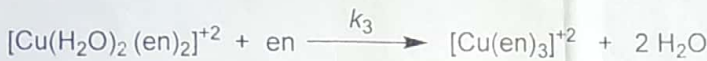
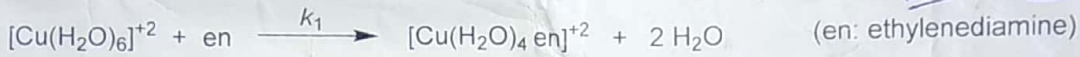
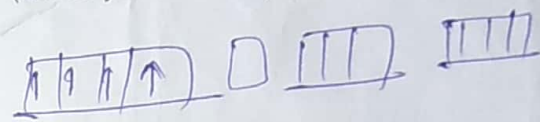


Answer all parts together.

- Three normal modes of vibration of CO₂ have $\Theta_{vib} = 3360, 954, 1890$. The second mode is doubly degenerate. Calculate the contribution to the heat capacity of these modes at 300 K. [2]
- Calculate the molar entropy of He gas at 0 K and 273.15 K, 1 bar. [3]
- Express the Helmholtz energy, $A = U - TS$ in terms of the partition function. [2]
- N₂ and CO are isoelectronic molecules but M-N₂ complexes are much weaker compared to M-CO complexes. Draw the MO diagram of both N₂ and CO and then explain why? (M is a transition metal ion) [2+2+2]
- In the following stepwise reactions, the order of the values of rate constants is $k_1 \approx k_2 \gg k_3$. Explain in details why? [3]



Cu⁺² 29



- Has FeCr₂O₄ normal or inverse spinel structure? Explain why? [1+1]
- Determine the total number of metal-metal bonds in $(\eta^4-C_4H_4)_2Fe_2(CO)_3$. [3]

Useful information

$$m_n = m_p = 1.67 \times 10^{-27} \text{ kg}; h = 6.626 \times 10^{-34} \text{ Js}; c = 2.998 \times 10^8 \text{ ms}^{-1}$$

$$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$$

Molar volume of an ideal gas = 22.4 L at STP.

$$\bar{C}_{V,vib} = \frac{d\langle \bar{E}_{vib} \rangle}{dT} = R \left(\frac{\beta h \nu}{2} \right)^2 \frac{1}{(1 - e^{-\beta h \nu})^2}$$

$\frac{0.514 \text{ J/C}}{R (\beta h \nu)^2 \frac{e^{-\beta h \nu}}{(1 - e^{-\beta h \nu})^2}}$

Monoatomic ideal gas

$$Q(N, V, T) = \frac{1}{N!} \left(\frac{2\pi M k_B T}{h^2} \right)^{3N/2} V^N \cdot g^N$$

$$S = k_B \ln Q + k_B T \left(\frac{\partial \ln Q}{\partial T} \right)_{N, V}$$

Stirling's approximation: $\ln N! = N \ln N - N$



$\frac{h\nu}{k_B}$