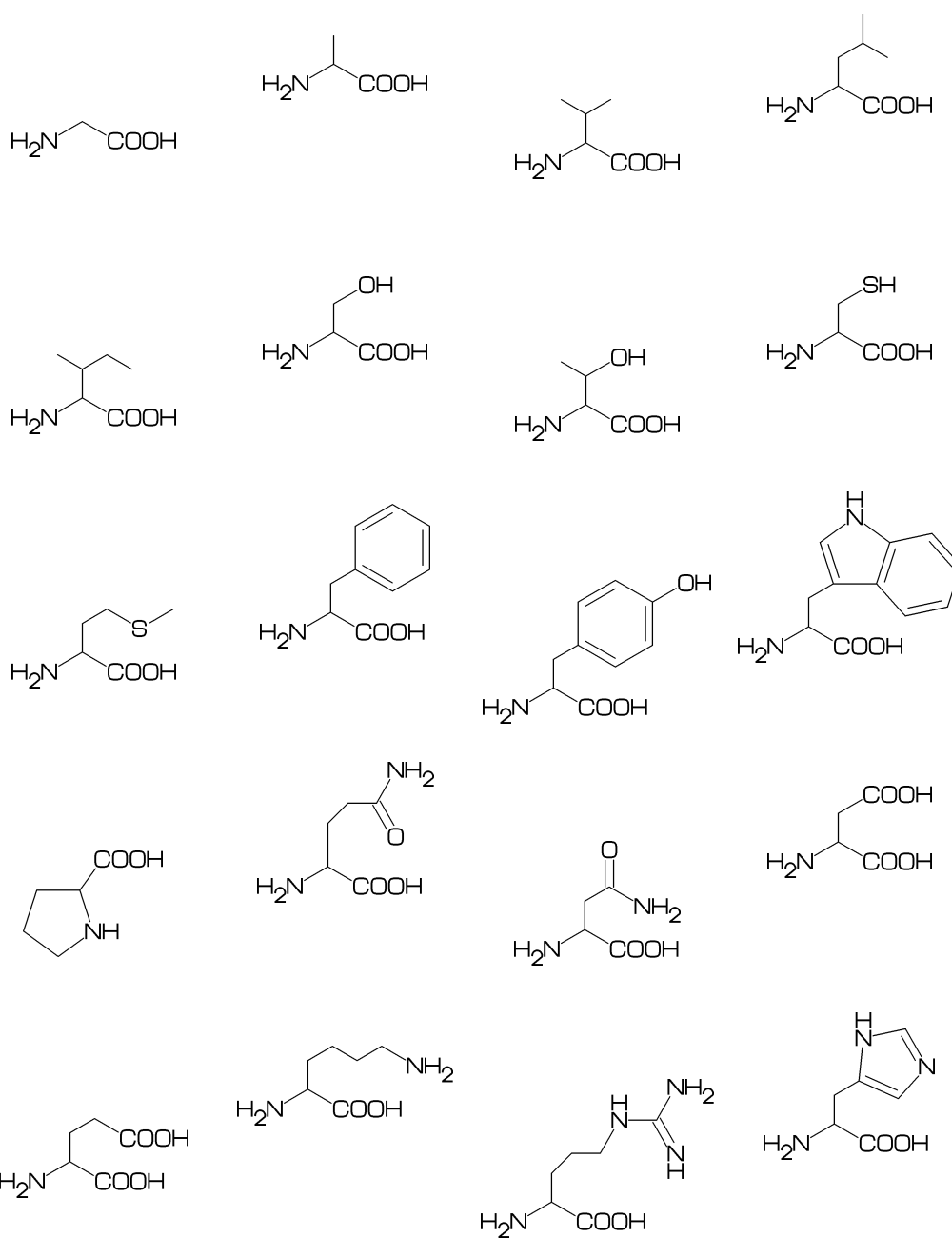


# Molecular Coding Format manual

Akira Yamaji

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



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# 1 Introduction

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

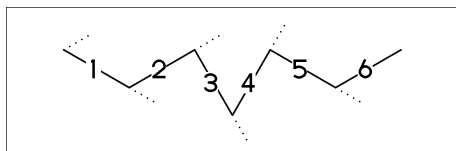
## 2 MCF syntax

### 2.1 Make bond

#### 2.1.1 Chain

real number plus (+): anticlockwise  
real number minus(-): clockwise

<30,-60,60,-90,120,-90,60

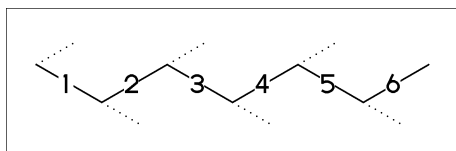


! : take value 60 or -60 depend on current angle and enviroment

!6 : !,!,!,!,!,!

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

<30,!6

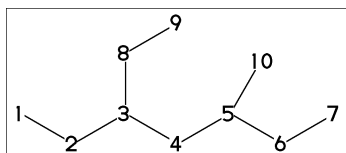


#### 2.1.2 Jump and branch bond

n\* : Jump to An

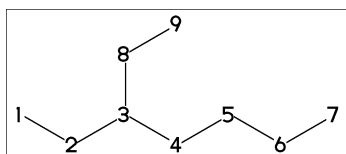
\*\* An: atom number(-999<=n<=4095)

<30,!6,3\*,0,!,5\*,-30



3\ : 3\*,0

<30,!6,3\,!



#### 2.1.3 Branch bond

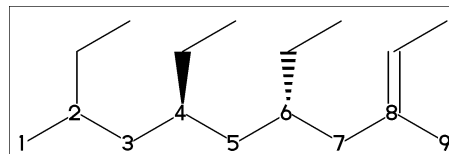
2\ : 2\*,0

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

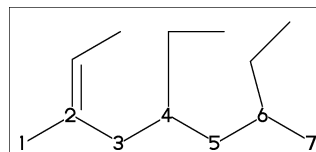
6\^15 : 6\*,0^15

<-30,!6,

2\~dr,!,

4\'1.5,-90,

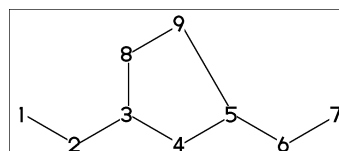
6\^15,-60



#### 2.1.4 Connect atom

&n : Connect to An

<30,!6,3\,!,&5

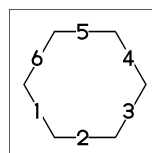


#### 2.1.5 Ring

?n : n membered ring(3<=n<=20)

?6 : <-120,60,60,60,60,60,&1

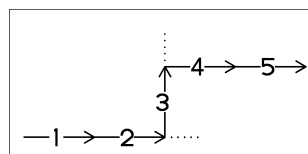
?6



#### 2.1.6 Rotate current angle

<angle : rotate current angle

0,0,<90,0,<-90,0,0,\$(1,2,3,4,5)vf

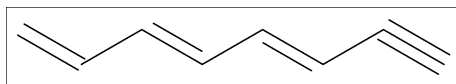


## 2.2 Change bond type

### 2.2.1 Double, triple

a~type : ~type,a  
dm : double middle  
dl : double left side  
dr : double right side  
tm : triple

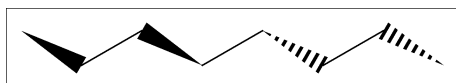
<30,!~dm,!~dl,!~dr,!~tm



### 2.2.2 Wedge

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

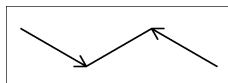
<30,!~wf,!~wb,!~zf,!~zb



### 2.2.3 Vector

vf : vector forward  
vb : vector backward

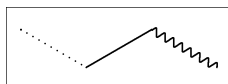
<30,!~vf,!~vb



### 2.2.4 Dotted, wave

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

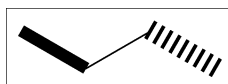
<30,!3,1=dt,3=wv



### 2.2.5 Broad

bd : broad  
bz : broad dotted

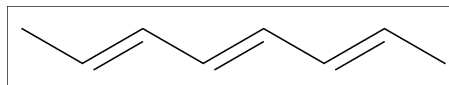
<30,!3,1=bd,3=bz



### 2.2.6 Change multi bond type

\$(2,4,6)dr : 2=dr,4=dr,6=dr

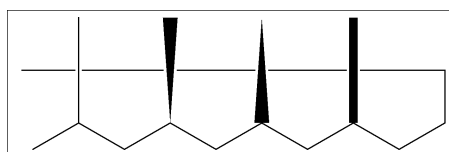
<30,!7,\$(2,4,6)dr



### 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\_)/Me'2



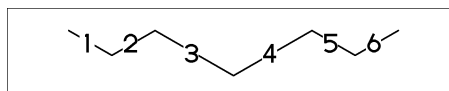
## 2.3 Change bond length

### 2.3.1 Chain length

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

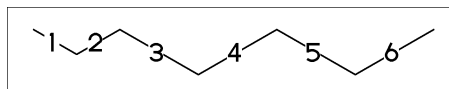
<30,!2,!2'1.2,!2

\*\* !2'1.2 : ''1.2,!2



''length : change all bond length after

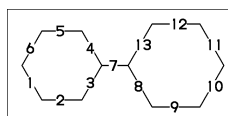
<30,!2, ''1.2,!4



### 2.3.2 Ring length

?n'length : change ring length

?6,4\,?6'1.2

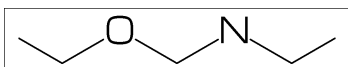


## 2.4 Change atom

### 2.4.1 Insert atom

Insert hetero atom

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

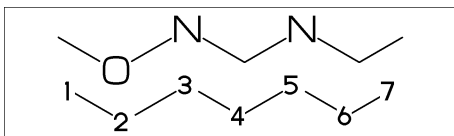


### 2.4.2 Addressed atom

2:0 : change A2 C to O

@(3,5)N : change A3,A5 C to N

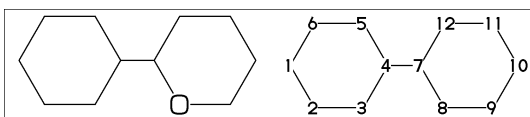
<30,!6,2:0,@(3,5)N



### 2.4.3 Brock address

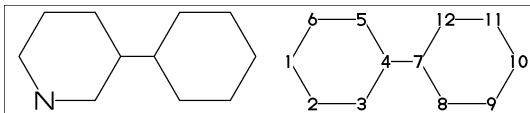
| : divide brock

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



|| : reset brock address

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

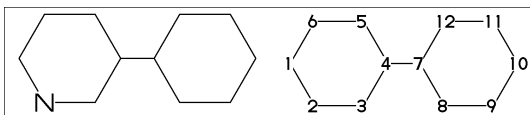


### 2.4.4 Absolute address

#2:N : change A#2 C to N

\*\* #n : (1<n<=3095)

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

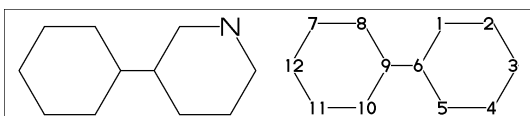


### 2.4.5 Relative address

-2:N : change A(-2) C to N

\*\* -n : (1<n<=999)

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



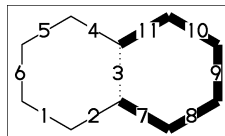
## 2.5 Fuse ring

### 2.5.1 Attached 1 bond

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

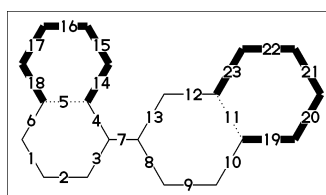
\*\* Bn(n:-999<n<=4095): bond number

?6,3=?6



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

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

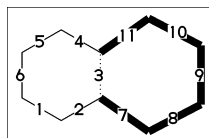


?6,3=?6[13] : fuse ?6[13] at B3

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

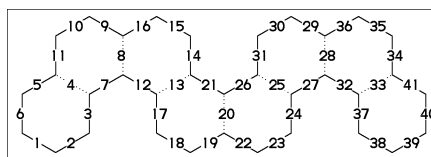
\*\* ?m[n] (5<=m<=8,11<=n<=15)

?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

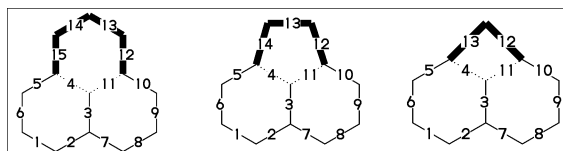
(4,11)=?4[2] : fuse 2/4 ring to B11..B4

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

MCd(1,.7)( 0,0)(<30,?6,3=?6,(11,4)=?6[4])

MCd(1,.6)(.54,1)(<30,?6,3=?6,(11,4)=?5[3])

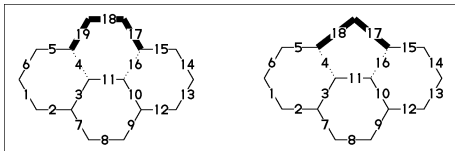
MCd(1,.6)( 1,0)(<30,?6,3=?6,(11,4)=?4[2])



### 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)

MCd(1,.55)(0,0)(?6,\$(3,10)?6,(16,4)=?6[3])  
 MCd(1,.55)(1,0)(?6,\$(3,10)?6,(16,4)=?5[2])

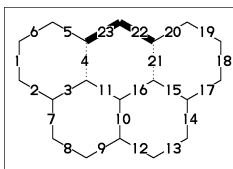


### 2.5.4 Attached 4 bond

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

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

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

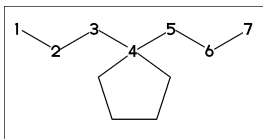


### 2.5.5 Spiro ring

4\*,?5 : add ?5(5 membered ring) at A4

<30,!6,4\*,?5

An\* : jump to An

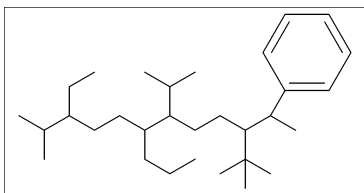


## 2.6 Substituent

### 2.6.1 Insert substituent

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

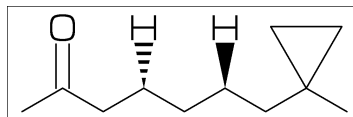
\*\* Me:methyl Et:ethyl  
 Pr:propyl iPr:isopropyl  
 tBu:tertial buthyl Ph:phenyl



### 2.6.2 Insert modified substituent

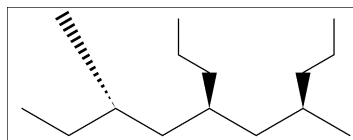
/ : single  
 // : double  
 \*/ : wedge forward  
 /\* : wedge dotted forward  
 \*\* : direct

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



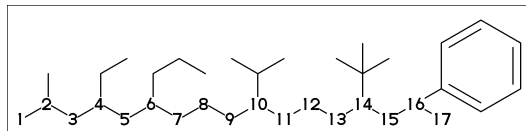
~ : change type  
 ^ : change angle  
 ' : change length  
 > : change enviroment

<30,'^1,!/,Me~zf^2^30,!/,Me~zf^2^30,  
 !2,\*/Pr>lr,!2,\*/Pr>rl,!)



### 2.6.3 Add substituent

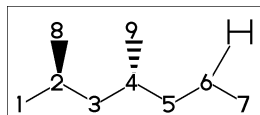
<-30,!17,2:/Me,4:/Et,6:/Pr,  
 10:/iPr,14:/tBu,16:/Ph^-60



### 2.6.4 Add modified substituent

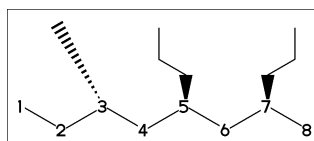
~,^,' : change type,angle,length

<-30,!6,  
 @(2~wf,4~zf,6^-30)/H



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

<30,!7^1,  
 3:/\*Me^2^30,5:\*/Pr>lr,7:\*/Pr>rl

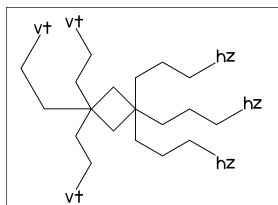


## 2.7 Chain environment

### 2.7.1 Horizontal,vertical

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

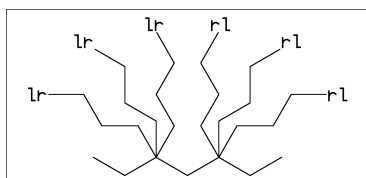
```
?4,@(3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,  
@(1^-60,1^2,1^60)/'(!2,"{vt}")>vt
```



### 2.7.2 Left-right,right-left

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

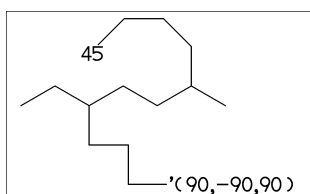
```
<30,!6,  
@(3^-30,3,3^30)/'(!3,"{lr}")>lr,  
@(5^-30,5,5^30)/'(!3,"{rl}")>rl
```



### 2.7.3 Fixed angle,multi angle

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

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

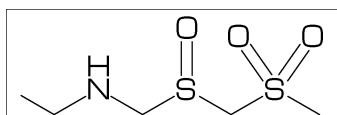


## 2.8 Miscellaneous

### 2.8.1 Change atom and Substituent

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

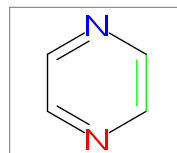
```
<30,!2,NH,! ,S0,! ,S00,!3
```



### 2.8.2 Change color

@(5)green : change color of A5 green  
\$(3)red : change color of B3 red  
\*\* METAFONT ignore color command

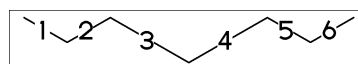
```
<30,Ph,@(2,5)N,2:red,5:blue,3=green
```



### 2.8.3 Make block

{ : start block  
} : end block

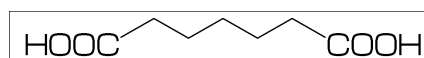
```
<30,!2,{,'1.2,!2},!2
```



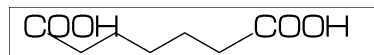
### 2.8.4 Chain start multiple characters

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

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



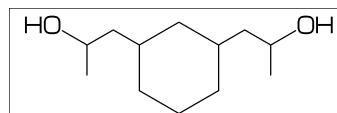
```
MCf(<30,COOH,!4,COOH)
```



### 2.8.5 User definition

iBuOH : user defined substructure

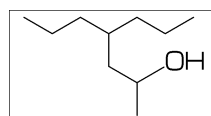
```
iBuOH:= '(!,/Me,!,OH)  
MCf(<30,?6,@(4,6)/iBuOH)
```



### 2.8.6 Inline definition

Insert user defined substructure

```
<30,!3,/ '(!,/Me,!,OH),!3
```

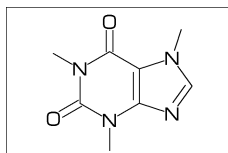


## 3 Option parameter

### 3.1 Size parameter

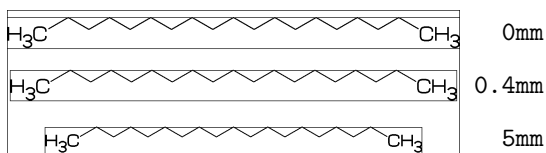
#### 3.1.1 Font size

```
beginfont("EN:Caffeine")
font_wd#:=30mm#; %<=font width
font_ht#:=20mm#; %<=font height
MCf(<30,?6,-4=?5,$(3,8)d1,@(2,6,7,9)N,
@(2,6,9)/Me,@(1,5)//0) endfont
```



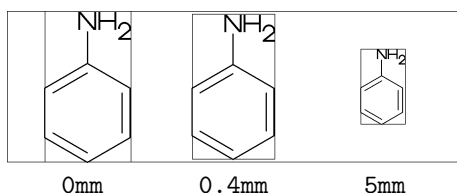
#### 3.1.2 Margin left and right

default: margin\_left\_right=0.4mm



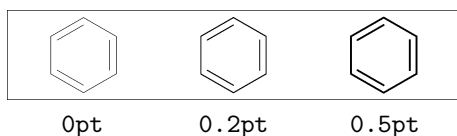
#### 3.1.3 Margin top and bottom

default: margin\_top\_bottom=0.4mm



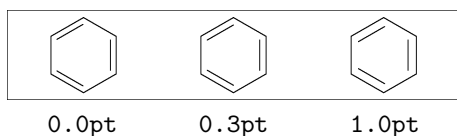
#### 3.1.4 Offset thickness of bond

default: offset\_thickness#=0.2pt#



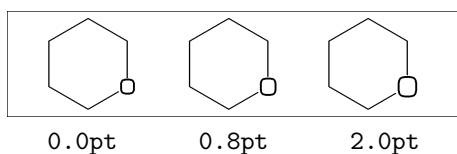
#### 3.1.5 Offset of doublebond gap

default: offset\_bond\_gap#=0.3pt#



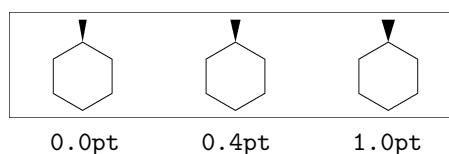
#### 3.1.6 Offset of atom width

default: offset\_atom#=0.8pt#



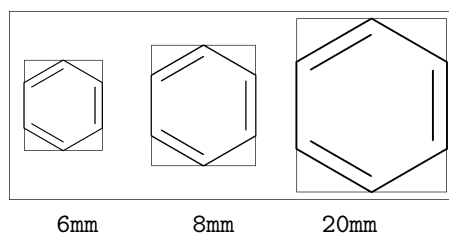
#### 3.1.7 Offset of wedge width

default: offset\_wedge#=0.4pt#



#### 3.1.8 Max bond length

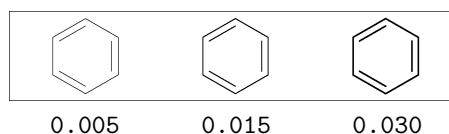
default: max\_bond\_length#=10mm#



## 3.2 Ratio parameter

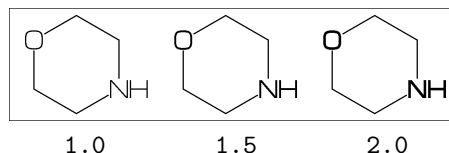
#### 3.2.1 Thickness/bond length

default: ratio\_thickness\_bond=0.015



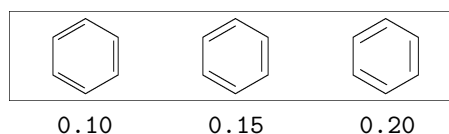
#### 3.2.2 Char/bond thickness

default: ratio\_char\_bond=1.5



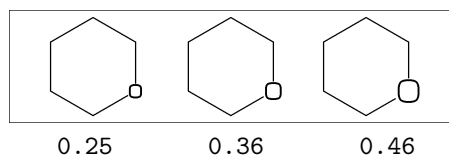
#### 3.2.3 Bondgap/bond length

default: ratio\_bondgap\_bond= 0.15



#### 3.2.4 Atom/bond length

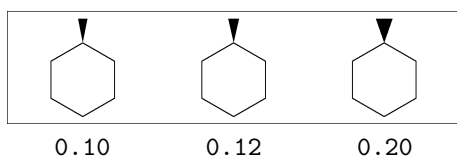
default: ratio\_atom\_bond= 0.36





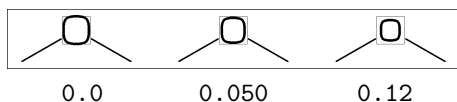
### 3.2.5 Wedge/bond length

default: ratio\_wedge\_bond=0.12



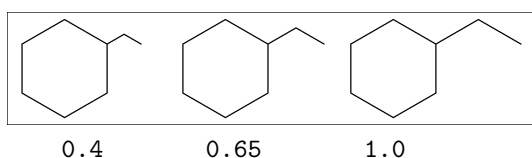
### 3.2.6 Font atom gap/atom length

default: ratio\_atomgap\_atom= 0.050



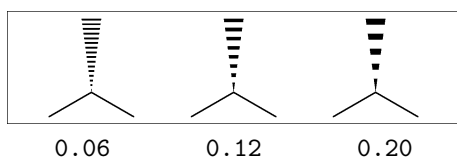
### 3.2.7 Chain/ring length

default: ratio\_chain\_ring= 0.66



### 3.2.8 Zebra gap/bond length

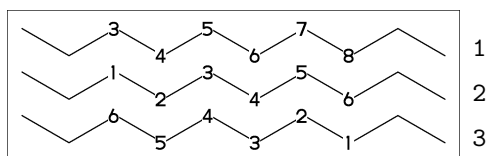
default: ratio\_zebragap\_bond=0.12



## 3.3 Drawing mode

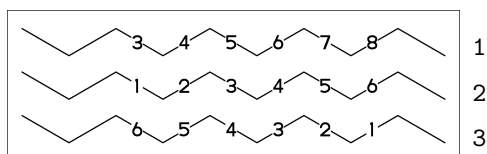
### 3.3.1 Numbering atom

numberA\_start:=3; numberA\_end:=8;  
default: sw\_numberA=0 :  
numberA\_start=1 numberA\_end=4095



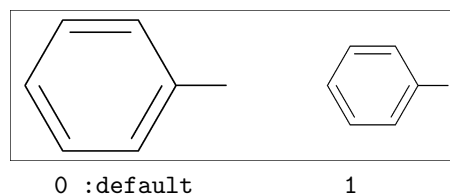
### 3.3.2 Numbering bond

numberB\_start:=3; numberB\_end:=8;  
default: sw\_numberB=0 :  
numberB\_start=1 numberB\_end=4095



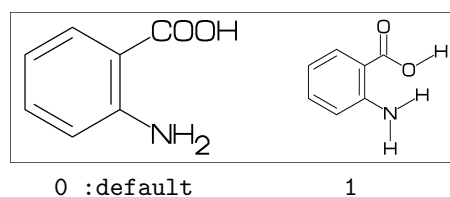
### 3.3.3 Solid mode

```
MCd(1,1)(0,.5)(Ph,4:/Me)  
sw_solid:=1;  
bond_len#:=6mm#;  
MCd(1,1)(1,.5)(Ph,4:/Me)
```



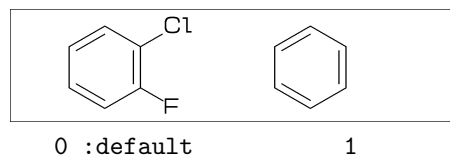
### 3.3.4 Expand mode

```
MCd(1,.5)(0,0.5)(<30,Ph,4:/COOH,3:/NH2)  
sw_expand:=1;  
MCd(1,.5)(1,0.5)(<30,Ph,4:/COOH,3:/NH2)
```



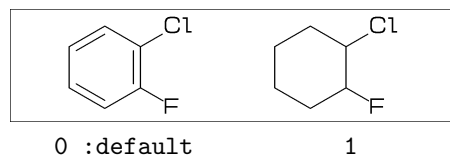
### 3.3.5 Substituent off mode

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



### 3.3.6 Single bond mode

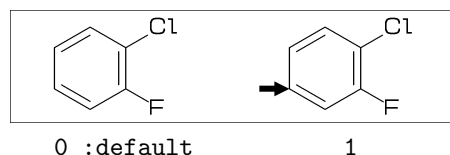
```
MCd(1,.5)( 0,0.5)(<30,Ph,4:/Cl,3:/F)  
sw_bond_single:=1;  
MCd(1,.5)( 1,0.5)(<30,Ph,4:/Cl,3:/F)
```



## 3.4 Frame,vector

### 3.4.1 Start vector

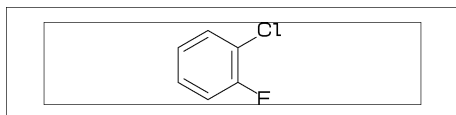
```
MCf(<30,Ph,4:/Cl,3:/F)  
sw_start_vector:=1;  
MCf(<30,Ph,4:/Cl,3:/F)
```



### 3.4.2 Font frame

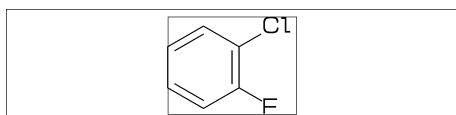
```
sw_font_frame=0 : no frame **default
sw_font_frame=1 : draw frame of font
sw_font_frame=2 : draw frame inside margin
sw_font_frame=3 : draw both
```

```
sw_font_frame:=3;
margin_left_right:=5mm;
margin_top_bottom:=2mm;
Mcf(<30,Ph,4:/Cl,3:/F)
```



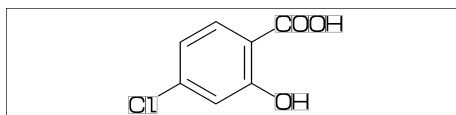
### 3.4.3 Molecular frame

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



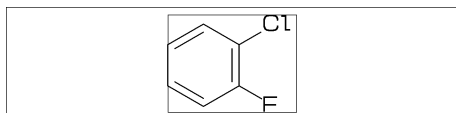
### 3.4.4 Atom frame

```
sw_atom_frame:=1;
Mcf(<30,Ph,1:/Cl,4:/COOH,3:/OH)
** default: sw_atom_frame=0
```

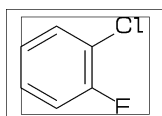


## 3.5 Clipping font

```
beginfont()
sw_clip:=0;
Mcf(<30,Ph,4:/Cl,3:/F) endfont
** default: sw_clip=0
```



```
beginfont()
sw_clip:=1;
Mcf(<30,Ph,4:/Cl,3:/F) endfont
```

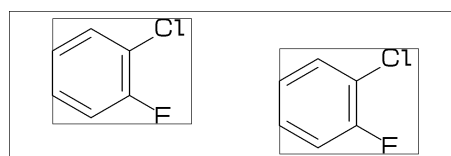


## 4 MCF draw function

### 4.1 Function MCd (draw)

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

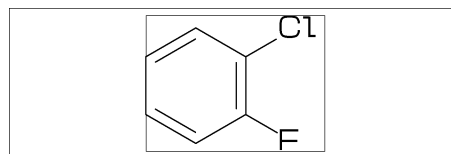
```
MCd(1,0.8)(0.2,0.9)(<30,Ph,3:/F,4:/Cl)
MCd(1,0.8)(0.8,0.1)(<30,Ph,3:/F,4:/Cl)
```



### 4.2 Function MCf (fit draw)

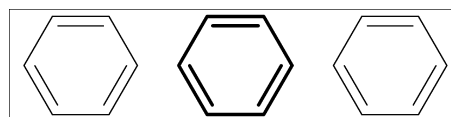
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)
```

```
sw_font_frame:=1;
sw_mol_frame:=1;
Mcf(<30,Ph,3:/F,4:/Cl)
```



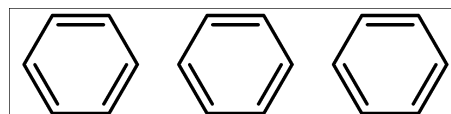
### 4.3 Local setting

```
beginfont() MCd(1,.4)(0,.5)(Ph) endfont
beginfont()
ratio_thickness_bond:=0.05;
MCd(1,.4)(0.5,.5)(Ph)
endfont
beginfont() MCd(1,.4)(1,.5)(Ph) endfont
```



### 4.4 Global setting

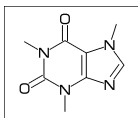
```
ratio_thickness_bond:=0.05;
beginfont() MCd(1,.4)(0,.5)(Ph) endfont
beginfont() MCd(1,.4)(.5,.5)(Ph) endfont
beginfont() MCd(1,.4)(1,.5)(Ph) endfont
```



## 4.5 Output molecular information

```
var3="calc_weight"; tag3="cMW";
var4="calc_formula"; tag4="cFM";
%% Output to mcf_man_soc-info.aux %%
..... ;C:85;cMW:194.19174;cFM:C8H10N4O2
```

cMW:calculated molecular weight  
cFM:calculated molecular formula

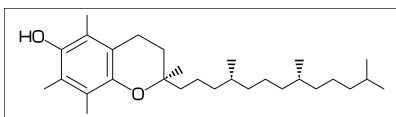


## 4.6 Output additional information

```
beginfont("EN:Tocopherol","CAS:59-02-9")
Mcf(...) endfont

%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc;C:86;EN:Tocopherol;CAS:59-02-9

*F:filename *C:char number EN:molecular name
CAS:CAS number *:default output
```

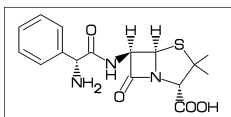


## 4.7 Change aux information delimiter

```
aux_delimiter:="/";
beginfont("EN:Ampicillin","CAS:69-53-4")
Mcf(...) endfont

%% Output to mcf_man_soc-info.aux %%
F:mcf_man_soc/C:90/EN:Ampicillin/CAS:69-53-4

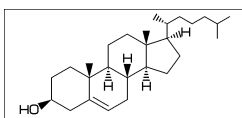
**default aux_delimiter=";"
```



## 4.8 Fixed aux information

```
tag3="NO"; var3="inf_NO";
tag4="EN"; var4="inf_EN";
sw_auxfix:=1; aux>tag_out;
beginfont("EN:Cholesterol","NO:1")
..... endfont
```

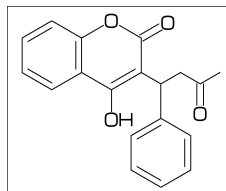
```
%% Output to mcf_man_soc-info.aux %%
F;C;NO;EN
mcf_man_soc;91;1;Ampicillin
```



## 5 MCF example

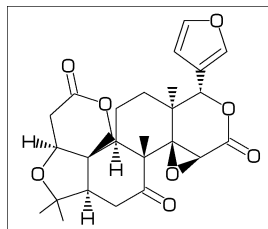
### 5.1 Warfarin

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



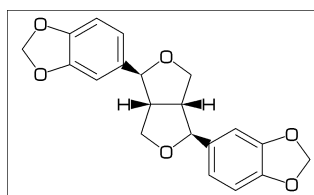
### 5.2 Limonin

```
<30,?6,$(-3,-4)?6,-5=?3,
-2=wf,-1=wb,6=?5,-4=?6,-5=wf,
@(13,15,17,20)0,@(3,12,21)//0,
@(4~wf^60,8~zf^60,18^35,18^-35)/Me,
@(1^60,5^180,16^60)*H,
14\*,|,?5,$(1,4)d1,3:0
```



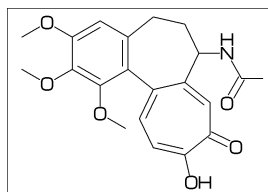
### 5.3 Sesamine

```
<54,?5,1=?5,
@(4,7)0,@(1^-54,2^54)*H,
#5*\^-12,Ph,|,-3=?5,@(-1,-3)0,
#8*\^-12,Ph,|,-3=?5,@(-1,-3)0
```



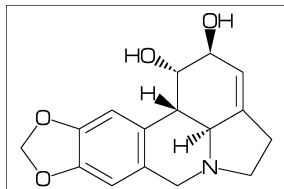
### 5.4 Colchicine

```
<30,Ph,@(1,2,6)/OMe,
-4=?7,-5=?7,
$(-1,-4,-6)d1,-2://0,-3:/OH,
9\,NH,!,//0,!
```



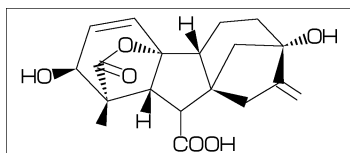
## 5.5 Lycorine

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



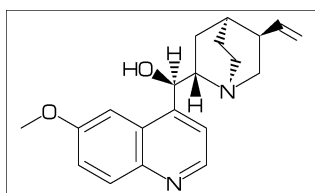
## 5.6 Gibberellin

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



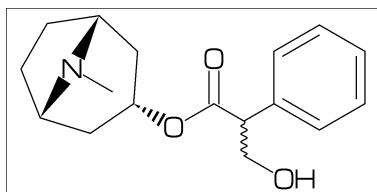
## 5.7 Quinine

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



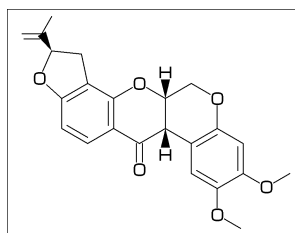
## 5.8 Atoropin

<-30, 0, !, //0, !, !, Ph,  
#1\~zb^120,  
|, ?7, 6\*\^190' 1.02, N, /Me, &3~wb,  
#3\~wv, !, OH



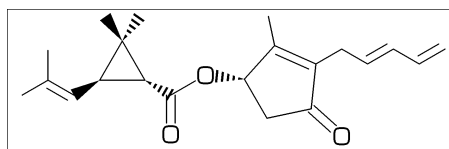
## 5.9 Rotenone

<-60, ?5, \$(-3, -2, -3, -4)?6,  
\$(7, 9, -2, -4)d1, \$(3, 17)dr,  
@(2, 13, 16)0, 10: //0, @(11^60, 12^60) \*/H,  
@(-2, -3)/OMe, 1\*\, /Me, !~d1



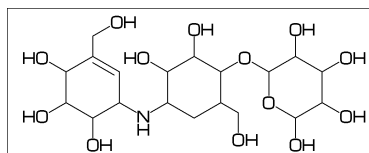
## 5.10 Pyrethrin I

<30, ?3, @ (3^35~wf, 3^35~zf) /Me,  
1\*\, !~d1, iPr, 2\*\, //0, !, 0, -36~zb, |,  
?5, -2=d, -1: /Me, -3: //0, -2\, !4, \$(-1, -3)d1



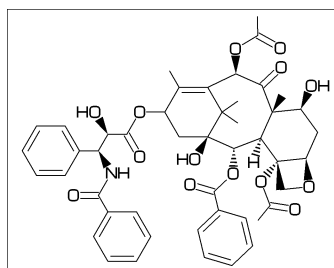
## 5.11 Validamycin

<30, ?6, @ (5, 6) /OH, 3\, -60, OH,  
#4\, 0, -60, |, ?6, 2: 0, @ (3, 4, 5, 6) /OH,  
#1\, NH, !, |, ?6, 2=d, @ (4, 5, 6) /OH, -4\, !, OH



## 5.12 Paclitaxel

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



## 6 Example to use mcf2graph

### 6.1 Molecular definition file

```
%-----  
input mcf2graph.mf;                                % input macro  
%-----  
sw_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";                            >  
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://0^15,5:/*COOH^-18,            >  
    @(6^35,6^-35)/Me,                                  >  
    4\^75,NH,! ,//0,! ,/*NH,! ,Ph)                   > end MCF  
endfont                                                > end font  
%-----  
beginfont("NO:2","EN:Cholesterol")                    > begin font(information)  
  MCF(<30,?6,$(-4,-2)?6,-4=?5,7=d1,                   > begin MCF (2)  
    1:*/OH,@(4,12)*/Me^60,9:*/H^60,                   >  
    10:*/H^180,@(11,-1)*/H^-60,                       >  
    -1\^17,/*Me,!4,/Me,! )                            > 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 ahandle=0 FILENAME (molecular difinition file)
```

(Output)

(sw\_auxfix=0)

```
F:mcf_man_soc;C:109;cMW:349.40462;cFM:C16H19N3O4S;EN:Ampicillin  
F:mcf_man_soc;C:110;cMW:386.6532;cFM:C27H46O;EN:Cholesterol  
.....  
.....
```

(sw\_auxfix=1)

```
F;C;cMW;cFM;EN  
mcf_man_soc;90;349.40462;C16H19N3O4S;Ampicillin  
mcf_man_soc;91;386.6532;C27H46O;Cholesterol  
.....  
.....
```

( tag : variable )

```
F : filename   C : char number   NO : serial number   EN : english name  
cMW : molecular weight calculated   cFM : molecular formula calculated  
MW  : molecular weight from literature data
```

### 6.3 Checklist output

(Insert option parameter setting)

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

(Command line)

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

(Output)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%  
% Molecular name = Caffeine  
% There were 0 warnings / Expanded command count= 75  
% width * height = 39.54677 * 36.84769  
% Shift width * height = -9.33592 * -12.77518  
% Bond length = 9.23628 Atom size = 4.12209  
% Atom count= 14 Bond count= 15 Ring count= 2 Hide H = 10  
%-----< atom >< bond >-----  
% 1 ( 0 ) ( 0 ) C 4  
% 2 ( 0.86603 ) ( -0.5 ) N 3  
% 3 ( 1.73206 ) ( 0 ) C 4  
% 4 ( 1.73206 ) ( 1 ) C 4  
% 5 ( 0.86603 ) ( 1.5 ) C 4  
% 6 ( 0 ) ( 1 ) N 3  
% 7 ( 2.6831 ) ( -0.30902 ) N 3  
% 8 ( 3.27089 ) ( 0.5 ) C 3  
% 9 ( 2.6831 ) ( 1.30902 ) N 3  
% 10 ( 0.86603 ) ( -1.38315 ) C 1  
% 11 ( -0.78764 ) ( 1.45474 ) C 1  
% 12 ( 2.95923 ) ( 2.15886 ) C 1  
% 13 ( -0.78764 ) ( -0.45474 ) O 2  
% 14 ( 0.86603 ) ( 2.38315 ) O 2  
%Bond list-----  
% 1 1 -> 2 ( 1)  
% 2 2 -> 3 ( 1)  
% 3 3 -> 4 ( 2)  
% 4 4 -> 5 ( 1)  
% 5 5 -> 6 ( 1)  
% 6 6 -> 1 ( 1)  
% 7 3 -> 7 ( 1)  
% 8 7 -> 8 ( 2)  
% 9 8 -> 9 ( 1)  
% 10 9 -> 4 ( 1)  
% 11 2 -> 10 ( 1)  
% 12 6 -> 11 ( 1)  
% 13 9 -> 12 ( 1)  
% 14 1 -> 13 ( 2)  
% 15 5 -> 14 ( 2)  
%Fomula / Molecular weight -----  
% C ( 12.0107 ) * 8 = 96.08557  
% H ( 1.00793 ) * 10 = 10.07935  
% N ( 14.0067 ) * 4 = 56.0268  
% O ( 15.9994 ) * 2 = 31.99881  
% Weight Calc: 194.19052 / Input: 194.19 / weight gap= 0.00052  
% Fomula Calc: C8H10N4O2 / Input: C8H10N4O2 / MACTCH  
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

## 6.4 Molfile output

(Insert option parameter setting)

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

(Command line)

```
>mpost -s ahangle=3 FILENAME (molecular difinition 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 D  0 0 0 0  
  0.86603    2.36383    0 D  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
```

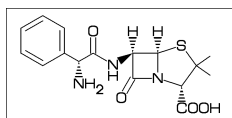
```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

## 6.5 L<sup>A</sup>T<sub>E</sub>X file example

```
%-----  
\documentclass[a4paper]{article}  
\usepackage{graphicx}  
\pagestyle{empty}  
\makeatletter%  
%-----  
\def\@F{F}\def\@C{C}\def\@EN{EN}\def\@NO{NO}\def\@MW{MW}\def\@FMc{FMc}%  
\def\@fst@param#1:#2;{#1}\def\@sec@param#1:#2;{#2}%  
\def\mol@sel#1{%  
\if#1empty\relax\else%  
  \edef\@tag{\expandafter\@fst@param#1;}%  
  \edef\@var{\expandafter\@sec@param#1;}%  
  \ifx\@tag\@F\edef\MOLfile{\@var}\fi%  
  \ifx\@tag\@C\edef\MOLchar{\@var}\fi%  
  \ifx\@tag\@EN\edef\MOLnameE{\@var}\fi%  
  \ifx\@tag\@NO\edef\MOLnum{\@var}\fi%  
  \ifx\@tag\@MW\edef\CALmw{\@var}\fi%  
  \ifx\@tag\@FMc\edef\CALfm{\@var}\fi%  
\fi}%  
\def\put@char{%  
  \begin{picture}(84,42)%  
    \put(0,38){\bf [MOLnum]\MOLnameE{ }\small\tt/FM:\CALfm/MW:\CALmw}%  
    \put(10,0){\font\@strufont=\MOLfile\relax%  
      \hbox{\@strufont\char\MOLchar}}%  
  \end{picture}%  
\def\INFO#1{\@for\@temp=#1\do{\mol@sel\@temp}\put@char}%  
\makeatother  
%-----  
\begin{document}  
\unitlength=1mm%  
\INFO{F:mcf_man_soc,C:103,NO:1,cMW:349.40462,cFM:C16H19N3O4S,EN:Ampicillin}%  
\INFO{F:mcf_man_soc,C:104,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

