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## 40 C.F.R. § 796.3500

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### Hydrolysis as a function of pH at 25 °C.

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(a) *Introduction* — (1) *Background and purpose.* (i) Water is one of the most widely distributed substances in the environment. It covers a large portion of the earth's surface as oceans, rivers, and lakes. The soil also contains water, as does the atmosphere in the form of water vapor. As a result of this ubiquitousness, chemicals introduced into the environment almost always come into contact with aqueous media. Certain classes of these chemicals, upon such contact, can undergo hydrolysis, which is one of the most common reactions controlling chemical stability and is, therefore, one of the main chemical degradation paths of these substances in the environment.

(ii) Since hydrolysis can be such an important degradation path for certain classes of chemicals, it is necessary, in assessing the fate of these chemicals in the environment, to know whether, at what rate, and under what conditions a substance will hydrolyze. Some of these reactions can occur so rapidly that there may be greater concern about the products of the transformation than about the parent compounds. In other cases, a substance will be resistant to hydrolysis under typical environmental conditions, while, in still other instances, the substance may have an intermediate stability that can result in the necessity for an assessment of both the original compound and its transformation products. The importance of transformation of chemicals via hydrolysis in aqueous media in the environment can be determined quantitatively from data on hydrolysis rate constants. This hydrolysis Test Guideline represents a test to allow one to determine rates of hydrolysis at any pH of environmental concern at 25 °C.

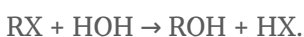
(2) *Definitions and units.* (i) “Hydrolysis” is defined as the reaction of an organic chemical with water, such that one or more bonds are broken and the reaction products of the transformation incorporate the elements of water (H<sub>2</sub>O).

(ii) “Elimination” is defined in this Test Guideline to be a reaction of an organic chemical (RX) in water in which the X group is lost. These reactions generally follow the same type of rate laws that hydrolysis reactions follow and, thus, are also covered in this Test Guideline.

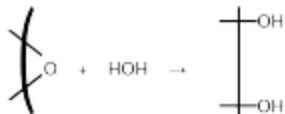
(iii) A “first-order reaction” is defined as a reaction in which the rate of disappearance of the chemical substance being tested is directly proportional to the concentration of the chemical substance and is not a function of the concentrations of any other substances present in the reaction mixture.

(iv) The “half-life” of a chemical is defined as the time required for the concentration of the chemical substance being tested to be reduced to one-half its initial value.

(v) “Hydrolysis” refers to a reaction of an organic chemical with water such that one or more bonds are broken and the reaction products incorporate the elements of water (H<sub>2</sub>O). This type of transformation often results in the net exchange of a group X, on an organic chemical RX, for the OH group from water. This can be written as:



(A) Another result of hydrolysis can be the incorporation of both H and OH in a single product. An example of this is the hydrolysis of epoxides, which can be represented by



(B) The hydrolysis reaction can be catalyzed by acidic or basic species, including  $\text{OH}^-$  and  $\text{H}_3\text{O}^+$  ( $\text{H}^+$ ). The promotion of the reaction by  $\text{H}_3\text{O}^+$  or  $\text{OH}^-$  is called specific acid or specific base catalysis, respectively, as contrasted with general acid or base catalysis encountered with other cationic or anionic species. Usually, the rate law for chemical RX can be written as:

Equation 1

$$-d[\text{RX}]/dt = k_h[\text{RX}] = k_A[\text{H}^+][\text{RX}] + k_B[\text{OH}^-][\text{RX}] + k'_N[\text{H}_2\text{O}][\text{RX}],$$

where  $k_A$ ,  $k_B$  and  $k'_N$  are the second-order rate constants for acid and base catalyzed and neutral water processes, respectively. In dilute solutions, such as are encountered in following this Test Guideline, water is present in great excess and its concentration is, thus, essentially constant during the course of the hydrolysis reaction. At fixed pH, the reaction, therefore, becomes pseudo first-order, and the rate constant ( $k_h$ ) can be written as:

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