

1120-37-23

Ali Allahem* (a.allahem@qu.edu.sa), Qassim University, Qassim, Buraydah, 81999, Saudi Arabia. *The concept of the dividing surface in collinear Hydrogen exchange reaction.*

Transition state theory (TST) describes the elementary chemical reaction rate. There are three main regions in the reaction: reactant, product and the transition state (TS). The transition state must have two properties to make the transition state theory exact: all reactive trajectories must cross the TS (dividing surface) and the reactive trajectories cross it only once. Dynamical effects recrossing is possible from coupling in kinetic energy where TST provides upper bound of the exact reaction rate. Historically, (Wigner 1938) developed the reaction rate theory and extended the idea from configuration space to phase space. (Pollak et al 1978) found the structure of the dividing surface in the collinear $H_2 + H$ reaction. It is well-known as unstable periodic orbit dividing surface (PODS). We are going to talk about the reactivity on the dividing surface of this reaction. (Received January 20, 2016)