)

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

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

c: x axis position d: y axis position

```
defaultsize:=5bp;
fsize:=(40mm,40mm); fmargin:=(3mm,3mm);
blength:=0.1; sw_fframe:=1;
mangle:=0;
for i=1 step -0.5 until 0:
  for j=0 step 0.5 until 1:
    MCat(j,i)(Ph,4:N)
    add(drawarrow((A1+A1up**aw)..A1);
        label(decimal(mangle),
            p0+(0.5w,0.5h));
    )
    mangle:=mangle+30;
  endfor
endfor
```



### 4.3 Function check\_mc()

(immediately compile)

```
beginfont("EN:Pyridine")
  MC(Ph,<30,2:N)
endfont
```

(check mcf and compile)

```
beginfont("EN:Pyridine",":<30,Ph,2:N")
  if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```

```
** error in mcf check_mc(mc)>=1
beginfont("EN:Pyridine",":<30,Ph,2):N")
  if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



check\_mc(mc)=0      check\_mc(mc)>=1

## 4.4 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

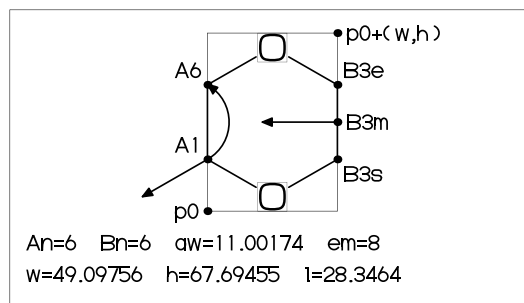
plus : '+' circled  
minus : '-' circled  
circlediam = 0.6aw (default)  
circlepen = 0.2bp (default)

lonpair r: ':' rotated r  
lonpairdiam = 0.3aw (default)  
lonpairspace = 0.7aw (default)

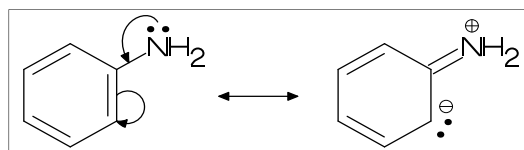
\*\* : scaled  
<< : rotated  
a /\* b : point b of a

```
beginfont("EN:add() 1")
  fsize:=(70mm,40mm);
  sw_aframe:=sw_mframe:=1;
  max_blength:=10mm;
  msize:=(.91,.9);
  MCat(.5,.85)<30,?6,{2,5}:0)
  add(
    defaultscale:=.8;
    labeloffset:=.3aw;
    dotlabel.lft("p0",p0);
    dotlabel.rft("p0+(w,h)",p0+(w,h));
    dotlabel.ulft("A1",A1);
    drawarrow A1..A1+__*l<<A1ang;
    dotlabel.lrt("B3s",B3s);
    dotlabel.rft("B3m",B3m);
    drawarrow B3m..B3m+__*l<<(B3ang+90);
    dotlabel.ulft("A6",A6);
```

```
drawarrow A1{A1down}..A6;
dotlabel.rft("B3e",B3e);
label.rft("An"&decimal(An)&
  " Bn"&decimal(Bn)&
  " aw"&decimal(aw)&
  " em"&decimal(em),
  p0+(-9em,-1.5em));
label.rft("w"&decimal(w)&
  " h"&decimal(h)&
  " l"&decimal(l),
  p0+(-9em,-3em));
)
endfont
```



```
beginfont("EN:add() 2")
  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.rft(minus,A3);
    label(lonpair A3ang,A3+A3up**1.7aw);
  )
  %-----
  ext(drawdblarrow (.4w,.4h)..(.55w,.4h));
  %-----
endfont
```



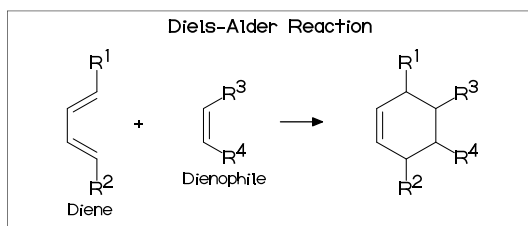
## 4.5 Function ext()

(Extra graphic to font)

```
w:      font width
h:      font height
w0:     font width-2xpart(fmargi
h0:     font height-2ypart(fmargi
aw:     atom font size
em:     label font size
p0:     fmargi

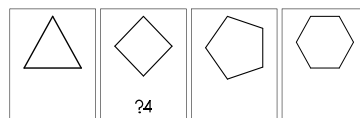
n:      molecular number
p[m]:   molecular origin position
w[m]:   molecular width
h[m]:   molecular height

ratio_thickness_char:
pen thickness / char width
%-----
beginfont()
  fsize:=(70mm,30mm);
  blength:=0.065;
%-----
MCat(0.1,0.5)(
  <-210,60'1,60'1,60'1,{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
```



### 4.5.1 Local ext() setting

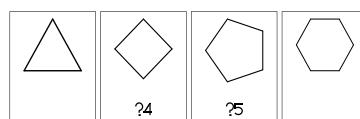
```
beginfont("EN:?3")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(<30,?3)
endfont
beginfont("EN:?4")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?4)
%-----
ext(label.top(inf_EN,(0.5w,0));)
%-----
endfont
beginfont("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?5)
endfont
beginfont("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?6)
endfont
```



### 4.5.2 Global ext() setting

ext\_clear: reset global ext()

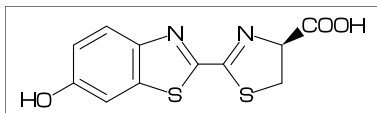
```
beginfont("EN:?3")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(<30,?3)
endfont
%-----
ext(label.top(inf_EN,(0.5w,0));)
%-----
beginfont("EN:?4")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?4)
endfont
beginfont("EN:?5")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?5)
endfont
%-----
ext_clear;
%-----
beginfont("EN:?6")
  fsize:=(12mm,15mm);
  MCat(0.5,1)(?6)
endfont
```



## 5 MCF example

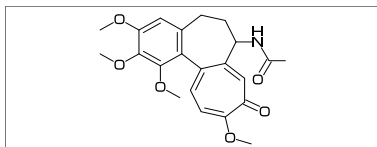
### 5.1 Luciferin

```
beginfont("EN:Luciferin","MW:280.33",
%-----
": <30,Ph,3=?5,@8,\,?5,{9,16}=d1,    ",
": {9,14}:N,{7,11}:S,1:/OH,-2:*/COOH ")
%-----
fsize:=(50mm,20mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



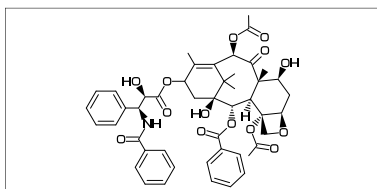
### 5.2 Colchicine

```
beginfont("EN:Colchicine","MW:385.41",
%-----
": <30,Ph,{1,2,6}:/O!,-4=?7,-5=?7,    ",
": {-1,-4,-6}=d1,-2://O,-3:/O!,      ",
": @9,\,NH,! ,//O,!                  ")
%-----
fsize:=(50mm,20mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



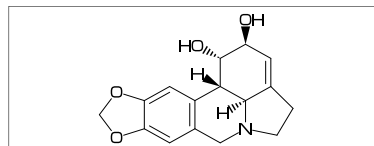
### 5.3 Paclitaxel

```
beginfont("EN:Paclitaxel","MW:853.91",
%-----
": ?6,5=d1,@3,#1,36,45,45,45,45,##, ",
": &.$5",
": -4=?6,-4=?4,-1=wb,-3=wf,-1:0,||, ",
": 4:??,6:/_,{3~-60,15}:*/OH,      ",
": 8:/*H~-60,"",
": 9:*/_~60,10://O,                ",
": @1,\,0,! ,//O,! ,*/OH,! ,/Ph,60~wf, ",
": NH,-60,//O,60,Ph,                ",
": @7,\*,0,-45,//O,60,Ph,           ",
": @11,\*,0,-60,//O,60,             ",
": @12,\*~-15,0,60,//O,-60         ")
%-----
fsize:=(50mm,25mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



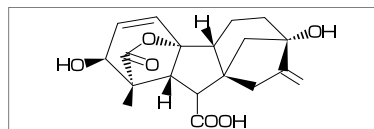
### 5.4 Lycorine

```
beginfont("EN:Lycorine","MW:287.31",
%-----
": 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:*/OH                      ")
%-----
fsize:=(50mm,20mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



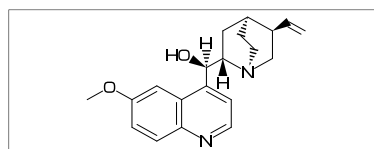
### 5.5 Gibberellin

```
beginfont("EN:Gibberellin A3","MW:346.37",
%-----
": <18,?5,3=?7,5=?6[12],@8,160'1.3,&3, ",
": 13=d1,6=wf,8=wb,                      ",
": @5,40~zf'1,0,50,//O^180,&14~zb,      ",
": 2:/COOH,7://_,13:*/OH,8:*/OH,        ",
": 14:*/_,{1,4}:*/H^60                    ")
%-----
fsize:=(50mm,18mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



### 5.6 Quinine

```
beginfont("EN:Quinine","MW:324.42",
%-----
": <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                    ")
%-----
fsize:=(50mm,20mm);
if check_mc(mc)=0: MC(scantokens(mc)) fi
endfont
```



## 6 Example to use mcf2graph

### 6.1 Molecular definition file

```

%-----
input mcf2graph.mf;                                     % input macro
%-----
sw_aux_out:=1;          % aux(information) file output on > Global setting
fsize:=(60mm,40mm);    % (font width,font height)      >
tag1:="F";              > AUX file table
tag2:="C";              >
tag3:="mw";             >
tag4:="fm";             >
%%% 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("EN:Ampicillin","MW:349.405",                > information
%-----
": <45,?4,-3=?5,2:N,7:S,                                ", >
": 3^45:/*H,1://0^15,5:/*COOH^-18,6:??, ",              > mc1
": @4,*\^15,NH,! ,//0,! ,/*NH2,! ,Ph                    ") > mc2
%-----
if check_mc(mc)=0: MC(scantokens(mc)) fi               > mc3
endfont                                                  > mc=mc1&mc2&mc3
%-----
beginfont("EN:Cholesterol","MW:386.65",                > information
%-----
": <30,?6,{-4,-2}=?6,-4=?5,7=d1,                        ", >
": 10:/*H^180,11:/*H^-60,17:/*H^-54, ",                 > mc1
": {4,12}:*/_ ^60,                                       ", > mc2
": @-1,18,/*_,-60,!3,?!                                ") > mc3
%-----
if check_mc(mc)=0: MC(scantokens(mc)) fi               > mc4
endfont                                                  > mc=mc1 - mc4
%-----
beginfont("EN:Limonin",                                > information
%-----
": <30,?6,{-3,-4}=?6,                                    ", >
": -5=?3,-2=wf,-1=wb,6=?5,-4=?6,-5=wf, ",              > mc1
": {13,15,17,20}:0,{3,12,21}://0,                        ", > mc2
": {4~wf^60,8~zf^60,18^35,18^-35}:/_ ,                  ", > mc3
": {1^60,5^180,16^60}:/*H,                               ", > mc4
": @14,\*,| ,?5,{1,4}=d1,3:0)                            ") > mc5
%-----
if check_mc(mc)=0: MC(scantokens(mc)) fi               > mc6
endfont                                                  > mc=mc1 - mc6
%-----
beginfont("EN:beta-carotene",                          > information
%-----
": <30,?6,3=d1,{3,5^35,5^-35}:/_ ,                      ", >
": @4,\,| ,!18,{1,3,5,7,9,11,13,15,17}=dr, ",            > mc1
": {3,7,12,16}:/_ ,                                     ", > mc2
": | ,?6,6=d1,2:??,6:/_ )                               ") > mc3
%-----
if check_mc(mc)=0: MC(scantokens(mc)) fi               > mc4
endfont                                                  > mc=mc1 - mc4
%-----
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")      .... endfont
beginfont("EN:Cholesterol")     .... endfont
beginfont("EN:Limonin")         .... endfont
beginfont("EN:beta-Carotene")   .... endfont
```

(Setting)

```
tag1:="F"; tag2:="C"; tag3:="mw"; tag4:="fm"; tag5:="EN";
```

(Output)

(sw\_aux\_out=1)

```
F:mcf_man_soc;C:1;mw:349.40462;fm:C16H19N3O4S;EN:Ampicillin
F:mcf_man_soc;C:2;mw:386.6532;fm:C27H46O;EN:Cholesterol
F:mcf_exa_soc;C:3;mw:470.5113;fm:C26H30O8;EN:Limonin
F:mcf_exa_soc;C:4;mw:536.8722;fm:C40H56;EN:beta-Carotene
```

(sw\_aux\_out=2)

```
F;C;mw;fm
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/mw:349.40462/fm:C16H19N3O4S/EN:Ampicillin
F:mcf_man_soc/C:2/mw:386.6532/fm:C27H46O/EN:Cholesterol
F:mcf_exa_soc/C:3/mw:470.5113/fm:C26H30O8/EN:Limonin
F:mcf_exa_soc/C:4/mw:536.8722/fm: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
MI  : monoisotopic mass from literature data
USE : the use
mw  : molecular weight calculated
mi  : monoisotopic mass calculated
fm  : molecular formula calculated
w   : font width
h   : font height
```



### 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)

```
=====
No.    1 / Name = Adenine
-----
<30,?6,3=?5,{1,3,5,9}=d1,{2,6,9}:N,5:/NH2,7:NH
-----
mc length= 46 / mc low= 1
-----
Warnings = 0 / Command count= 65
Width * Height = 44.41766 * 44.96748
Shift width * height = -2.69456 * -12.02556
Bond length = 12.75589 Atom size = 5.38914
Atom count= 11 Bond count= 12 Ring count= 2 Hide H count= 2
-----
< NO. ><atom(s) >( x axis , y axis )<bond><hideH><chg>
A1 C ( 0 , 0 ) 3 1
A2 N ( 0.866 , -0.5 ) 3
A3 C ( 1.732 , 0 ) 4
A4 C ( 1.732 , 1 ) 4
A5 C ( 0.866 , 1.5 ) 4
A6 N ( 0 , 1 ) 3
A7 N ( 2.683 , -0.309 ) 3
A8 C ( 3.271 , 0.5 ) 3 1
A9 N ( 2.683 , 1.309 ) 3
A10 NH2 ( 0.866 , 2.371 ) 1
A11 H ( 2.683 , -0.732 ) 1
-----
< 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 3 -> 7 ( 1) 342 ( -18) 1 ( 12.76)
B8 7 -> 8 ( 1) 54 ( 54) 1 ( 12.76)
B9 8 -> 9 ( 2) 126 ( 126) 1 ( 12.76)
B10 9 -> 4 ( 1) 198 ( -162) 0.66 ( 8.42)
B11 5 -> 10 ( 1) 90 ( 90) 0.66 ( 8.42)
B12 7 -> 11 ( 1) 270 ( -90) 0.36 ( 4.59)
-----
<atom>( atom wt ) [ mi wt ] < cnt > < sum wt > [ sum mi wt ]
C ( 12.0107) [ 12 ] * 5 60.05348 [ 60 ]
H ( 1.00793) [ 1.00783 ] * 5 5.03967 [ 5.03914 ]
N ( 14.0067) [ 14.00307 ] * 5 70.0335 [ 70.01534 ]
Molecular Weight [Mono Isotopic] = 135.1266 [ 135.05447 ]
-----
Weight Calc: 135.1266 / Input: 135.13 / weight gap= -0.00336
Fomula Calc: C5H5N5 / 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  FILENAME      % MOL(V2000)
>mpost -s ahlength=6  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}%
\usepackage[T1]{fontenc}%
\usepackage{textcomp}%
\mplibcodeinherit{enable}%
\mplibverbatim{enable}%
\mplibnumbersystem{double}%
\everymplib{%
  if unknown Ph1: input mcf2graph.mf; fi
  sw_calc:=1; sw_fframe:=4; max_blength:=4.5mm;
  defaultfont:="uhvr8r"; defaultsize:=8bp; defaultscale:=1;
}%
\begin{document}
\noindent%
%-----
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfont("N0:1","EN:Limonin","MW:470.51",
    %-----
    ": <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 ")
    %-----
  if check_mc(mc)=0: MC(scantokens(mc)) fi
  endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
  fsize:=(80mm,50mm);
  beginfont("N0:2","EN:beta-carotene","MW:536.87",
    %-----
    ": <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}:/_ ")
    %-----
  if check_mc(mc)=0: MC(scantokens(mc)) fi
  endfont
\end{mplibcode}\\
%-----
\begin{mplibcode}
  fsize:=(50mm,50mm);
  beginfont("N0:3","EN:Gibberellin A3","MW:346.37",
    %-----
    ": <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 ")
    %-----
  if check_mc(mc)=0: MC(scantokens(mc)) fi
  endfont;
%-----
\end{mplibcode}\\
\end{document}

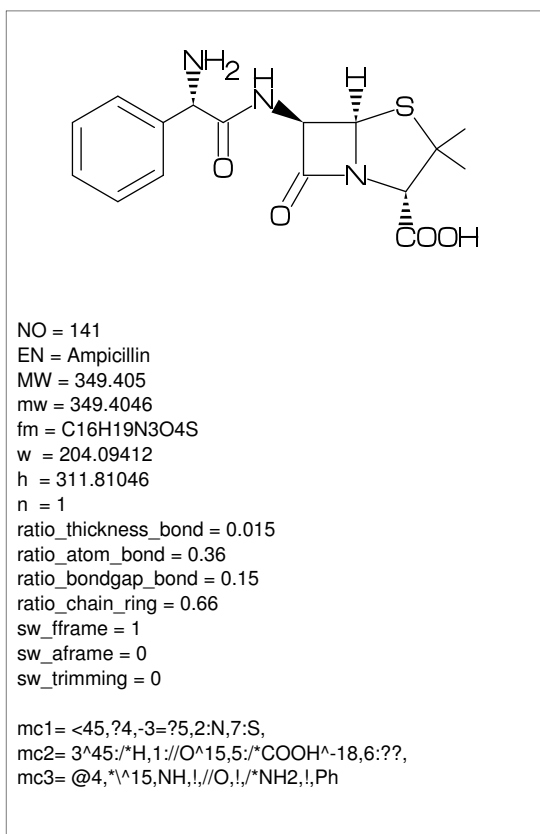
```

## 6.6 LaTeX file example

```
%-----
\documentclass[a4paper]{article}
\usepackage{graphicx}
%-----
\usepackage{mcf_setup}
%-----
\pagestyle{empty}
\makeatletter%
%-----
\def\put@char{%
  \begin{picture}(84,42)%
    \put(0,38){\bf [MOLnum]\EN{ }\small\tt/FM:\fm/MW:\mw}%
    \put(10,0){\font\@strufont=\File\relax%
      \hbox{\@strufont\char\Char}}}%
  \end{picture}%
}%
\def\INFO#1{\@for\@temp:=#1\do{\tag@var\@temp}\put@char}%
\makeatother
%-----
\begin{document}
\unitlength=1mm%
\INFO{F:mcf_man_soc,C:141,NO:1,mw:349.40462,fm:C16H19N3O4S,EN:Ampicillin}%
\INFO{F:mcf_man_soc,C:142,NO:2,mw:386.6532,fm:C27H46O,EN:Cholesterol}%
\end{document}
%-----
```

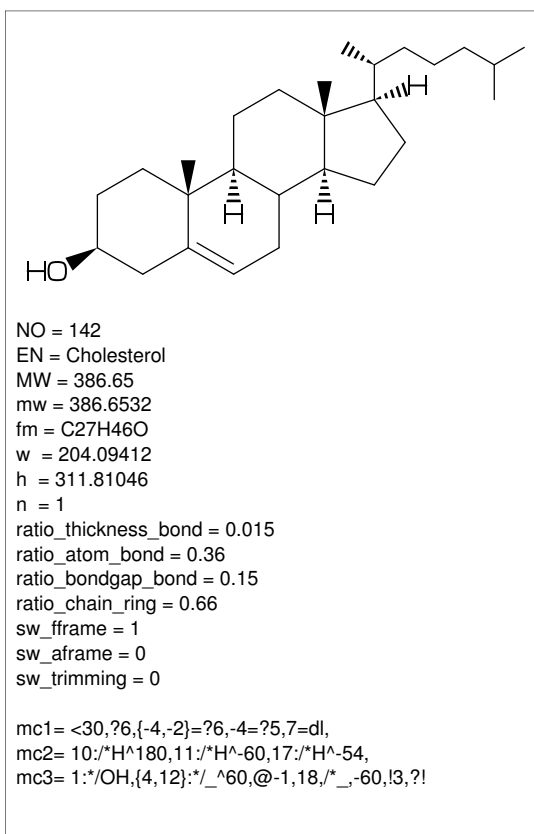
### [1]Ampicillin

FM:C16H19N3O4S MW:349.40462



### [2]Cholesterol

FM:C27H46O MW:386.6532



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