

REGULAR ARTICLE

Accurate vibration-rotation spectra of $X^1\Sigma^+$ and $A^1\Pi$ in BH molecule with explicitly correlated method

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Abstract High-level *ab initio* calculations on the ground state $X^1\Sigma^+$ and the excited state $A^1\Pi$ of the BH molecule were carried out by using the explicitly correlated multireference configuration interaction method (MRCI-F12) plus Davidson correction (+Q) and scalar relativistic correction (+SR). The potential energy curves (PECs) of the $X^1\Sigma^+$ and $A^1\Pi$ states were obtained. From the computed PECs, the spectroscopic constants were determined, which are close to the observed values. Further comparisons show that the spectroscopic results determined by the MRCI-F12+Q+SR method have the best accuracy. Therefore, the PECs from the MRCI-F12+Q+SR calculation are used for the determination of the vibrational wavefunctions for the $X^1\Sigma^+$ and $A^1\Pi$ states. And the corresponding vibrational levels ΔG_v , vibration-dependent rotational constant B_v and centrifugal distortion constant D_v were calculated. Finally, the transition properties of the $A^1\Pi-X^1\Sigma^+$, including Franck-Condon factors, transition energies and radiative lifetimes of the $A^1\Pi$ state, were obtained and found to be in good agreement with the available experiments. The computed results are helpful to further experimental study of laser cooling BH molecule.

AMS subject classifications: 81V45, 81V55, 70F07

Key Words: MRCI-F12, Spectroscopic constant, Vibration levels, Radiative lifetime.

1 Introduction

Boron compounds have a wide range of applications in many technological areas such as separations, catalyst promoters, radiation therapy and potential high-energy fuels [1, 2]. And

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the diatomic boron hydride (BH), one of the simplest molecules in nature, is also the subject of several spectroscopic studies in the gas phase [3-9]. In addition, BH is also the candidate molecule for the laser cooling which has been applied with great success to a wide variety of atomic species and achieves huge advances in many fields including metrology, sensing, interferometry, tests of fundamental physics, ultracold collisions and studies of quantum degenerate gases [10]. Therefore, the BH, as well as other hydrides or diatomic system [11-14], has become the subject of a large number of theoretical and experimental studies for several decades.

The BH molecule was first studied in 1931 by Lochte-Holtgreven and van der Vleugel, who recorded the optically allowed $A^1\Pi-X^1\Sigma^+$ transition at 433 nm [15]. Sahni carried out the first *ab initio* study on the $X^1\Sigma^+$ state of the BH molecule in 1956 [16]. Since then, a lot of theoretical and experimental investigations have been reported mainly on the $X^1\Sigma^+$ state of BH. Many investigations have focused on the equilibrium internuclear distance R_e and the dissociation energy D_e . For example, in 1967 Cade and Huo computed the $R_e=1.220 \text{ \AA}$, $D_e=64.108 \text{ kcal/mol}$ [17] and Miliordos and Mavridis obtained the dissociation energy $D_e=84.78 \text{ kcal/mol}$ by using the restricted coupled cluster theory with single-double and perturbative triple excitation (RCCSDT) in 2008 [18]. Recently, the D_e was calculated to be 84.92 kcal/mol by Koput with multi-reference averaged coupled-pair function (MR-ACPF) method [19]. And several reports concerning the potential energy curves of low-lying electronic states, as well as the spectroscopic constants of BH, were found during 1970-1975 [20-22]. The potential energy curves and spectroscopic constants of the $X^1\Sigma^+$ and $A^1\Pi$ states for BH have been studied by Luh in 1983 [23]. The Fourier transforms spectrum of the $A^1\Pi-X^1\Sigma^+$ transition of BH were recorded near 4330 \AA by Fernando [4], and the some vibration levels ΔG_v of the $X^1\Sigma^+$ and $A^1\Pi$ states were obtained. The radiative lifetimes that 116 ns ($v'=0$), 137 ns ($v'=1$) and 176 ns ($v'=2$) for the $A^1\Pi$ state were calculated by Diercksen in 1987 [24]. In 1989, the radiative lifetimes [25] of the $A^1\Pi$ state were measured to be $127\pm 10 \text{ ns}$ ($v'=0$), $146\pm 12 \text{ ns}$ ($v'=1$) and $172\pm 14 \text{ ns}$ ($v'=2$), respectively. Since BH molecule is a candidate molecule for laser cooling [11], the detailed rotation-vibration spectroscopic information is therefore important. Very recently, some theoretical efforts [19] have been made to reproduce the experimental ground-state G_v values [3] given by Pianalto et al via computed high-level PEC of $X^1\Sigma^+$ state

In present work, we carried out the high-level *ab initio* calculations on two low-lying electronic states of BH to obtain the accurate spectroscopic constants and rotation-vibration levels. The PECs of two electronic states, $X^1\Sigma^+$ and $A^1\Pi$, were calculated with explicitly correlated multireference methods. The Davidson correction (+Q) and scalar relativistic (mass-velocity and Darwin term) corrections were taken into account. On the basis of computed PECs, the spectroscopic constants were determined by solving the nuclear-motion Schrödinger equations. Then, the vibrational energy levels ΔG_v , the vibration-dependent