Chem 30324, Spring 2020, Homework3

Due February 5, 2020

Heat capacity of solids

1. In Einstein's original paper on the heat capacity of solids, he compared his m
diamond, using a frequency for the vibrating C atoms $\nu = 2.75 \times 10^{13}\mathrm{s}^{-1}$. W
about the vibrating C atoms to describe the heat capacity of diamond?

1. Each solid is composed of a lattice structure consisting of N atoms. Each atom is treated as moving inde
degrees of freedom). The entire lattice's vibrational motion could be described by a total of 3N motions, o
2. The atoms inside the solid lattice do not interact with each other.
3. All of the atoms inside the solid vibrate at the same frequency.

2. Plot the Einstein model for the heat capacity of diamond from 0 to 1500 K.

```
import numpy as np
import matplotlib.pyplot as plt
h = 6.626e-34 #Planck constant in m^2*kg/s
f = 2.75e13 #Vibrating frequency of carbon in s^-1
kB = 1.38e-23 #Boltzmann const in m^2*kg/s^2/K
T = np.arange(0,1500,1) # Temperature range from 0 to 1500 K
R = 8.314 #Gas constant m^2*kg/s^2/K/mol
def Cv(T):
  return (3*R)*(h*f/kB/T)**2*np.exp(h*f/kB/T)/(np.exp(h*f/kB/T)-1)**2
plt.plot(T,Cv(T))

plt.title('Einstein model for the heat capaciyt of diamond from 0 to 1500K')
plt.xlabel('T(K)')
plt.ylabel('Heat capacity(J/(mol*K)')
plt.show()
```

```
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:9: RuntimeWarning
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