DFT (B3LYP) COMPUTATIONAL STUDY ON THE MECHANISMS OF FORMATION OF SOME SEMICARBAZONES

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Abstract. Thermodynamic and kinetic mechanisms of forming six semicarbazones have been investigated computationally by DFT B3LYP method. All the reactions proceed *via* two transitions and include two consecutive steps: bimolecular and unimolecular. The computed transition steps have varying equilibrium constants values, enthalpy of activation and Gibbs energy of activation, depending on the semicarbazone involved. Also depending on the semicarbazones involved some of the consecutive steps are found to have varying enthalpy of reactions and spontaneity.

Keywords: semicarbazone, kinetics, bi- and unimolecular step, transition step, spontaneity.

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