Kinetic Solvent Deuterium Isotope Effects on the Micellar-Catalyzed Hydrolysis of Trisubstituted Phosphate Esters

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Functional micelles of hexadecyl(2-hydroxyethyl)dimethylammonium bromide (I) are better catalysts than hexadecyltrimethylammonium bromide (CTABr) for the alkaline hydrolysis of diethyl and di-n-hexyl p-nitrophenyl phosphate (IIIa,b). The kinetic solvent deuterium isotope effects for reactions catalyzed by CTABr are very similar to those for reaction in water, but for reaction of Mb in the presence of I the inverse isotope effect gradually disappears with increasing concentration of hydroxide ion. These results show that the inverse isotope effect is due to the ionization of I to its zwitterion II at high pH. They are consistent with nucleophilic attack by the alkoxide moiety in II but not with general acid or base catalysis. © 1976, American Chemical Society. All rights reserved.