ADVANCED CHEMISTRY

QUANTUM MECHANICS - WINTER - WEEK 4 HOMEWORK

Chapter 9

(18) $$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

n_x	n_y	n_z	degeneracy	Energy
1	1	1	1	$3h^2/8ma^2$
1	2	1	3	$6h^2/8ma^2$
2	1	1		
1	1	2		
2	2	1	3	$9h^2/8ma^2$
1	2	2		
2	1	2		

(23) $$\tilde{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{12 \times 16}{(12+16)} \text{ amu}$$

$$= 6.857 \text{ amu} \times \frac{1.661 \times 10^{-27} \text{ kg}}{1 \text{ amu}}$$

$$\mu = 1.139 \times 10^{-26} \text{ kg}$$

$$\tilde{\nu}^2 = \frac{1}{4\pi^2 c^2}\left(\frac{k}{\mu}\right) \Rightarrow k = 4\pi^2 c^2 \tilde{\nu}^2 \mu$$

$$k = 4\pi^2 \left(2.99\times10^{8}\, m s^{-1}\right)^2 \left(2169.814\, cm^{-1} \times \frac{100\, cm}{m}\right)^2 \left(1.139\times10^{-26}\, kg\right)$$

$$= 1892.65 \ \frac{m^2 s^{-2}}{m^2}\ kg$$

$$kg \cdot s^{-2} = N \cdot m^{-1}$$

$$k = \underline{\underline{1892.65\ N m^{-1}}}$$

(24) $\mu = \frac{12 \times 18}{(12+18)}\, amu = 7.2\, amu \times \frac{1.661\times10^{-27}\, kg}{1\, amu} = 1.196\times10^{-23}\, kg.$

$$\tilde{\nu}_1 = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu_1}} \quad \text{—①} \qquad \tilde{\nu}_2 = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu_2}}$$

for $^{12}C^{16}O$ — for $^{12}C^{18}O$

$$① \div ② \Rightarrow \frac{\tilde{\nu}_1}{\tilde{\nu}_2} = \sqrt{\frac{\mu_2}{\mu_1}} \Rightarrow \tilde{\nu}_2 = \tilde{\nu}_1 \sqrt{\frac{\mu_1}{\mu_2}}$$

$$\tilde{\nu}_2 = \left(2169.814\, cm^{-1}\right)\sqrt{\frac{6.857\, amu}{7.2\, amu}} = \underline{\underline{2117.499\, cm^{-1}}}$$

(26) (a) $k = 4\pi^2 c^2 \tilde{\nu}^2 \mu$

$$\mu(Cl_2) = \frac{35 \times 35}{(35+35)}\, amu = 17.5\, amu \times \frac{1.661\times10^{-27}\, kg}{1\, amu}$$

$$= 2.907\times10^{-26}\, kg$$

$$k = 4\pi^2 \left(2.99\times10^{8}\, m s^{-1}\right)^2 \left(560\, cm^{-1} \times \frac{100\, cm}{m}\right)^2 \left(2.907\times10^{-26}\, kg\right)$$

$$k = \underline{\underline{321.75\ Nm^{-1}}}$$

$$\mu(KCl) = \frac{(39 \times 35)}{(39+35)} amu \times \frac{1.661 \times 10^{-27} kg}{1 amu} = 3.064 \times 10^{-26} kg$$

$$k = 4\pi^2 (2.99 \times 10^{8} ms^{-1})^2 \left(281 cm^{-1} \times \frac{100 cm}{m}\right)^2 (3.064 \times 10^{-26} kg)$$

$$= \underline{\underline{85.39\ Nm^{-1}}}$$

$$\mu(H_2) = \frac{1 \times 1}{(1+1)} amu \times \left(\frac{1.661 \times 10^{-27} kg}{1 amu}\right) = 8.305 \times 10^{-28} kg$$

$$k = 4\pi^2 (2.99 \times 10^{8} ms^{-1})^2 \left(4401 cm^{-1} \times \frac{100 cm}{m}\right)^2 (8.305 \times 10^{-28} kg)$$

$$= \underline{\underline{567.73\ Nm^{-1}}}$$

(b) $$\mu(^{37}Cl_2) = \frac{37 \times 37}{(37+37)} amu = 18.5\ amu$$

For two molecules with the same force constant

$$\frac{\tilde{\nu}_1}{\tilde{\nu}_2} = \sqrt{\frac{\mu_2}{\mu_1}} \qquad \tilde{\nu}_2 = \tilde{\nu}_1 \sqrt{\frac{\mu_1}{\mu_2}}$$

$$\tilde{\nu}_2(^{37}Cl_2) = \tilde{\nu}_1(^{35}Cl_2) \sqrt{\frac{\mu(^{35}Cl_2)}{\mu(^{37}Cl_2)}}$$

$$= 560 cm^{-1} \sqrt{\frac{17.5 amu}{18.5 amu}} = \underline{\underline{544.65 cm^{-1}}}$$

(39) $100W = 100\ J/s$

$\text{Energy} = \frac{(100W)}{s}(1s) = 100J$

$E = nh\nu = \frac{nhc}{\lambda}$

$n = \frac{E\lambda}{hc} = \frac{(100J)(694nm \times \frac{10^{-9}m}{nm})}{(6.626\times10^{-34}Js)(2.99\times10^{8}ms^{-1})}$

$= \underline{\underline{3.50\times10^{20}}}$ photons

$\text{Power} = 0.1GW = 0.1\times10^{9}W = 0.1\times10^{9}J/s$

$\text{Energy} = 0.1\times10^{9}W\times(5\times10^{-9}s) = 0.5J$

$n = \frac{E\lambda}{hc} = \frac{(0.5J)(694\times10^{-9}m)}{(6.626\times10^{-34}Js)(2.99\times10^{8}ms^{-1})}$

$= \underline{\underline{1.751\times10^{18}\text{ photons}}}$

(43) (a) $\text{energy} = (1000V)(1.602\times10^{-19}C) = 1.602\times10^{-16}J$

$\lambda = \frac{h}{mV} = \frac{h}{P}$

$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{P^2}{2m}$

$P^2 = 2mE \Rightarrow P = \sqrt{2mE}$

$P = \sqrt{2(9.109\times10^{-31}\,kg)(1.602\times10^{-16}\,J)} = 1.708\times10^{-23}\,kg\,m\,s^{-1}$

$\lambda = \dfrac{6.626\times10^{-34}\,Js}{1.708\times10^{-23}\,kg\,m\,s^{-1}} = 3.879\times10^{-11}\,m = \underline{\underline{0.0388\,nm}}$

(b) energy $= (1000\,V)(1.602\times10^{-19}\,C) = 1.602\times10^{-16}\,J$

$P = \sqrt{2(1.673\times10^{-27}\,kg)(1.602\times10^{-16}\,J)} = \cancel{5.380\times10^{-43}\,kg\,m\,s^{-1}}$

$= 7.321\times10^{-22}\,kg\,m\,s^{-1}$

$\lambda = \dfrac{6.626\times10^{-34}\,Js}{7.321\times10^{-22}\,kg\,m\,s^{-1}} = 9.0502\times10^{-13}\,m = \underline{\underline{9.0502\times10^{-4}\,nm}}$

(45) $\lambda = \dfrac{h}{p}$ $\quad p = \dfrac{h}{\lambda} = \dfrac{6.626\times10^{-34}\,Js}{500\times10^{-9}\,m} = 1.325\times10^{-27}\,\dfrac{Js}{m}$

$\underline{\underline{P = 1.325\times10^{-27}\,kg.m\,s^{-1}}}$

$\dfrac{Js}{m} = \dfrac{kg\,m^2\,s^{-2}\,s}{m} = kg\,m\,s^{-1}$

Amount of momentum is transferred to $^{35}Cl_2$

momentum of $^{35}Cl_2 = 1.325\times10^{-27}\,kg\,m\,s^{-1}$

$= m.\,V.$

$$v = \frac{1.325\times10^{-27}\ \text{kg m s}^{-1}}{m} = \frac{1.325\times10^{-27}\ \text{kg m s}^{-1}}{70\ \text{amu}} \times \frac{\text{amu}}{1.661\times10^{-27}\ \text{kg}}$$

$$= \underline{\underline{1.139\times10^{-2}\ \text{m s}^{-1}}}$$

(47) $\psi = R + iI \qquad \psi^* = R - iI$

$$\psi^*\psi = (R - iI)(R + iI) = R^2 + iRI - iRI - i^2 I^2$$

$$= \underline{\underline{R^2 + I^2}}$$ real since there are no imaginary components.

(48) (a)
$$\frac{d^2}{dx^2}\psi = \frac{d}{dx}\left(\frac{d}{dx}\, x e^{-ax^2}\right) = \frac{d}{dx}\left[x\left(-2ax\, e^{-ax^2}\right) + e^{-ax^2}\right]$$

$$= \frac{d}{dx}\left[-2ax^2 e^{-ax^2} + e^{-ax^2}\right]$$

$$= -2ax^2\left(-2ax\, e^{-ax^2}\right) + e^{-ax^2}(-4ax) + (-2ax)\, e^{-ax^2}$$

$$= +4a^2x^3 e^{-ax^2} - 4ax\, e^{-ax^2} - 2ax\, e^{-ax^2}$$

$$= \left(4a^2x^2 - 4a - 2a\right) x\, e^{-ax^2}$$

$$= \left(4a^2x^2 - 6a\right)\psi = 4a^2x^2\psi - 6a\psi \quad \text{—①}$$

$$\left(\frac{d^2}{dx^2} - 4a^2x^2\right)\psi = \frac{d^2}{dx^2}\psi - 4a^2x^2\psi$$

$$= 4a^2x^2\psi - 6a\psi - 4a^2x^2\psi$$ (substitute from ①)

$$= -6a\psi$$

$\therefore$ ψ is an eigen function of the operator $\left(\frac{d^2}{dx^2} - 4a^2x^2\right)$ with the eigen value $-6a$

(b) $\frac{d}{dr}\psi = \frac{d}{dr}\left(K e^{-r/k}\right) = K\left(-\frac{1}{k}\right)e^{-r/k}$

$$= \left(-\frac{1}{k}\right) K e^{-r/k} = \left(-\frac{1}{k}\right)\psi$$

$\therefore$ ψ is an eigen function of $\frac{d}{dr}$ with the eigen value $\left(-\frac{1}{k}\right)$

49 $\lambda = \frac{h}{p}$ $\quad p = \frac{h}{\lambda}$ de Brglie formula

$$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} = \frac{h^2}{\lambda^2 2m}$$

For a particle in a box of length a; $\therefore a = \frac{n\lambda}{2} \Rightarrow \lambda = \frac{2a}{n}$

$$E = \frac{h^2}{\left(\frac{2a}{n}\right)^2(2m)} = \frac{n^2h^2}{8ma^2}$$

51) $$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

n_x	n_y	n_z	E	degeneracy	# of states
1	1	1	$3h^2/8ma^2$	1	1
2	1	1	$6h^2/8ma^2$	3	3
1	2	1			
1	1	2			
1	2	2	$9h^2/8ma^2$	3	3
2	1	2			
2	2	1			
~~2~~	~~2~~	~~2~~	$\cancel{12h^2/8ma^2}$	~~1~~	~~1~~
3	1	1	$11h^2/8ma^2$	3	3
1	3	1			
1	1	3			

10 states total