

عنوان مقاله:

Study on kinetic & thermodynamic control with increase temperature reaction (1,3-butadiene addition hydrogen bromid) in gaz phase

محل انتشار:

همایش ملی نانو فناوری و شیمی سبز (سال: 1391)

تعداد صفحات اصل مقاله: 3

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خلاصه مقاله:

In response to conjugate Diene thermodynamic stability is high, but in the presence of the electrophilic reaction kinetics activation. At temperatures 273.15 K and 1.00 atmospheric pressure to produce a 70% 3-Bromo-1-Butene and 30% 1-Bromo-2-Butene also in 313.15 K and 1 atmosphere pressure 15% to first product and 85% of the second product. with Gaussian calculate and DFT , aspect thermodynamic result -113735.4029 Kcal mol⁻¹ at 273.15 Kelvin amount -113734.5338 Kcal mol⁻¹ in 313.15 K for the Enthalpy and 0.047420831 Kcal mol⁻¹ in 273.15 K and 0.050387034 Kcal mol⁻¹ in 313.15 K for the Eentropy is obtained. at higher temperatures isomers equilibrium is reached and reflects the thermodynamic stability . Although the stability of 3-Bromo-1-Butene is lower but the rate is higher than other products, that result reflects the Kinetic control

کلمات کلیدی:

Isomer thermodynamic & kinetic controls

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