

Kinetic and Quantum-Chemical Study of Oxirane Ring Cleavage with Acids

P. V. Nikolaev and M. K. Islyaikin

Ivanovo State University of Chemical Engineering, Ivanovo, Russia

Received May 24, 2001

Abstract - Kinetic and thermodynamic parameters of the reactions of phenyl glycidyl ether and epichlorohydrin with bis(alkylpolyethylene glycol) ether of orthophosphorus acid (oxyphos KD-6) are established. It is shown that the difference in the reactivity of the oxiranes is caused by the electronic effects of substituents and the protonation by the phenolic oxygen atom of phenyl glycidyl ether. Basic solvents decrease the reactivity of the systems. Based on AM1 semiempirical quantum-chemical calculations, a hydroxycarbocation mechanism of the oxirane ring opening was proposed, involving initial formation of unstable *cis*- and *trans*-oxonium structures.