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Effect of Iodide Ion Concentration on the Equilibrium Position of the Iodine Reaction

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ABSTRACT

Chemical equilibrium is a reversible condition in which the rates of the forward and reverse reactions are equal, resulting in constant concentrations of reactants and products. This dynamic state, represented by a bidirectional arrow (⇌), continues at the molecular level without observable macroscopic changes. According to Le Chatelier's principle, any change in concentration, temperature, pressure, or volume causes the equilibrium to shift in a direction that counteracts the disturbance. The equilibrium constant (K) quantitatively expresses the ratio of product and reactant concentrations at equilibrium, indicating the reaction's extent. This study aimed to determine the equilibrium constant (Kc) for the reaction $I_2 + I^- \leftrightarrow I_3^-$ through solvent distribution and iodometric titration methods. The experiment investigated how varying KI concentrations affect iodine solubility and triiodide ion formation. Results revealed that higher KI concentrations increased iodine solubility, favoring I_3^- formation and shifting the equilibrium toward the products. The equilibrium constant (Kc) at 30°C was calculated to be 48, indicating a strong tendency for triiodide ion formation under the given conditions. These findings demonstrate that iodide ion concentration plays a crucial role in determining iodine solubility and the equilibrium position of the reaction system.

Keywords: Chemical equilibrium; Le Chatelier's principle; equilibrium constant; iodine; iodide.

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1. Introduction

Chemical equilibrium is defined as a reversible reaction in which products can revert to reactants until the concentrations of both remain constant [1]. A system at

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equilibrium tends to maintain its balance; thus, when subjected to external disturbances such as changes in concentration, pressure, or temperature, it adjusts to restore equilibrium [8]. Chemical equilibrium can be classified into two types based on system characteristics: static equilibrium and dynamic equilibrium [2]. Static equilibrium exists when all acting forces are balanced and no resultant force is produced, whereas dynamic equilibrium occurs when forces remain balanced but molecular motion continues [3]. In chemical systems, the equilibrium constant quantitatively represents the ratio between the concentrations of products and reactants at equilibrium, providing insight into the reaction's extent [4].

Chemical equilibrium occurs when the rates of the forward and reverse reactions become equal, resulting in no observable macroscopic changes in the system [5]. In chemical notation, equilibrium reactions are represented by a double arrow (↔), signifying the bidirectional nature of the process [6]. In the forward reaction, product concentration increases while reactant concentration decreases; conversely, in the reverse reaction, reactants are regenerated from products, maintaining dynamic balance between both directions [7]. In general, a chemical equilibrium reaction can be represented as: $aA + bB = cC + dD$ [8]. According to the law of mass action proposed by Guldberg and Waage, at equilibrium and a constant temperature, the ratio of the product of the concentrations of products (each raised to its stoichiometric coefficient) to that of the reactants remains constant [9]. Therefore, the equilibrium constant (K) quantitatively defines the ratio of product concentrations to reactant concentrations at equilibrium [10].

Variations in external conditions can shift the position of equilibrium, influencing the extent of product formation and reaction direction [11]. According to Le Chatelier's principle, when a system at equilibrium is subjected to an external disturbance, it responds in a way that minimizes the effect of that disturbance and restores a new equilibrium state [12]. Several external parameters, including concentration, pressure, volume, and temperature, can alter equilibrium conditions and determine the direction of the shift [13]. Increasing the concentration of a reactant drives the equilibrium toward product formation, whereas decreasing it shifts the equilibrium toward the reactants [14]. Pressure and volume are inversely related: an increase in volume (decrease in pressure) shifts equilibrium toward the side with more gas molecules, while a decrease in volume (increase in pressure) favors the side

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with fewer gas molecules [15]. Temperature changes influence equilibrium by favoring the endothermic direction when heat is absorbed ($\Delta H > 0$) and the exothermic direction when heat is released ($\Delta H < 0$) [16]. Catalysts accelerate both forward and reverse reactions equally, thereby reducing the time required to reach equilibrium without affecting its position or the equilibrium constant [17].

In most chemical systems, reactions rarely proceed to complete conversion; instead, they reach a state in which both reactants and products coexist in measurable amounts [18]. At a specific temperature and pressure, the ratio between the concentrations of products and reactants becomes constant, marking the attainment of chemical equilibrium [19]. In this condition, the forward and reverse reactions occur at identical rates, resulting in a dynamic equilibrium where no net change in concentration is observed [20]. Based on the physical phases involved, equilibrium can be classified into homogeneous equilibrium—when all substances are in the same phase—and heterogeneous equilibrium—when more than one phase is present within the system [21]. Therefore, the classification of equilibrium into homogeneous and heterogeneous types provides a fundamental framework for understanding phase interactions in chemical systems [22].

2. Materials and Method

Tools and Materials

The apparatus utilized in this experiment included Erlenmeyer flasks (200 and 250 mL), graduated cylinders (10, 25, and 250 mL), volumetric pipettes (5 and 25 mL), a 25 mL burette, and a wash bottle. The chemical reagents were a saturated solution of I_2 in $CHCl_3$, 0.1 M standard KI solution, 0.02 M standard $Na_2S_2O_3$ solution, 1% starch indicator solution, and crystalline KI.

Experimental Procedure

Two Erlenmeyer flasks, labeled A and B, were prepared, each containing 4 mL of a saturated iodine (I_2) solution in chloroform ($CHCl_3$). Flask A was used for determining the distribution coefficient (KD), while flask B was used for calculating the equilibrium constant (KC).

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1. Measurement of the distribution coefficient (KD)

   To determine the distribution coefficient, flask A was filled with 40 mL of distilled water. The flask was then sealed, vigorously shaken, and placed in a thermostat at 30°C for 30 minutes. Once equilibrium was reached, 1 mL of the $CHCl_3$ layer was withdrawn with a pipette. Then, 0.4 g of KI crystals and 4 mL of water were added. The mixture was titrated with 2 mL of a 0.02 M $Na_2S_2O_3$ solution containing a starch indicator until the color turned pale yellow. The $Na_2S_2O_3$ volume utilized (V_1) was measured and recorded. Additionally, 10 mL of the aqueous layer was titrated, and the volume consumed (V_2) was recorded to calculate the KD.

2. Measurement of the equilibrium constant (KC)

   To determine the equilibrium constant (KC), flask B contained 40 mL of a 0.1 M KI solution. The flask was then shaken, thermostated at 30°C for 30 minutes, and left to attain equilibrium. The $CHCl_3$ layer (1 mL) was sampled, followed by the addition of 0.4 g KI crystals and 4 mL of water, then titrated with $Na_2S_2O_3$ using starch as an indicator. The volume of titrant (V_3) was recorded. Similarly, 10 mL of the aqueous layer was titrated, and the volume consumed (V_4) was recorded to calculate KC.

3. Result

Table 1. Experimental Data

Time (minutes)	Suhu (^{o}C)	
	Sample A	Sample B
5	30	30
10	30	30
15	30	30
20	30	30
25	30	30
30	30	30

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Measured volumes:

- V1 = 4.4 mL
- V2 = 5.85 mL
- V3 = 2 mL
- V4 = 135 mL

$$
\begin{aligned}
[KI] &= \frac{n}{v} \\
&= \frac{mass}{Mr/0.3\ l} \\
&= \frac{3\ gr}{166\frac{gr}{mol}/0.3\ l} \\
&= 0.46\ \mathrm{M}
\end{aligned}
$$

1. Determination of Distribution Coefficient (KD) in Erlenmeyer

   The reactions involved are as follows:

   $I_2 + I^- \rightarrow I_3^-$

   $\underline{I_3^- + 2S_2O_3^{2-} \leftrightarrow 3I^- + S_4O_6^{2-}}$

   $I_2 + 2S_2O_3^{2-} \leftrightarrow 2I^- + S_4O_6^{2-}$

   Mol $S_2O_3^{2-}$ = 2 mol I_2

   $[S_2O_3^{2-}] \times V\ S_2O_3^{2-} = 2 \times [I_2] \times V\ I_2$

   a. In the CCl_4 layer

      $$[I_2] = \frac{[S_2O_3^{2-}]\ x\ Vtitration}{2\ x\ VI_2} = \frac{0.02M\ x\ 4.4mL}{2\ x\ 4mL} = 0.0110\ \mathrm{M}$$

   b. In the aqueous layer

      $$[I_2]_{CCl_4} = \frac{[S_2O_3^{2-}]\ x\ Vtitration}{2\ x\ VI_2} = \frac{0.02M\ x\ 5.85mL}{2\ x\ 20mL} = 0.0029\ \mathrm{M}$$

   c. Distribution Coefficient (KD)

      $$KD = \frac{[I_2]\ CCl_4}{[I_2]\ air} = \frac{0.0110\ M}{0.0029\ M} = 3.8\ \mathrm{M}$$

2. Determination of $[I_2]$, $[I^-]$, and $[I_3^-]$ in Erlenmeyer

   In the CCl_4 layer

   $$[I_2]_{CCl_4} = \frac{[S_2O_3^{2-}]\ x\ Vtitration}{2\ x\ VI_2} = \frac{0.02M\ x\ 2mL}{2\ x\ 4mL} = 0.0050\ \mathrm{M}$$

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In the aqueous layer

$$[I_2]_{H_2O} = \frac{[S_2O_3{}^{2-}]\ x\ Vtitration}{2\ x\ VI_2} = \frac{0.02M\ x\ 12.35mL}{2\ x\ 20mL} = 0.0061\ M$$

a. Free $[I_2]$ concentration in water

$$[I_2] = \frac{[I_2]\ CCl_4}{KD} = \frac{0.0050\ M}{3.8\ M} = 0.0013\ M$$

b. Triiodide ion concentration $[I_3^-]$

$$[I_3^-] = [I_2]_{H_2O} - [I_2]_{free}$$
$$= 0.0061\ M - 0.0048\ M$$
$$= 0.0952\ M$$

c. Iodide ion concentration $[I^-]$

$$[I^-] = [KI] - [I_3^-]$$
$$= 0.1\ M - 0.0048\ M$$
$$= 0.0952\ M$$

3. Equilibrium Constant KC

$$KC = \frac{I_3{}^-}{[I_2][I^-]}$$
$$= \frac{0.0048\ M}{0.0013M\ .\ 0.0952M}$$
$$= 48\ M$$

Thus, the value of the equilibrium constant (Kc) for $I_2 + I^- \leftrightarrow I_3^-$ is 48.

4. Discussion

This research examines the chemical equilibrium of the reaction $I_2 + I^- \leftrightarrow I_3^-$. The primary objective was to determine the equilibrium constant by evaluating the distribution coefficient of iodine in various solvents and the subsequent equilibrium concentrations of iodine species. Chemical equilibrium is defined as a dynamic condition in which the rates of the forward and reverse reactions are equal, resulting in constant concentrations of reactants and products. Several factors, such as concentration, temperature, and pressure, affect equilibrium, while a catalyst merely accelerates the attainment of equilibrium without altering its position [7, 9].

In this experiment, iodine was dissolved in two immiscible solvents: water (a polar solvent) and chloroform ($CHCl_3$, a non-polar solvent). The experiment showed that iodine dissolves better in $CHCl_3$ than in water because the molecules of iodine and chloroform have similar polarities [2,7]. The shaking process ensured a proper

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distribution of iodine molecules between the two phases, while allowing the system to stand for a period of time enabled the reorganization of molecules to achieve equilibrium. The results confirmed that $CHCl_3$ formed the lower layer due to its higher density (1.49 $g·cm^{-3}$), whereas water constituted the upper phase. The distribution coefficient (KD) was determined to be 3.8, indicating a strong preferential partitioning of iodine into the chloroform phase [3, 8].

In the subsequent stage, the addition of potassium iodide (KI) to the aqueous phase facilitated the formation of triiodide ions (I_3^-) via the reversible reaction between molecular iodine (I_2) and iodide ions (I^-), as expressed by the equilibrium $I_2 + I^- \rightleftharpoons I_3^-$ [5,7]. The titration of iodine with standardized sodium thiosulfate solution ($Na_2S_2O_3$, 0.02 M) in the presence of starch as an indicator confirmed the quantitative distribution of iodine species. The experimental results showed that the concentration of free iodine in water was 0.0013 M, while the concentration of complexed iodine (as I_3^-) was 0.0048 M, with the corresponding iodide concentration being 0.0952 M. Based on these data, the equilibrium constant (KC) of the reaction was calculated to be 48.

The relatively high equilibrium constant (KC = 48) indicates that, under the experimental conditions, the formation of triiodide ions (I_3^-) is thermodynamically favored, consistent with previous findings on halogen–halide equilibria [7,8]. The findings are consistent with the theoretical understanding of iodine solubility and equilibrium processes in polar and non-polar systems. Overall, the experiment not only demonstrates the concept of phase distribution but also highlights the importance of equilibrium constants in predicting the extent of complex ion formation in solution.

5. Conclusions

Chemical equilibrium is a dynamic process in which the rates of the forward and reverse reactions are equal, resulting in constant concentrations of reactants and products. In this study, iodine (I_2) was less soluble in water but dissolved more effectively in chloroform ($CHCl_3$) because of the similarity in polarity between the solute and solvent. Adding potassium iodide (KI) to the aqueous phase significantly increased iodine's solubility by forming triiodide ions (I_3^-). This illustrates the role of complex ion formation in phase distribution equilibria. The experimentally

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determined equilibrium constant (K_c = 48) for the reaction $I_2 + I^- \rightleftharpoons I_3^-$ indicates that the system strongly favors the production of triiodide ions under the experimental conditions. These findings reinforce the theoretical understanding of chemical equilibrium and demonstrate how solvent polarity and ionic interactions influence equilibrium in heterogeneous systems.

6. Patents

This investigation did not result in a patent. Instead, the findings enrich the theoretical perspective on chemical equilibrium by offering experimental insights into determining the equilibrium constant for $I_2 + I^- \leftrightarrow I_3^-$. The results highlight fundamental concepts in phase distribution, solubility, and ion complex formation. These concepts can serve as valuable references in educational and research contexts. However, they do not generate intellectual property rights in the form of a patent.

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