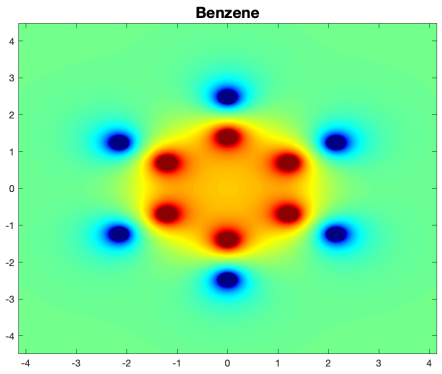
Home work 11

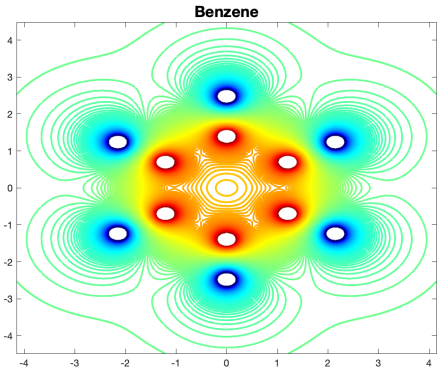
Calculate and draw the electrostatic potential around the benzene molecule. The file *benzene.dat* contains the data about the atom, coordinates (x, y, z) and the charge (5th column).

```
C   0.000   1.396   0.000   -0.1
C   1.209   0.698   0.000   -0.1
C   1.209  -0.698   0.000   -0.1
C   0.000  -1.396   0.000   -0.1
C  -1.209  -0.698   0.000   -0.1
C  -1.209   0.698   0.000   -0.1
H   0.000   2.479   0.000    0.1
H   2.147   1.240   0.000    0.1
H   2.147  -1.240   0.000    0.1
H   0.000  -2.479   0.000    0.1
H  -2.147  -1.240   0.000    0.1
H  -2.147   1.240   0.000    0.1
```

Write a script that reads the data from the file and uses this data to calculate the electrostatic potential. Use a **<u>for loop</u>** to calculate the electrostatic potential.

a) Calculate the electrostatic potential in the 2D plane – XY - and plot it. For plotting use the Matlab functions *contourf* and *contour*.





b) Calculate the electrostatic potential in 3D space and plot it. Use the Matlab function *isosurface* for plotting. Draw three isosurfaces (positive, zero and negative).