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Diels-Alder reaction between naphthalene and N-phenylmaleimide under mild conditions

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Abstract

The rate and equilibrium constants for the Diels-Alder reactions between benzene or naphthalene and several dienophiles at 25°C were calculated from the data on the ionization potentials of dienes and electron affinity energies of dienophiles, as well as the reaction enthalpies. The highest yield of the adduct was predicted for the reaction of naphthalene with N-phenylmaleimide. However, the time of its formation in 50% yield exceeds 30 years. The use of gallium chloride as a catalyst affords the endo-adduct for seven days at room temperature in 30% yield. The rate ((2±0.5)·10-6 L mol-1 s-1) and equilibrium constants (5±2 L mol-1) of the reaction were determined.

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Keywords

Catalysis, Diels-Alder reaction, Kinetics, N-phenylmaleimide, Naphthalene