Commun. Comput. Chem.
doi: 10.4208/cicc.2016.v4.n4.1

Vol.4, No.4, pp.109-119
Dec 2016

REGULAR ARTICLE

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

Pei-yuan Yan, and Bing Yan*

Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, China

Received 15 Dec 2016; Accepted (in revised version) 30 Dec 2016

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

* Corresponding author *E-mail address*: yanbing@jlu.edu.cn (B. Yan).

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 Å, D_e=64.108 kcal/mol [17] and Miliordos and Mavridis obtained the dissociation energy D_e=84.78 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 Å 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±10 ns (v'=0), 146±12 ns (v'=1) and 172±14 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

rotational constant B_v and centrifugal distortion constant D_v of the two electronic states were also obtained by numerically solving the one-dimensional ro-vibrational Schrödinger equations. The transition properties including the transition dipole moment (TDM), Franck-Condon factors, and the radiative lifetimes of the excited state $A^1\Pi$ were also predicted.

2 Computational Method

In the present work, *ab initio* calculations on the electronic structure of the $^{11}B^1H$ were performed with MOLPRO 2012 quantum chemistry program package [26]. The spectroscopic constants are determined by solving the radial Schrödinger equation with the aid of the LEVEL program [27].

The correlation-consistent basis sets cc-pwCV5Z-MP2FIT [28] for B atom and cc-pVQZ-MP2FIT [29] for H atom were selected in our calculation. In order to obtain the high-level PECs of BH, the Hartree-Fock calculation has been firstly carried out to generate the single-configuration wavefunction of the ground state for the BH molecule; then, the multi-configuration wavefunction was generated and optimized by using complete active space self-consistent field (CASSCF) [30, 31] method; finally, based on the CASSCF wavefunction, the dynamic correlation energies have been computed by using the explicitly correlated multi-reference configuration interaction (MRCI-F12) [32] approach. The Davidson (+Q) correction [33] was considered in order to treat the size-consistency error due to the truncated MRCI method. And the relativistic effect (SR) was estimated with Douglas-Kroll-Hess approach in combination with uncontracted cc-pVQZ basis [34].

In the current calculations, the C_{2v} ($a_1/b_1/b_2/a_2$) point group was chosen in the electronic structure computations, which is the Abelian subgroup of the $C_{\infty v}$ ($\sigma/\pi/\delta/...$) point group. And the corresponding relationships between the reducible representations are $\sigma^+=a_1$, $\pi=b_1+b_1$, $\delta=a_1+a_2$ and $\sigma^-=a_2$, respectively. For the BH molecule, $5a_1$, $2b_1$ and $2b_2$ molecular orbitals are selected as the active space to construct the wavefunctions of the electronic states. The active space corresponds to the $2s2p3s3p$ shells of B atom and the $1s$ shell of H atom. The outermost $2s^22p^1$ electrons of the B atom and $1s^1$ electrons of the H atom were placed in the active space. It must be mentioned that the electrons of n=1 shell for the B atom were correlated via singly and doubly electron excitation in the following MRCI-F12 computation.

At last, by solving the corresponding nuclear Schrödinger equation, the spectroscopic constants including adiabatic excitation energy T_e, equilibrium internuclear distance R_e, vibrational constants ω_e, inharmonic coefficient $\omega_e\chi_e$, rotational constant B_e and vibration rotating coupling constant α_e, were determined. Moreover, it should be pointed out that the calculations of spectroscopic constants were based on the lowest four vibrational levels for the $X^1\Sigma^+$ state and two for the $A^1\Pi$ state. The dissociation energy D_e was obtained by subtracting

the molecular energy at R_e from the energy at a large separation. From the PECs of the $X^1\Sigma^+$ and $A^1\Pi$ states, we predicted the vibrational levels ΔG_v, the vibration-dependent rotational constant B_v and the centrifugal distortion constant D_v. The TDM and the Franck-Condon factors were determined. Furthermore, the radiative lifetimes of $A^1\Pi$-$X^1\Sigma^+$ transition, based on the calculated TDM and Franck-Condon factors, were predicted.

3 Results and discussion

3.1 The spectroscopic constants of BH

In this work, the electronic structure calculations were performed at the different levels of theory, MRCI-F12, MRCI-F12+Q and MRCI-F12+Q+SR. In the calculation of the PECs, we spacing the calculated electronic states was 0.05 Å for R=0.8-4 Å, 0.1 Å for R= 4-4.5 Å and 1 Å for 5-10 Å. From the PECs, the spectroscopic constants (T_e, R_e, ω_e, $\omega_e\chi_e$, B_e, α_e, D_e) of the $X^1\Sigma^+$ and $A^1\Pi$ states have been determined and tabulated in **Table 1**. At the same time, the previous theoretical and the experimental findings are also listed in Table 1 for comparison.

As tabulated in **Table 1**, for the ground state $X^1\Sigma^+$, the spectroscopic constants we determined by the three theoretical methods are close to each other. However, our computed spectroscopic constants including Davidson correction are somewhat improved by comparing with the MRCI-F12 method. At the same time, our computed R_e and ω_e are in better agreement with the corresponding these experimental values [2-4]. However, the values of $\omega_e\chi_e$ derived from these experiment measurements [2-4] exhibit the great deviations. The latest experimental value of $\omega_e\chi_e$ was determined to be 47.710 cm^{-1} [2], which is apparently smaller than the other experimental values of 49.338 cm^{-1} and 49.326 cm^{-1} [3, 4]. Our calculations with the three methods all support the latest experimental result [2]. Moreover, the calculated vibrational constant ω_e with different methods are also very close to the results determined from the experiment [2]. In contrast, the result from the MRCI-F12 with Davidson correction and SR effect calculation has the smallest deviation with the observed value [2], and the difference between them is only 1.03 cm^{-1}. Therefore, the R_e we evaluated using the MRCI-F12+Q+SR method is also reliable. Compared with the experimental and the previous theoretical, the R_e we evaluated is well excellently with experimental result [4] and the computation values with the methods including the CV effect such as CCSD(T)/cc-pCV5Z [35] and MR-ACPF/cc-pCV7Z [19]. It demonstrates that the CV effect has the great effect on the BH molecule. Our D_e value with MRCI-F12+Q+SR method differs from that determined with the Rydberg-Klein-Rees (RKR) method by 2.48 kcal/mol. In contrast, our computed D_e value (84.98 kcal/mol) is in accordance with the theoretical result (84.92 kcal/mol) [19] at the MR-ACPF/cc-pCV7Z level of theory. At the same time, our other computed spectroscopic

constants with MRCI-F12+Q+SR method excellently reproduce the observed values [2], the largest deviations are only 0.0541, 0.006 cm^{-1} for the B_e, α_e, respectively.

Table 1. The spectroscopic constants of the Λ-S states

Λ-S State	Method	T_e (cm^{-1})	R_e (Å)	ω_e (cm^{-1})	$\omega_e\chi_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	D_e (kcal/mol)
$X^1\Sigma^+$	MRCI-F12	0	1.2289	2369.50	47.170	12.0879	0.432	84.96
	MRCI-F12+Q	0	1.2293	2366.28	47.232	12.0800	0.416	85.00
	MRCI-F12+Q+SR	0	1.2293	2365.69	47.231	12.0801	0.416	84.98
Expt.[2]				2364.66	47.710	12.026	0.422	
Expt.[3]		0	1.2322	2366.73	49.338	12.026	0.421	82.50
Expt.[4]		0	1.2295	2368.62	49.326			
Calc.[11]								85.01
Calc.[35]	FCI/cc-pV5Z		1.2329	2358.21	49.2	12.013		
	CCSD(T)/cc-pV5Z		1.2327	2360.27	49.0	12.016	0.420	
	CCSD(T)/cc-pCV5Z		1.2295	2370.30	49.3	12.079		
	CCSD(T)/cc-pV6Z		1.2325	2360.25	49.3	12.019		
Calc.[19]	cc-pCV7Z		1.2293					84.92
$A^1\Pi$	MRCI-F12	23355.814	1.2214	2343.52	127.974	12.2798	0.733	20.598
	MRCI-F12+Q	23089.329	1.2212	2344.67	127.889	12.2830	0.739	20.659
	MRCI-F12+Q+SR	23099.838	1.2212	2343.96	128.178	12.2836	0.740	20.612
Expt.[2]		23105		2342.41	127.8	12.2		
Expt.[36]		23136	1.2186	2251		12.295	0.835	
Calc.[11]		22997.9	1.2210	2404.6	147.3	12.2795		20.980
Calc.[18]		23144	1.222	2341			0.851	
Calc.[37]			1.2492	2118				

Turning to the $A^1\Pi$ state, the T_e values evaluated using the MRCI-F12 method without and with the Davidson correction differs from experimental measurements [2] by 250.814 and 15.671 cm^{-1}, respectively. Obviously, the Davidson correction leads to the great improvement of the T_e for the $A^1\Pi$ state. Furthermore, the inclusion of the SR effect makes the deviation decrease to 5.162 cm^{-1}. Similarly, among the calculated spectroscopic constants from the

different theoretical methods, both the R_e and ω_e determined by the MRCI-F12+Q+SR method are in the best accuracy (1.2212 Å and 2343.96 cm^{-1}) comparing with the previous measurements [2]. The dissociation energy of the $A^1\Pi$ state, to the best of the knowledge, has never been studied in experiment. Our predicted D_e is 20.612 kcal/mol in the preset work, which is very close to the theoretical value [11] of 20.980 cm^{-1}. Therefore, comparing with experimental results, the MRCI-F12 method in combination with the Davidson and SR corrections leads to the best accuracy. On the other hand, as shown in **Table 1,** good agreements with the experiments [2] and other computations [11] could be found for the $\omega_e\chi_e$, B_e, α_e. Therefore, the PECs with MRCI-F12+Q+SR method were chosen for the vibration-rotation levels calculations of the $X^1\Sigma^+$ and $A^1\Pi$ states.

3.2 Rotation-vibration spectrum

Table 2. Vibrational levels ΔG_v and rotational constants (B_v, 10^3D_v) of the $X^1\Sigma^+$ state (all data are in units of cm^{-1})

$X^1\Sigma^+$	ΔG_v				B_v		10^3D_v	
V	This work	Expt.[4]	Errors (%)	Calc.[19]	This work	Expt.[4]	This work	Expt.[4]
0	0	0			11.8718	11.8157	1.2455	1.2237
1	2271.59	2269.3	0.10104	2269.60	11.4551	11.4009	1.2223	1.2020
2	4447.64	4443.1	0.10207	4443.66	11.0449	10.9926	1.1987	1.1786
3	6530.30	6523.6	0.10277	6524.36	10.6407	10.5898	1.1737	1.1418
4	8521.82	8513.1	0.10241		10.2422		1.1455	
5	10424.42				9.8479		1.1120	
6	12240.22				9.4561		1.0703	
7	13971.26				9.0648		1.0195	
8	15619.15				8.6715		9.6027	
9	17184.90				8.2741		8.9571	
10	18668.83				7.8713		8.3069	
11	20070.40				7.4616		7.7302	
12	21387.97				7.0433		7.2709	
13	22618.96				6.6154		7.0061	
14	23759.46				6.1737		6.9784	
15	24804.20				5.7135		7.2618	
16	25746.12				5.2264		7.9236	
17	26576.17				4.7004		9.1116	
18	27282.72				4.1177		1.1071	

19	27851.13	3.4503	1.4349
20	28263.26	2.6501	2.0496
21	28497.80	1.6084	3.7983

On the basis of the PECs obtained from the MRCI-F12+Q+SR calculations, the vibrational levels ΔG_v, vibration-dependent rotational constants B_v and centrifugal distortion constants D_v for both $X^1\Sigma^+$ and $A^1\Pi$ states were evaluated and tabulated in **Table 2** and **3**, respectively. We list the data of D_v results using the style of 10^3D_v, because the D_v results are so small. As listed in **Table 2** and **3**, totally 22 and 4 vibrational levels have been found for the $X^1\Sigma^+$ and $A^1\Pi$ states, respectively. Meanwhile, the corresponding ΔG_v, B_v and D_v are also determined. However, the corresponding experimental data including only 5 and 3 vibrational levels are available. For the $X^1\Sigma^+$ state, the largest deviations of ΔG_v, B_v and D_v from experimental values [4] are only 8.72 cm^{-1}, 0.0561 cm^{-1}, and 0.0319 cm^{-1}, respectively. The relative errors for all available vibrational levels are in the range of 0.10104%-0.10277%. This comparison indicates that our computed values are pretty close to the experimental values. And our calculated results are also in good agreement with the other theoretical values [19]. For $A^1\Pi$ state, our computed values, ΔG_v, B_v and D_v differ from the experimental values [4] by 0.72, 0.0071 and 0.0193 cm^{-1}, respectively. The comparison also manifests that our calculated values are in excellent agreement with the experimental ones. Moreover, our computed ΔG_v, B_v and D_v will be helpful for the further experiments.

Table 3. Vibrational levels ΔG_v and rotational constants (B_v, 10^3D_v) of the $A^1\Pi$ state (all data are in units of cm^{-1}).

$A^1\Pi$	ΔG_v		B_v		10^3D_v	
v	This work	Expt.[4]	This work	Expt.[4]	This work	Expt.[4]
0	0	0	11.9134	11.9063	1.4386	1.4385
1	2087.61	2086.89	11.1729	11.1680	1.6040	1.5986
2	3918.86	3918.26	10.2283	10.2282	1.9986	2.0179
3	5398.87		8.7692		3.7026	

3.3 Transition dipole moments and radiative lifetimes of BH

The Franck-Condon factors $q_{v'v''}$ represent the overlap of the two vibrational wave functions $\phi_{v'}$ and $\phi_{v''}$ of the upper to lower states. In this work, we evaluated the Franck-Condon factors from the vibration levels v'=0-2 of the upper electronic state ($A^1\Pi$) to the vibrational levels v''= 0-5 of the lower ground state ($X^1\Sigma^+$) with the aid of the LEVEL

program, as listed in **Table 4**. From the **Table 4**, it is found that the maximum values of FCFs for v'- v'' are 0.9992 (0-0), 0.9905 (1-1), 0.9193 (2-2), which are in excellent agreement with the corresponding experimental measurements [23], 0.9987, 0.9911, 0.9209, respectively. Thus, the diagonal Δv= 0 bands have the strongest transition probability. Our calculated data are also in accordance with the recent theoretical data [11]. Moreover, since the FCFs are highly diagonal, the BH molecule should be one of the good candidates for laser cooling. Furthermore, we also list the transitional energy $T_{v'v''}$ in the **Table 4**, which are also valuable for selecting proper wavelength in further laser cooling experiments.

For the aforementioned transitions, the radiative lifetimes of the selected vibrational level v' have been computed by the following formula:

$$\tau_{v'} = \left(A_{v'}\right)^{-1} = \frac{3hg'}{64\pi^4 \left|a_0 \cdot e \cdot TDM\right|^2 \sum_{v''} q_{v',v''} \left(\Delta E_{v',v''}\right)^3}$$

where $A_{v'}$ is the Einstein coefficient; $q_{v',v''}$ is the Franck-Condon factor (FCF); TDM is averaged transition dipole moment in atomic units (a.u.); ΔE is the energy difference between vibration level v' and v''.

Table 4. Franck-Condon factors of the $A^1\Pi$-$X^1\Sigma^+$ transition of BH

v'		v''=0	1	2	3	4	5
0	FCFs	0.9992	0.000046	0.000800	0.000000	0.000001	0.000000
	Expt.[23]	0.9987	0.00027	0.000983	0.000000	0.000000	0.000000
	Calc.[11]	0.9992					
	$T_{v'v''}$	23012	20732	18548	16458	14400	12551
1	FCFs	0.000022	0.9905	0.005072	0.004295	0.000073	0.000018
	Expt.[23]	0.000275	0.9911	0.004172	0.004430	0.000073	0.000013
	Calc.[11]		0.9908				
	$T_{v'v''}$	25109	22828	20644	18554	16556	14648
2	FCFS	0.000778	0.007145	0.9193	0.04907	0.02111	0.002083
	Expt.[23]	0.000958	0.006074	0.9209	0.04787	0.02147	0.002178
	Calc.[11]			0.9235			
	$T_{v'v''}$	26947	24667	22483	20393	18395	16486

The calculated radiative lifetimes for the $A^1\Pi$ state were listed in **Table 5**. As shown in **Table 5**, we can get the lifetime 125 ns (v'=0), 168 ns (v'=1), 193 ns (v'=2) are in reasonable agreement with the experimental values [25, 38], respectively. These calculation results are

also very close to the theoretical value [23].

Table 5. The radiative lifetimes of the $A^1\Pi$ state

Transition	Radiative lifetime (ns)		
	v'=0	v'=1	v'=2
This work	125	168	193
Expt.[25]	127±10	146±12	172±14
Expt.[38]	152±6	167±7	198±8
Calc.[23]	123	141	170

4 Conclusions

In the present work, the $X^1\Sigma^+$ and $A^1\Pi$ states for the BH molecule have been investigated by using the MRCI-F12 method. In order to obtain the high-level PECs, the Davidson correction and the scalar relativistic effect were taken into account in calculation. From the PECs, the spectroscopic constants of the corresponding states were evaluated, and the results from the MRCI-F12+Q+SR calculation exhibit the best accuracy. The ΔG_v, B_v and D_v for each vibrational state of the $X^1\Sigma^+$ and $A^1\Pi$ were also determined based on the computed PECs from the MRCI-F12+Q+SR calculation, which are in good agreement with the available measurements. The Franck-Condon factors of spin-allowed transition $A^1\Pi$-$X^1\Sigma^+$ were calculated. Finally, the radiative lifetimes of $A^1\Pi$ state were evaluated and the results are in accordance with the experiment data. The presently computed results should be valuable for the further experimental studies on the electronic states and laser cooling of BH molecule.

Acknowledgments

This work was supported by National Natural Science Foundation of China (Grand No.11574114) and the Natural Science Foundation of Jilin Province, China (Grand No. 2015101003JC).

References

[1] D. Feller, D. A. Dixon, Heats of Formation of Simole Boron Compounds, J. Phys.Chem. A, 102 (1998) 7053-7059.

[2] J. Clark, M. Konopka, L. M. Zhang, E. R. Grant, The A 1Π-X1Σ+ (2,0) transition in 11BH and 10BH observed by (1+2)-photon resonance-enhanced multiphoton ionization spectroscopy, Chem. Phys. Lett., 340 (2001) 45-54.

[3] F. S. Pianalto, L. C. O'Brien, P. C. Keller, P. F. Bernath, Vibration-rotation spectrum of BH X1Σ+ by Fourier transform emission spectroscopy, J. Mol. Spectrosc., 129 (1988) 348-353.

[4] W. T. M. L. Fernando, P. F. Bernath, Fourier transform spectroscopy of the A1Π-X1Σ transition of BH and BD, J. Mol. Spectrosc., 145 (1991) 392-402.

[5] I. D. Petsalakis, G. Theodorakopoulos, Multireference configuration interaction and quantum defect calculations on the Rydberg states of the BH molecule, Mol. Phys., 104 (2006) 103-113.

[6] B. P. L. Lavrov, M. Osiac, A. V. Pipa, On the spectroscopic detection of neutral species in a low-pressure plasma containing boron and hydrogen, Plasma Sources Sci. Technol., 12 (2003) 576-589.

[7] A. Shayesteh, E. Ghazizadeh, Dunham coefficients for the X1Σ+ ground state of BH and BD, J. Mol. Spectrosc., 312 (2015) 110-112.

[8] S. H. Bauer, G. Herzberg, J. W. C. Johns, The absorption spectrum of BH and BD in the vacuumultraviolet, J. Mol. Spectrosc., 13 (1964) 256-280.

[9] J. W. C. Johns, On the spectrum of BH in the near ultraviolet, J. Mol. Spectrosc., 22 (1967) 435-451.

[10] R. J. Hendricks, D. A. Holland, Vibrational branching ratios and hyperfine structure of 11BH and its suitability for laser cooling, Physics, 2 (2014) 1-8.

[11] Y. F. Gao, T. Gao, Laser cooling of BH and GaF: insights from an ab initio study, Phys. Chem. Chem. Phys., 17 (2015) 10830-10837.

[12] X. T. Liu, G. Y. Liang, X. M. Zhang, B. Yan, Rotation-vibration spectra for ground state of NaH and its isotopes with explicitly multireference configuration interaction method, Journal of Atomic and Molecular Sciences, 7 (2016) 125-134.

[13] J. Guo, B. Yan, D. L. Zeng, Accurate ab initio potential energy curve of X2Π state and high-temperature A2Δ-X2Π fluorescence spectra for CH radical, Journal of Atomic and Molecular Sciences, 4 (2013) 183-192.

[14] J. Liu, M. Wang, J. Li, M. Ma, C. Yang, Ab initio study of spectroscopic constants and anharmonic force field of hypochlorous acid HO35Cl, Journal of Atomic and Molecular Sciences, 6 (2015) 103-112.

[15] W. L. Holtgreven, V. d. Vleugel, Uber ein Bandespektrum des Borhydrides, Z.Phys, 70 (1931) 188-203.

[16] R. C. Sahni, Electronic States of Molecules. I. Electronic Structure of BH, J. Chem. Phys., 25 (1956) 332-336.

[17] P. E. Cade, W. M. Huo, Electronic Structure of Diatomic Molecules. VI.A. Hartree-Fock Wavefunctions and Energy Quantities for the Ground States of the First-Row Hydrides, AH, J. Chem. Phys., 47 (1967) 614-648.

[18] E. Miliordos, A. Mavridis, Ab initio investigation of the electronic structure and bonding of BH, BH-, and HBBH molecules, J. Chem. Phys., 128 (2008) 144308.

[19] J. Koput, Ab Initio spectroscopic characterization of borane, BH, in its X1Σ+ electronic state, J. Comput. Chem., 36 (2015) 2219-2227.

[20] W. Meyer, P. Rosmus, PNO–CI and CEPA studies of electron correlation effects. III. Spectroscopic constants and dipole moment functions for the ground states of the first-row and second-row diatomic hydrides, J. Chem. Phys., 63 (1975) 2356-2375.

[21] L. A. Curtiss, J. A. Pople, A theoretical study of the dissociation energy of BH using quadratic configuration interaction, J. Chem. Phys., 90 (1989) 2522-2523.

[22] C. W. Bauschlicher, S. R. Langhoff, P. R. Taylor, On the dissociation energy of BH, J. Chem. Phys., 93 (1990) 502-506.

[23] W. T. Luh, W. C. Stwalley, The X1Σ+, A1Π ,B1Σ+ potential energy curves and spectroscopy of BH, J. Mol. Spectrosc., 102 (1983) 212-223.

[24] J. R. Sabin, J. Oddershede, The Radiative lifetime of the A1Π state of BH, Chem. Phys., 115 (1987) 15-21.

[25] C. H. Douglass, H. H. Nelson, J. K. Rice, Spectra, radiative lifetimes, and band oscillator strengths of the A 1Π-X1Σ+ transition of BH, J. Chem. Phys., 90 (1989) 6940-6948.

[26] H. J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, Molpro: a general-purpose quantum chemistry program package, WIREs Comput. Mol. Sci., 2 (2012) 242-253.

[27] R. Le Roy, LEVEL 8.0: A computer program for solving the radial Schrödinger equation for bound and quasibound levels, University of Waterloo Chemical Physics Research Report CP-663, (2007).

[28] C. Hättig, Optimization of auxiliary basis sets for RI-MP2 and RI-CC2 calculations: Core–valence and quintuple-ζ basis sets for H to Ar and QZVPP basis sets for Li to Kr, Phys. Chem. Chem. Phys., 7 (2005) 59-66.

[29] F. Weigend, A. Kohn, C. Hättig, Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations, J. Chem. Phys., 116 (2002) 3175-3183.

[30] H. J. Werner, P. J. Knowles, A second order multiconfiguration SCF procedure with optimum convergence, J. Chem. Phys., 82 (1985) 5053-5063.

[31] H. J. Werner, P. J. Knowles, An efficient internally contracted multiconfiguration–reference configuration interaction method, J. Chem. Phys., 89 (1988) 5803-5814.

[32] T. Shiozaki, G. Knizia, H. J. Werner, Explicitly correlated multireference configuration interaction: MRCI-F12, J. Chem. Phys., 134 (2011) 034113.

[33] S. R. Langhoff, E. R. Davidson, Configuration interaction calculations on the nitrogen molecule, Int. J. Quantum Chem, 8 (1974) 61-72.

[34] M. Douglas, N. M. Kroll, Quantum electrodynamical corrections to the fine structure of helium, Annals of Physics, 82 (1974) 89-155.

[35] B. Temelso, E. Valeev, A Comparison of One-Particle Basis Set Completeness, Higher-Order Electron Correlation, Relativistic Effects, and Adiabatic Corrections for Spectroscopic Constants of BH,CH+, and NH+, J.Phys.Chem.A, 108 (2004) 3068-3075.

[36] Gerhard.Herzberg. Molecular Spectra and Molecular Structure1979.

[37] L. Gagliardi, G. L. Bendazzoli, S. Evangelisti, A full configuration interaction study of the low-lying states of the BH molecule, Mol. Phys., 91 (1997) 861-872.

[38] O. Gustafsson, M. Rittby, A study of the predissociation in the A1Π state of BH, J. Mol. Spectrosc., 131 (1988) 325-339.