CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME II

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Department of Biotechnology Engineering
Faculty of Engineering
International Islamic University Malaysia

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POTENTIAL ENERGY SURFACES FOR REACTIONS AMONG HYDROGEN FLUORIDE MOLECULES

Ibrahim Ali Noorbatcha[1], Borhannuddin Arifin[2] and Sharifudin M Zain[3]

[1]Department of Biotechnology Engineering, Faculty of Engineering,
International Islamic University Malaysia, P.O. Box 10, 50728 Kuala Lumpur, Malaysia
[2]Faculty of Applied Sciences, University Technology MARA, 40450 Shah Alam, Selangor
[3]Department of Chemistry, Faculty of Science, University Malaya, 50603 Kuala Lumpur

ABSTRACT

A global potential energy surface (PES) for the hydrogen fluoride trimer $(HF)_3$ system has been modeled using the LEPS (London-Eyring-Polanyi-Sato) semi-empirical formulation. Both the six-centered (6C) and four centered (4C) reactions among the three HF molecules are considered. We find that the correct energy barriers for both 6C and 4C processes taking place via the formation of trimers and dimers respectively, can be obtained using the Pedersen-Porter anti-Morse function with scaling of the triplet dissociation energies of the F_2 and HF molecules. The calculated PES gives an energy barrier for 6C reaction of 5.2 kcal/mol above the HF trimer and an energy barrier for 4C reaction of 36.7 kcal/mol above the HF dimer. These results are in good agreement with previous ab initio and DFT calculations. This global PES can be used to carry out dynamical study of the 6C processes that are possible among the three HF molecules.

Keywords: PES, LEPS, Six-Centered and Four-Centered reactions, HF trimer

INTRODUCTION

The London-Eyring-Polanyi-Sato (LEPS) semi-empirical potential energy surfaces (PES) have been widely used in quasiclassical trajectory (QCT) calculations (Parr and Truhlar, 1971; Porter, 1974). Although there are some limitations, it seems to be a well-established fact that given reasonable adjustments of parameters, the calculated surfaces are realistic and provides a reasonably good representation of the PES.

There have been many studies using the LEPS formulation to describe three- and four-atom systems (Thompson, 1976). Raff *et al.* first used this method to describe the interaction potential of the H_2I_2 reaction (Raff et al 1970). Shock tube (Bauer and Ossa, 1966) and stimulated Raman (Schwartz and Schaad, 1968) experiments on $H_2 + D_2$ reaction suggested a four-centered (4C) process with activation energy of 42 kcal/mol. However Wright (1975) proposed a six centered transition state with an energy barrier of 90 kcal/mol (Wright, 1975). Further work using