Visualizing Acid-Base Chemistry for Environmental Scientists and Engineers

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Motivation- How to turn:

$$[H_2A] = \alpha_0 A_T, \text{ where } \alpha_0 = [H^+]^2 / ([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})$$

$$[HA^-] = \alpha_1 A_T, \text{ where } \alpha_1 = K_{a,1}[H^+] / ([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})$$

$$[A^{2-}] = \alpha_2 A_T, \text{ where } \alpha_2 = K_{a,1}K_{a,2} / ([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})$$

Ionization Fraction Equations for Diprotic Acid

Into a visual experience with on-line calculator?
Background:
Everything involves Chemistry, acids, bases, and pH
What is pH?
- A measure of $\text{H}^+$ in liquid.
- $\text{H}^+$ is measured in moles per liter.
  - pH below 7 = acidic
  - pH 7 = neutral
  - pH above 7 = basic

What is an acid?
- A molecule that can release $\text{H}^+$.

pH and acids are interrelated.

Why does pH matter?

• It’s a like temperature
  • at different temperatures, different reactions happen
    • Water freezes at 32 °F or 0 °C
    • Water boils at 212°F or 100 °C
  • temperature indicates human health
    • 98.6 °F or 37 °C is about normal

• At different pH values, different reactions happen
  • pH indicates human health
    • blood pH is about 7.4
  • The relative amounts of **acid** and **conjugate base species** change with pH
  • These species react differently

Blood pH Levels

<table>
<thead>
<tr>
<th>pH</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Death</td>
</tr>
<tr>
<td>7</td>
<td>Acidosis</td>
</tr>
<tr>
<td>7.35</td>
<td>Normal pH</td>
</tr>
<tr>
<td>7.45</td>
<td>Alkalosis</td>
</tr>
<tr>
<td>7.8</td>
<td>Death</td>
</tr>
</tbody>
</table>

Species are important

Animal SPECIES
• a group of living organisms capable of exchanging genes.

Acid-Conjugate Base SPECIES
• a chemical consisting of similar atomic structure capable of exchanging $\text{H}^+$.  
• When have $\text{H}^+$, are the acid  
• When do not have $\text{H}^+$, are the base  
• SIMPLE- only **two species**

$$\text{H}_2\text{CO}_3 \leftrightarrow \text{HCO}_3^- + \text{H}^+$$

Carbonic Acid  
Bicarbonate  
(conjugate base)

Source: https://www.winnipegsd.ca/schools/RalphBrown/StudentResources/eal/Pages/Default.aspx [Fair Use]
Moving from the global scale to small scale

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VT
VIRGINIA TECH.
An acid and its conjugate base species always exist – relative amounts of each matters.

Carbonic Acid loses $\text{H}^+$ to become Bicarbonate

$$\text{H}_2\text{CO}_3 \leftrightarrow \text{HCO}_3^- + \text{H}^+ \quad \text{pK}_{a,1} = 6.3$$
Carbonic Acid \hspace{1cm} Bicarbonate (conjugate base)

Bicarbonate loses $\text{H}^+$ to become Carbonate

$$\text{HCO}_3^- \leftrightarrow \text{CO}_3^{2-} + \text{H}^+ \quad \text{pK}_{a,2} = 10.3$$
Bicarbonate \hspace{1cm} Carbonate (conjugate base)

$pK_a$ is a constant and property of an acid/conjugate base
pKAnalyzer is an on-line visual calculator to show acid/conjugate species changes with pH.

\[ \text{pK}_{a,1} = 6.3 \]

\[ \text{pK}_{a,2} = 10.3 \]
pKAnalyzer

Link to App:
https://databridgevt.github.io/pka-analyzer/

Copy and paste into Firefox or Chrome. Make sure JAVA is installed.
First, performed usual acid-base species calculations with algebraic equations using Excel or calculator.

\[
[H_2A] = \alpha_0 A_T, \text{ where } \alpha_0 = \frac{[H^+]^2}{([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})}
\]

\[
[HA^-] = \alpha_1 A_T, \text{ where } \alpha_1 = \frac{K_{a,1}[H^+]}{([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})}
\]

\[
[A^{2-}] = \alpha_2 A_T, \text{ where } \alpha_2 = \frac{K_{a,1}K_{a,2}}{([H^+]^2 + K_{a,1}[H^+] + K_{a,1}K_{a,2})}
\]

Second, a month later, students introduced to pKAnalyzer software tool for acid-base species calculations.
How to Use pKAnalyzer

1. Click “Select Acid” button

2. Click; acid & base distributions appear
Question: When using the pKAnalyzer tool to calculate acid-base ionization fractions, what score would you give it out of 7, 7 being the highest?
Student Survey, Fall 2019

- **Question:** Now that you have access to the pKAnalyzer tool, which technique would you choose to use to calculate ionization fractions for in-class assignments and homework?
  - 100% pKAnalyzer
  - 0% for Calculator
  - 0% for Excel

- **Question:** Any other comments you care to share?
Student Survey, Fall 2019

**Question:** How did using pKAnalyzer improve your visualization and understanding of acid-base species distribution as a function of pH?

- The changing of color allows you to visualize how the species change over changing pH, in an exact and smooth way that would be very difficult for me to draw on my own.
- It allowed me to better understand the graphs we have seen in class and see how the ionization fractions change over pH.
- It was helpful to see how the alpha values change in relation to each other instead of just getting one output from my calculator.
- The graph shows the trend and change in dominate species.
- It was helpful to see an immediate response to a change in pH or different acid all together. The ability to play around with different acids and pH's really helped describe how this all works.
- It gave a visual understanding as a function of pH instead of just a numerical value that calculations output.
- It helped me to visualize the alphas, and how they behave relative to pH and each other. It was very helpful to have instant visualization.
- It allowed me to see the percentage of each species at a given pH.
- pKAnalyzer provides direct results of acid dissociation conditions. It looks simpler and explicit The feature of using the mouse to go over the graph and see how all the alphas change with pH understand the a value.
- Graphical descriptions make it easier to understand the pattern of different things when all of those are changing simultaneously.
ICAT SUCCESS!

Visualizing Acid-Base Chemistry for Environmental Scientists and Engineers produced the on-line software tool pKAnalyzer that students rate nearly 7 out of 7 and will use both academically and professionally.