CHEMISTRY (CYL1010) Minor

1. Threshold frequency for electrons to be emitted from Na metal is 665×10^{12} Hz. Calculate the kinetic energy of electrons (in J) emitted from Na metal when radiation of wavelength 200 nm falls on it.

(3 points)

2. Show that the wavefunctions $\psi_1(x)$ and $\psi_2(x)$ of particle in a 1D box problem are orthogonal. Particle in a 1D box wavefunctions are given by $\psi_n(x) = (\sqrt{2/l})\sin(n\pi x/l)$.

(3 points)

3. Consider an electron moving in a 1D box bound by infinite potential energy walls. When the electron jumps from $n = 5$ level to $n = 2$ level, it emits a photon of frequency $6 \times 10^{14} s^{-1}$. Find the length of the box.

(3 points)

4. Vibrational motion of a diatomic molecule such as HCl can be modeled using quantum harmonic oscillator. Suppose HCl molecule shows a vibrational frequency of 54.322×10^{13} Hz when it jumps from $v = 1$ to $v = 0$ level, calculate its force constant. Also calculate the zero point energy of HCl molecule. (mass of H atom, $m_H = 1.674 \times 10^{-27}$ kg, mass of Cl atom, $m_{Cl} = 5.887 \times 10^{-26}$ kg)

(4 points)

5. Show that the particle in a ring wavefunctions $\left(\psi_{m_l}(\phi) = \frac{e^{im_l\phi}}{\sqrt{2\pi}}\right)$ are normalized.

(2 points)

6. Identify whether the following ions are Hydrogenic or not. (a) Li^+ (b) Li^{2+} (c) Be^{3+} (d) C^{5+}

(2 points)

Useful Information

Planck's constant, $h = 6.626 \times 10^{-34}$ J.s

Speed of light, $c = 3 \times 10^8$ m.s^{-1}

Mass of electron, $m_e = 9.109 \times 10^{-31}$ kg

Mass of proton, $m_p = 1.673 \times 10^{-27}$ kg

Rydberg constant, $R_H = 109677.6$ cm^{-1}

1 eV $= 1.602 \times 10^{-19}$ J

1

① $h\nu = h\nu_0 + KE$ (1 mark for formula) 3 points

$$KE = \frac{hc}{\lambda} - h\nu_0$$

$$= \frac{6.626\times10^{-34}\ Js \times 3\times10^{8}\ ms^{-1}}{200\times10^{-9}\ m} - 6.626\times10^{-34}\ Js \times 665\times10^{12}\ s^{-1}$$ (1 mark for correct substitutions)

$KE = 5.533\times10^{-19}\ J$ (1 mark for final answer, less $\frac{1}{2}$ mark if unit is not written)

2) 3 points

$$\psi_1(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi x}{l}\right)$$

$$\psi_2(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{2\pi x}{l}\right)$$

orthogonality

$$\int_0^l \psi_1^*(x)\,\psi_2(x)\,dx = 0$$ (1 mark)

$$\frac{2}{l}\int_0^l \sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{2\pi x}{l}\right)dx = \frac{1}{l}\int_0^l\left[\cos\left(\frac{\pi x}{l}\right) - \cos\left(\frac{3\pi x}{l}\right)\right]dx$$ (1 mark)

$[2\sin A\sin B = \cos(A-B) - \cos(A+B)]$

$$= \frac{1}{l}\left[\left(\frac{l}{\pi}\right)\sin\left(\frac{\pi x}{l}\right)\Big|_0^l - \left(\frac{l}{3\pi}\right)\sin\left(\frac{3\pi x}{l}\right)\Big|_0^l\right]$$

$$= \underline{\underline{0}}$$ (1 mark)

3) 3 points

$$E_n = \frac{n^2h^2}{8ml^2}$$

$$\Delta E = h\nu = E_5 - E_2 = \frac{25h^2}{8ml^2} - \frac{4h^2}{8ml^2} = \frac{21h^2}{8ml^2}$$ (1 mark)

$$\Rightarrow l^2 = \frac{21h}{8m\nu}$$

$$= \frac{21\times6.626\times10^{-34}\ Js}{8\times9.109\times10^{-31}\ kg\times6\times10^{14}\ s^{-1}}$$

$$l^2 = 3.18\times10^{-18}\ m^2$$

$\underline{\underline{l = 1.78\ nm}}$ (2 marks, less 1 mark for wrong un

(4) $\omega = \sqrt{\frac{k}{\mu}}$

4 Points

$$\mu = \frac{m_H \, m_{Cl}}{m_H + m_{Cl}}$$

$$= \frac{1.674 \times 10^{-27} \times 58.87 \times 10^{-27}}{60.544 \times 10^{-27}}$$

$$\mu = 1.628 \times 10^{-27}\,kg$$ (1 mark)

$$k = \mu \omega^2 = 1.628 \times 10^{-27}\,kg \times 54.322^2 \times 10^{26}\,s^{-2}$$

$k = 480\,kg\,s^{-2}$ (or) $N m^{-1}$ (2 marks, less 1 mark for wrong unit)

$$ZPE = \frac{1}{2}\hbar\omega = \frac{h\omega}{4\pi}$$

$$= \frac{6.626 \times 10^{-34}\,Js \times 54.322 \times 10^{13}\,s^{-1}}{4 \times 3.14}$$

$ZPE = 28.7 \times 10^{-21}\,J$ (1 mark, less $\frac{1}{2}$ mark for wrong unit)

---

(5) Normalization $\int_{-\infty}^{+\infty} \psi^*(x)\, \psi(x)\, d\tau = 1$

2 points

$$\int_0^{2\pi} \frac{1}{\sqrt{2\pi}} e^{-im\phi} \frac{1}{\sqrt{2\pi}} e^{im\phi}\, d\phi = \frac{1}{2\pi}\int_0^{2\pi} d\phi$$

(1 mark)

$$= \frac{1}{2\pi}[\phi]_0^{2\pi}$$

$$= \frac{1}{2\pi}[2\pi - 0]$$

$= \underline{1}$ (1 mark)

---

(6)

2 Points

(a) NO $\left(\frac{1}{2}\right)$

(b) YES $\left(\frac{1}{2}\right)$

(c) YES $\left(\frac{1}{2}\right)$

(d) YES $\left(\frac{1}{2}\right)$

7 (a)

TRUE

$\nu_H B_1 t_p = \theta$ (0.5 mark)

$\Rightarrow \nu_H B_1 t_p = \frac{\pi}{2}$ (0.5 mark)

$\frac{\nu_H B_1}{2\pi} t_p = \frac{1}{4}$

$\frac{\nu_H B_1}{2\pi} = \frac{1}{4 t_p} = 10\,kHz$

$\Rightarrow t_p = \frac{1}{4 \times 10 \times 10^3\,Hz} = 25 \times 10^{-6}\,s = \underline{25\,\mu s}$ (0.5 mark)

$KE = \frac{1}{2} mv^2$

$\boxed{1.5 \text{ points}}$

- final ans = 1 mark
- no unit cut ½ mark

(b)

TRUE

$s = \frac{1}{2}$

$$\left.\begin{aligned} \vec{\mu_s} &= \frac{-e\hbar}{2m_e}\vec{s} \\ \mu_{sz} &= \frac{-e\hbar}{2m_e} s_z \end{aligned}\right\} \text{(0.5 mark)}$$

$\boxed{1.5 \text{ points}}$

$$\left.\begin{aligned} |\mu_{sz}| &= \frac{-e\hbar}{2m_e} s_z = \frac{-e\hbar}{2m_e}\frac{1}{2} \\ |\vec{\mu_s}| &= \frac{-e\hbar}{2m_e}\sqrt{s(s+1)} = \frac{-e\hbar}{2m_e}\frac{\sqrt{3}}{2} \end{aligned}\right\} \text{(0.5 mark)}$$

$$\Rightarrow \left.\frac{|\mu_{sz}|}{|\vec{\mu_s}|} = \frac{1}{\sqrt{3}}\right\} \text{(0.5 mark)}$$

Minor-2 | **CYL1010_Chemistry** | **23-03- 2024**
Duration 60 Min | | **Marks 30**

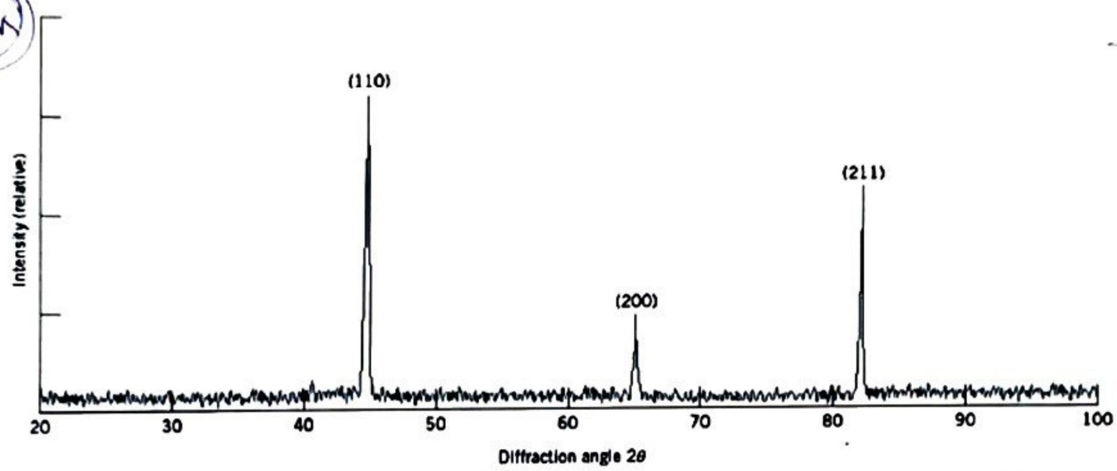
All questions are compulsory.

Q.1. Describe the process of adsorption from thermodynamic point of view. Describe all the parameters that influence the process of adsorption **[2+3=5 marks]**

Q.2. Explain surface tension. Describe capillary rise method for the determination of surface tension. A capillary tube of internal diameter 0.21 mm is dipped into a liquid whose density is 0.79 g cm^3. The liquid rises in this capillary to a height of 6.30 cm. Calculate the surface tension of the liquid. (g = 980 cm sec^{-2}).
[1+2+2=5 Marks]

Q.3. Write the information we get from XRD pattern. How can you calculate crystallite size from peak width of a XRD pattern. Below is the typical diffraction pattern for polycrystalline α-iron **(BCC)**

$\frac{10^5}{10^2}$



Calculate the d-spacing for (110) and (200) planes (given 2θ values for (110) and (200) are 45, 65 respectively; λ=1.5406 Å. **[2+2+2 =6 Marks]**

Q.4. Why is the edge centered cubic cell not considered a Bravais lattice? Why are there only 14 Bravais lattices. **[2+2 =4 Marks]**

Q.5. Explain how Bloch theorem and Kronig-Penney Model help to understand the formation of electronic band structure in metals and semiconductors. **[3+3=6 marks]**

Q.6. Write short notes on surface plasmon and quantum confinement. **[2+2=4 Marks]**

$h = 2T$ $\rho g h (\pi r^2) = (2\pi r)(\gamma \cos\theta)$