PLOTTING THE BORN-MAYER POTENTIAL FOR 1:1 IONIC COMPOUND AND ALSO FINDING THE EQUILIBRIUM INTERNUCLEAR DISTANCE

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1 Theory

The Born-Mayer potential(U) for 1:1 ionic compound is given by

$$U = -\frac{e^2}{4\pi\varepsilon_0 r} + b\exp{-ar} \tag{1}$$

where, e is the charge of an electron (=1.6x10^{-19} C), ε_0 is the permittivity of free space(= 8.84x10$^{-12}C^2N^{-1}m{-2}$), r is the distance between the nucleus of anion and cation and a and b constants which vary with different compounds.

The first term in equation (1) represents the 'attractive term' while the second term represents the 'repulsive term'. When the resultant of the two i.e. U is plotted against r the shape of the curve is as shown below:

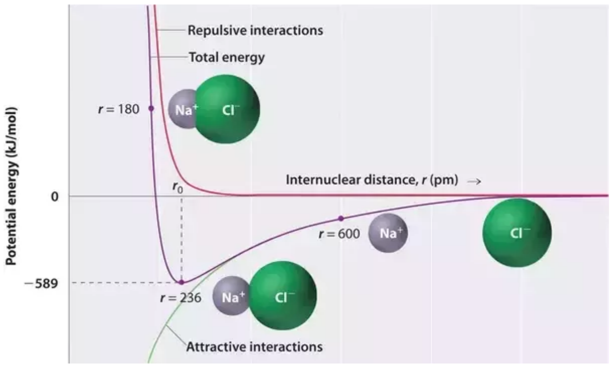

Figure 1: Born Mayer Potential

However from such a plot i.e. from the plot of U against r, one can obtain the approximate value of equilibrium internuclear distance r_e for which U is minimum. To obtain the value of r_e, one applies the concept that $\frac{dU}{dr}$ vanishes at $r = r_e$. Differentiating equation (1) and setting it to zero gives

$$\frac{e^2}{4\pi\varepsilon_0 r^2} - ab\exp{-ar} = 0 \tag{2}$$

$$\frac{e^2}{4\pi\varepsilon_0 r^2} = ab\exp{-ar} \tag{3}$$

But it is not possible to obtain an analytical solution of r_e from the above equation. However a graphical solution is possible. For that the left and right hand side of equation are plotted against r on the same graph. Their intersection point represents the corresponding r_e

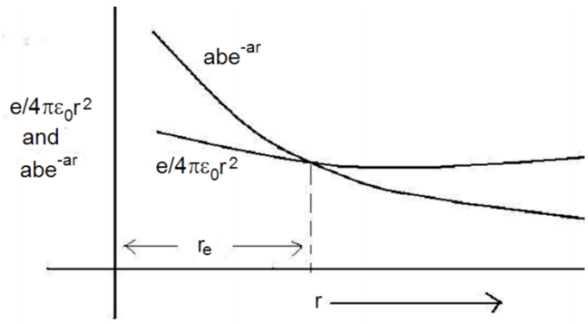

Figure 2: Derivative Terms Curve

1.1 NaCl crystal

The value of the constants a and b for NaCl crystal are 3.3x10^{1}0 m^{-1} and 3.237x10^{-16} J/molecule respectively.

2 Calculations

The value of potential U is calculated for varying 'r' from 160 pm to 450 pm at a regular interval of 10 pm. Then U is plotted against r.

To calculate internuclear equilibrium distance r_e, the value of $\frac{e^2}{4\pi\varepsilon_0 r^2}$ and $ab\exp{-ar}$ is plotted against r from 180 pm to 278 pm at an interval of 2 pm.

The calculations are carried out with the Python codes attached with this report.

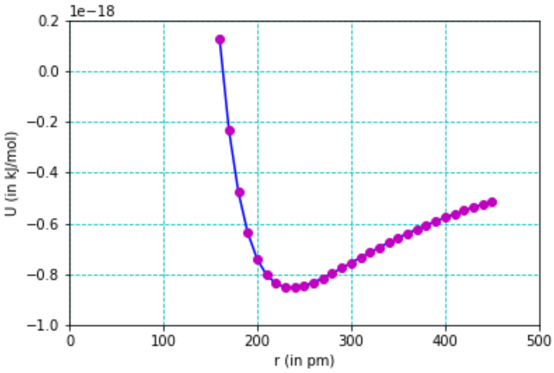

Figure 3: U(r) Vs r

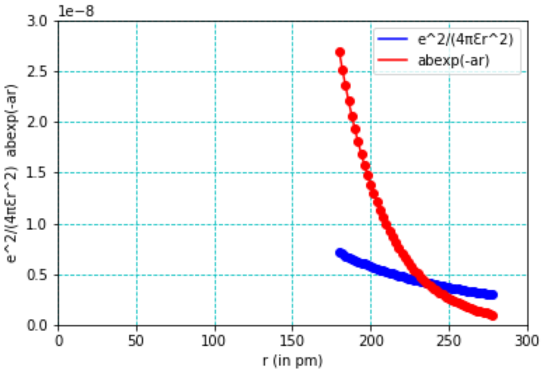

Figure 4: Derivative Terms Curve

3 Results

The equilibrium distance is 236 pm

The value of U at r_e is -8.54 x 10^{-19} J.

Codes of Born-Mayer Potential

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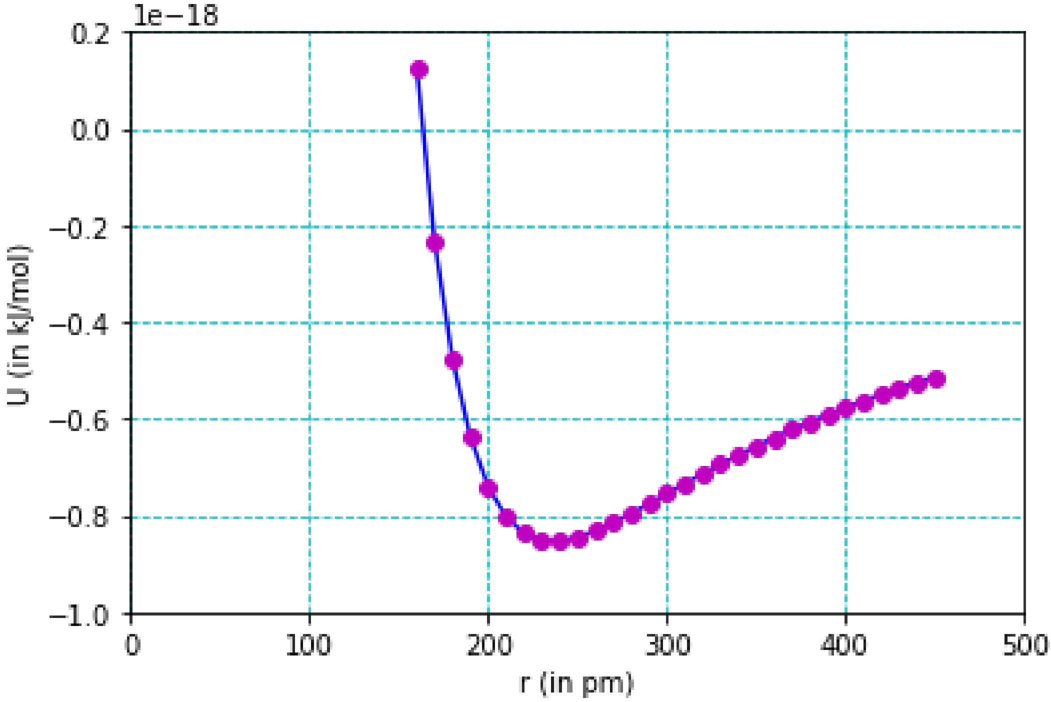
```
In [88]: import matplotlib.pyplot as plt
         import numpy as np
         import math
         U=[]
         r=[]
         e=1.602*(10**(-19))
         ep=8.84*(10**(-12))
         a=3.33*(10**(10))
         b=3.237*(10**(-16))
         k=0
         for i in range (160, 451,10):
             r_pm=i*(10**(-12))
             r.append(i)
             u=(-(e*e)/(4*math.pi*ep*r_pm))+(b*math.exp(-(a*r_pm)))
             U.append(u)
         fig1=plt.figure()
         axes = plt.gca()
         axes.set_ylim([(-1*(10**(-18))),(0.2*(10**(-18)))])
         axes.set_xlim([0,500])
         plt.grid(color='c', linestyle='--', linewidth=0.8)
         plt.ylabel("U (in kJ/mol)")
         plt.xlabel("r (in pm)")
         plt.plot(r,U,c='b')
         plt.plot(r,U,'mo')
         plt.savefig("U_r.png",format="png")
         plt.show()
```



In [101]:
```
import matplotlib.pyplot as plt
import numpy as np
import math
r=[]
REP=[]
ATT=[]
e=1.602*(10**(-19))
ep=8.84*(10**(-12))
a=3.33*(10**(10))
b=3.237*(10**(-16))
k=0
for i in range (180, 280,2):
    r_pm=i*(10**(-12))
    r.append(i)
    att=((e*e)/(4*math.pi*ep*r_pm*r_pm))
    rep=(a*b*math.exp(-(a*r_pm)))
    ATT.append(att)
    REP.append(rep)
fig2=plt.figure()
plt.grid(color='c', linestyle='--', linewidth=0.8)
axes = plt.gca()
axes.set_ylim([0,(3*(10**(-8)))])
axes.set_xlim([0,300])
plt.ylabel("e^2/(4πr^2)  abexp(-ar)")
```

```
plt.xlabel("r (in pm)")
plt.plot(r,ATT,c='b',label="e^2/(4πr^2)")
plt.plot(r,ATT,'bo')
plt.plot(r,REP,c='r',label="abexp(-ar)")
plt.plot(r,REP,'ro')
plt.legend()
plt.savefig("ATRE.png",format="png")
plt.show()
```