

The Effects of pH on Acid Behavior

Deprotonation is a molecular mechanism that illustrates how, under certain conditions, acids can lose a hydrogen ion. In many circumstances, an acid can exist in a sample in both protonated (no H⁺ donation) and deprotonated forms. In many compounds or formulations that utilize an acid active ingredient, a measurement of "total acid" includes both forms of the acid.

Free acid, conversely, is a measurement solely of acid molecules that have not yet been deprotonated (donated an H⁺ ion). While free acids remain protonated and are chemically reactive, deprotonated acids are less able to bond or react with other molecules. Thus, acidic formulations with lower percentages of free acid have decreased activity and reactivity.

The relationship between free acid and deprotonation illustrates how increasing the pH of an acidic compound will decrease the ability of the acid to react with other molecules. An

increase of pH in a formulation is indicative of an increasing percentage of the acid becoming deprotonated, thereby decreasing its reactivity and subsequently its efficiency.

In order to demonstrate this principle, an experiment was conducted in which a number of 10% glycolic acid ($C_2H_4O_3$) sample solutions with a baseline pH of approximately 1.70, were treated with varying amounts of 25% sodium hydroxide (NaOH) solution to increase the pH of the samples to a set of values between approximately 2 and 5.5 pH (**Figure 1**). These were then analyzed to calculate the percentage of free acid at the differing pH values in each sample.

As the data indicates **(Figure 2)**, increasing the pH of the glycolic acid solutions drastically decreases the amount of free acid present in the sample. When sodium hydroxide, a base, is introduced into the solution, the sodium hydroxide can dissociate into Na⁺ and OH⁻ ions.

Figure 1 Free Acid Experimental Data

SAMPLE	SAMPLE PH GOAL	SAMPLE PH ACTUAL	FREE ACID (%)
S1	2.0	2.01	8.89
S2	2.5	2.50	8.10
S 3	3.0	3.00	6.87
S4	3.5	3.49	4.62

SAMPLE	SAMPLE PH GOAL	SAMPLE PH ACTUAL	FREE ACID (%)	
S 5	4.0	4.04	2.47	
S6	4.5	4.53	0.96	
S 7	5.0	5.01	0.48	
S8	5.5	5.51	0.24	

Deprotonation of the glycolic acid follows as the sodium hydroxide and glycolic acid react in an acid-base neutralization reaction. The Na⁺ ion from sodium hydroxide will react with deprotonated glycolic acid to form sodium glycolate, a compound that does not share the chemical activity of protonated glycolic acid. Thus, the amount of free acid present is reduced, as the increasing levels of sodium hydroxide base in the solution will convert a larger percentage of the free acid into a deprotonated form (Figure 3). This indicates that those glycolic acid solutions with higher pH's will be less effective than those with lower pH.

Conclusion

In summation, this experiment validates the principal that greater acid reactivity corresponds to lower formulation pH. An increase of pH in an acidic compound indicates greater concentrations of deprotonated acid molecules in the formulation. This in turn decreases the amount of free acid present, and diminishes the reactivity of the acidic compound.

Figure 2 Sample pH and Free Acid %

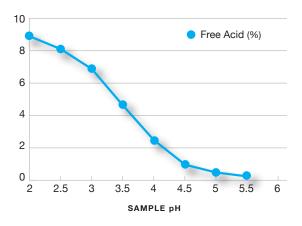
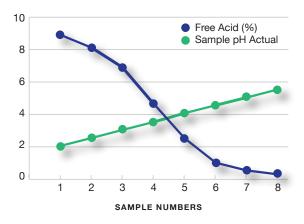


Figure 3 Sample pH and Free Acid % for Samples





CROSSCHEM LIMITED | 100 WESTWOOD PLACE STE 430 | BRENTWOOD TN 37027 USA | +1 615 716 3510

©2020 CrossChem LP All statements in this publication are believed to be accurate and reliable. The user assumes all risks and liability for results obtained by use of the products or applications of the suggestions described. SELLER MAKES NO WARRANTY OF ANY KIND, EITHER EXPRESS OR IMPLIED, BY FACT OR LAW, INCLUDING WARRANTIES OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE. Statements or suggestions concerning possible use of the products are made without representation or warranty that any such use is free of patent infringement and are not recommendations to infringe any patent. The claims and supporting data provided in this publication have not been evaluated for compliance with any jurisdiction's regulatory requirements and the results reported may not be generally true under other conditions. Users must evaluate what claims and information are appropriate and comply with a jurisdiction's regulatory requirements. Recipients of this publication agrees to (i) indemnify and hold harmless CrossChem LP for any and all regulatory action arising from recipient's use and any claims or information in this publication including but not limited to use in advertising and finished product claims, and (ii) not present this publication as evidence of finished product claim substantiation to any regulatory authority.