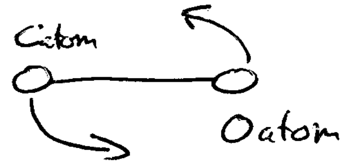
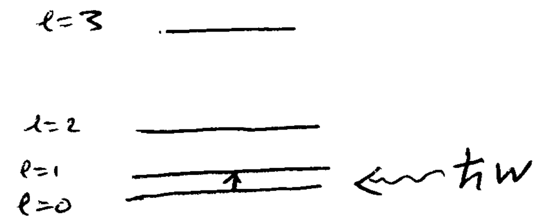
Tute 8

Q1

"dumbell"





$\ell=0 \rightarrow \ell=1$ is an increase in energy of the CO molecule, so the energy that is added to the system must have come from an incident photon of energy $\hbar\omega$. (note $\hbar\omega = \frac{h}{2\pi} \cdot 2\pi f = hf$).
The $\ell=0$ rotational state has no energy $E_{\ell=0} = 0$, i.e. the dumbell is not spinning. After it has absorbed the photon, it is yet spinning.

We can draw the energy level diagram above by using the expression for the energy of the states.

① $$E_\ell = \frac{\hbar^2}{2I}\,\ell(\ell+1)$$

② $$I = m_1 r_1^2 + m_2 r_2^2 = \mu R_0^2$$

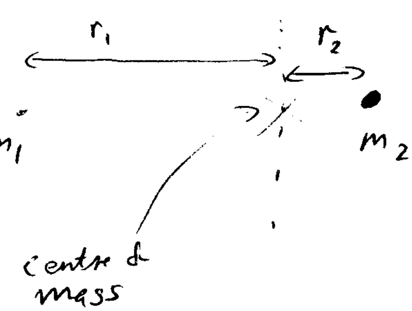
where r_1 and r_2 are the distances of the masses m_1 and m_2 from the center of mass

reduced mass $$\mu = \frac{m_1 m_2}{m_1+m_2}$$ ③

we can derive this by noting that $R_0 = r_1 + r_2$ and

④ $$r_2 = \frac{m_1}{m_1+m_2} R_0$$

⑤ $$r_1 = \frac{m_2}{m_1+m_2} R_0$$



Put ④ & ⑤ into ② ...

Tute 8 Q1 continued.

$$I = m_1 \cdot \frac{m_2^2}{(m_1+m_2)^2} R_0^2 + \frac{m_2 m_1^2}{(m_1+m_2)^2} R_0^2$$

$$= \frac{m_1 m_2^2 + m_2 m_1^2}{(m_1+m_2)^2} R_0^2$$

$$= \frac{(m_1+m_2)\, m_1 m_2}{(m_1+m_2)^2} R_0^2 = \frac{m_1 m_2}{m_1+m_2} R_0^2 \quad \text{as required.}$$

The energy required to go from the $l=0$ state to the $l=1$ state is

$$E_{l=1} - E_{l=0} = \frac{\hbar^2}{2I} 1(1+1) = \frac{\hbar^2}{I}$$

which is equal to the energy of the absorbed photon $hf (= \hbar\omega)$

$$I = \frac{\hbar}{\omega} = \frac{1.055 \times 10^{-34}}{7.23 \times 10^{11}} = 1.46 \times 10^{-46} \ kg/m^2$$

notice that this is a very small number - appropriate given the tiny mass of atoms.

We have already got $I = \mu R_0^2$

$$\mu = \frac{12 \times 16}{12+16} \text{ amu}$$

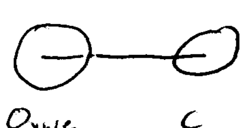
mass of carbon atom = 12 atomic mass units, i.e. the total mass of the protons and the neutrons in the nucleus.

mass of proton ≈ mass of neutron = 1 amu.

mass of oxygen atom = 16 amu

$1 \text{amu} = 1.66 \times 10^{-27}$ kg

$$R_0 = \sqrt{\frac{I}{\mu}} = 0.113 \text{nm}$$



so the separation between the atoms is very small: 1.13 Å, which is roughly the size of a H atom. Note that if we had got an answer of an order of magnitude smaller, we should start looking for a mistake in our calculations.

$\nu = 2$

$\nu = 1$ 

$\nu = 0$

↑

greek letter 'nu'. Denotes the ν^{th} state. Note the even spacing of the energy levels

$$E_\nu = \left(\nu + \tfrac{1}{2}\right)\hbar w$$

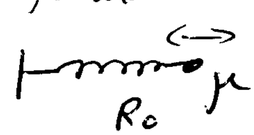
The atoms are considered to be masses connected by a spring with spring constant k. We know from classical mechanics that the potential energy stored in a spring is $\frac{1}{2}kx^2$, where x is the displacement from equilibrium (unstretched). The masses have kinetic energy which transfers into potential energy at the maximum amplitude $x = A$. We can say that all of the E_ν is in the spring at $x = A$, i.e.

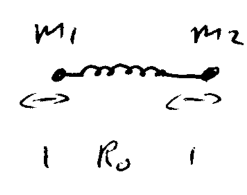
$$\frac{1}{2}kA^2 = \left(\nu + \tfrac{1}{2}\right)\hbar w$$

We know that $\nu = 0$ in this case, so we can solve for A:

$$A = \sqrt{\frac{hf}{k}}$$

For the first part of the question, we know from classical mechanics that for a spring $k = m w^2$.

↑ We use the reduced mass μ here, because we are using the equivalent system 

to solve the system 

Pset8 Q2 cont'd

To understand when $k = m w^2$ comes from, recall that

$F = -kx$ and $F = ma$

$$= m \frac{d^2x}{dt^2}$$

so $m \frac{d^2x}{dt^2} = -kx$ which has solutions $x = \cos wt$

$$\frac{dx}{dt} = w \sin wt$$

$$\frac{d^2x}{dt^2} + \frac{k}{m} x = 0$$

$$\frac{d^2x}{dt^2} = -w^2 \sin wt$$

sub in to get

$$-w^2 \cos wt + \frac{k}{m} \cos wt = 0$$

$$\left(\frac{k}{m} - w^2\right) \cos wt = 0$$

$$\frac{k}{m} - w^2 = 0$$

$$k = m w^2$$ QED.

Psheet 8 Q3

We use

$$\frac{1}{2}\hbar w = \frac{1}{2}kA^2$$

$$A = \sqrt{\frac{hf}{k}}$$ from before (Q2) and plug in the numbers.

Which bond is weaker? $E_v = (n+\frac{1}{2})\hbar w$ gives the energy that is lost by the system as a result of the bond. In other words, bonds form because the total energy of the system is lowered as a result of the bond formation. So the

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See the 'old solutions' for the rest of the problem sheet.