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Research highlight

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Theoretical study with dipole moment calculation of new electronic states of the molecule BF

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Abstract: The potential energy curves for the 45 singlet, triplet, and quintet electronic states in the representation $^{2s+1}\Lambda^{(+/-)}$ of the BF molecule have been investigated using the complete active space self-consistent field (CASSCF) method with multireference configuration interaction (MRCI). The internuclear distance R_e, the harmonic frequency ω_e, the static dipole moment μ, the rotational constants B_e, and the electronic transition energy with respect to the ground state T_e have been calculated for the considered electronic states. The comparison between the values of the present work and those available in the literature for several electronic states shows a very good agreement. Twelve electronic states of BF molecule are reported here for the first time that are not yet observed experimentally.

Keywords: *ab initio* calculation; dipole moments; electronic structure; potential energy curves; spectroscopic constants.

1 Introduction

The scientific community became interested in boron monofluoride (BF) molecules at the beginning of the 20th century. Between 1957 and 1985, many electronic states have been investigated by using different experimental techniques [1–10]. Between 1988 and 2011, 22 singlet and triplet electronic states have been studied theoretically [11–36]. Recently, Magoulas et al. [37] have added, to these states, the study of 11 new singlet and triplet electronic states with a complete and detailed description of the studies on this molecule since 1927.

Based on our previous theoretical calculations [38–46], we investigate in the present work, the electronic structure of new higher singlet and triplet, along with new 14 quintet electronic, states of the BF molecule. By using an *ab initio* calculation, the potential energy curves (PECs) as well as the permanent dipole moment curves (DMCs) are investigated for 45 electronic states along with the equilibrium internuclear distance R_e, the transition energy with respect to the minimum energy of the ground state T_e, the harmonic frequencies ω_e, and the rotational constant B_e.

2 Method of calculations

We investigate the low-lying singlet, triplet, and quintet electronic states of the molecule BF using complete active space self-consistent field (CASSCF) procedure followed by a multireference configuration interaction (MRCI with the Davidson correction) treatment for the electron correlation. The entire CASSCF configuration space was used as the reference in the MRCI calculations, which were done via the computational chemistry program MOLPRO [47] taking advantage of the graphical user interface GABEDIT [48]. The boron species is treated as a system of five electrons by using the aug-cc-pCVTZ; c basis set for s, p, and d functions. The nine electrons of the fluorine atom are considered using the DGauss-a1-Xfit; c basis set for s, p, and d functions. The very good quality of the selected basis sets for the BF molecule is checked by comparing our CI calculations for the ground and several excited states of isolated boron and fluorine atoms to the experimental data in NIST atomic spectra database from literature where the relative difference for the two atoms ranges between $0.91\% \leq \Delta E_e/E_e \leq 3.90\%$. Among the 14 electrons explicitly considered for the BF molecule, eight inner electrons were frozen in subsequent calculations so that six valence electrons were explicitly treated corresponding to 16 active orbitals. All computations were performed according to the C_{2v} symmetry. Three high-power

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computing tools were used for performing the calculations: two local machines – Ankabut HPC Cluster (Abu-Dhabi, UAE), Khalifa University HPC (Abu-Dhabi, UAE) shared facility, and the Amazon Elastic Cloud Computing (EC2, Ashburn, VA, USA) facility.

The Ankabut HPC cluster is a 2U four-node server system that includes four Intel® Server Board S2600JF. It consists of a master node (2×Intel Xeon X5675 six cores) that has a memory storage of 48 GB. There is a total number of 16 processes per node, with two cores per process, equating to a total number of 32 cores per node.

The Khalifa University HPC Cluster facility compromises 25 IBM x3755 M3 servers. Each node is configured with 4×AMD 12-core CPUS giving a total of 48 cores. Each server has 128 GB of RAM. Disk storage is proved with a pair of 250-GB STA disks mirrored in a RAID1 configuration. A single port 4X QDR Qlogic Infiniband adapter provides the high-speed interconnect between the cluster nodes. The storage and the management nodes are of the X3550 M3 Intel server-type. The Intel nodes contain two (for the management node) or one (for the storage) Intel CPUs.

The Amazon EC2 instance that we used is of the cc2.8xlarge type (Amazon Web Services, Ashburn, VA, USA). This instance sports two eight-core intel Xeon processors and 32 hardware execution threads. It has 60.5 GB of RAM and 3.37 TB of instance storage.

3 Results and discussion

The potential energy curves (PECs) for the 45 singlet, triplet, and quintet electronic states, in the representation $^{2s+1}\Lambda^{(+/-)}$, of the molecule BF were generated for 76 internuclear distance calculations in the range 0.85 Å ≤ R ≤ 2.8 Å (Figures 1–4). Some curves are dotted or dashed for clarity. We calculated the harmonic vibrational frequencies ω_e,

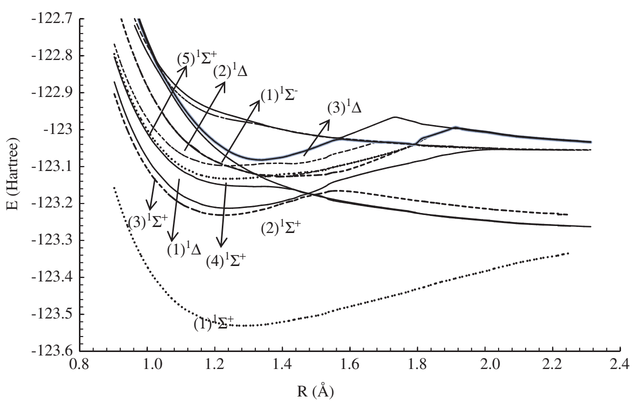

Figure 1: Potential energy curves of the electronic states $^1\Sigma^{\pm}$ and $^1\Delta$ of the molecule BF.

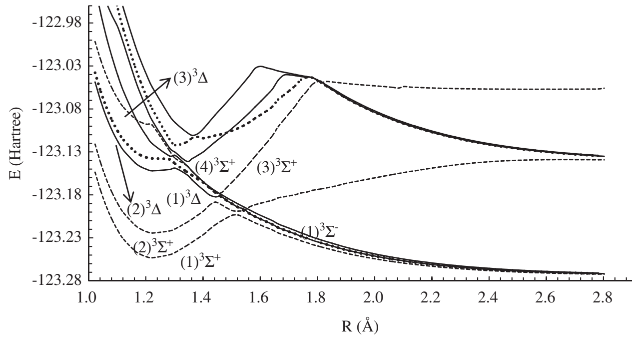

Figure 2: Potential energy curves of the electronic states $^3\Sigma^{\pm}$ and $^3\Delta$ of the molecule BF.

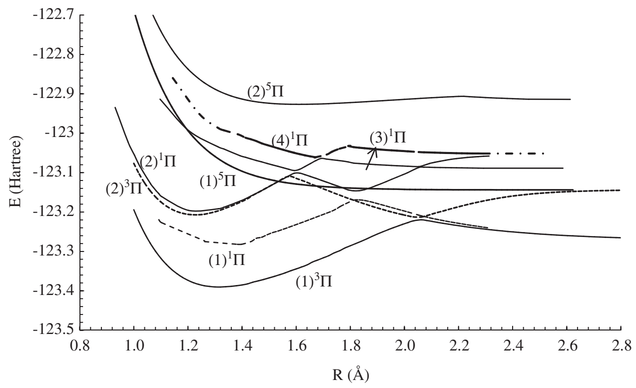

Figure 3: Potential energy curves of the electronic states $^{1,3,5}\Pi$ of the molecule BF.

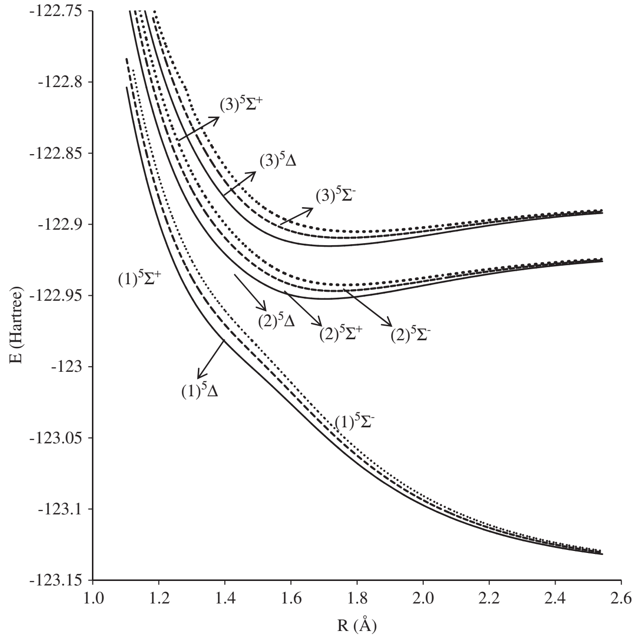

Figure 4: Potential energy curves of the electronic states $^5\Sigma^{\pm}$ and $^5\Delta$ of the molecule BF.

the relative energy separations with respect to the ground state T_e, and the rotational constants B_e of the different electronic states by fitting their potential energy curves into a polynomial in R, around the internuclear distance at equilibrium R_e. These values with the available data in literature are given in Table 1. For the ground state, the relative differences between our calculated spectroscopic constants and those obtained experimentally in literature are 1.5% (Ref. [17])$<\Delta R_e/R_e<$1.7% (Ref. [52]), 2.8% (Ref. [49])$<\Delta\omega_e/\omega_e<$5.7 (Ref. [52]), and 1.5% (Ref. [52])$<\Delta B_e/B_e<$8.7% (Ref. [49]). These relative differences show that the agreement for the R_e values that we obtained, with those given in literature is very good, while those of ω_e and B_e vary between very good [49, 52] and acceptable [49, 52]. Similarly, our calculated ground state R_e values are close with those obtained theoretically in literature, as the relative differences are in the order of 1.1% (Ref. [28])$<\Delta R_e/R_e<$3.0% (Ref. [17]). Also, the agreements for ω_e and B_e vary between excellent [28, 49] and acceptable [17, 51], as the relative differences are, respectively, 0.1% (Ref.

Table 1: Spectroscopic constants of the molecule BF.

States	T_e (cm^{-1})	R_e (Å)	ω_e (cm^{-1})	B_e (cm^{-1})
$X^1\Sigma^+$	0.0^a	1.284	1486.8	1.485
		1.245^b	1496^b	1.559^b
		1.265^c	1402^c	1.510^c
		1.26271^d	1445.666^d	1.6123^d
		$1.2486\leq R_e\leq 1.3037^e$	$1245\leq\omega_e\leq 1493^e$	$1.423\leq B_e\leq 1.551^e$
		$1.2502\leq R_e\leq 1.2697^f$	$1402.1\leq\omega_e\leq 1488.8^f$	
		$1.2625\leq R_e\leq 1.2673^g$	$1391.43\leq\omega_e\leq 1405.15^g$	$1.050633\leq B_e\leq 1.51593^g$
		1.2635^h	1408.57^h	
		1.2625^i	1402.1^i	1.5072^i
$(1)^3\Pi$	30,988.4^a	1.309	1312.2	1.4091
	$34{,}427\leq T_e\leq 39{,}597^g$	$1.3076\leq R_e\leq 1.3151^g$	$1293.40\leq\omega_e\leq 1334.80^g$	$1.39069\leq B_e\leq 1.41641^g$
	29,355.63^h	1.3049^h	1350.68^h	
		1.3081^i	1323.86^i	1.4135^i
$(1)^1\Pi$	54,597.2^a			
	51,009.6^h	1.3076^h	1240.41^h	
$(1)^3\Sigma^+$	60,949.9^a	1.231	1753.2	1.615
	60,140.7^h	1.218^h	1659.8^h	
$(2)^1\Sigma^+$	65,725.6^a	1.228		1.623
	64,438.6^h	1.2099^h	1697.76^h	
$(2)^3\Sigma^+$	67,197.9^a	1.239	1738.6	1.595
	66,082.1^h	1.225^h	1591.9^h	
$(3)^1\Sigma^+$	69,816.9^a	1.242	1686.6	1.585
	68,066.2^h	1.223^h	1617.4^h	
$(2)^3\Pi$	71,066.4^a			
	69,429.7^h	1.2136^h	1696.87^h	
$(2)^1\Pi$	74,428.6^a			
	70,685.2^h	1.2255^h	1682.84^h	
		1.2188^i	1661.96^i	
$(4)^1\Sigma^+$	87,288.6^a	1.251	1222.4	1.535
	88,453.7^h	1.567^h	1863.9^h	
$(2)^1\Delta$	88,535.8^a	1.387	1756.0	1.272
	91,722.2^h	1.447^h	1363.9^h	
$(5)^1\Sigma^+$	95,044.5^a			
$(3)^1\Delta$	98,540.7^a	1.336	2123.6	1.370
Σ^+, Δ	99,463.5^a			
$(2)^5\Sigma^+$	126,967.8^a	1.703	662.6	0.8447
$(2)^5\Delta$	128,195.7^a	1.735	620.0	0.8127
$(2)^5\Sigma^-$	129,126.7^a	1.765	574.4	0.7854
$(3)^5\Sigma^+$	135,120.6^a	1.715	578.2	0.8321
$(3)^5\Delta$	136,390.2^a	1.7610	517.9	0.7891
$(3)^5\Sigma^-$	137,344.3^a	1.8030	475.0	0.7527

^{a}Present work, ^{b}Ref^{theo}. [17], ^{c}Ref^{exp}. [1], ^{d}Ref^{exp}. [49], ^{e}Ref^{theo}. [50], ^{f}Ref^{theo}. [28], ^{g}Ref^{theo}. [51], ^{h}Ref^{theo}. [37], ^{i}Ref^{exp}. [52].

[28])<$\Delta\omega_e/\omega_e$<6.4 (Ref. [51]) and 1.1% (Ref. [49])<$\Delta B_e/B_e$<3.0% (Ref. [17]). One can notice that, the two values, ω_e=1245 cm^{-1} [50] and B_e=1.050633 cm^{-1} [51] are very small with respect to ours and to others obtained in the literature. This can be explained by the difference in the theoretical calculation technique used to obtain these constants. For the first excited state, the present work values of R_e, ω_e, and B_e are in complete accordance with the experimental data [52], with the relative differences 0.1%, 0.9%, and 0.0%, respectively. Good accuracy is obtained by comparing the values that we computed, for the same constants, with those obtained theoretically in literature [37, 51], as in these cases, the relative differences are as follows: 1.1% [51]<$\Delta R_e/R_e$<0.3% [37], 1.4% [51]<$\Delta\omega_e/\omega_e$<2.9% [37] and 0.5% [51]<$\Delta B_e/B_e$<1.3 [51].

By comparing our calculated values for T_e with those obtained theoretically in literature [37] for the excited electronic states, one can find a relative difference that varies between $\Delta T_e/T_e$=1.22% for $(3)^1\Sigma^+$ and $\Delta T_e/T_e$=6.6% for $(1)^1\Pi$. The comparison with those of De-Heng et al. [51] for the electronic state $(1)^3\Pi$ gives a larger relative difference where 10%<$\Delta T_e/T_e$<21.7%.

From the overall agreement between our data and that in literature, either theoretical or experimental, we confirm the validity of our technique of calculation. Consequently, we expect the same precision for the new results that we obtained, i.e. for the 12 previously uninvestigated electronic states. We are looking forward to future experimental studies on the high electronic states of the BF molecule to confirm the precision of our data.

We were able to determine the spectroscopic constants of nine excited states, out of the original new 12; actually, the three remaining states, and some of the previously seen in literature, are either unbound states or states that show an avoided crossing. In such cases, no spectroscopic constants can be determined. The avoided crossing between the adiabatic potential energy curves takes place usually at the position of, or near, the internuclear distance at the equilibrium distance R_e. The existence of this phenomenon is related to the interaction between the adiabatic potential curves of the corresponding states. When two wavefunctions of two electronic states belonging to the same symmetry mix with each other to give two adiabatic solutions, the corresponding potential energy curves no longer cross, and the crossing becomes avoided between them. It then becomes impossible to calculate the corresponding spectroscopic constant of such states.

On the other hand, the crossing between two potential energy curves of two electronic states of different symmetry is usually allowed, and the electronic state wavefunctions are adiabatic solutions of the Schrödinger equation.

An avoided crossing between two states causes an important change in their dipole moment, where the electronic character of the atom is interchanged in this region, and its polarity reversed. Such crossings or avoided crossings can dramatically alter the stability of the molecule. The dipole moments of the 45 lowest electronic states of the BF molecule are analyzed. The dipole moment operator is among the most reliably demanded as it helps predict important physical properties of molecules. The expectation value of this operator is sensitive to the nature of the least energetic and most chemically relevant valence electrons. The Hartree-Fock dipole moment (HF) is usually large, as the HF wavefunction overestimates the ionic contribution. All our calculations were also performed with the MOLPRO [38] program. The permanent dipole moments have been calculated by taking the boron atom at the origin, and the fluorine atom moves along the positive z-axis. These dipole moment curves are given in Figures 5–8. At large internuclear separations, all dipole moment curves asymptotically reach a zero value reflecting the proper dissociation of the molecule into neutral species.

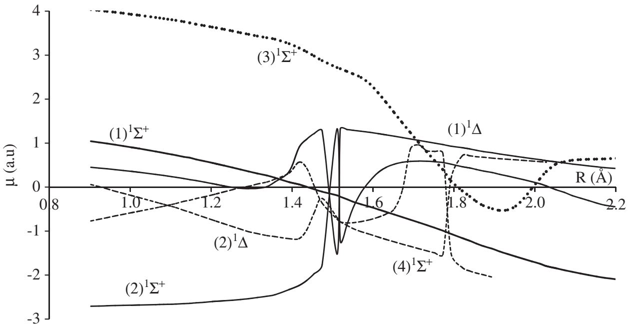

Figure 5: Dipole moment curves of the electronic states $^1\Sigma^\pm$ and $^1\Delta$ of the molecule BF.

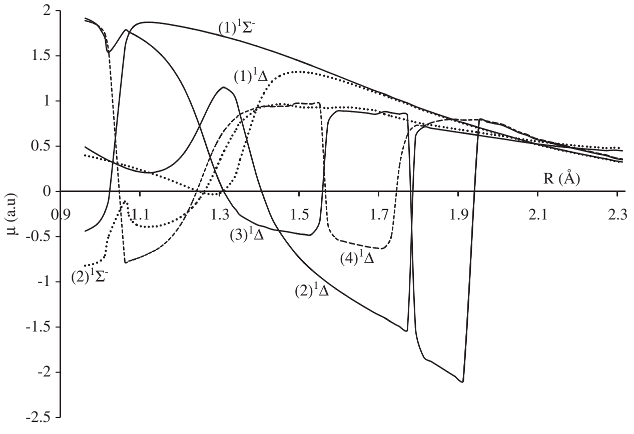

Figure 6: Dipole moment curves of the electronic states $^1\Sigma^-$ and $^1\Delta$ of the molecule BF.

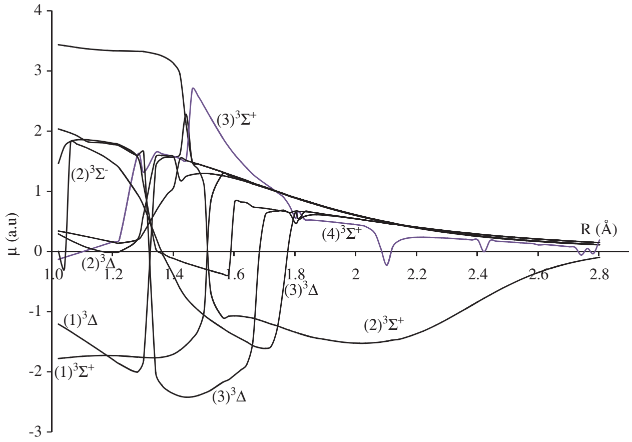

Figure 7: Dipole moment curves of the electronic states $^3\Sigma^\pm$ and $^3\Delta$ of the molecule BF.

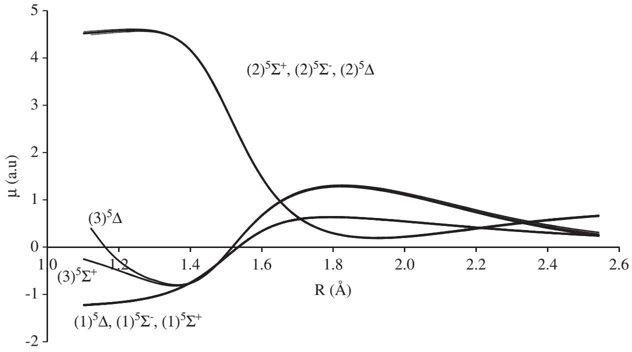

Figure 8: Dipole moment curves of the electronic states $^5\Sigma^\pm$ and $^5\Delta$ of the molecule BF.

4 Conclusion

In the present work, an *ab initio* calculation of 45 singlet, triplet, and quintet lowest electronic states in the $^{2s+1}\Lambda^\pm$ representation has been performed via CASSCF/MRCI methods. The potential energy curves have been calculated along with the spectroscopic constants T_e, R_e, B_e, and ω_e for these states and the static dipole moment μ. The comparison of our calculated values with either the theoretical or the experimental data available in the literature demonstrated an overall good agreement. The electronic structure of new higher singlet and triplet along with new 14 quintet electronic states of the BF molecule have been studied in the present work for the first time. The investigated data in the present work may help for more experimental or theoretical studies in the future for higher electronic states.

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