Introducing a simplified terminology for conjugate acids and bases

To avoid the confusion introduced by traditional HA & A terminology, we suggest the following abbreviations:

- Conjugate acid: CA
- Conjugate base: CB

Thus strong acids can dissociate in water as follows:

\[ H_2O + CA \rightarrow H^+ + H_2O^+ + CB \]

Weak acids can form the following equilibrium:

\[ H_2O + CA \leftrightarrow H_2O^+ + CB \]

The equilibrium formed between a weak acid and its conjugate base forms the basis for how buffers work. When the CA and CB terminology is used, there is no implication that CA must be neutral as was conveyed in the old HA terminology. Similarly, use of CB to represent the conjugate base does not imply a negatively charged species, as was often mistakenly implied by the A terminology.

Applying the simplified terminology to the titration of a tripotric amino acid

If an amino acid has a titratable side chain, it is an example of a tripotric acid, designated as CA with our simplified terminology. To demonstrate how changes in pH affect the ionization states of the three titratable groups, students are asked to draw the amino acid in its most protonated state and then titrate it sequentially from pH zero to 14.

Example: titration of lysine

Starting at the left, at pH zero, the CA form of lysine has a net charge of +2. The group with the lowest pK, is the α-carboxylate group, which is the first group to lose its proton as the pH increases. When the equilibrium for CA formation is considered, the protonation of lysine occurs, which has a net charge of +1. The α-amino group has the next lowest pK and loses its proton next to produce CA, a conjugate form with a net charge of 0. The side chain amino group has the highest pK and releases and releases the final proton to produce the CB form with a net charge of -1 charge.

Development of an interactive Java Applet for visualizing the distribution of CA and CB forms of amino acids as a function of pH

We have developed a Java Applet to allow students to visualize the changes in amino acid protonation states as a function of pH. Students have responded extremely positively to the intuitive graphical “pH ruler” that is used to interactively control pH, as well as the pK, values of different titratable groups. The Henderson-Hasselbach equation is used to calculate the concentrations of CA and CB forms, and bar graphs provide a visual representation of these concentrations. The three screenshots below illustrate how changes in the pH slider affect the distribution of CA and CB for the simple case of alanine.

Students can construct a titration curve using a 5-point approach, based on calculations they perform with the Henderson-Hasselbach equation. Each functional group is titrated separately and in sequence starting with the most acidic pK, and ending with the most alkaline pK. The titration curve for the amino acid lysine constructed using the 5-point approach is shown below.

The interactive nature of the applet provides students with a self-directed, inquiry-based learning experience that requires minimal instruction. The applet can be easily modified to accommodate more complex systems with additional titratable groups, including interesting cases like lysine, where the two amino groups have similar pK, values. Instructors can also use the applet to develop cases to test students understanding of pH, buffers and net charge, as well as more advanced concepts central to protein-ligand interactions, enzyme catalysis and protein purification via ion exchange chromatography.

Key concept: The pH ruler Java applet provides students with a simple graphical interface for exploring how changes in pH and pK, values in the pK, of functional groups affect the concentrations of CA and CB forms in solution.