2/22/2019

— SO MUCH POTENTIAL —

1) Reduced mass of CO molecule in atomic units.

$$M = \frac{mc * mo}{mc + mo} = \frac{(12.0107) * (15.9994)}{(12.0107) + (15.9994)} = \frac{192.1639936}{28.0101}$$

$= 6.8605$ amu

$mc = 12.0107$ amu

$mo = 15.9994$ amu

$6.8605 \text{ amu} \rightarrow 12504.237592$ ↓ electron mass

In our calculations we assumed that the reduced mass of CO = 13625 election mass

2) Vibrational frequency of CO → ω

$$\omega = \sqrt{\frac{k}{M}}$$

k → Force constant = atomic units

M → reduced mass = atomic units

$$\omega = \sqrt{\frac{1.9097856889891685 6}{13625}} = 0,011839246473330577 \text{ atomic units}$$

$$t.a.u = 2.418 * 10^{-17} s$$

$$\omega * \frac{Hz}{a.u \text{ of freq.}} \qquad Hz = \frac{1}{s} \qquad \omega * \frac{a.u. \text{ of time}}{s} = 0,011839\ldots * \frac{1}{2.418 * 10^{-17} s}$$

$$= 4.8962 * 10^{14} \text{ Hertz} \left(\frac{1}{s}\right)$$

3) The accelaration of the bond stretch when C is separated by O by 3 atomic units will be $-2.0614464965843 89 * 10^{-5}$ atomic units.

$$\text{accelaration} = a = -1 * fE(3) / mu$$

$$a = -2.06144\ldots * 10^{-5} \text{ atomic unit}$$