Task 1. Dimerization of Acetic Acid

1.1) The reaction can be represented as $2CH_3COOH \rightleftharpoons (CH_3COOH)_2$.

If we begin with, say, 100.0 mol CH_3COOH and 92.0% dimerizes, then 8.0 mol will be present at equilibrium. The 92.0 mol that react give rise to 46.0 mol dimers. The total number of moles present is therefore 54.0. Hence using the data at 298 K, the equilibrium constant, K_p, is given by

$$K_p = \frac{P_{(CH_3COOH)_2}}{(P_{CH_3COOH})^2} = \frac{X_{(CH_3COOH)_2} P_{tot}}{(X_{CH_3COOH} P_{tot})^2} = \frac{(46.0/54.0)(0.200)}{[(8.0/54.0)(0.200]^2} = 194$$

From equation $\Delta G° = -RT \ln K_p$,

At 298 K, $\Delta G° = -RT \ln K_p$

$= -(8.314 \text{ J K}^{-1}\text{mol}^{-1})(298 \text{ K}) \ln (194)$

$= -13.0 \text{ kJ mol}^{-1}$

At 318 K, $\Delta G° = -RT \ln K_p$

$= -(8.314 \text{ J K}^{-1}\text{mol}^{-1})(318 \text{ K}) \ln (37.3)$

$= -9.57 \text{ kJ mol}^{-1}$

Applying the equation $\Delta G° = \Delta H° - T\Delta S°$:

The method for the calculation is to write the two equations

$\Delta G°(298 \text{ K}) = -13.0 \text{ kJ mol}^{-1} = \Delta H° - (298)\, \Delta S°$

$\Delta G°(318 \text{ K}) = -9.57 \text{ kJ mol}^{-1} = \Delta H° - (318)\, \Delta S°$

and solve the equations simultaneously.

Then $\Delta H° = -64.1 \text{ kJ mol}^{-1}$ and $\Delta S° = -170 \text{ J K}^{-1} \text{ mol}^{-1}$.

1.2) Applying the Le Chatelier's principle, an increase of pressure should favor the dimerization.

1.3) The extent of dimerization decreases with increasing the temperature.

Task 4. Vibrational Frequency of a Diatomic Molecule

4.1) To find the reduced mass of CX, μCX:

$$E_0 = \left(0 + \frac{1}{2}\right) h\nu \quad = \frac{1}{2} h\nu$$

$$E_1 = \left(1 + \frac{1}{2}\right) h\nu \quad = \frac{3}{2} h\nu$$

$$\Delta E = E_1 - E_2 = \left(\frac{3}{2} - \frac{1}{2}\right) h\nu \quad = h\nu$$

$$\Delta E = hc\left(\frac{1}{\lambda}\right) = h\frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \quad ; \quad \nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

$$c\left(\frac{1}{\lambda}\right) = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

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

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

$$\mu = \frac{1.903 \times 10^3}{4(3.14)^2 (2.9979 \times 10^{10}\, cm \times s^{-1})^2 \left(2170.0\ cm^{-1}\right)^2}$$

μ = 1.140 × 10^{-26} kg = 6.866 amu

$\mu = 6.866$ amu

4.2) To find mass of the atom X, m_x:

$$\mu_{CX} = \frac{m_C m_X}{m_C + m_X}$$

$$\mu_{CX}(m_C + m_X) = m_C m_X$$

$$\mu_{CX} m_C + \mu_{CX} m_X = m_C m_X$$

$$m_C m_X - \mu_{CX} m_X = \mu_{CX} m_C$$

$$m_X = \frac{\mu_{CX} m_C}{m_C - \mu_{CX}}$$

$$m_X = \frac{6.866 \times 12.011}{12.011 - 6.866} = \frac{82.47}{5.145} = 16.03$$

Thus, atom **X** should be oxygen.

Task 24. Compound Identification and Related Chemistry

24.1) MCl_3 and M = Al

Theoretically, the maximum amount of the product is obtained when the mole fraction of M and Cl_2 are in the correct stoichiometric ratio. Based on the experiments, M:Cl_2 = 0.4:0.6 or 2/3 is the stoichiometric ratio needed to form M_xCl_y. Thus, the equation is as follows:

$$2\ M + 3\ Cl_2 = 2\ MCl_3.$$

The chemical formula of M_xCl_y = MCl_3

Since 0.4 mole of M generates 0.4 mole of MCl_3, the molar mass of MCl_3 and atomic mass of M can be derived:

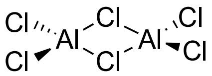
Molar mass of MCl_3 = 53.3 g/0.40 mol = 133 g mol^{-1}

A(M) = 133 – (3 * atomic mass Cl) = 133.3 – (3 * 35.45) = 26.9 g mol^{-1}

M = Al

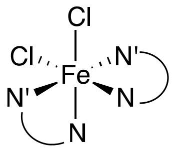
24.2) (i) $AlCl_3 + 3\ H_2O = Al(OH)_3 + 3\ HCl$

(ii) $2\ AlCl_3 + 3\ H_2SO_4 = Al_2(SO_4)_3 + 6\ HCl$

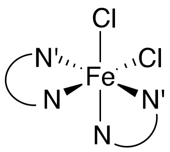
24.3) 

Task 25. Isomerism of Octahedral Fe(II) Complexes

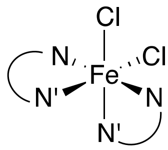
25.1)



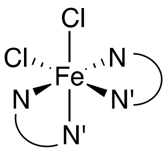
isomer **A**
cis(Cl,Cl)
trans(N',N'), *cis*(N,N)



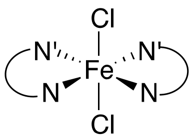
isomer **A***
cis(Cl,Cl)
trans(N',N'), *cis*(N,N)



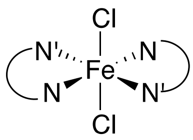
isomer **B**
cis(Cl,Cl)
cis(N',N'), *trans*(N,N)



isomer **B***
cis(Cl,Cl)
cis(N',N'), *trans*(N,N)



isomer **C**
trans(Cl,Cl)
cis(N',N'), *cis*(N,N)



isomer **D**
trans(Cl,Cl)
trans(N',N'), *trans*(N,N)

25.2) isomers A, A*, B, and B*

SOLUTION

4.1 $n(\text{CO}, \beta) = 3/2 \times n(\text{CH}_3\text{OH}, \gamma) = 1500 \text{ mol s}^{-1}$

$n(\text{H}_2, \beta) = 3 \times n(\text{CO}, \beta) = 4500 \text{ mol s}^{-1}$

4.2 $n(\text{CO}, \gamma) = n(\text{CO}, \beta) - n(\text{CH}_3\text{OH}, \gamma) = (1500 - 1000) \text{ mol s}^{-1} = 500 \text{ mol s}^{-1}$

$n(\text{H}_2, \gamma) = \text{n}(\text{H}_2, \beta) - 2 \times n(\text{CH}_3\text{OH}, \gamma) = (4500 - 2 \times 1000) \text{ mol s}^{-1} = 2500 \text{ mol s}^{-1}$

4.3 $n(\text{CH}_4, \alpha) = n(\text{CO}, \beta) = 1500 \text{ mol s}^{-1}$

$n(\text{H}_2\text{O}, \alpha) = n(\text{CO}, \beta) = 1500 \text{ mol s}^{-1}$

4.4 $n_{tot} = (1000 + 500 + 2500) \text{ mol s}^{-1} = 4000 \text{ mol s}^{-1}$

$p_i = p_{tot} \cdot (n_i/n_{tot})$

$p(\text{CO}, \gamma) = 10 \text{ MPa} \times (500/4000) = 1{,}25 \text{ MPa}$

$p(\text{H}_2, \gamma) = 10 \text{ MPa} \times (2500/4000) = 6{,}25 \text{ MPa}$

$p(\text{CH}_3\text{OH}, \gamma) = 10 \text{ MPa} \times (1000/4000) = 2{,}50 \text{ MPa}$