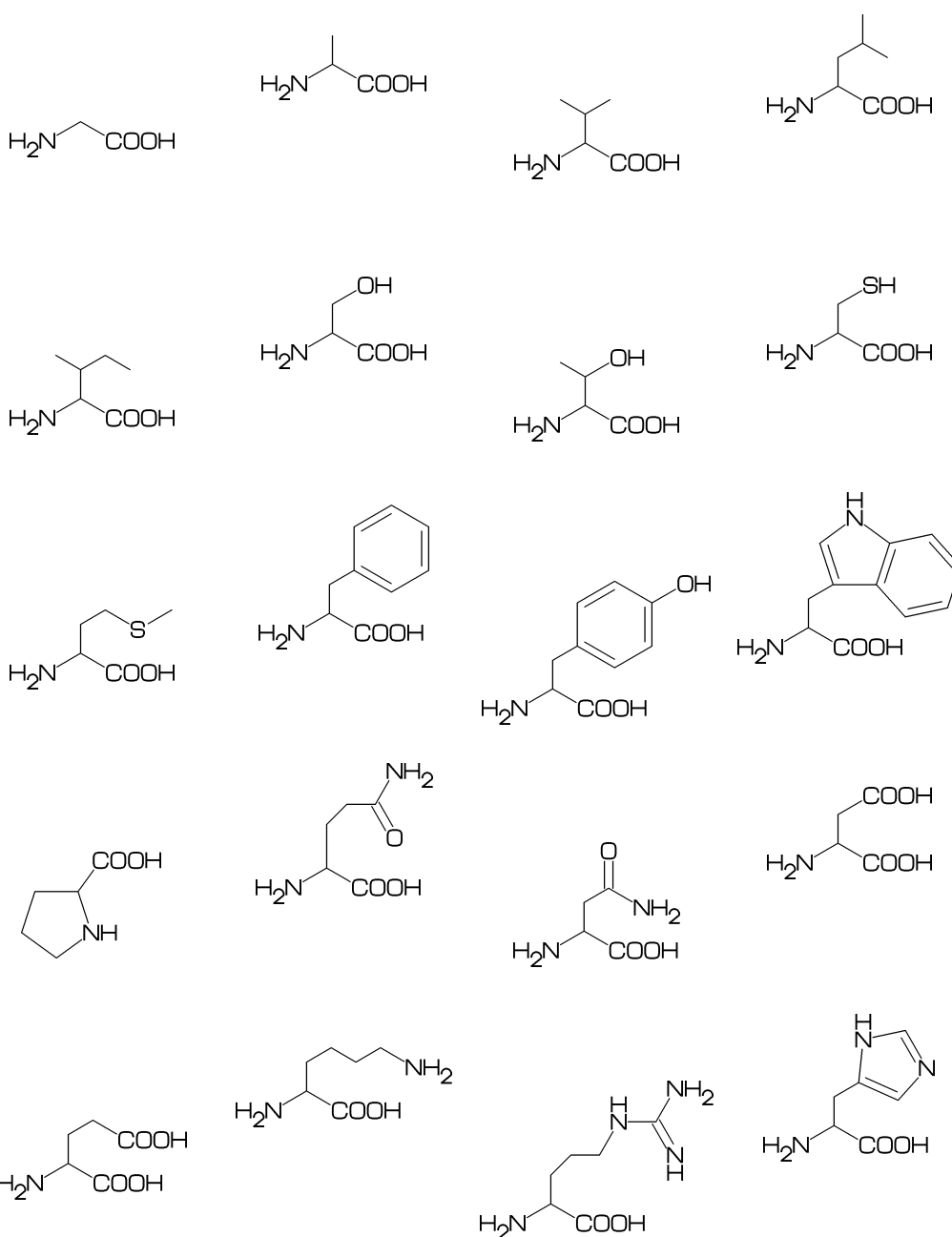


Molecular Coding Format manual

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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).

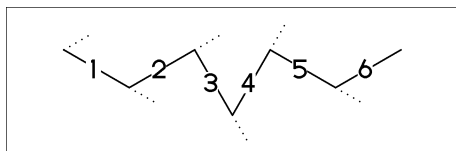
2 MCF syntax

2.1 Make bond

2.1.1 Chain

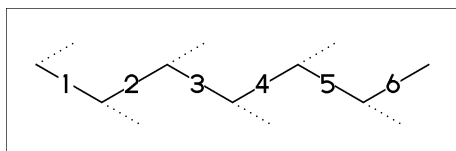
real number plus (+): anticlockwise
real number minus(-): clockwise

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



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

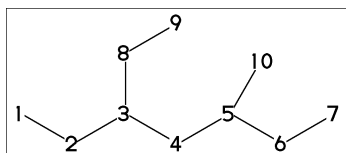
<30,! ,! ,! ,! ,! ,!
<30,!6



2.1.2 Jump and branch bond

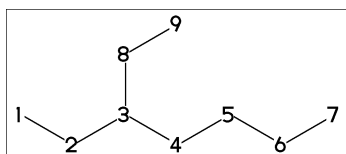
n* : Jump to An
** An: atom number(-999<=n<=4095)

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



3\ : 3*,0

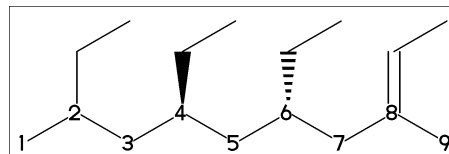
<30,!6,3\,! ,



2.1.3 Branch bond

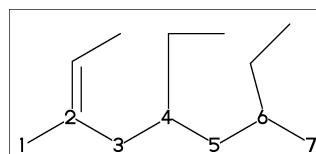
2\ : 2*,0
4*\ : 4*,0~wf
6* : 6*,0~zf
8\\ : 8*,0~dm

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



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

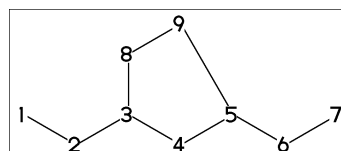
<-30,!6,
2\~dr,! ,
4\'1.5,-90,
6\^15,-60



2.1.4 Connect atom

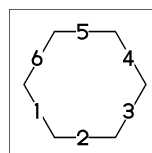
&n : Connect to An

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



2.1.5 Ring

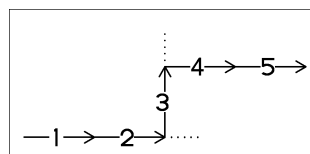
?n : n membered ring(3<=n<=20)
?6 : <-120,60,60,60,60,60,&1
?6



2.1.6 Rotate current angle

<angle : rotate current angle

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

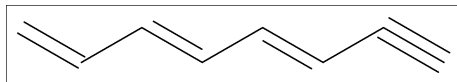


2.2 Change bond type

2.2.1 Double, triple

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

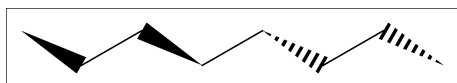
<30,!~dm,!~dl,!~dr,!~tm



2.2.2 Wedge

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

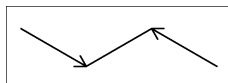
<30,!~wf,!~wb,!~zf,!~zb



2.2.3 Vector

vf : vector forward
vb : vector backward

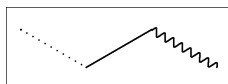
<30,!~vf,!~vb



2.2.4 Dotted, wave

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

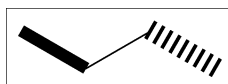
<30,!3,1=dt,3=wv



2.2.5 Broad

bd : broad
bz : broad dotted

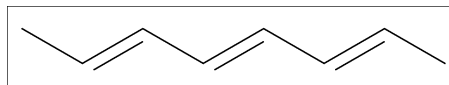
<30,!3,1=bd,3=bz



2.2.6 Change multi bond type

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

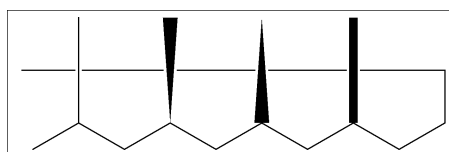
<30,!7,\$(2,4,6)dr



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



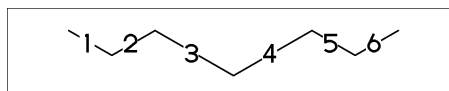
2.3 Change bond length

2.3.1 Chain length

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

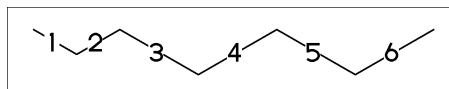
<30,!2,!2'1.2,!2

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



''length : change all bond length after

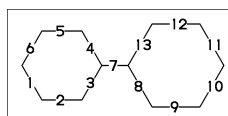
<30,!2, ''1.2,!4



2.3.2 Ring length

?n'length : change ring length

?6,4\,?6'1.2

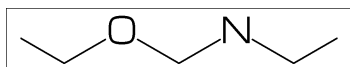


2.4 Change atom

2.4.1 Insert atom

Insert hetero atom

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

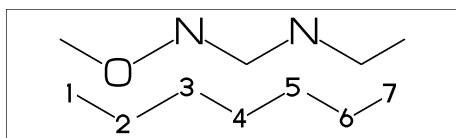


2.4.2 Addressed atom

2:0 : change A2 C to O

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

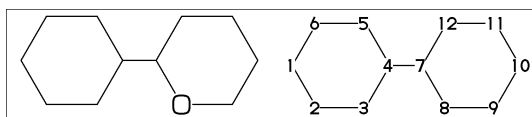
<30,!6,2:0,@(3,5)N



2.4.3 Brock address

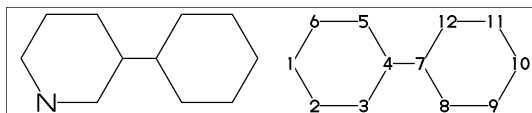
| : divide brock

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



|| : reset brock address

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

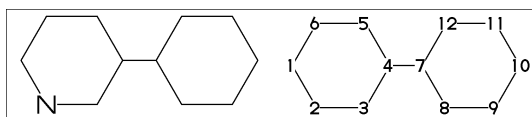


2.4.4 Absolute address

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

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

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

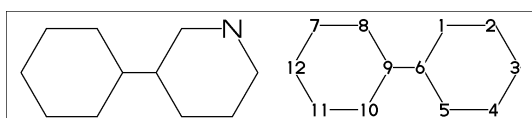


2.4.5 Relative address

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

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

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



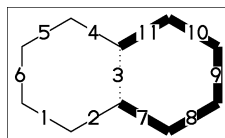
2.5 Fuse ring

2.5.1 Attached 1 bond

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

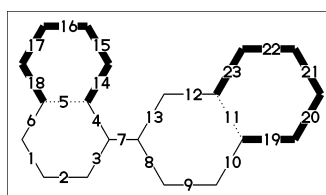
** Bn(n:-999<=n<=4095): bond number

?6,3=?6



** fused ring size depend on attached bond length

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

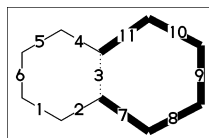


?6,3=?6[13] : fuse ?6[13] at B3

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

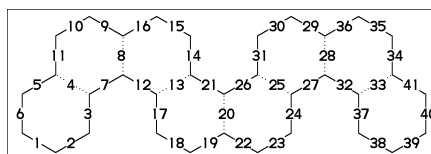
** ?m[n] (5<=m<=8,11<=n<=15)

?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

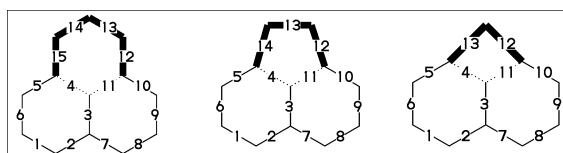
(4,11)=?4[2] : fuse 2/4 ring to B11..B4

** ?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])

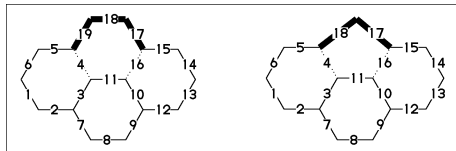
MCd(1,.6)(1,0)(<30,?6,3=?6,(11,4)=?4[2])



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])

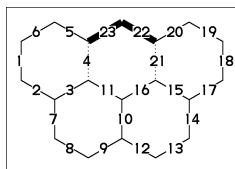


2.5.4 Attached 4 bond

(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)

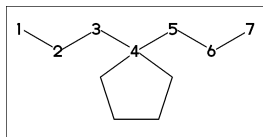


2.5.5 Spiro ring

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

<30,!6,4*,?5

An* : jump to An

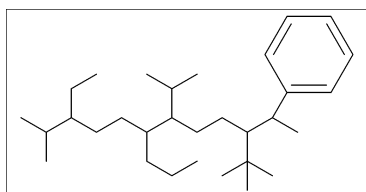


2.6 Substituent

2.6.1 Insert substituent

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

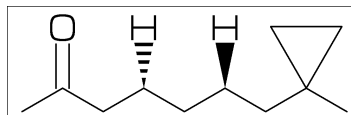
** Me:methyl Et:ethyl
 Pr:propyl iPr:isopropyl
 tBu:tertial buthyl Ph:phenyl



2.6.2 Insert modified substituent

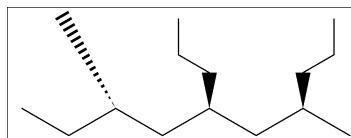
/ : single
 // : double
 */ : wedge forward
 /* : wedge dotted forward
 ** : direct

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



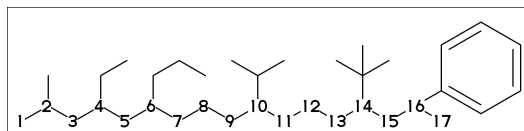
~ : change type
 ^ : change angle
 ' : change length
 > : change enviroment

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



2.6.3 Add substituent

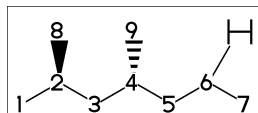
<-30,!17,2:/Me,4:/Et,6:/Pr,
 10:/iPr,14:/tBu,16:/Ph^-60



2.6.4 Add modified substituent

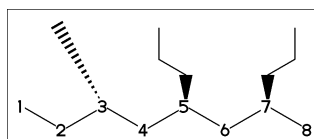
~,^,' : change type,angle,length

<-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

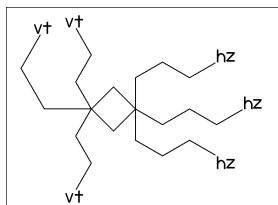


2.7 Chain environment

2.7.1 Horizontal,vertical

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

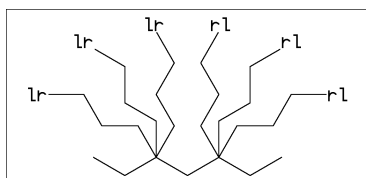
```
?4,@(3^-90,3^-30,3^90)/'(!3,"{hz}")>hz,  
  @(1^-60,1'^2,1^60)/'(!2,"{vt}")>vt
```



2.7.2 Left-right,right-left

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

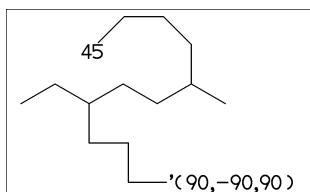
```
<30,!6,  
  @(3^-30,3,3^30)/'(!3,"{lr}")>lr,  
  @(5^-30,5,5^30)/'(!3,"{rl}")>rl
```



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)}")
```

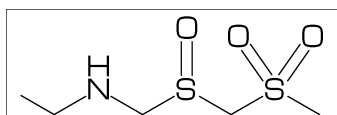


2.8 Miscellaneous

2.8.1 Change atom and Substituent

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

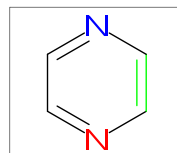
```
<30,!2,NH,! ,S0,! ,S00,!3
```



2.8.2 Change color

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

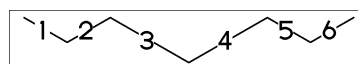
```
<30,Ph,@(2,5)N,2:red,5:blue,3=green
```



2.8.3 Make block

{ : start block
} : end block

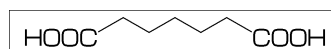
```
<30,!2,{,'1.2,!2,},!2
```



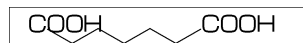
2.8.4 Chain start multiple characters

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

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



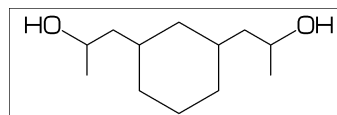
```
MCf(<30,COOH,!4,COOH)
```



2.8.5 User definition

iBuOH : user defined substructure

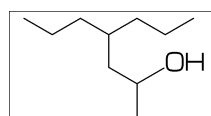
```
iBuOH:= '(!,/Me,! ,OH)  
MCf(<30,!6,@(4,6)/iBuOH)
```



2.8.6 Inline definition

Insert user defined substructure

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

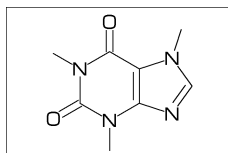


3 Option parameter

3.1 Size parameter

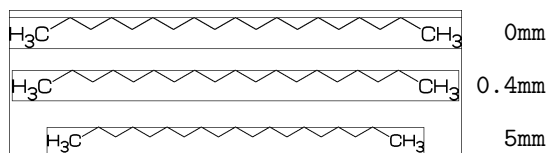
3.1.1 Font size

```
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)//O) endfont
```



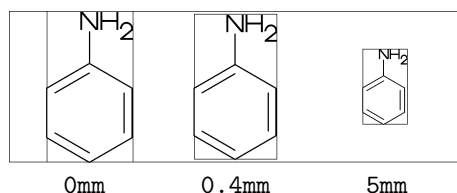
3.1.2 Margin left and right

default: margin_left_right=0.4mm



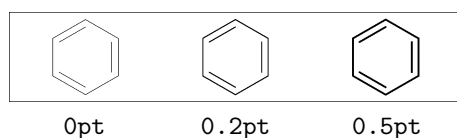
3.1.3 Margin top and bottom

default: margin_top_bottom=0.4mm



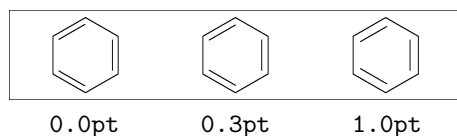
3.1.4 Offset thickness of bond

default: offset_thickness#=0.2pt#



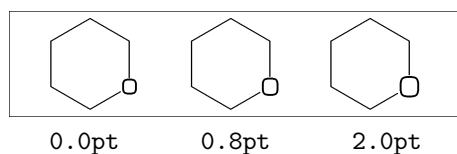
3.1.5 Offset of doublebond gap

default: offset_bond_gap#=0.3pt#



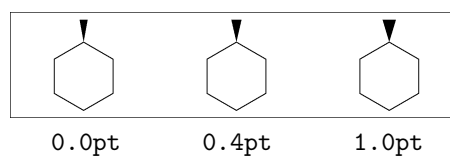
3.1.6 Offset of atom width

default: offset_atom#=0.8pt#



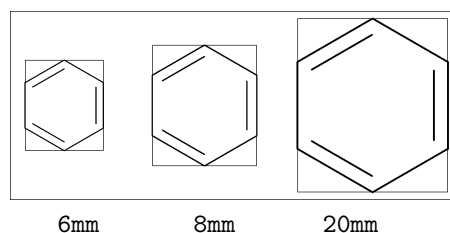
3.1.7 Offset of wedge width

default: offset_wedge#=0.4pt#



3.1.8 Max bond length

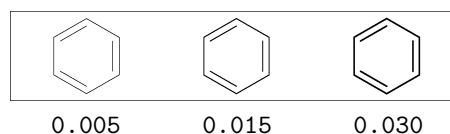
default: max_bond_length#=10mm#



3.2 Ratio parameter

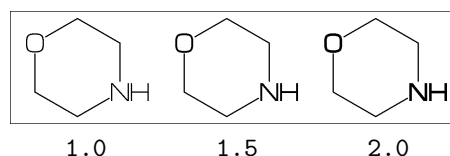
3.2.1 Thickness/bond length

default: ratio_thickness_bond=0.015



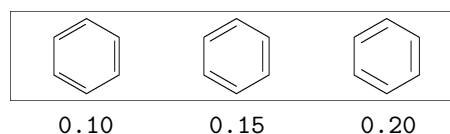
3.2.2 Char/bond thickness

default: ratio_char_bond=1.5



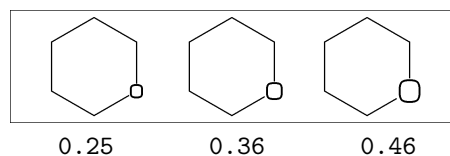
3.2.3 Bondgap/bond length

default: ratio_bondgap_bond= 0.15



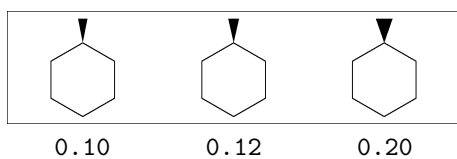
3.2.4 Atom/bond length

default: ratio_atom_bond= 0.36



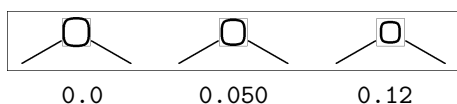
3.2.5 Wedge/bond length

default: ratio_wedge_bond=0.12



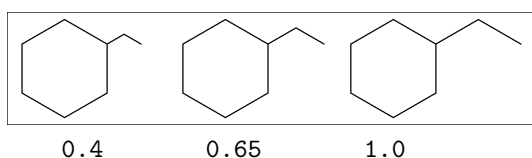
3.2.6 Font atom gap/atom length

default: ratio_atomgap_atom= 0.050



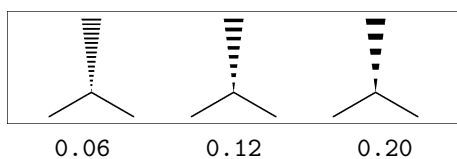
3.2.7 Chain/ring length

default: ratio_chain_ring= 0.66



3.2.8 Zebra gap/bond length

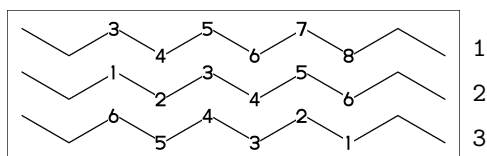
default: ratio_zebragap_bond=0.12



3.3 Drawing mode

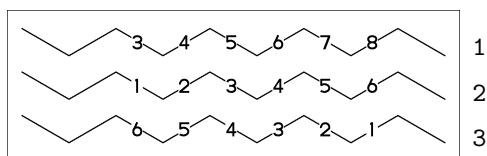
3.3.1 Numbering atom

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



3.3.2 Numbering bond

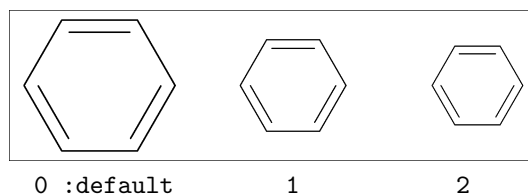
```
numberB_start:=3; numberB_end:=8;  
default: sw_numberB=0 :  
    numberB_start=1 numberB_end=4095
```



3.3.3 Solid mode

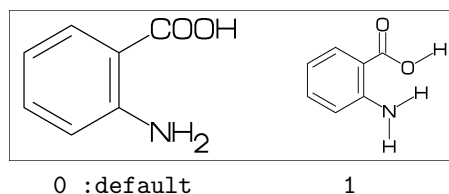
```
sw_solid=1 :  
    ratio_bond_width=0.1  
    font_width=70mm  
    (bond_len#=70mm*0.1=7mm)  
    ** ignore bond_len#
```

```
sw_solid=2 :  
    bond_len#=6mm#  
    ** ignore ratio_bond_width
```



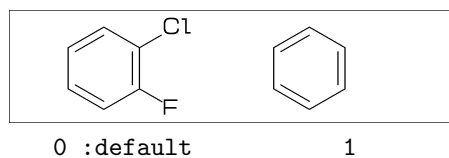
3.3.4 Expand mode

default: sw_expand=0



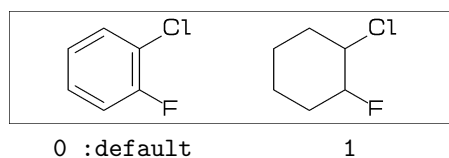
3.3.5 Substituent off mode

default: sw_subst_off=0



3.3.6 Single bond mode

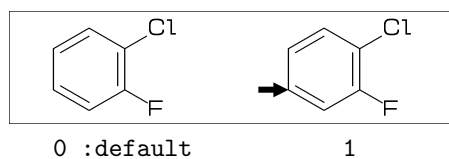
default: sw_bond_single=0



3.4 Frame,vector

3.4.1 Start vector

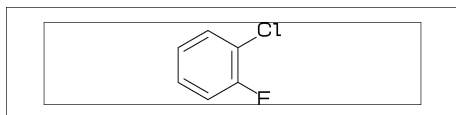
default: sw_start_vector=0



3.4.2 Font frame

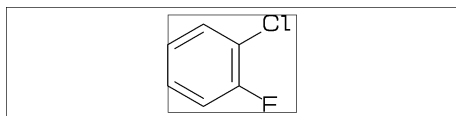
```
sw_font_frame=0 : no frame **default
sw_font_frame=1 : draw frame of font
sw_font_frame=2 : draw frame inside margin
sw_font_frame=3 : draw both
```

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



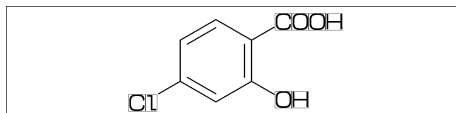
3.4.3 Molecular frame

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



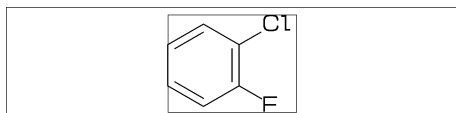
3.4.4 Atom frame

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

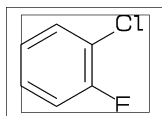


3.5 Clipping font

```
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
```

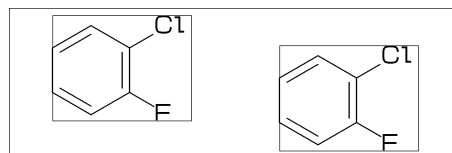


4 MCF draw function

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
```

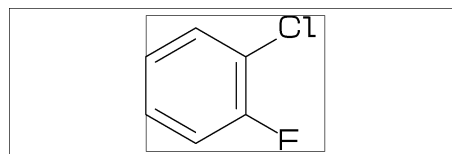
```
MCd(1,0.8)(0.2,0.9)(<30,Ph,3:/F,4:/Cl)
MCd(1,0.8)(0.8,0.1)(<30,Ph,3:/F,4:/Cl)
```



4.2 Function MCf (fit draw)

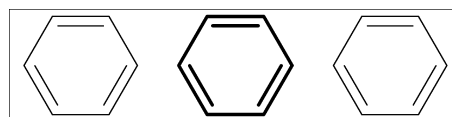
```
MCf(...) : MCd(1,1)(0.5,0.5)(...)
```

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



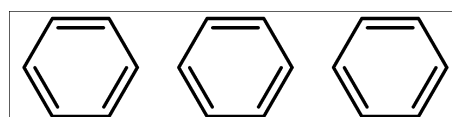
4.3 Local setting

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



4.4 Global setting

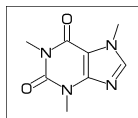
```
ratio_thickness_bond:=0.05;
beginfont() MCf(Ph) endfont
beginfont() MCf(Ph) endfont
beginfont() MCf(Ph) endfont
```



4.5 Output molecular information

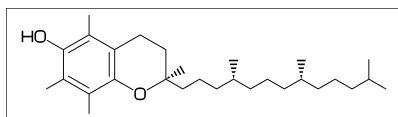
```
var3="calc_weight"; tag3="cMW";  
var4="calc_formula"; tag4="cFM";  
%% Output to mcf_man_soc-info.aux %%  
..... ;C:85;cMW:194.19174;cFM:C8H10N4O2
```

cMW:calculated molecular weight
cFM:calculated molecular formula



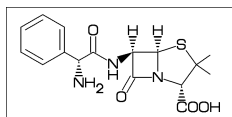
4.6 Output additional information

```
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

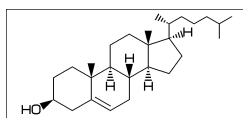
```
aux_delimiter="/";  
beginfont("EN:Ampicillin","CAS:69-53-4")  
Mcf(...) endfont  
  
%% Output to mcf_man_soc-info.aux %%  
F:mcf_man_soc/C:90/EN:Ampicillin/CAS:69-53-4  
  
**default aux_delimiter=";"
```



4.8 Fixed aux information

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

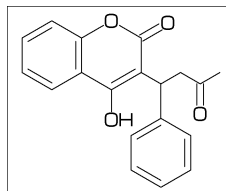
```
%% Output to mcf_man_soc-info.aux %%  
F;C;NO;EN  
mcf_man_soc;91;1;Ampicillin
```



5 MCF example

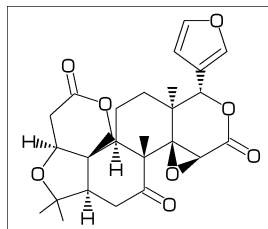
5.1 Warfarin

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



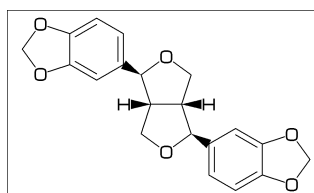
5.2 Limonin

```
<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
```



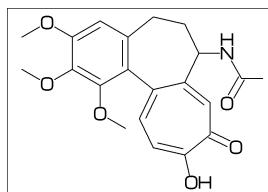
5.3 Sesamine

```
<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
```



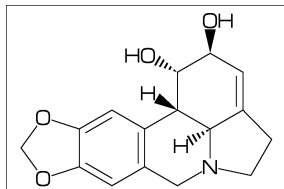
5.4 Colchicine

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



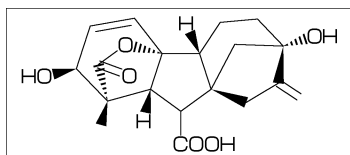
5.5 Lycorine

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



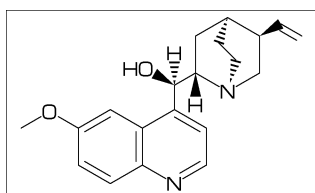
5.6 Gibberellin

<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



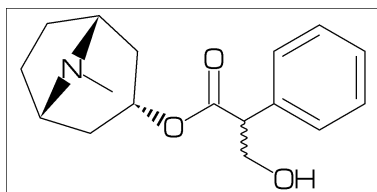
5.7 Quinine

<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



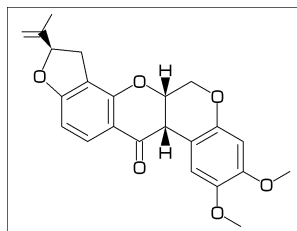
5.8 Atoropine

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



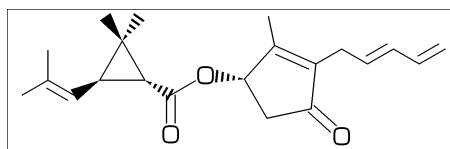
5.9 Rotenone

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



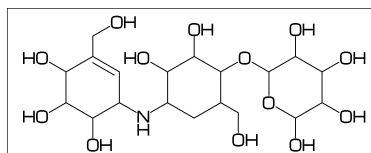
5.10 Pyrethrin I

<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



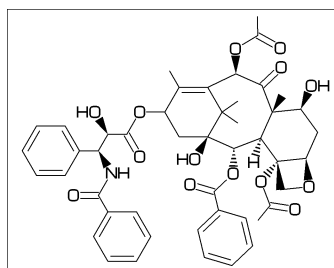
5.11 Validamycin

<30, ?6, @(5, 6)/OH, 3\, -60, OH,
#4\, 0, -60, |, ?6, 2:O, @(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, }, ,
-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\, 0, !, //O, !, /*OH, !, /Ph,
60~wf, NH, -60, //O, 60, Ph,
7*\, 0, -45, //O, 60, Ph, 11*\, 0, -60, //O, 60,
12*\^-15, 0, 60, //O, -60



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://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=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)  
%Formula / 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  
% Formula Calc: C8H10N4O2 / Input: C8H10N4O2 / MACTCH  
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

6.4 Molfile output

(Insert option parameter setting)

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

(Command line)

```
>mpost -s ahandle=3  FILENAME (molecular difinition file)
```

(Output)

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

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

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

```
M  END
```

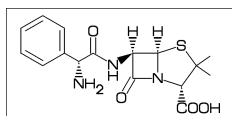
```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

6.5 L^AT_EX 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

