Determination of the equilibrium constant for esterification essay sample

Esterification is the reaction of a carboxylic acid with an alcohol.

This experiment is an esterification reaction between ethanoic acid and propan-1-ol when heated:

CH3COOH(aq) + CH3CH2CH2OH(aq) <=> CH3COOCH2CH2CH3(aq) + H2O(l)

The formation of propyl ethanoate is particularly well-suited to the determination of the equilibrium constant. The reaction is slow enough at room temperature so the order of mixing, temperature fluctuations over the reaction time and even a final titration with a strong base only have little effect on the reaction. Since this is a homogeneous reaction with the same number of moles of reactants and products, the equilibrium constant (Kc) is generally expressed in terms of molarity or can be calculated in terms of moles alone which is more convenient.

Because the reaction is very slow at room temperature, it is sped up by addition of catalyst (concentrated sulphuric(VI) acid). But the catalyst does not take part in the overall reaction.

The analysis of the equilibrium mixtures is based on a simple titration with standardized NaOH. Since the initial amounts of all materials are known and the overall changes in the reaction can be reflected by the determination of the final amount of acid. The concentrated H2SO4 catalyst remains unchanged and once an amount of acid is subtracted out, there is only ethanoic acid. If less acid is detected than original addition, the reaction has moved in the forward direction. If more acid is detected, the reaction has moved in the reverse direction. Since the stoichiometric ratios in the reaction

are all unity, the loss or gain in ethanoic acid can be used to figure the loss or gain in everything else.

6. Relevant Equations/Chemical Reactions Involved :

(1) Esterification reaction between ethanoic acid and propan-1-ol:

CH3COOH(aq) + CH3CH2CH2OH(aq) <=> CH3COOCH2CH2CH3(aq) + H2O(l)

(2) Titration:

CH3COOH(aq) + NaOH(aq) –> CH3COONa(aq) + H2O(aq)

7. Chemicals :

Glacial ethanoic acid 10. 5 g

Propan-1-ol 10. 0 cm3

0. 50 M sodium hydroxide 50. 0 cm3

Concentrated sulphuric(VI) acid 8 drops

Phenolphthalein indicator

8. Apparatus and equipment :

Quickfit set

1

Safety spectacle

1

Burette

1

Wash bottle

1

Filter funnel

1

1. 0 cm3 pipette

1

White tile

1

Measuring cylinder

1

250 cm3 conical flask

2

Heat-proof mat

1

250 cm3 beaker

2

Anti-bumping granules

Bunsen burner

1

Ice

9. Procedure :

1. 10. 5 g of glacial ethanoic acid and 10. 0 cm3 of propan-1-ol are put into a clean and dry peer-shaped flask. And then those were mixed thoroughly.

2. 1. 0 cm3 of the mixture was transferred by pipette to a 250 cm3 conical flask that about 25 cm3 of deionized water and 2 drops of phenolphthalein indicator were contained. The solution was then titrated to the end point with 0. 50 M sodium hydroxide solution.

3. The volume (V1 cm3) of titre was recorded.

4. 8 drops of concentrated sulphuric(VI) acid were added to the remainder of the acid-alcohol solution and the flask was swirled continuously.

5. Step 2 was repeated immediately.

6. The volume (V2 cm3) of titre was recorded.

7. A few anti-bumping granules were added to the flask and then it was attached to a water-cooled reflux condenser.

8. The solution was refluxed for 30 minutes. Then, the flask was cooled by an ice bath.

9. Step 2 was repeated again.

10. The volume (V3 cm3) of titre was recorded.

11. The solution was refluxed continuously for additional 20 minutes. Then, the flask was also cooled by an ice bath.

12. Step 2 was repeated again.

13. The volume (V4 cm3) of titre was recorded.

10. Observations :

The reaction mixture changed from colourless to red in titration.

11. Data, Calculation and Results :

Titration

1

2

3

4

Final burette reading (cm3)

22. 00

41. 50

6. 55

12. 00

Initial burette reading (cm3)

2. 90

22. 00

0. 85

6. 55

Volume of titre (cm3)

19. 10

19. 50

5. 70

5. 45

V1 = 19. 10 cm3

V2 = 19. 50 cm3

V3 = 5. 70 cm3

V4 = 5. 45 cm3

Volume of sodium hydroxide required for neutralizing concentrated sulphuric(VI) acid

= V2 – V1

= 19. 5 – 19. 1

= 0. 40 cm3

Volume of sodium hydroxide required for neutralizing remained ethanoic acid after refluxing for 30 minutes

= V3 – (V2 – V1)

= 5. 70 – 0. 40

= 5. 30 cm3

Volume of sodium hydroxide required for neutralizing remained ethanoic acid after refluxing for 50 minutes

= V4 – (V2 – V1)

= 5. 45 – 0. 40

= 5. 05 cm3

12. Conclusion :

The equilibrium constant of esterification was found to be 7. 74.

13. Discussion :

1. Small amount of concentrated sulphuric(VI) acid was added to the reaction mixture at the beginning of the experiment as a catalyst in order to speed up the reaction.

2. Anti-bumping granules should be added to the reaction mixture before refluxing so as to prevent super-heating. It can ensure smooth boiling.

3. The refluxing should be continued in step (11) until the titre of sodium hydroxide used approaching constantso as to ensure equilibrium is reached.

4. Equation for the esterification reaction between ethanoic acid and propan-1-ol:

CH3COOH(aq) + CH3CH2CH2OH(aq) <=> CH3COOCH2CH2CH3(aq) + H2O(l)

5. No. of moles of ethanoic acid = no. of moles of sodium hydroxide used

= 0. 5 x 5. 05 x 10-3

= 2. 525x 10-3 mol

Concentration of ethanoic acid remaining at the end of the reflux

= 2. 525x 10-3 / (1 x 10-3)

= 2. 525 M

6. Concentration of propan-1-ol = Concentration of ethanoic acid

= 2. 525 M

Concentration of propyl ethanoate

= 0. 5 x (V2 – V4) / (1 x 10-3)

= 0. 5 x [(19. 5 – 5. 45) x 10-3] / (1 x 10-3)

= 7. 025 M

Concentration of water = Concentration of propyl ethanoate

= 7. 025 M

7. Kc = [CH3COOCH2CH2CH3(aq)] [H2O(l)] [CH3COOH (aq)]

[CH3CH2CH2OH (aq)]

8. Kc = (7. 025/2. 525)2

= 7. 74

9. If the concentration of the sodium hydroxide solution is not known exactly, it would not have any effect on the determination of the equilibrium constant for the esterification reaction.

Since Kc = [CH3COOCH2CH2CH3(aq)] [H2O(l)]

[CH3COOH (aq)][CH3CH2CH2OH (aq)]

Kc = { [NaOH](V2- V4) / [NaOH] [V4 – (V2 – V1)]}2

= { (V2- V4) / [V4 – (V2 – V1)] }2

Thus, Kc is not affected by the concentration of sodium hydroxide.

10. There is error in this experiment.

(1) Taking reading in titration.

Error estimation –

When taking initial reading, error is + 0. 05 cm3.

When taking final reading, error is also + 0. 05 cm3.

Therefore, error is + 0. 1 cm3.