

Calculate The Equilibrium Concentrations Of All Chemical Species Present In A 0.10 M H₂CO₃(aq) Solution.

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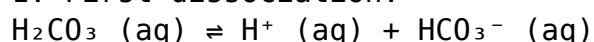
Understanding the equilibrium concentrations in a carbonic acid solution is fundamental to many fields, including environmental chemistry, physiology, and industrial processes. When carbonic acid (H₂CO₃) dissolves in water, it undergoes dissociation into various species, primarily bicarbonate (HCO₃⁻) and carbonate (CO₃²⁻) ions, depending on the pH of the solution. Calculating the equilibrium concentrations of all species present involves applying principles of chemical equilibrium, acid-base chemistry, and stoichiometry. In this article, we will walk through the detailed process of determining these concentrations in a 0.10 M H₂CO₃ solution.

Understanding the Chemistry of Carbonic Acid in Water

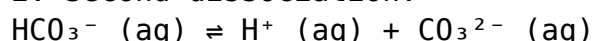
The Dissociation Equilibria of H₂CO₃

Carbonic acid is a weak acid that exists in equilibrium with water and dissolved CO₂. Its dissociation occurs in two primary steps:

1. First dissociation:



2. Second dissociation:



Each of these steps has an associated acid dissociation constant (K_a), which quantifies the extent of dissociation:

- First dissociation constant (K_{a1}): approximately 4.3×10^{-7}
- Second dissociation constant (K_{a2}): approximately 5.6×10^{-11}

These values indicate that the first dissociation is much more significant than the second under typical conditions, but both influence the overall

speciation in solution.

Initial Conditions and Assumptions

Before setting up the equilibrium expressions, it's crucial to specify initial conditions and assumptions:

- Initial concentration of H_2CO_3 : 0.10 M
- The solution is initially only composed of H_2CO_3 , with no bicarbonate or carbonate ions present.
- The dissociation is at equilibrium, and activity coefficients are assumed to be close to 1 for dilute solutions.
- Temperature is assumed to be 25°C, where the given K_a values are valid.

Setting up the Equilibrium Expressions

To find the equilibrium concentrations, we need to write the equilibrium equations based on the dissociation steps.

First Dissociation Equilibrium

Let's define:

- Initial concentration of H_2CO_3 : $[\text{H}_2\text{CO}_3]_0 = 0.10 \text{ M}$
- Change in concentration due to dissociation: x (extent of dissociation into H^+ and HCO_3^-)

At equilibrium:

- $[\text{H}_2\text{CO}_3] = 0.10 - x$
- $[\text{H}^+] = x$
- $[\text{HCO}_3^-] = x$

The equilibrium expression:

$$K_{a1} = [\text{H}^+][\text{HCO}_3^-] / [\text{H}_2\text{CO}_3] = x^2 / (0.10 - x)$$

Given the small value of K_{a1} , we can often approximate $(0.10 - x) \approx 0.10$, simplifying calculations.

Second Dissociation Equilibrium

Let's define:

- y = amount of HCO_3^- that dissociates further into CO_3^{2-}

At equilibrium:

- $[\text{HCO}_3^-] = x - y$
- $[\text{CO}_3^{2-}] = y$
- $[\text{H}^+] = x + y$ (since both dissociations produce H^+ ions)

The second equilibrium expression:

$$K_{a2} = [\text{H}^+][\text{CO}_3^{2-}] / [\text{HCO}_3^-] = (x + y) y / (x - y)$$

Because K_{a2} is very small, the concentration of CO_3^{2-} (y) is typically much less than $[\text{HCO}_3^-]$, and the approximation $y \approx 0$ can sometimes be used. However, for accuracy, especially in a detailed calculation, we should include y explicitly.

Calculating the Equilibrium Concentrations

The calculation proceeds in steps, starting with the first dissociation, then addressing the second.

Step 1: Calculate $[\text{H}^+]$ and $[\text{HCO}_3^-]$ from the First Dissociation

Using K_{a1} and the approximation:

$$K_{a1} \approx x^2 / 0.10$$

$$x^2 \approx K_{a1} \times 0.10 = (4.3 \times 10^{-7}) \times 0.10 = 4.3 \times 10^{-8}$$

$$x \approx \sqrt{(4.3 \times 10^{-8})} \approx 6.56 \times 10^{-4} \text{ M}$$

Therefore:

- $[\text{H}^+] \approx 6.56 \times 10^{-4} \text{ M}$
- $[\text{HCO}_3^-] \approx 6.56 \times 10^{-4} \text{ M}$
- $[\text{H}_2\text{CO}_3] \approx 0.10 - 6.56 \times 10^{-4} \approx 0.0993 \text{ M}$

This indicates that most of the initial H_2CO_3 remains undissociated, with a

small fraction dissociated.

Step 2: Determine the Extent of Second Dissociation

Next, analyze the second dissociation:

$$K_{a2} = 5.6 \times 10^{-11}$$

Assuming:

- $[\text{HCO}_3^-]$ at this point is approximately 6.56×10^{-4} M minus y
- $[\text{CO}_3^{2-}] = y$
- $[\text{H}^+] = 6.56 \times 10^{-4} + y$

Since y is expected to be very small compared to 6.56×10^{-4} M, we can approximate:

- $[\text{HCO}_3^-] \approx 6.56 \times 10^{-4}$ M
- $[\text{H}^+] \approx 6.56 \times 10^{-4}$ M (from first dissociation) plus a negligible amount from second dissociation

Now, set up the second equilibrium:

$$K_{a2} \approx (6.56 \times 10^{-4}) y / (6.56 \times 10^{-4}) \approx y$$

Thus:

$$y \approx K_{a2} \approx 5.6 \times 10^{-11} \text{ M}$$

This extremely small value suggests that the second dissociation contributes negligibly to the overall H^+ concentration and species distribution.

Final Species Concentrations at Equilibrium

Summarizing the calculations:

- H_2CO_3 (aq): approximately 0.0993 M (remaining undissociated)
- H^+ (aq): approximately 6.56×10^{-4} M (from first dissociation)
- HCO_3^- (aq): approximately 6.56×10^{-4} M (from first dissociation)
- CO_3^{2-} (aq): approximately 5.6×10^{-11} M (from second dissociation)

The minor amount of CO_3^{2-} indicates that the solution is predominantly characterized by undissociated H_2CO_3 and bicarbonate ions, with negligible carbonate formation under these conditions.

pH Calculation of the Solution

The pH of the solution can be derived from the concentration of H^+ :

$$pH = -\log [H^+] \approx -\log (6.56 \times 10^{-4}) \approx 3.18$$

This pH indicates an acidic solution, consistent with the presence of undissociated carbonic acid and bicarbonate ions acting as a buffer.

Implications and Applications

Understanding the equilibrium speciation of carbonic acid solutions is essential in various contexts:

- Environmental Chemistry: The buffering capacity of natural waters depends on bicarbonate and carbonate concentrations.
- Physiology: Blood plasma maintains pH through bicarbonate buffering, with equilibrium calculations informing about CO_2 transport.
- Industrial Processes: Carbonate systems are used in carbonation, water treatment, and chemical manufacturing.

Summary and Key Takeaways

- The dissociation of H_2CO_3 in water involves two steps with distinct K_a values, with the first being much more significant.
- Approximate calculations based on equilibrium expressions and assumptions about small dissociation extents provide reasonable estimates of species concentrations.
- The dominant species in a 0.10 M H_2CO_3 solution are undissociated H_2CO_3 and HCO_3^- ions, with negligible CO_3^{2-} under standard conditions.
- The pH of the solution is approximately 3.18, reflecting its acidity.

By systematically applying equilibrium principles and approximations, we can accurately determine the distribution of chemical species in complex aqueous systems like carbonic acid solutions. This approach is fundamental in analytical chemistry, environmental science, and biochemistry

Frequently Asked Questions

How do I set up the equilibrium expressions for a 0.10 M H₂CO₃ solution?

Start by writing the dissociation reactions: $\text{H}_2\text{CO}_3 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$ and $\text{HCO}_3^- \rightleftharpoons \text{H}^+ + \text{CO}_3^{2-}$. Then, apply the equilibrium constants (K_{a1} and K_{a2}) to express the concentrations of each species in terms of H^+ concentration, and set up equations based on initial concentrations and dissociation.

What is the initial concentration of H₂CO₃ in the solution, and how does it affect the equilibrium calculations?

The initial concentration of H_2CO_3 is given as 0.10 M. Since it is a weak acid, only a portion dissociates at equilibrium. This initial value serves as the starting point for calculating the extent of dissociation and the concentrations of all species at equilibrium.

How do I use the acid dissociation constants (K_{a1} and K_{a2}) to find the equilibrium concentrations?

Use the expressions: $K_{a1} = [\text{H}^+][\text{HCO}_3^-]/[\text{H}_2\text{CO}_3]$ and $K_{a2} = [\text{H}^+][\text{CO}_3^{2-}]/[\text{HCO}_3^-]$. Set up equations considering the degree of dissociation, then solve for $[\text{H}^+]$, and subsequently find the concentrations of all species using these relationships.

Can I assume complete dissociation of H₂CO₃ in dilute solutions like 0.10 M?

No, H_2CO_3 is a weak acid with partial dissociation. Assuming complete dissociation would lead to inaccurate results. Instead, use the K_a values to determine the actual equilibrium concentrations.

What are the typical values of K_{a1} and K_{a2} for carbonic acid, and how do they influence the calculations?

K_{a1} is approximately 4.3×10^{-7} , and K_{a2} is about 5.6×10^{-11} . These small values indicate weak dissociation, and they help determine the extent of ionization and the relative concentrations of H^+ , HCO_3^- , and CO_3^{2-} at equilibrium.

How do I determine the pH of the 0.10 M H₂CO₃ solution?

Calculate the concentration of H^+ ions from the dissociation of H_2CO_3 using the equilibrium expressions. Once $[\text{H}^+]$ is known, find $\text{pH} = -\log[\text{H}^+]$.

Typically, for weak acids like this, the pH will be slightly acidic, around 4.2 to 4.4.

What steps should I follow to find the equilibrium concentrations of all species in this problem?

First, write the dissociation reactions and expressions for K_{a1} and K_{a2} . Set up an ICE table to track initial, change, and equilibrium concentrations. Use the K_a values to create equations, solve for $[H^+]$, then calculate the concentrations of H_2CO_3 , HCO_3^- , and CO_3^{2-} at equilibrium. Finally, check the consistency of your results.

Additional Resources

Calculate The Equilibrium Concentrations Of All Chemical Species Present In A 0.10 M $H_2CO_3(aq)$ Solution

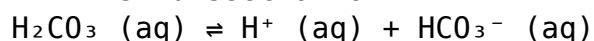
Understanding the equilibrium concentrations of all species in a solution of carbonic acid (H_2CO_3) is a classic problem in chemical equilibria and acid-base chemistry. This analysis provides insights into the behavior of weak acids in aqueous solutions, their dissociation patterns, and how to quantitatively determine the concentrations of all species at equilibrium. This article offers a comprehensive review of how to calculate the equilibrium concentrations of H_2CO_3 and its related ions in a 0.10 M solution, integrating theoretical principles, step-by-step calculations, and contextual explanations.

Introduction to Carbonic Acid in Aqueous Solution

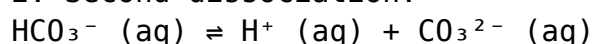
Carbonic acid (H_2CO_3) is a weak, diprotic acid that naturally exists in equilibrium with dissolved carbon dioxide (CO_2) and water. Its importance extends beyond simple acid-base chemistry; it plays a vital role in physiological processes such as blood buffering and in geological carbon cycles.

When H_2CO_3 dissolves in water, it undergoes two primary dissociation steps:

1. First dissociation:



2. Second dissociation:



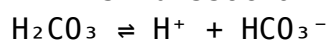
However, at typical aqueous conditions, especially at low concentrations (~ 0.10 M), the dominant species are H_2CO_3 (or more accurately, dissolved CO_2), H^+ , and HCO_3^- . The carbonate ion (CO_3^{2-}) is present in negligible amounts unless the pH is sufficiently high to favor its formation.

Fundamental Concepts and Equilibrium Constants

Understanding the dissociation constants (K_a):

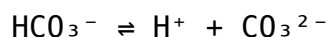
The acid dissociation constants quantify the strength of an acid. For H_2CO_3 , two dissociation constants are relevant:

- First dissociation constant (K_{a1}):



$K_{a1} \approx 4.3 \times 10^{-7}$ at 25°C .

- Second dissociation constant (K_{a2}):



$K_{a2} \approx 5.0 \times 10^{-11}$ at 25°C .

Note:

The concentrations of each species at equilibrium depend on these constants, initial concentration of H_2CO_3 , and the pH of the solution.

Setting Up the Problem: Initial Conditions and Assumptions

In this scenario:

- Initial concentration of H_2CO_3 (C_0): 0.10 M
- Initial concentrations of other species: 0 M (assuming no initial ions other than H_2CO_3)
- Temperature: 25°C (standard conditions)
- Ionic activity: Assumed ideal solution
- Negligible CO_2 hydration effects: For simplicity, the solution is assumed to be equilibrated with atmospheric CO_2 , and the dissolved CO_2 is in rapid equilibrium with H_2CO_3 .

Step-by-Step Calculation of Equilibrium Concentrations

The goal: Find the equilibrium concentrations of H_2CO_3 (or dissolved CO_2), H^+ , and HCO_3^- .

1. Defining Variables

Let:

- x : The amount of H_2CO_3 dissociated into H^+ and HCO_3^- during equilibrium.
- $[\text{H}^+]$: The concentration of hydrogen ions at equilibrium.
- $[\text{HCO}_3^-]$: The concentration of bicarbonate ions at equilibrium.
- $[\text{H}_2\text{CO}_3]$: The remaining undissociated carbonic acid.

Initial concentrations:

- $[\text{H}_2\text{CO}_3]_{\text{initial}} = 0.10 \text{ M}$
- $[\text{H}^+]_{\text{initial}} = 0 \text{ M}$
- $[\text{HCO}_3^-]_{\text{initial}} = 0 \text{ M}$

At equilibrium:

- $[\text{H}_2\text{CO}_3] = 0.10 - x$
- $[\text{H}^+] = x$ (from first dissociation)
- $[\text{HCO}_3^-] = x$

Given that the second dissociation is negligible at this pH (which is typical for a 0.10 M solution), we can ignore CO_3^{2-} for simplicity.

2. Expressing Equilibrium Constants

Using the definition of K_{a1} :

$$K_{a1} = \frac{[\text{H}^+][\text{HCO}_3^-]}{[\text{H}_2\text{CO}_3]}$$

Substituting the equilibrium concentrations:

$$4.3 \times 10^{-7} = \frac{x \times x}{0.10 - x}$$

Or,

$$4.3 \times 10^{-7} = \frac{x^2}{0.10 - x}$$

Given the small value of K_{a1} , x will be very small compared to 0.10, allowing the approximation:

$$0.10 - x \approx 0.10$$

Thus,

$$4.3 \times 10^{-7} \approx \frac{x^2}{0.10}$$

Solving for x :

$$x^2 = 4.3 \times 10^{-7} \times 0.10$$

$$x^2 = 4.3 \times 10^{-8}$$

$$x = \sqrt{4.3 \times 10^{-8}}$$

$$x \approx 6.56 \times 10^{-5} \text{ M}$$

3. Determining pH and Species Concentrations

- Hydrogen ion concentration:

$$[H^+] \approx 6.56 \times 10^{-5} \text{ M}$$

- pH of the solution:

$$pH = -\log [H^+]$$

$$pH \approx -\log (6.56 \times 10^{-5})$$

$$pH \approx 4.18$$

- Concentration of HCO_3^- :

$$[HCO_3^-] = x \approx 6.56 \times 10^{-5} \text{ M}$$

- Remaining undissociated H_2CO_3 :

$$[H_2CO_3] \approx 0.10 - x \approx 0.10 \text{ M}$$

Thus, at equilibrium, the dominant species are:

Species	Concentration (M)
H_2CO_3 (or dissolved CO_2)	≈ 0.10 M (since x is negligible)
HCO_3^-	$\approx 6.56 \times 10^{-5}$ M
H^+	$\approx 6.56 \times 10^{-5}$ M
CO_3^{2-}	Negligible under these conditions

Considering the Second Dissociation and Its Impact

While the second dissociation ($\text{HCO}_3^- \rightleftharpoons \text{H}^+ + \text{CO}_3^{2-}$) is characterized by a much smaller K_{a2} ($\approx 5 \times 10^{-11}$), its contribution is minimal at this pH (~ 4.2). The pH is well below the point where carbonate becomes significant, and thus, for most practical purposes, the carbonate concentration remains negligible.

However, for completeness, a similar approach can be employed if the pH were higher, indicating significant carbonate formation.

Implications and Real-World Significance

Understanding the pH of the solution:

The pH of approximately 4.18 indicates a mildly acidic solution, consistent with the properties of carbonic acid. This pH aligns with typical physiological blood pH (~ 7.4), but in this simplified calculation, the pH is lower because the initial concentration is relatively high and no buffering agents are present.

Relevance to biological systems:

In blood, the bicarbonate buffer system maintains tight pH regulation. The calculations here reflect the equilibrium state of a dilute solution of carbonic acid, providing a foundation for understanding how shifts in concentrations affect pH and species distribution.

Environmental and industrial context:

In ocean chemistry, atmospheric CO_2 dissolves into seawater, forming H_2CO_3 and bicarbonate ions, which regulate ocean acidity. Accurate calculations of species concentrations are critical for modeling climate change impacts and ocean health.

Advanced Considerations: Activity Coefficients and Temperature Effects

While the calculations above assume ideal behavior, real solutions exhibit activity coefficients that slightly modify effective concentrations. These coefficients depend on ionic strength, temperature, and other factors. For high-precision work, incorporating activity corrections via Debye-Hückel theory or Extended Debye-Hückel equations is necessary.

Temperature also influences dissociation constants. Typically, K_{a1} and K_{a2} increase with temperature, leading to greater dissociation

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