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Diels-Alder reaction between naphthalene and N-phenylmaleimide under ambient and high pressure conditions

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Abstract

The rate and equilibrium constants for the Diels-Alder reactions between benzene and naphthalene as dienes and tetracyanoethylene, maleic anhydride and N-phenylmaleimide as dienophiles at 25°C were estimated from empirical rule. The highest yield of the adduct was predicted for the reaction of naphthalene with N-phenylmaleimide. The time of adduct formation in 50% yield exceeds 30 years. The use of gallium chloride as a catalyst affords the exo-adduct for seven days at room temperature. The rate $((2 \pm 0.5) \cdot 10^{-6} \text{ L mol}^{-1} \text{ s}^{-1})$ and equilibrium constants $(5 \pm 2 \text{ L mol}^{-1})$ of this reaction were determined. Under high pressure conditions (8kbar) reaction occurs with formation of both stereo isomers at 100°C during 80 hours. © ARKAT.

Keywords

Catalysis, Diels-alder reaction, High pressure, Naphthalene