161-1

DATA EVALUATION RECORD

Study Identification

Paul, L., Szaer, G., and Walters, M. 1989. Hydrolysis of Duomeen-C Diacetate. Akzo Chemical Inc. McCook, Illinois. MRID No. 40062413.

Reviewer

Roy Bingham, Biologist
Monitoring Section

Type of study

Hydrolysis (161-1)

Conclusions

This study was conducted in accordance with 40 CFR 158.108 [subdivision N (161-1)]. The study was found to be acceptable and provided information regarding the hydrolysis of Duomeen-C Diacetate (Akzo Chemicals, Inc.), the trade name for 1-(alkyl*amino)-3-aminopropane diacetate (* alkyl groups derived from coconut oil fatty acids).

From the above hydrolysis study it can be concluded that Duomeen-C Diacetate, at pHs of 5 and 7, is hydrolytically stable. More than 90% of Duomeen-C Diacetate has remained intact at neutral or acid pH aqueous systems over a 30-day period. At pH 9 hydrolysis did not occur due to the conversion of the acidic salt to free diamine.

Materials and Methods

Test Compounds

Duomeen-C Diacetate [1-(alkyl-amino)-3-aminopropane diacetate (alkyl-coco)] was prepared from a fatty diamine containing one long chain (primarily C_{12}) and derived from coconut oil and acetic acid. The stock solution was prepared 51.9% active by dissolving 1-(alkyl-amino)-3-aminopropane in isopropanol and neutralizing with concentrated acetic acid. The active concentration was confirmed by titration of the amine portion (2.752 meq/g) and the acid portion (2.738 meq/g) of the compound.

Test Solution Preparation

All four test solutions were prepared in a similar fashion. A 1.0017 gram sample of Duomeen-C Diacetate (51.9% active solution in isopropyl alcohol) was added to a 100 ml volumetric flask and diluted to volume with deionized water giving a concentration of 0.005199 grams of Duomeen-C Diacetate per ml. To each of four glass 250ml bottles was added 2.0 ml of the Duomeen-C Diacetate solution and 98.0 ml of the appropriate buffer solution (pH 5, pH 7, and pH 9, or deionized water). A 1.0017 gram sample after dilutions generated a concentration of 104.0 µg/ml of Duomeen-C Diacetate. Each of these bottles was sealed with airtight polyethylene-lined caps and stored in a closed waterbath at approximately 25 ± 1°C.

Buffer Preparation

All solutions were prepared using reagent grade chemicals and deionized water. A buffer system at pH 5 was prepared using 0.2 M acetic acid and 0.2 M sodium acetate. A buffer system at pH 7 was prepared using 0.2 M Tris(hydroxymethyl)aminomethane and 0.2 M HCl. A buffer system at pH 9 was prepared using 0.2 M boric acid and 0.2 M sodium borate The pH of each buffer was measured using a Lltex 60 pH meter with a Corning pH electrode and standard calomel reference electrode. The pH value of each buffer was adjusted to within 0.02 pH units by adjusting ratios of buffer components.

Sampling and Testing Procedures

Sampling was conducted on days 0, 8, 15, 23, and 30 of the study. Sample solutions were shaken for 20 to 30 seconds before sampling to ensure homogeneity. A one-gram sample (weighed to the fourth decimal place on an analytical balance) was then placed in a four-ounce jar. To the jar was added 5.0 ml of saturated sodium chloride solution, 10.0 ml of reagent grade chloroform, and 20.0 ml of a buffer solution. The jar was capped and shaken for 20 to 30 seconds. The layers were then allowed to settle for one minute, followed by two more shake and settling periods. When the final settling period had elapsed, approximately three mls of the lower chloroform layer was drawn from the bottle with a plastic pipet and placed in a one-centimeter quartz cuvette. The absorbance of the chloroform layer was determined using a Bauch and Lomb Spectronic 2000 spectrophotometer set at 425 nm. A blank containing no sample was run through the same procedure and used to zero the instrument.

Results and Discussion

The objective of the study was to evaluate the hydrolysis rate and/or potential of Duomeen-C Diacetate as a function of pH.

The hydrolysis study of Duomeen-C Diacetate was conducted under dark conditions using three buffer solutions and one unbuffered solution at 25 ± °C: pH 5 (acetic acid/sodium acetate), pH 7 [Tris(hydroxymethyl)-aminomethane/HCl], pH 9 (boric acid/sodium borate), and a solution containing deionized water (pH of approximately 6.2). The buffer solutions were spiked at approximately 100 ppm levels (based on 100% activity of the Duomeen-C Diacetate).

Each of the four solutions was sampled on days 0, 8, 15, 23, and 30. The pH of each solution remained within 0.2 pH units of the starting value throughout the thirty day sampling period. Each buffer solution was analyzed in duplicate.

Results of the pH 5 hydrolysis study showed less than 10% hydrolysis of Duomeen-C Diacetate occurred. The compound is hydrolytically stable at pH 5. This is in accordance with the criteria outlined in Data Reporting Guidelines for Hydrolysis Studies (161-1) .

Results of the pH 7 hydrolysis study showed that Duomeen-C Diacetate is hydrolytically stable at pH 7.

Results of the hydrolysis study at pH 9 (day 0) Duomeen-C Diacetate levels were initially found to be lower than the levels measured in pH 5 and pH 7 tests although the amount of material added was identical in all tests. Acetic acid salts of amines exist at acidic or neutral pH values. At pH 9 the Duomeen-C Diacetate is converted to free diamine which may combine with buffer salts or become insoluble in water. Therefore, at this pH, the decreased levels of diamine diacetate found resulted from the conversion of Duomeen-C Diacetate to another form rather than hydrolysis.

Results of the unbuffered hydrolysis study agree well with pH 5 and pH 7 studies. They again show Duomeen-C Diacetate to be hydrolytically stable.