

The effect of external electric field on AlH radical

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Received 5 May 2014; Accepted (in revised version) 18 July 2014

Published Online 29 October 2014

Abstract. Using the density functional B3P86/cc-PV5Z method, the geometric structure of AlH molecule under different external electric fields are optimized, and the bond lengths, dipole moments, vibration frequencies and other physical properties parameters are obtained. The potential energy curves under different external fields are also obtained by CCSD(T) method with the same basis set. These results show that the properties parameters and potential energy curves may change with different external electric field, especially in the reverse electric fields. The potential energy function without external electric field is fitted by Morse potential, and the potential energy curves under different external fields are fitted using constructed potential model, which adopted the dipole approximation theory. It is found that the fitting parameters are good agreement with experimental values and the critical dissociation electric parameter is consistent with numerical calculation. These results will provide important theoretical and experimental reference for further studying the molecular spectrum, dynamics and molecular cooling with Stark effect.

PACS: 31.15.E-, 31.50.Bc-, 33.15.Fm

Key words: AlH radical, potential function, external electric field

1 Introduction

AlH is the main reaction products of aluminum atoms in the hydrogenation reaction, moreover, is the main component of sun shading too. It widely exists in the upper atmosphere, interstellar space, discharge and the combustion process, which is the intermediates in many chemical reactions. Aluminium hydride is a white to gray powder, they can be attached with plastic, metal, fiber and textile, flammable, explosive and corrosive, is harmful to the human body. Hydride AlH radical as the typical hybrid molecule has been made many studies. In experiment, Huber [1], Kurth [2], Gurvich *et al.* [3], measured the

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formation enthalpy, entropy, heat capacity at constant pressure, vibration frequency, zero point energy, rotational constants and bond length of AlH molecule at 0K and 298.15K; In theory, Cobos [4] further studied the standard heat of formation, structure and optical properties of AlH and its cation using G3, CBS and density functional method [5-7]; Pople *et al.* [8] calculated the electronic affinity energy of AlH molecule by molecular orbital theory; Rice *et al.* [9] measured the Einstein transition probability of AlH molecule $A^1\Pi - X^1\Sigma$ transition; Qian *et al.* [10] observed six emission bands of AlH molecule by Fu Liye optical transform method; Yan *et al.* [11] studied the potential energy function of ground state, the first and third excited states of AlH molecule by SAC/SAC-CI method; Shen *et al.* [12] studied the structure and thermodynamic stability of AlH molecule using density functional theory [13-15] and two configuration interaction method. In these literatures, they are not related to AlH free radical molecular structure and potential energy function under an external electric field.

Due to the effect of external electric field, the molecular Hamiltonian system energy based on no external electric field, increases the interaction Hamiltonian of external electric field and molecular systems, then the problem becomes more complicated, but in the dipole approximation, the energy of molecular system can be divided into zero-field potential energy and the interaction potential of external field with molecule [16-18].

2 Theoretical details

In this letter, we accurately construct the potential model adopting dipole approximation theory. At zero-field, the potential energy function is fitted by Morse potential model. The Morse potential is applied to three-parameter function of stable diatomic molecule [18]

$$V(r) = D_e [1 - e^{-a(r-R_e)}]^2, \quad (1)$$

where D_e is the dissociation energy, a is the Morse parameter, R is the inter-nuclear distance, and R_e is its equilibrium distance.

Under an external electric field, the Hamiltonian of molecular system energy will increase the interaction between external electric field and molecular system, and H is given as [19, 20]

$$H = H_0 + H_{int}, \quad (2)$$

where H_0 is the Hamiltonian at zero-field, and H_{int} is the interaction Hamiltonian between external electric field and molecular system. Thus the Hamiltonian of external field F and molecular system interaction can be expressed as

$$H_{int} = -\mu \cdot F. \quad (3)$$

Here, μ is the dipole moment and F is the external electric field. Therefore, the molecular potential energy under an external field can be divided into zero-field potential energy