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MECHANISM OF CHEMICAL REACTIONS

AT HIGH PRESSURES

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Pages 10

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One of the important fields of chemistry at high and ultra-high pressures is the study of reaction rates and courses in order to elucidate the mechanism. Recently this field has been developed considerably, especially in its application to the study of liquid phase organic reaction mechanism.

A simple case is the study of pressure effect on the rate and course of chemical processes in the gaseous phase at temperatures much above the critical. Under such conditions the partial pressures of the components are approximately proportional to their concentrations. Furthermore, the amount of any component in the gas mixture can be varied by adding this component (or any other component) to the mixture with corresponding pressure increase. In such a fashion the pressure effect is equivalent to changing the concentration ratio of reactants and products, i. e. the usual methods of reaction mechanism study may be applied. In these methods it is customary to compare the empirical reaction rate and product composition with theoretical values derived from an assumed reaction mechanism.

As an example for applying high pressure to reaction mechanism study in the gaseous phase at high temperatures we may bring the homogeneous destructive hydrogenation of alkylbenzenes, a reaction of practical significance. In this reaction an alkyl radical is cleaved from the alkylbenzene at 500-800 ° under hydrogen pressure in the absence of catalysts.

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C15