

# Potential Energy Surface Topology

## I. Correlations with the Diatomic Constants

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### Abstract

The semi-empirical method is used to calculate potential energy surfaces. The linear  $H_3$  and rectangular  $H_4$  systems have been chosen as standard surfaces in order to compare the surface features. Relationships between diatomic constants and topological features along a minimum energy path, and the height and location of the barrier, are demonstrated.

### 1. Introduction

The knowledge of the relation between the effect of vibrational and translational energies on the reaction cross section and the topological features of potential energy surfaces have provided valuable information in understanding the fundamental nature of collision dynamics<sup>1,2,3</sup>. We are seeking additional insight into this relation. In this attempt, we investigate correlations between the features of the potential energy surfaces and the characters of the reactant molecules. With the understanding of the correlations, the effect of the two kinds of energies on the chemical reaction can be estimated directly from the characters of the reactant molecules.

Recently, more accurate ab initio potential energies have been calculated for many reaction systems, using fast computers. Even though the potential energies calculated by ab initio method are accurate, it is difficult to relate the potential energies with the character of reactant molecules because of the complicated calculation method. On the other hand, a semi-empirical method can relate directly the potential energies with the character without complicated calculations. Commonly used semiempirical methods<sup>4,8,10</sup> employ the diatomic constants as the characteristics of reactant molecules.

This report investigates the relation between diatomic constants and features of potential energy surfaces, using our semiempirical method<sup>5</sup>. In this article, such simple models as linear  $H_3$  and rectangular  $H_4$  will be chosen. Varying the values of the diatomic constants which are used to calculate potential energies in the both systems, we observe the changes of the topological features along minimum energy path, and height and location of the barrier.

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