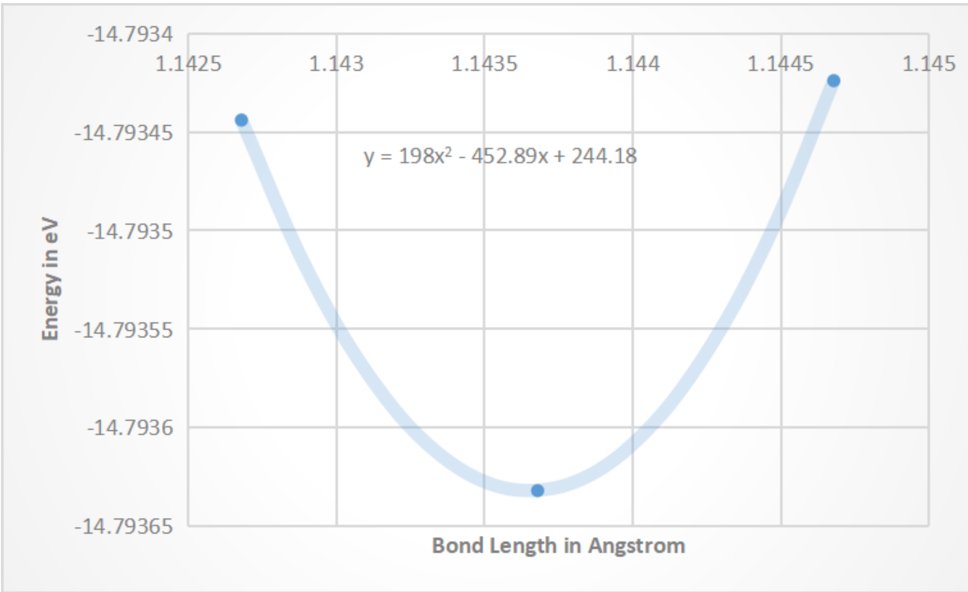
Hands on Assignment 2

MM19B027 Bhuvanesh P

(i) The equilibrium bond length of CO as calculated from the program is 1.143679155 A° units

(ii) By stretching the bond length by 0.001 A° units we get energy plot as



The equation that can be fitted is given by **y = 198x^2 - 452.89x + 244.18**

In order to find the frequency

$$\omega = \sqrt{\frac{\alpha(w1 + w2)}{w1\,w2}}$$

The equation above gives the vibrational frequency between atoms.

We get α after double differentiating the energy equation with respect t o distance

$\alpha = \frac{d^2E}{dx^2}$ = 2 x 198 = 369

This is not in SI units to convert it we need to multiply by 1.6 X 10^{-19} in numerator and 10^{-20} in the denominator

$$\alpha = \frac{396X1.6X\ 10^{-19}}{10^{-20}} = 6336$$

$$w1 = \frac{12}{6.023X10^{-23}}$$

$$w2 = \frac{16}{6.023X10^{-23}}$$

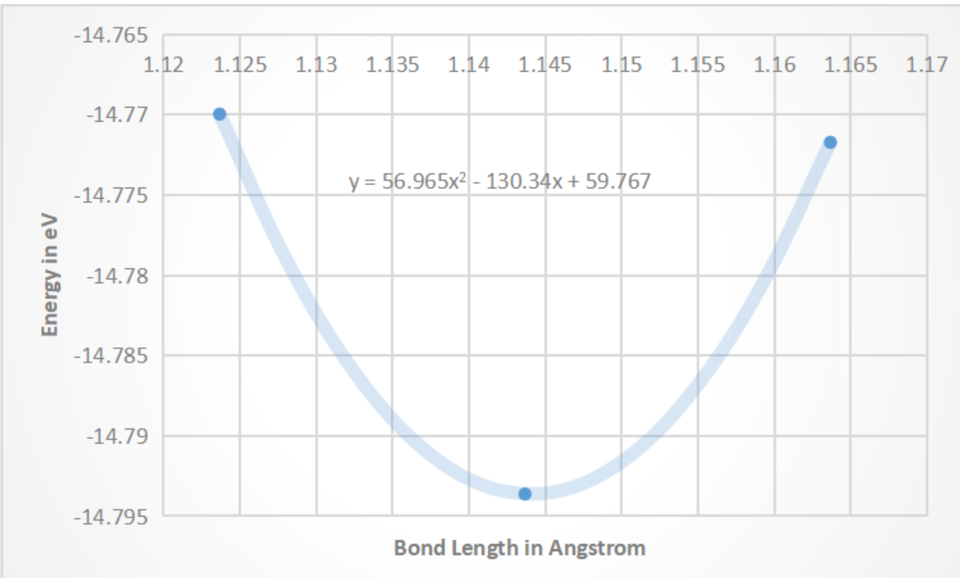
After substituting ω is given by

$$\omega = \sqrt{\frac{6336(\frac{12}{6.023X10^{23}} + \frac{16}{6.023X10^{23}})}{\frac{16}{6.023X10^{23}}\ \frac{12}{6.023X10^{23}}}}$$

$$= \sqrt{\frac{63360\quad X\quad (28)\quad X\quad 6.023}{192}}\ X\ 10^{12}$$

$$= 235.907\ X\ 10^{12}\ \ Hz$$

(iii) By stretching the bond length by 0.02 A° units we get energy plot as



The equation that can be fitted is given by **$y = 56.965x^2 - 130.34x + 59.767$**

In order to find the frequency

$$\omega = \sqrt{\frac{\alpha(w1 + w2)}{w1\, w2}}$$

The equation above gives the vibrational frequency between atoms.

We get α after double differentiating the energy equation with respect t o distance

$\alpha = \frac{d^2E}{dx^2}$ = 2 x 56.965 = 113.93

This is not in SI units to convert it we need to multiply by 1.6 X 10^{-19} in numerator and 10^{-20} in the denominator

$\alpha = \frac{113.93X1.6X\ 10^{-19}}{10^{-20}} = 1822.88$

$w1 = \frac{12}{6.023X10^{-23}}$

$w2 = \frac{16}{6.023X10^{-23}}$

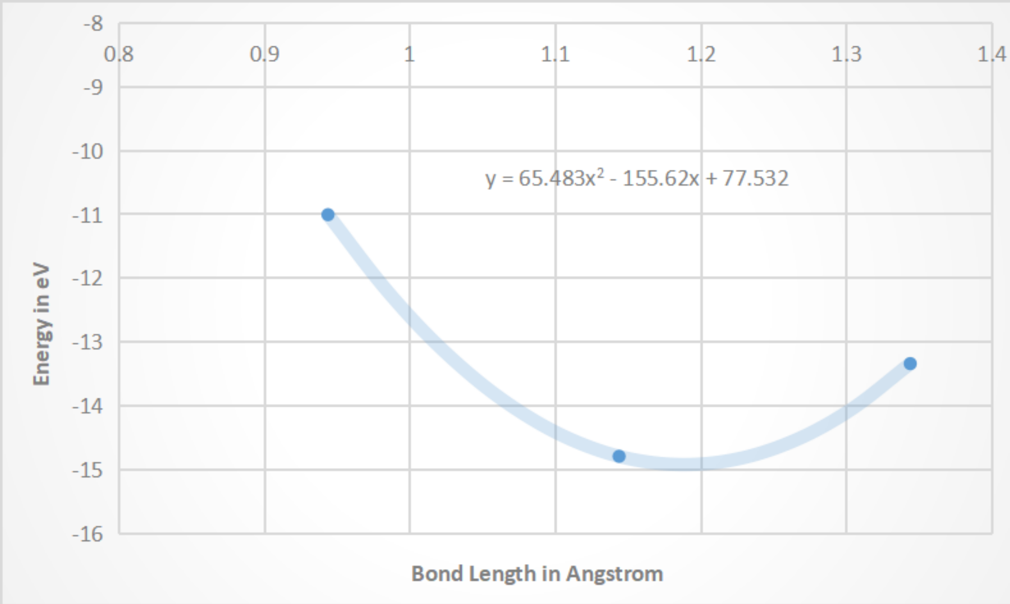
After substituting ω is given by

$$\omega = \sqrt{\frac{1822.88(\frac{12}{6.023X10^{23}} + \frac{16}{6.023X10^{23}})}{\frac{16}{6.023X10^{23}}\ \frac{12}{6.023X10^{23}}}}$$

$$= \sqrt{\frac{18228.8 \quad X \quad (28) \quad X \quad 6.023}{192}}\ X\ 10^{12}$$

$$= 126.539\ X\ 10^{12}\ \ Hz$$

(iv) By stretching the bond length by 0.2 A° units we get energy plot as



The equation that can be fitted is given by **y = 65.483x^2 - 155.62x + 77.532**

In order to find the frequency

$$\omega = \sqrt{\frac{\alpha(w1 + w2)}{w1\, w2}}$$

The equation above gives the vibrational frequency between atoms.

We get α after double differentiating the energy equation with respect t o distance

$\alpha = \frac{d^2E}{dx^2}$ = 2 x 65.483= 130.966

This is not in SI units to convert it we need to multiply by 1.6 X 10^{-19} in numerator and 10^{-20} in the denominator

$$\alpha = \frac{130.966X1.6X\ 10^{-19}}{10^{-20}} = 2095.456$$

$$w1 = \frac{12}{6.023X10^{-23}}$$

$$w2 = \frac{16}{6.023X10^{-23}}$$

After substituting ω is given by

$$\omega = \sqrt{\frac{2095.496\left(\frac{12}{6.023X10^{23}} + \frac{16}{6.023X10^{23}}\right)}{\frac{16}{6.023X10^{23}} \quad \frac{12}{6.023X10^{23}}}}$$

$$= \sqrt{\frac{20954.96 \quad X \quad (28) \quad X \quad 6.023}{192}} \; X \; 10^{12}$$

$$= 135.668 \, X \, 10^{12} \;\; Hz$$