Energy levels or water molecule:

Rotational energy:

$$\vec{L} = \vec{r} \times \vec{p}$$

form quantum dynamics we know the momentum vector is: $\vec{p} = -i\hbar\vec{\nabla}$

so that $\vec{L} = -i\hbar\left(\vec{r} \times \vec{\nabla}\right) \Rightarrow |L| = \left|\hbar\left(\vec{r} \times \vec{\nabla}\right)\right| \Rightarrow |L| = |\hbar\vec{r} \times \vec{p}|$

$$|L| = |rmv| = mr^2 \frac{v}{r} = I\omega$$

$$E = \frac{mv^2}{2} = \frac{L^2}{2I} = \frac{\hbar^2}{2I} = \frac{\left(\frac{6.63\times10^{-34}{}_{js}}{2\pi}\right)^2}{2\cdot1.6\times10^{-27}{}_{kg}\left(\sin(52)\cdot1\times10^{-10}{}_{m}\right)^2} = \frac{1.11\times10^{-68}{}_{j^2s^2}}{1.987\times10^{-47}{}_{m^2kg}} = 5.58\times10^{-22}{}_{J}$$

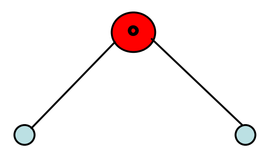
$$E = h\nu \Rightarrow \nu = \frac{E}{h} = \frac{5.58\times10^{-22}{}_{J}}{6.63\times10^{-34}{}_{js}} = 8.41\times10^{11}{}_{Hz}$$

Molecular Vibration:

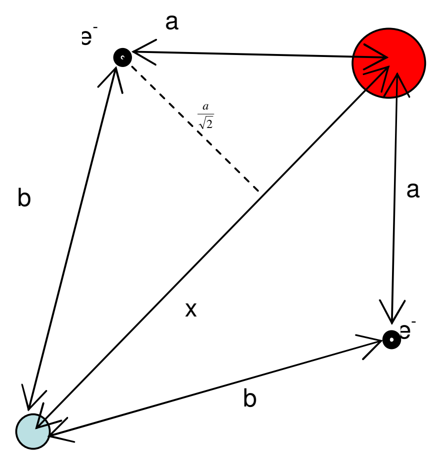
The method:

- to calculate the frequency using $\omega = \sqrt{\frac{k}{\mu}}$ we need to find "k" :
- creating a potential curve
- finding the minimum
- expending the force around the minimum
- taking the linear constant in the expansion to find the "k"
- calculating $\omega = \sqrt{\frac{k}{\mu}}$

we'll use water molecule for the example,



and look at one of the O-H bonds in particular:



The potential of the system is:

$$U = -2\frac{kq^2}{a} + \frac{kq^2}{a\sqrt{2}} + \frac{kq^2}{x} - 2\frac{kq^2}{\underbrace{\sqrt{\left(x - \frac{a}{\sqrt{2}}\right)^2 + \frac{a^2}{2}}}_{b}}$$

Using 1Å for the "a" the distance to the electrons, we can plot the potential curve:

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Plot[U, {x, 3 10^-11, 8 10^-10}]
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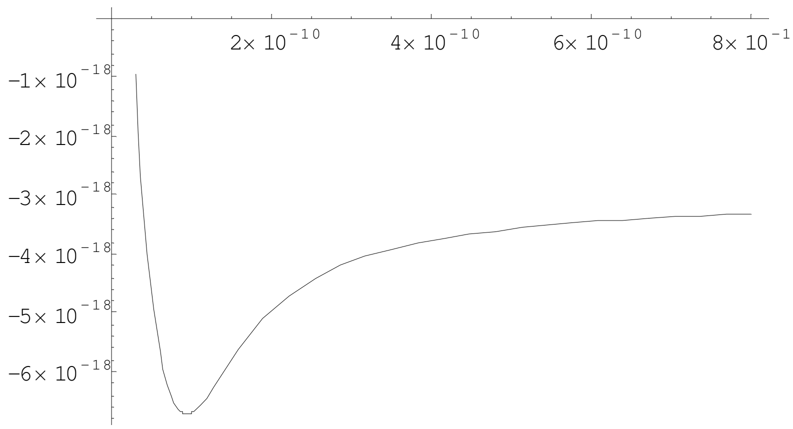

Using Mathematica (or any other program) we can easily get:

$$F = \frac{\partial U}{\partial x} = -\frac{k\,q^2}{x^2} + \frac{2\,k\,q^2\left(-\frac{a}{\sqrt{2}} + x\right)}{\left(\frac{a^2}{2} + \left(-\frac{a}{\sqrt{2}} + x\right)^2\right)^{3/2}}$$

F = ∂ₓ U

Again using Solve[F==0,x] we get the minimum value: $x \to 9.40493 \times 10^{-11}$

Expanding the force around this point Series[F,{x,9.40493 10^-11,3}] we get:

$1.70386 \times 10^{-14} + 1341.08\,(x - 9.40493 \times 10^{-11}) + \ldots\ldots..$

Therefore "k" is 1341.08.

the reduced mass is ($\mu = \frac{M_1 M_2}{M_1 + M_2} = \frac{16}{17} = 0.94$) so that:

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{1341.08}{0.94 \cdot 1.6 \times 10^{-27}\,kg}} = 9.44 \times 10^{14}$$

the frequency $\nu = \frac{\omega}{2\pi} = 1.5 \times 10^{14}\,Hz \to \lambda = 2\mu m$