Partition coefficient K – Worksheet Partition coefficients describe how a solute is distributed between two immiscible solvents. Solubility of Solute in Organic Layer Partition coefficient K = Solubility of Solute in Aqueous Layer ● The partition coefficient (Kpc) is the ratio of the concentrations of a solute in two different immiscible solvents in contact with each other when equilibrium has been established (at a particular temperature) ● For example, methylamine (CH3NH2) is dissolved in two immiscible solvents: o Water o An organic solvent ● A separating funnel is shaken with the organic solvent and aqueous methylamine ● The methylamine is soluble in both solvents, so when the mixture is left to settle an equilibrium is established o The rate of methylamine molecules moving from the organic layer into the aqueous layer is equal to the rate of molecules moving from the aqueous layer to the organic layer CH3NH2(aq) CH3NH2(organic solvent) ● The value of its equilibrium constant is also called the partition coefficient Kpc = Calculating Partition Coefficients ● The partition coefficient (Kpc) for a system in which the solute is in the same physical state in the two solvents can be calculated using the equilibrium expression Worked example Calculating the partition coefficient 100 cm3 of a 0.150 mol dm–3 solution of aqueous methylamine (CH3NH2) was shaken with 75.0 cm3 of an organic solvent and left in the separating funnel to allow an equilibrium to be established. Only 50.0 cm3 of the aqueous layer was run off and titrated against 0.225 mol dm–3 hydrochloric acid (HCl) with an end-point of 14.1 cm3 of HCl. Calculate the partition coefficient of methylamine the organic solvent and water. Answer ● Step 1: Write down the equilibrium equation: CH3NH2 (aq) CH3NH2 (organic solvent) ● Step 2: Write down the equilibrium expression: Kpc = CH3NH2 (Organic solvent) CH3NH2 (aq) ● Step 3: Determine how many moles of CH3NH2 has reacted with HCl at the end-point: o At the end-point, all CH3NH2 (aq) has been neutralised by HCl (aq) CH3NH2 (aq) + HCl (aq) ⍰ CH3NH3Cl (aq) o CH3NH2 and HCl react in a ratio of 1:1 o Mol (HCl) = mol (CH3NH2) = 0.225 x 0.0141 = 0.00318 = 3.18 x 10–3 mol ● Step 4: Determine the number of moles of CH3NH2 present in the aqueous layer o Only 50.0 cm3 of the aqueous layer was used to titrate against HCl o Thus, 3.18 x 10–3 mol of CH3NH2 was present in only 50.0 cm3 of the aqueous layer o The number of moles of CH3NH2 in 100 cm3 aqueous layer is, therefore: o Mol (CH3NH2 aqueous layer) = 3.18 x 10–3 x 2 = 6.34 x 10–3 mol ● Step 5: Determine the number of moles of CH3NH2 in the organic layer: o Mol CH3NH2 (organic layer) = mol CH3NH2 (total) – mol CH3NH2(aqueous layer) o Mol CH3NH2 (total) = 0.100 x 0.150 = 0.015 mol o Mol CH3NH2 (organic layer) = 0.015 – 6.34 x 10–3 = 8.67 x 10–3 mol ● Step 6: Change the number of moles into concentrations: o Concentration (CH3NH2 in aqueous layer) =6.34 x 10–3 /0.100= 0.063 mol dm–3 o Concentration (CH3NH2 in organic layer) =8.67 x 10–3 /0.075= 0.116 mol dm–3 ● Step 7: Substitute the values into the Kpc expression: o Kpc = 0.116/0.063 = 1.83 o Since the value of Kpc is larger than 1, methylamine is more soluble in the organic solvent than in water Problem 1 1.0g of a compound dissolved in 100ml of water. If the Partition coefficient K is 5, how much of the compound will you extract by doing one extraction with 25ml of dichloromethane? Set the compound you will extract as X g. If you start with 1g of compound, the amount of compound left in the aqueous layer at the end of one extraction will be (1–X)g. Volume of aqueous = 100ml H2O, Volume of organic = 25ml CH2Cl2 K = 5= X/25 (1–X)/100 X 25 K= 5= X = 0.55 100 1–X This means you extract 0.55g of the compound using 25ml of CH2Cl2 by doing only one extraction Problem 2 1.0g of a compound dissolved in 100ml of water. If the Partition coefficient K is 5, how much of the compound will you extract by doing one extraction with 50ml of dichloromethane? Set the compound you will extract as X g. If you start with 1g of compound, the amount of compound left in the aqueous layer at the end of one extraction will be (1–X)g. Volume of aqueous = 100ml $H_2O$, Volume of organic = 50ml $CH_2Cl_2$ K = 5= X/50 (1–X)/100 X 50 K= 5= X = 0.71 1– X 100 This means you extract 0.71g of the compound using 50ml of $CH_2Cl_2$ by doing only one large extraction Factors Affecting the Partition Coefficient ● The partition coefficient (Kpc) depends on the solubilities of the solute in the two solvents ● The degree of solubility of a solute is determined by how strong the intermolecular bonds between solute and solvent are ● The strength of these intermolecular bonds, in turn, depends on the polarity of the solute and solvent molecules ● For example, ammonia is more soluble in water than in an organic solvent such as carbon tetrachloride ($CCl_4$) o Ammonia and water are both polar molecules that form hydrogen bonds with each other o Ammonia forms permanent dipole–induced dipole forces with the non–polar $CCl_4$ molecules o Since these forces are much weaker than hydrogen bonding, ammonia is less soluble in $CCl_4$ ● When Kpc is1 the solute is more soluble in water than the organic solvent ● When Kpc is1 the solute is more soluble in the organic solvent than the water