Molecular Coding Format manual

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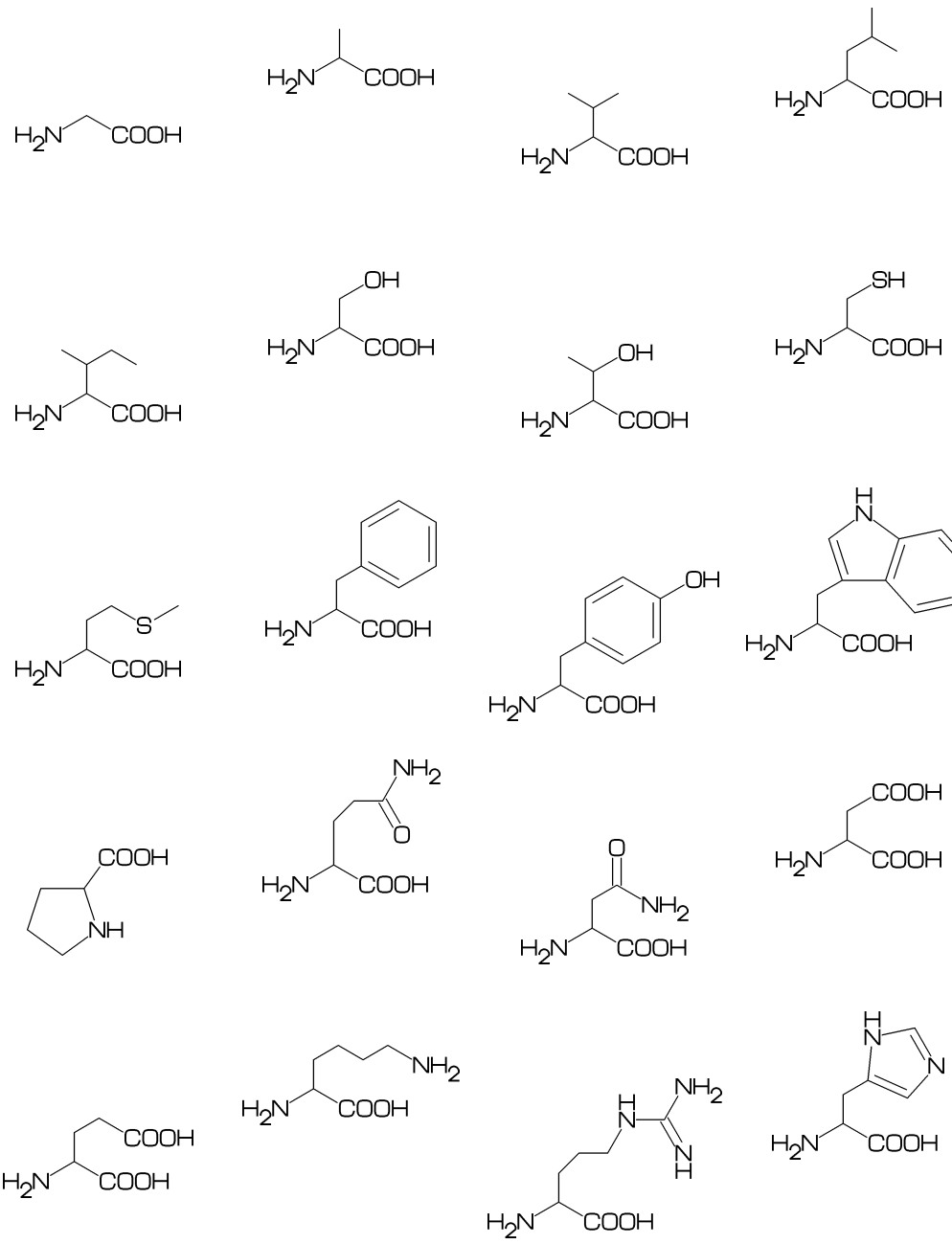
Located at http://www.ctan.org/pkg/mcf2graph



Contents

1 Introduction

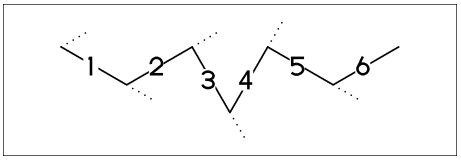
Molecular Coding Format(MCF) is new linear notation represent chemical structure diagrams. This 'Coding' is named from coding(programing) technique like adressing,grouping,macro,etc. There are no Meta language commands in MCF. mcf2graph.m convert MCF file to graphics file pk font,PNG,SVG,EPS or MDL MOL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

2 MCF syntax

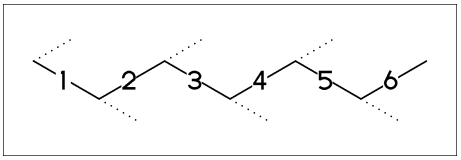
2.1 Make bond

2.1.1 Chain

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

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

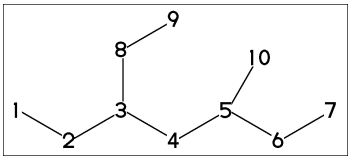



```
! : take value 60 or -60 depend on
      current angle and enviroment
!6 : !,!,!,!,!,!

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

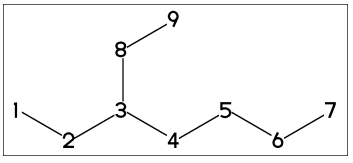


2.1.2 Jump and branch bond

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

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

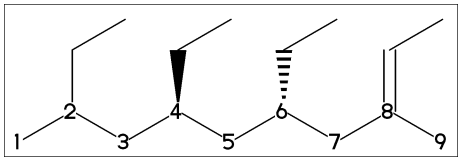



```
3\ : 3*,0

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

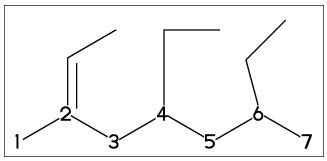


2.1.3 Branch bond

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

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

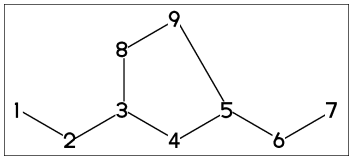



```
2\~dr  : 2*,0~dr
4\‘1.5 : 4*,0‘1.5
6\^15  : 6*,0^15

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



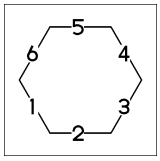
2.1.4 Connect atom

```
&n : Connect to An

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



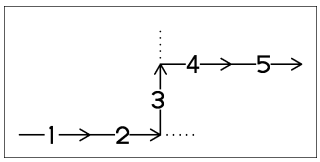
2.1.5 Ring

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



2.1.6 Rotate current angle

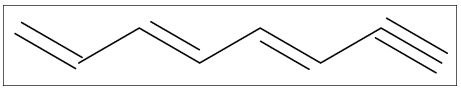
```
<angle : rotate current angle

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



2.2 Change bond type

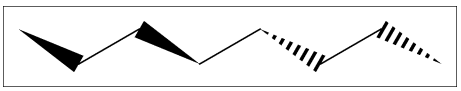
2.2.1 Double,triple

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

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



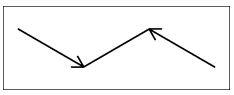
2.2.2 Wedge

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

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



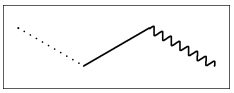
2.2.3 Vector

```
vf : vector forward
vb : vector backward

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



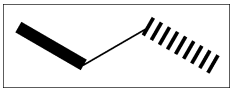
2.2.4 Dotted,wave

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

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



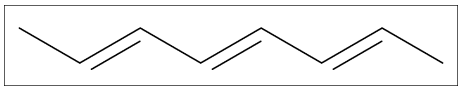
2.2.5 Broad

```
bd : broad
bz : broad dotted

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



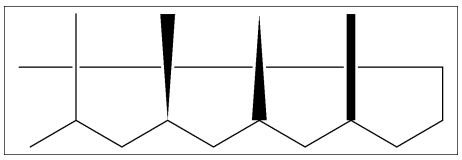
2.2.6 Change multi bond type

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

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



2.2.7 Over line

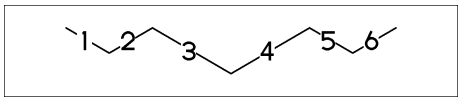
```
si_ : single over line
wf_ : wedge forward over line
wb_ : wedge backward over line
bd_ : broad over line

<-30,!8,!,60,90‘8,
@(2~si_,4~wf_,6~wb_,8~bd_)/Me‘2
```



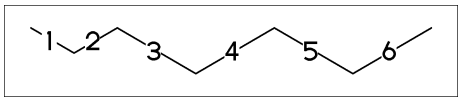
2.3 Change bond length

2.3.1 Chain length

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

<30,!2,!2‘1.2,!2

** !2‘1.2 : ’‘1.2,!2
```

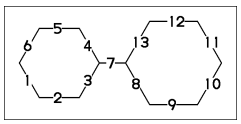



```
‘‘length : change all bond length after

<30,!2,‘‘1.2,!4
```



2.3.2 Ring length

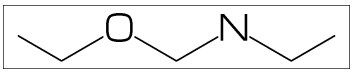
```
?n‘length : change ring length

?6,4\,?6‘1.2
```



2.4 Change atom

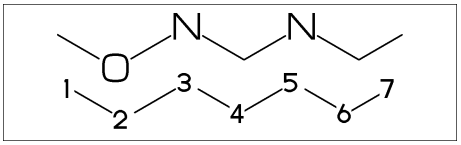
2.4.1 Insert atom

```
Insert hetero atom

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



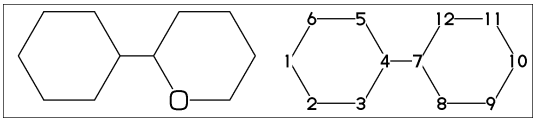
2.4.2 Addressed atom

```
2:O : change A2 C to O
@(3,5)N : change  A3,A5 C to N

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

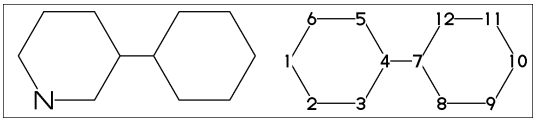


2.4.3 Brock address

```
| : divide brock

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

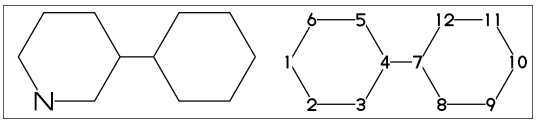


```
|| : reset brock adress

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



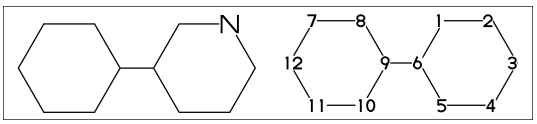
2.4.4 Absolute address

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

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



2.4.5 Relative address

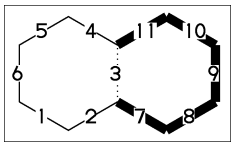
```
-2:N : change A(-2) C to N
** -n : (1<=n<=999)

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



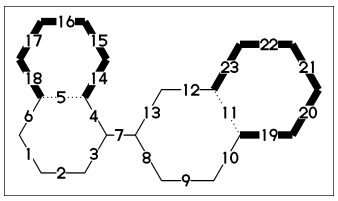
2.5 Fuse ring

2.5.1 Attached 1 bond

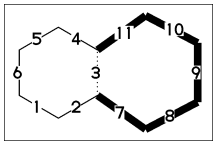
```
?6,3=?6 : fuse ?6 at B3
** Bn(n:-999<=n<=4095): bond number

?6,3=?6
```



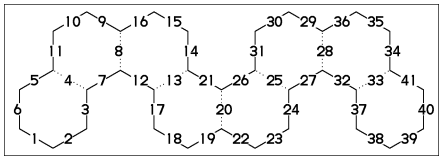
```
** fused ring size depend on
attached bond length

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



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

?6,3=?6[13]
```

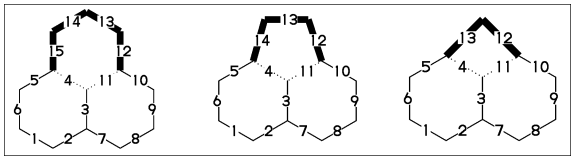


```
?6,$(-3,-4,-4,-2,-2,-4,-4)?6
?6,$(4,8,13,20,25,28,33)?6
```



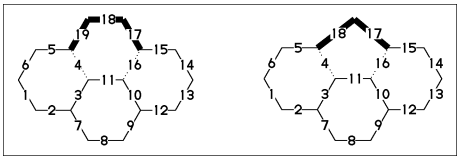
2.5.2 Attached 2 bond

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

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])
```



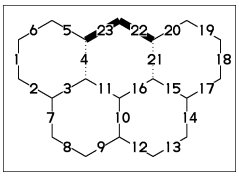
2.5.3 Attached 3 bond

```
(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])
```



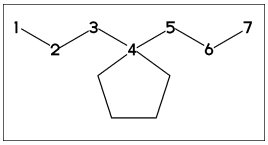
2.5.4 Attached 4 bond

```
(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

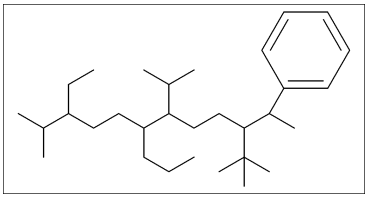
```
4*,?5 : add ?5(5 membered ring) at A4

<30,!6,4*,?5

An* : jump to An
```



2.6 Substituent

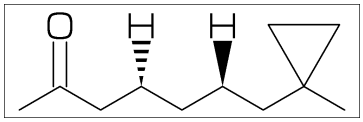
2.6.1 Insert substituent

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

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

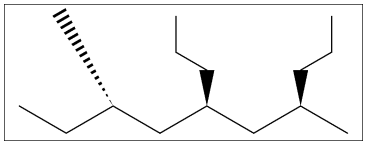


2.6.2 Insert modified substituent

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

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

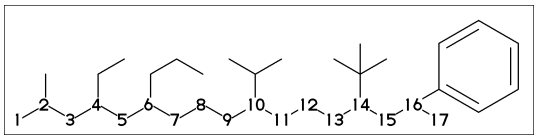


```
~ : change type
^ : change angle
‘ : change length
> : change enviroment

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



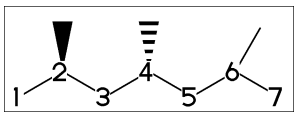
2.6.3 Add substituent

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

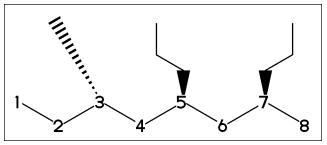


2.6.4 Add modified substituent

```
~,^,‘ : change type,angle,length

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



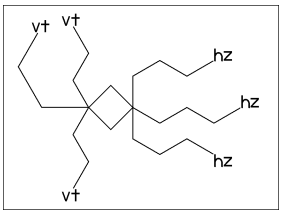
```
^,‘,> : change angle,length,environment

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



2.7 Chain environment

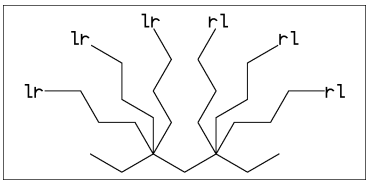
2.7.1 Horizontal,vertical

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

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



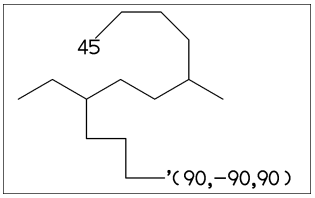
2.7.2 Left-right,right-left

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

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



2.7.3 Fixed angle,multi angle

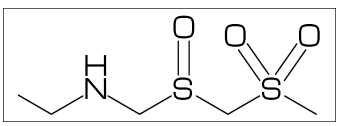
```
>45 : fixed angle enviroment
>'(-90,90,-90) : multi angle enviroment

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



2.8 Miscellaneous

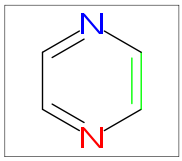
2.8.1 Change atom and Substituent

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

<30,!2,NH,!,SO,!,SOO,!3
```



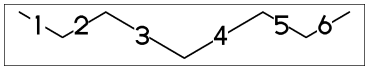
2.8.2 Change color

```
@(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
```



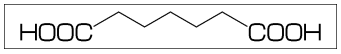
2.8.3 Make block

```
{ : start brock
} : end brock

<30,!2,{,‘‘1.2,!2,},!2
```

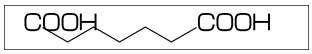


2.8.4 Chain start multiple characters

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

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

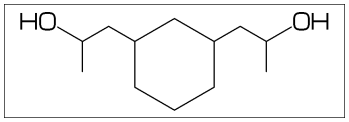



```
MCf(<30,COOH,!4,COOH)
```



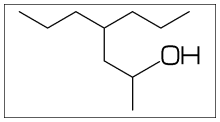
2.8.5 User definition

```
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
```

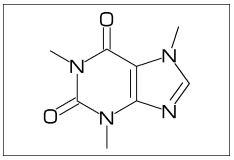


3 Option parameter

3.1 Size parameter

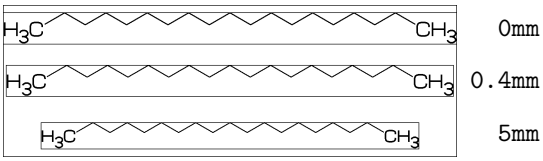
3.1.1 Font size

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



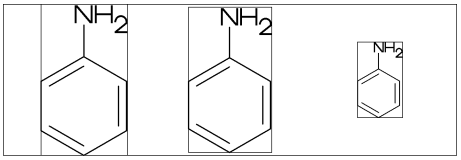
3.1.2 Margin left and right

default: margin_left_right=0.4mm



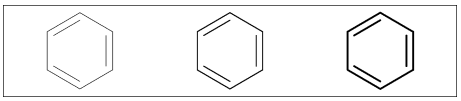
3.1.3 Margin top and bottom

default: margin_top_bottom=0.4mm



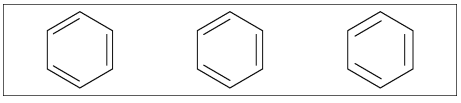
3.1.4 Offset thickness of bond

default: offset_thickness#=0.2pt#



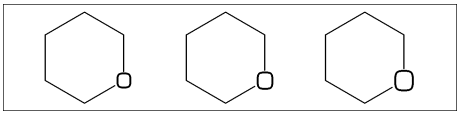
3.1.5 Offset of doublebond gap

default: offset_bond_gap#=0.3pt#



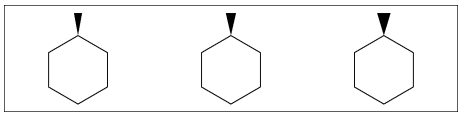
3.1.6 Offset of atom width

default: offset_atom#=0.8pt#



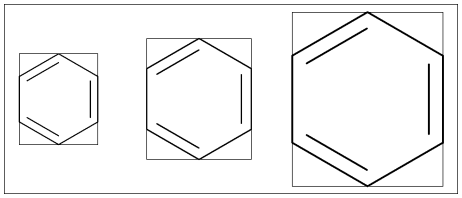
3.1.7 Offset of wedge width

default: offset_wedge#=0.4pt#



3.1.8 Max bond length

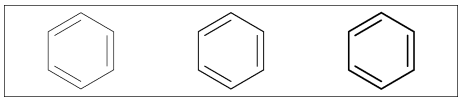
default: max_bond_length#=10mm#



3.2 Ratio parameter

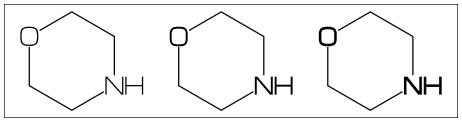
3.2.1 Thickness/bond length

default: ratio_thickness_bond=0.015



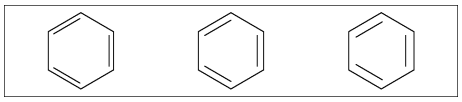
3.2.2 Char/bond thickness

default: ratio_char_bond=1.5



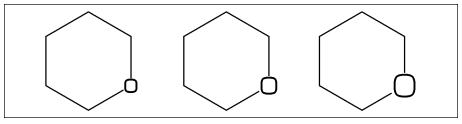
3.2.3 Bondgap/bond length

default: ratio_bondgap_bond= 0.15



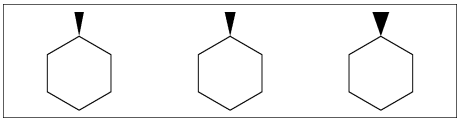
3.2.4 Atom/bond length

default: ratio_atom_bond= 0.36



3.2.5 Wedge/bond length

default: ratio_wedge_bond=0.12

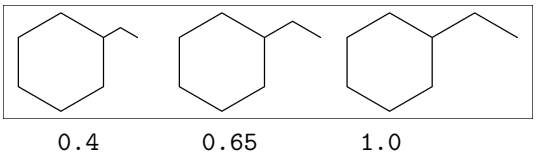


3.2.6 Font atom gap/atom length

default: ratio_atomgap_atom= 0.050

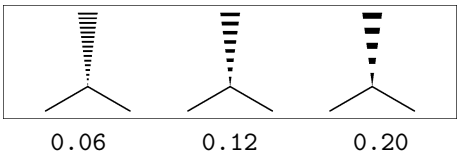
3.2.7 Chain/ring length

default: ratio_chain_ring= 0.66



3.2.8 Zebra gap/bond length

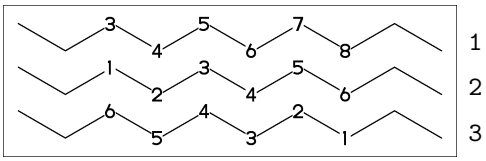
default: ratio_zebragap_bond=0.12



3.3 Drawing mode

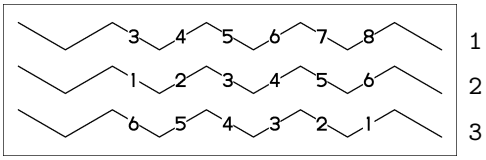
3.3.1 Numbering atom

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



3.3.2 Numbering bond

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



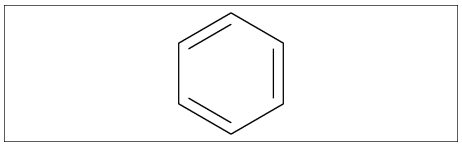
3.3.3 Clipping mode

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

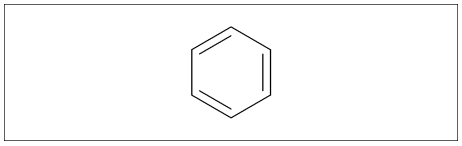
sw_clip:=1;
MCd(1,0.7)(0.2,0.3)(Ph)
MCd(1,0.7)(0.8,0.7)(Ph)

3.3.4 Solid mode

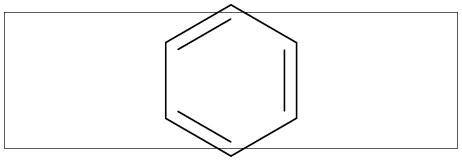
(fit to font size)
sw_solid=0 ** default



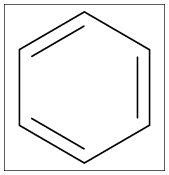
(solid ratio bond/font width)
sw_solid:=1;
ratio_bond_width=0.1
font_width=60mm
(bond_len#=60mm#*0.1=6mm#)
** ignore bond_len#



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

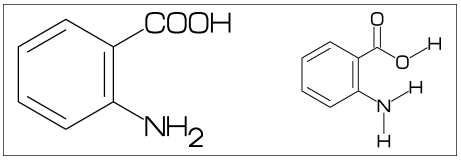


(solid bond length and clip)
sw_solid:=2;
sw_clip:=1;
bond_len#=10mm#



3.3.5 Expand mode

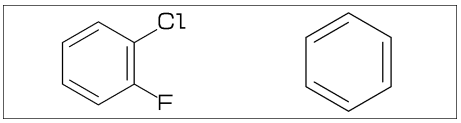
```
default:  sw_expand=0
```



0 :default 1

3.3.6 Substituent off mode

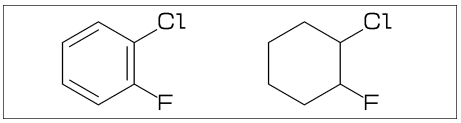
```
default:  sw_subst_off=0
```



0 :default 1

3.3.7 Single bond mode

```
default:  sw_bond_single=0
```

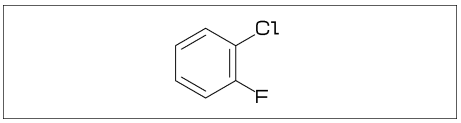


0 :default 1

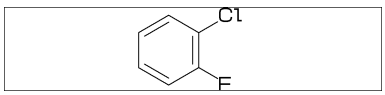
3.4 Frame

3.4.1 Font frame

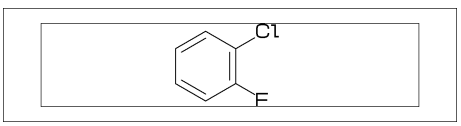
```
(Draw font frame)
margin_left_right:=5mm;
margin_top_bottom:=2mm;
sw_font_frame:=1;
MCf(<30,Ph,4:/Cl,3:/F)
```




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

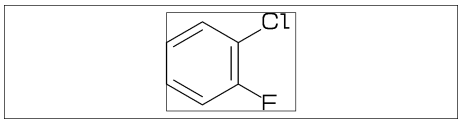



```
(Draw both frame)
sw_font_frame=3
```



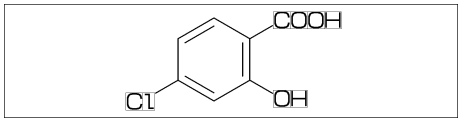
3.4.2 Molecular frame

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



3.4.3 Atom frame

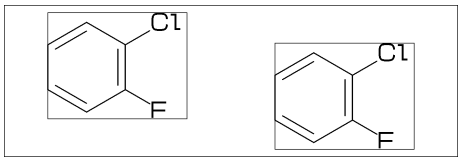
```
sw_atom_frame:=1;
MCf(<30,Ph,1:/Cl,4:/COOH,3:/OH)
** default: sw_atom_frame=0
```



4 Function

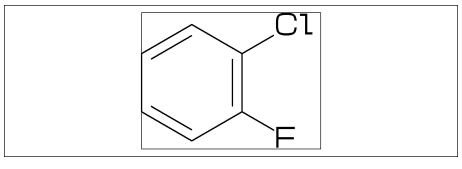
4.1 Function MCd()

```
(Draw molecular structure)

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

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



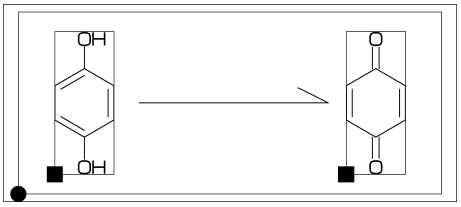
4.2 Function MCf()

```
(Draw fit to font size)

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

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



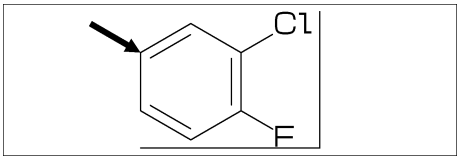
4.3 Function EXT()

```
(Extra graphic to font)
  w:  font width
  h:  font height
  wd: font width-margin_left_right*2
  ht: font height-margin_top_bottom*2
  p0: x=margin_left_right
      y=margin_top_bottom
  n:  molecular number
  p[m]: molecular origin position
        (1<=m<=molecular count)

  beginfont()
  sw_mol_frame:=1;
  MCd(1,0.8)(0.1,0.5)(<30,Ph,2:/OH,5:/OH)
  MCd(1,0.8)(0.9,0.5)
    (<30,?6,$(3,6)dl,@(2,5)//O)
  EXT(
  draw ((0,0)--(25mm,0)--(21mm,2mm))
       shifted (0.3w,0.5h);
  drawdot p0 withpen pencircle scaled 2mm;
  drawdot p1 withpen pensquare scaled 2mm;
  drawdot p2 withpen pensquare scaled 2mm;
  )
  endfont
```



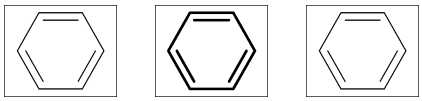
4.4 Function ext()

```
(Extra graphic to molecule)
  wd: molecular width
  ht: molecular height
  p0: origin of molecular structure
  n:  atom number
  l:  bond length
  p[m]: atom position of A[m]
  a[m]: branch angle of A[m]
        (1<=m<=atom count)
  draw_vector(position,angle,length)

  beginfont()
    MCf(<30,Ph,3:/F,4:/Cl)
    ext(draw p0--(p0+(wd,0))
             --(p0+(wd,ht);
        draw_vector(p6,a6-180,l);
    )
  endfont
```



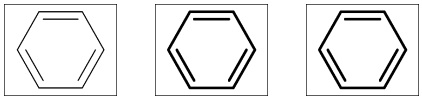
4.5 Local parameter setting

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



4.6 Global parameter setting

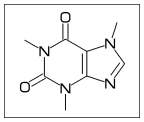
```
  beginfont() MCf(Ph) endfont
  ratio_thickness_bond:=0.05;
  beginfont() MCf(Ph) endfont
  beginfont() MCf(Ph) endfont
```



5 Output information

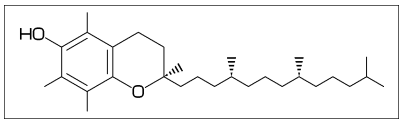
5.1 Output molecular information

```
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
```



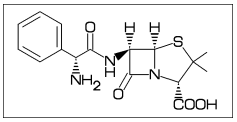
5.2 Output additional information

```
beginfont("EN:Tocopherol","CAS:59-02-9")
  MCf(<30,Ph,3=?6,
     7:O,@(1,2,5)/Me,8:/*Me^60,6:/OH,
     8\,|,!12,@(4,8)/*Me,12:/Me)
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
```



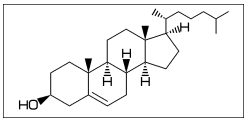
5.3 Change aux information delimiter

```
aux_delimiter:="/";
beginfont("EN:Ampicillin","CAS:69-53-4")
  MCf(<45,?4,2:N,2=?5,-1:S,
    @(3^45,4^-45)/*H,1://O^15,
    5:/*COOH^-18,@(6^35,6^-35)/Me,
    4*\^75,NH,!,//O,!,/*NH2,!,Ph)
endfont
beginfont(......)
  ..........
endfont
..............

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

  **default  aux_delimiter=";"
```



5.4 Fixed aux information

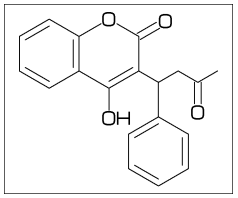
```
  tag3:="NO"; var3:="inf_NO";
  tag4:="EN"; var4:="inf_EN";
  sw_auxfix:=1; auxtag_out;
  beginfont("EN:Cholesterol","NO:1")
  MCf(<30,?6,$(-4,-2)?6,-4=?5,7=dl,
      1:*/OH,@(4,12)*/Me^60,9:*/H^60,
      10:/*H^180,11:/*H^-60,17:/*H^-54,
      -1\^18,/*Me,-60,!3,/Me,!)
  endfont
  beginfont(......)
    ..........
  endfont
  ..............

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



6 MCF example

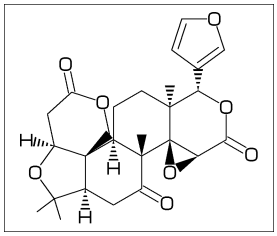
6.1 Warfarin

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



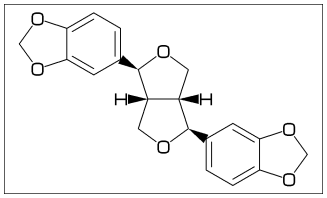
6.2 Limonin

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



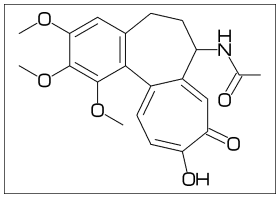
6.3 Sesamine

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



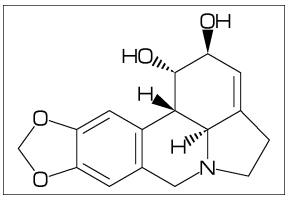
6.4 Colchicine

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



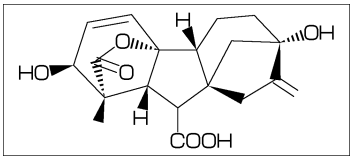
6.5 Lycorine

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



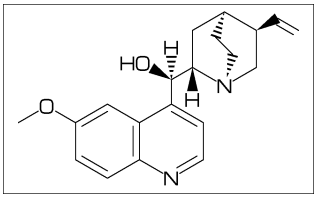
6.6 Gibberellin

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



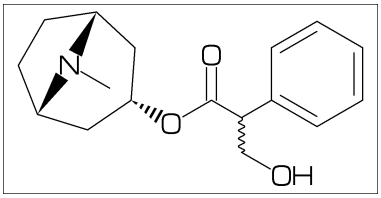
6.7 Quinine

```
<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
```



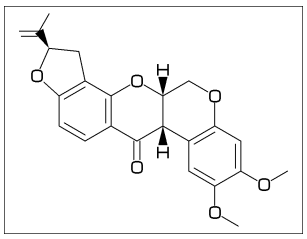
6.8 Atoropin

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



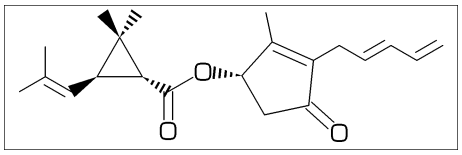
6.9 Rotenone

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



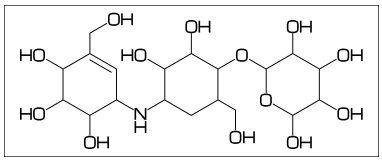
6.10 Pyrethrin I

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



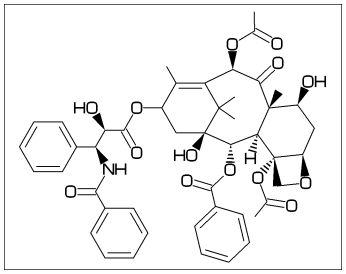
6.11 Validamycin

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



6.12 Paclitaxel

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



7 Example to use mcf2graph

7.1 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://O^15,5:/*COOH^-18,             >
     @(6^35,6^-35)/Me,                                   >
     4\^75,NH,!,//O,!,/*NH,!,Ph)                         > end MCF
endfont                                                  > end font
%-------------------------------------------------------------------------
beginfont("NO:2","EN:Cholesterol")                 > begin font(information)
  MCf(<30,?6,$(-4,-2)?6,-4=?5,7=dl,                      > begin MCF (2)
      1:*/OH,@(4,12)*/Me^60,9:*/H^60,                    >
      10:/*H^180,@(11,-1)/*H^-60,                        >
      -1\^17,/*Me,!4,/Me,!)                              > end MCF
endfont                                                  > end font
%-------------------------------------------------------------------------
bye
```

7.2 Information auxfile output

(Insert option parameter setting)

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

(Command line)

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

(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
```

7.3 Checklist output

(Insert option parameter setting)

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

(Command line)

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

(Output)

```
%-------------------------------------------------------------------
%  Molecular name = Caffeine
%  Warnings =   0 / Expanded command = 75
%  Width * Height =  39.5496 * 36.85023
%  Shift width * height  = -9.33653 * -12.77606
%  Bond length = 9.23695   Atom size   = 4.12231
%  Atom count= 14 Bond count= 15 Ring count=  2 Hide H count= 10
%-------------------------------------------------------------------
%< NO.  >< x axis  , y axis >< atom  >< bond >< hide_H >
%  A1    (      0 ,       0 )  C           4
%  A2    (  0.866 ,    -0.5 )  N           3
%  A3    (  1.732 ,       0 )  C           4
%  A4    (  1.732 ,       1 )  C           4
%  A5    (  0.866 ,     1.5 )  C           4
%  A6    (      0 ,       1 )  N           3
%  A7    (  2.683 ,  -0.309 )  N           3
%  A8    (  3.271 ,     0.5 )  C           3       1
%  A9    (  2.683 ,   1.309 )  N           3
%  A10   (  0.866 ,  -1.383 )  C           1       3
%  A11   ( -0.788 ,   1.455 )  C           1       3
%  A12   (  2.959 ,   2.159 )  C           1       3
%  A13   ( -0.788 ,  -0.455 )  O           2
%  A14   (  0.866 ,   2.383 )  O           2
%-------------------------------------------------------------------
%< NO.  ><  bond   (sdt)><angle + (  +-  )><length (   pt   )>
%  B1     1 ->   2 (  1)      330 (   -30)       1 (    9.24)
%  B2     2 ->   3 (  1)       30 (    30)       1 (    9.24)
%  B3     3 ->   4 (  2)       90 (    90)       1 (    9.24)
%  B4     4 ->   5 (  1)      150 (   150)       1 (    9.24)
%  B5     5 ->   6 (  1)      210 (  -150)       1 (    9.24)
%  B6     6 ->   1 (  1)      270 (   -90)       1 (    9.24)
%  B7     3 ->   7 (  1)      342 (   -18)       1 (    9.24)
%  B8     7 ->   8 (  2)       54 (    54)       1 (    9.24)
%  B9     8 ->   9 (  1)      126 (   126)       1 (    9.24)
%  B10    9 ->   4 (  1)      198 (  -162)    0.66 (     6.1)
%  B11    2 ->  10 (  1)      270 (   -90)    0.66 (     6.1)
%  B12    6 ->  11 (  1)      150 (   150)    0.66 (     6.1)
%  B13    9 ->  12 (  1)       72 (    72)    0.66 (     6.1)
%  B14    1 ->  13 (  2)      210 (  -150)    0.66 (     6.1)
%  B15    5 ->  14 (  2)       90 (    90)    0.66 (     6.1)
%-------------------------------------------------------------------
% 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
%===================================================================
```

7.4 Molfile output

(Insert option parameter setting)

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

(Command line)

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

(Output)

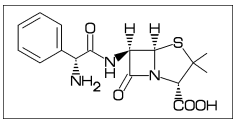
```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  -MCFtoMOL- EN:Caffeine

 14 15  0  0  0  0  0  0  0  0999 V2000
        0         0         0 C   0  0  0  0
   0.86603      -0.5         0 N   0  0  0  0
   1.73206         0         0 C   0  0  0  0
   1.73206         1         0 C   0  0  0  0
   0.86603       1.5         0 C   0  0  0  0
        0         1         0 N   0  0  0  0
    2.6831  -0.30902         0 N   0  0  0  0
   3.27089       0.5         0 C   0  0  0  0
    2.6831   1.30902         0 N   0  0  0  0
   0.86603  -1.36383         0 C   0  0  0  0
  -0.76894   1.44394         0 C   0  0  0  0
  -0.76894  -0.44394         0 O   0  0  0  0
   0.86603   2.36383         0 O   0  0  0  0
   2.95299    2.1396         0 C   0  0  0  0
  1  2  1  0     0  0
  2  3  1  0     0  0
  3  4  2  0     0  0
  4  5  1  0     0  0
  5  6  1  0     0  0
  6  1  1  0     0  0
  3  7  1  0     0  0
  7  8  2  0     0  0
  8  9  1  0     0  0
  9  4  1  0     0  0
  2 10  1  0     0  0
  6 11  1  0     0  0
  1 12  2  0     0  0
  5 13  2  0     0  0
  9 14  1  0     0  0
M  END
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

7.5 LaTeX file example

```
%-----------------------------------------------------------------------
\documentclass[a4paper]{article}
\usepackage{graphicx}
\pagestyle{empty}
\makeatletter%
%-----------------------------------------------------------------------
\def\@F{F}\def\@C{C}\def\@EN{EN}\def\@NO{NO}\def\@MW{MW}\def\@FMc{FMc}%
\def\@fst@param#1:#2;{#1}\def\@sec@param#1:#2;{#2}%
\def\mol@sel#1{%
\if#1\empty\relax\else%
  \edef\@tag{\expandafter\@fst@param#1;}%
  \edef\@var{\expandafter\@sec@param#1;}%
  \ifx\@tag\@F\edef\MOLfile{\@var}\fi%
  \ifx\@tag\@C\edef\MOLchar{\@var}\fi%
  \ifx\@tag\@EN\edef\MOLnameE{\@var}\fi%
  \ifx\@tag\@NO\edef\MOLnum{\@var}\fi
  \ifx\@tag\@MW\edef\CALmw{\@var}\fi
  \ifx\@tag\@FMc\edef\CALfm{\@var}\fi
\fi}%
\def\put@char{%
  \begin{picture}(84,42)%
     \put(0,38){\bf [\MOLnum]\MOLnameE{ }\small\tt/FM:\CALfm/MW:\CALmw}%
     \put(10,0){\font\@strufont=\MOLfile\relax%
                \hbox{\@strufont\char\MOLchar}}%
  \end{picture}%
\def\INFO#1{\@for\@temp:=#1\do{\mol@sel\@temp}\put@char}%
\makeatother
%-----------------------------------------------------------------------
\begin{document}
\unitlength=1mm%
\INFO{F:mcf_man_soc,C:114,NO:1,cMW:349.40462,cFM:C16H19N3O4S,EN:Ampicillin}%
\INFO{F:mcf_man_soc,C:115,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