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Activation energetic spectra of concerted molecular decomposition of unsaturated compounds and nitrocompounds

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Abstract

Experimental data on reactions of molecular concerted decomposition of unsaturated compounds, esters, and nitrocompounds were analysed in the parabolic model. The following factors that influence activation energy of these reactions were identified: enthalpy of reaction, inductive effect of substituents, the aryl substituent nearby the reaction center, steric effect, influence of force constants of reacting bonds, the transference of π-electrons in elementary act. The energetic spectrum of activation of these reactions was calculated using two-center model of reaction with concerted transformation of bonds. This energetic spectrum includes the values of partial activation energies of each elementary step in composite transformation.