Transition-state analysis of esterification of adipic acid with various polyethylene glycols: Effect of molecular size of polyethylene glycol on the reaction rate

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The esterification rate of adipic acid with polyethylene glycol is interpreted using transition-state theory. The esterification of adipic acid was carried out with various polyethylene glycols whose average molecular weights were ranged from 106 to 991 (the degree of polymerization of polyethylene glycol was 2 ~ 22.). In addition, the ratio of the equivalent of hydroxy group ([OH]) to the carboxylic acid group ([COOH]) was set to 2.0, so the degree of the esterification product was limited to ~3.0. To minimize the temperature dependency of the activation energy and the frequency factor, the esterification temperature range was restricted from 428K to 443K. The conversion of adipic acid, the limiting reactant, was calculated with the acid value data of the reactant-product mixtures. The molar mass of the esterification product was determined from the hydroxy value of the product. With the controlled esterification data, the effect of molecular size of the polyethylene glycol on the reaction rate was interpreted in terms of standard enthalphy and entropy of activation.