



Simulation Study of alkylation reaction of resorcinol

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ABSTRACT

Study of alkylation reaction of resorcinol has been carried out theoretically using semi-empirical methods (PM3). Four transition states have been suggested and examined to check up the most probable transition state that gives the most probable pathway of the reaction. Geometrical properties and vibration spectrums have been calculated and compare with their practical spectra. Calculus indicate two transition state which are most probable than other states due to its energetic values of total energy, binding energy, heat of formation, zero point energy, and imaginary frequency that's equal to -62727.105, -2661.13, -200.104, 132.038 respectively by Kcal mol⁻¹ units. The pathway of alkylation reaction is spontaneous and exothermic with the change in Gibes energy value and heat of formation value equal to -62620.4 and -200.104 Kcal mol⁻¹ units respectively.

Keywords: Semi empirical calculations, transition state, resorcinol, alkylation Al₂ (SiO₃)₃.
