Chapter 3. Molecular rendering (or graphics)

Molecular graphics (MG) is the discipline and philosophy of studying molecules and their properties through graphical representation. It might be considered as an alternative to the construction of physical real models.

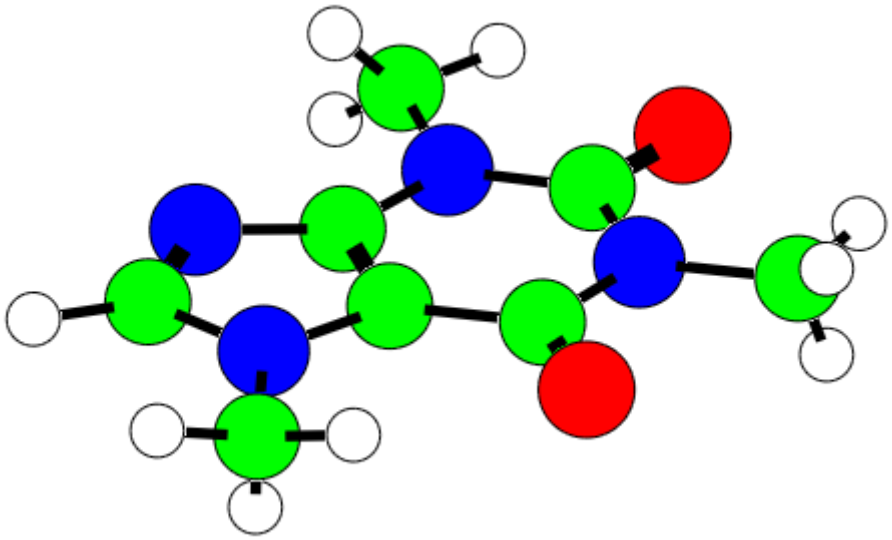

Fig. 3.1 caffeine (or theine) molecule. Red atom is oxygen, green carbon, blue nitrogen, and finally white hydrogen.

```
clear all;clc;format short;format compact;
figure(1,'position',[100 100 1000 800]);

function lineBond (c1,c2,r2,bondOrder)
  r3 = r2./100; % bring r2 in scale with axis
  dist = sqrt((c2(1)-c1(1))^2 + (c2(2)-c1(2))^2 + (c2(3)-c1(3))^2);
  x1 = (c2(1)*r3(1) - c1(1)*r3(1) + c1(1)*dist)/dist;
  y1 = (c2(2)*r3(1) - c1(2)*r3(1) + c1(2)*dist)/dist;
  z1 = (c2(3)*r3(1) - c1(3)*r3(1) + c1(3)*dist)/dist;
  x2 = (c1(1)*r3(2) - c2(1)*r3(2) + c2(1)*dist)/dist;
  y2 = (c1(2)*r3(2) - c2(2)*r3(2) + c2(2)*dist)/dist;
  z2 = (c1(3)*r3(2) - c2(3)*r3(2) + c2(3)*dist)/dist;
  line([x1,x2],[y1,y2],[z1,z2],'Color','black','LineWidth',1 + bondOrder*3);
endfunction

% insert here the file name here below
S = importdata("caffeine.txt","\n"); % line separator is \n (new line, ascii code
10)
% it may be downloaded from   'cactus.nci.nih.gov/chemical/structure/xxxxxxx/file?
format=sdf&get3d=True'
% where xxxxxxx is the name of the molecule

dN = S{4};dN = strtrunc(dN,20);
X = str2num(dN);
nAtom = X(1);
nBond = X(2);j = 0;
for i = 5:(5 + nAtom - 1)
  dM = S{i};dN = strtrunc(dM,30);dA = substr(dM,32,1)
  X = str2num(dN);
  ++j;x(j) = X(1);y(j) = X(2);z(j) = X(3);
  switch dA
    case "H";r(j) = 20;cr(j) = 'w';
```

```
    case "O";r(j) = 36;cr(j) = 'r';
    case "C";r(j) = 32;cr(j) = 'g';
    case "N";r(j) = 34;cr(j) = 'b';
    case "S";r(j) = 40;cr(j) = 'y';
  endswitch
endfor  % coordinates loaded in x() y() z() and radius in r()

j = 0;
for i = (5 + nAtom):(5 + nAtom + nBond -1)
  ++j;dM = S{i};X = str2num(dM);conn(j,1) = X(1);conn(j,2) = X(2);conn(j,3) =
X(3);
endfor  % connectivity loaded in conn()

for i = 1 : nAtom
  plot3(x(i),y(i),z(i),"ok",'markersize',r(i),'markerfacecolor',cr(i)); hold on;
endfor

axis([-5 5 -5 5 -5 5]);axis off
% axis on;grid on;grid minor on;  % choose if display axis
view(3);

for i = 1 : nBond
  h = conn(i,1);k = conn(i,2);
  lineBond([x(h),y(h),z(h)],[x(k),y(k),z(k)],[r(h),r(k)],conn(i,3));
endfor
```

The file containing the atomic coordinates and connectivity is conform to the standard molfile (MDL molfile) format. It can be downloaded from the web from many different repository; one of the most visited is '*cactus.nci.nih.gov/chemical/structure/xxxxxxx/file?format=sdf&get3d=True*' where *xxxxxxx* is the name of the molecule.

An example of such file format follows (caffeine molecule portrayed in fig. 3.1)

```
C8H10N4O2
APtclcactv11192101413D 0   0.00000     0.00000

 24 25  0  0  0  0  0  0  0  0999 V2000
    1.3120   -1.0479    0.0025 N   0  0  0  0  0  0  0  0  0  0  0  0
    2.2465   -2.1762    0.0031 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7906    0.2081    0.0010 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9938    0.3838    0.0002 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.9714    1.2767   -0.0001 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.5339    2.6294   -0.0017 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4026    1.0989   -0.0001 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4446    1.9342   -0.0010 N   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5608    1.2510   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2862   -0.0680    0.0015 N   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2614   -1.1612    0.0029 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9114   -0.1939    0.0014 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0163   -1.2853   -0.0022 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4380   -2.4279   -0.0068 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.2697   -1.8004    0.0022 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.0830   -2.7828    0.8938 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.0821   -2.7846   -0.8862 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.6223    2.5703   -0.0019 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1987    3.1611   -0.8923 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1990    3.1632    0.8877 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5520    1.6797   -0.0001 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5037   -1.4333   -1.0244 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   -2.8389   -2.0244    0.5173 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1672   -0.8395    0.5168 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  3  4  2  0  0  0  0
  3  5  1  0  0  0  0
  5  6  1  0  0  0  0
  5  7  1  0  0  0  0
  7  8  1  0  0  0  0
  8  9  2  0  0  0  0
  9 10  1  0  0  0  0
 10 11  1  0  0  0  0
 10 12  1  0  0  0  0
  7 12  2  0  0  0  0
 12 13  1  0  0  0  0
  1 13  1  0  0  0  0
 13 14  2  0  0  0  0
  2 15  1  0  0  0  0
  2 16  1  0  0  0  0
  2 17  1  0  0  0  0
  6 18  1  0  0  0  0
  6 19  1  0  0  0  0
  6 20  1  0  0  0  0
  9 21  1  0  0  0  0
 11 22  1  0  0  0  0
 11 23  1  0  0  0  0
 11 24  1  0  0  0  0
M  END
$$$$
```

The file was downloaded with .txt extension in the working directory. Double bonds are thicker than single bonds.