

Potential Energy Surface Topology

III. A Method of Graphical Analysis to Deduce Potential Energy Surface

Noboru TANAKA

Abstract

We have been proposed a new semi-empirical method (referred to as MT method) to calculate potential energy surfaces (PES). At first, characteristic of MT method is introduced, in detail. Next, by using MT method, a method of graphical analysis to deduce the features of PES is presented. Last, one of applications of the graphical analysis method is demonstrated to investigate topological feature of PES on linear triatomic A-B-C models.

1. INTRODUCTION

The topological features of potential energy surfaces (PES), such as height and location of the barrier, reaction-path curvature, etc. are fundamental to understand chemical and physical processes. For example, it is well-known that, in dynamical studies, the positions of the barrier is concerned with translational or vibrational enhancement whether the barrier locates “early” or “late”, respectively.

In additional points of view, it is interesting to investigate correlations between the feature of the potential energy surface and the parameters relating with the properties of the reactant molecules. From the correlations, it is possible to estimate the feature of the potential energy surfaces and to obtain useful guidelines in the computation of the surfaces. To calculate the surfaces, the energy formula not only need a tractable analytical form which is available to various reaction systems, but also a form combined with the parameters. Although there have been remarkable recent advances in computations of the potential energy surfaces with ab initio method, it is difficult to expect that ab initio computations will fulfill the above needs. For this reason, we have proposed a new semi-empirical method^{1,2)}, herein referred to as the MT method. MT method can be applied to calculate the potential energy surfaces composed of a n -electron n -atom system. The energy formula in MT method is expressed in analytical form of internuclear distance and connected, directly, with the parameters characterized by diatomic constants. The diatomic constants are dissociation energy D , range parameter α , and equilibrium distance R_e .

In previous papers^{3,4)}, using the MT method, we analyzed the features of potential energy surfaces on three or four identical atomic systems. As a result, we have found the characteristic relations between diatomic constants and the feature of the potential energy surfaces.

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* Hachinohe Institute of Technology, Hachinohe 031