



A theoretical study of the kinetics and mechanism of second-order intermolecular Cycloaddition of Norbornene and Phenyl Azide was performed using DFT methods at B3LYP levels of theory with 6-311++G(d,p) and 6-311G(d,p) basis sets at 298.15K and 313.45 K. Equilibrium molecular geometries and harmonic vibrational frequencies of the reactants, transition state and product were calculated. Solvent effect on the kinetic and thermodynamic parameters of reaction of 1,3- Dipolar Cycloadditions of Norbornene and Phenyl Azide was investigated too. The calculated rate constants and activation thermodynamics parameters showed a good agreement with experimental results. These calculations indicated that the reaction proceeds through a synchronous concerted mechanism.



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