

# Spin-Orbit Electronic Structure of the ScBr Molecule

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Received April 2, 2011; revised May 3, 2011; accepted June 1, 2011

## Abstract

A theoretical investigation of the spin-orbit electronic states of the molecule ScBr has been performed via CASSCF and MRCI (single and double excitations with Davidson correction) calculations. Spin-orbit effects have been introduced through semi-empirical spin orbit pseudo-potential for scandium while they have been neglected for bromine. Potential energy curves for 42 electronic states in the representation  $\Omega^{(\pm)}$  have been determined along with the corresponding spectroscopic constants. The comparison of the present results with those available in the literature shows a good agreement. New results have been investigated in present work for 30 electronic states in the representation  $\Omega^{(\pm)}$  for the first time.

**Keywords:** ScBr Molecule, *ab Initio* Calculation, Spin-Orbit Calculation, Potential Energy Curves, Spectroscopic Constants

## 1. Introduction

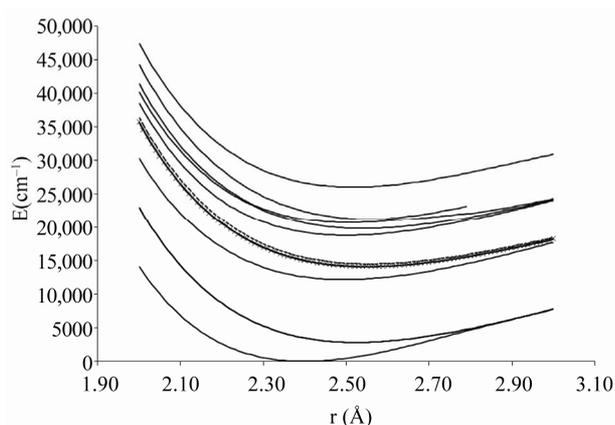
Scandium is the first of the transition metal atoms which has only one *d*-electron in the ground electronic state. Interest in its compounds thus arises because they can be considered as prototypes for understanding the role that *d*-orbitals play in chemical bonding and chemiluminescence reactions [1]. The spectra and structure of scandium monochloride ScCl and scandium monofluoride ScF have been the subject of many theoretical and experimental studies while scandium monobromide ScBr is the least studied spectroscopically. In literature the experimental and theoretical data in the representation  $^{2s+1}\Lambda^{(\pm)}$  of the molecule ScBr have been previously reported by Fischell *et al.* [2], Langhoff *et al.* [3] and Lin *et al.* [3]. The only investigated electronic states of this molecule with spin orbit effect are those calculated by Bencheikh [4] using the ligand field theory. Recently [5] we studied the electronic structure of 23 electronic states of the molecule ScBr without spin-orbit effect. In the present work, an *ab initio* investigation of 42 low-lying electronic states with spin-orbit effect of the molecule ScBr has been performed. The potential energy curves (PECs) along with the transition energy with respect to the minimum energy of the ground state  $T_e$ , the equilibrium internuclear distance  $R_e$ , the harmonic frequency  $\omega_e$ , the permanent dipole moment and the rotational constant  $B_e$ , have been calculated for these spin-orbit electronic states.

## 2. Computational Approach

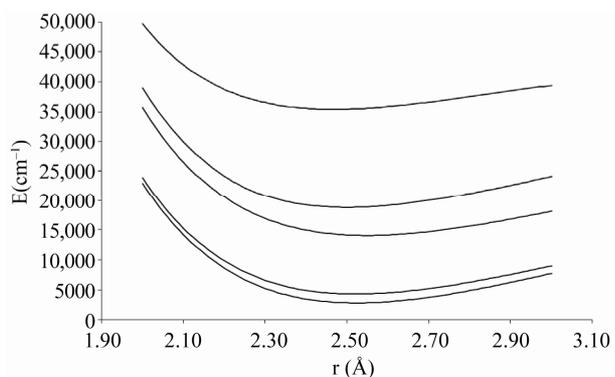
The PECs of the lowest-lying electronic states of the molecule ScBr have been investigated via CASSCF method. Multireference CI calculations (single and double excitations with Davidson corrections) were performed to determine the correlation effects. The entire CASSCF configuration space was used as the reference in the MRCI calculations. These calculations have been performed via the computational chemistry program MOLPRO [6] taking advantage of the graphical user interface GABEDIT [7]. Scandium species is treated in all electron scheme, the 21 electrons of the scandium atom are considered using a contracted Gaussian basis set used by Langhoff *et al.* [3] for s, d, and f functions then we added p function from 6-31G\*\* basis set [8] which has 16 diffused functions contracted set of Gaussian functions. The bromine species is treated as a system with 28 inner electrons taken into account through pseudo potential  $W_{SO}^{PS}$  [9] together with the corresponding Gaussian basis set from the basis LANL2DZ-ECP for s, p functions and we have added d function from 6-311G basis set [10] which has five d functions contracted to two functions, also we added f function from SDB-aug-cc-pVTZ basis set [11] which has two f diffused functions contracted to one f function given a final [2s 2p 2d 1f] contracted basis. The energies for  $\Omega^{(\pm)}$  states have been obtained from the diagonalization of the matrix energy corresponding to a total hamiltonian,

which is the sum of the electrostatic hamiltonian previously treated at the CASSCF/MRCI level [5] and the SO pseudo-potential  $W_{SO}^{PS}$ . This matrix was built up on the basis of CASSCF wave functions, while diagonal matrix elements came from CI plus Davidson correction calculations. Among the 28 electrons explicitly considered for ScBr (21 electrons for Sc and 7 for Br) 18 inner electrons were frozen in subsequent calculations so that 10 valance electrons were explicitly treated. The active space contains  $3\sigma(Sc:4s,3d_0;Br:4s)$ ,  $1\pi(Sc:3d_{\pm 1})$  and  $1\delta(Sc:3d_{\pm 2})$  orbitals in the  $C_{2v}$  symmetry; this corresponds to 7 active molecular orbitals distributed into irreducible representation  $a_1$ ,  $b_1$ ,  $b_2$  and  $a_2$  in the following way:  $4a_1$ ,  $1b_1$ ,  $1b_2$ ,  $1a_2$ , noted [4,1,1,1], while the doubly occupied orbitals  $1\sigma(Br:4p_0)$  and  $1\pi(Br:4p_{\pm 1})$  of bromine have been considered as inactive in the CAS-SCF calculations.

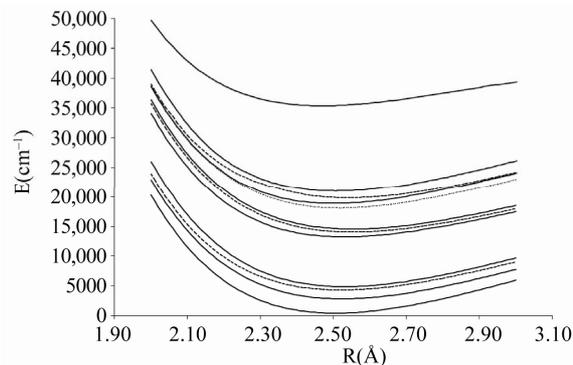
The calculations have been performed for 100 internuclear distances in the range  $2.00\text{\AA} \leq R \leq 3.00\text{\AA}$  for 42 states in the representation  $\Omega^{(\pm)}$ . The PECs for the symmetries  $\Omega = 0^+$ ,  $0^-$ , 1, 2, 3, 4 are drawn respectively in the Figures 1-5.



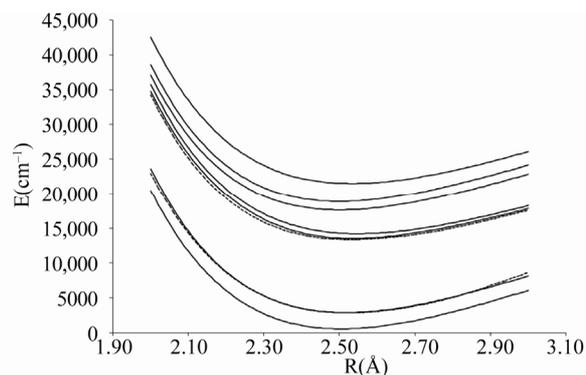
**Figure 1.** Potential energy curves of the lowest electronic states  $\Omega = 0^+$  of the molecule ScBr.



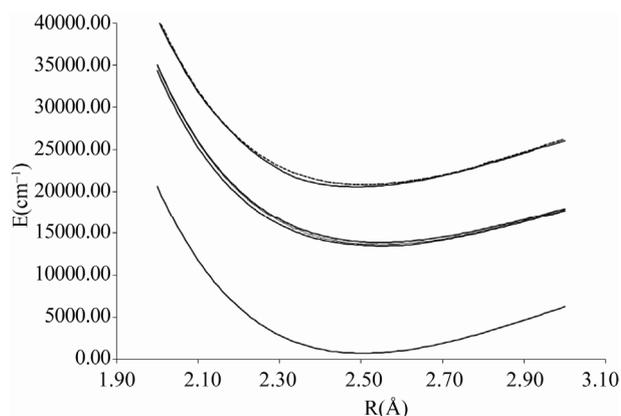
**Figure 2.** Potential energy curves of the lowest electronic states  $\Omega = 0^-$  of the molecule ScBr.



**Figure 3.** Potential energy curves of the lowest electronic states  $\Omega = 1$  of the molecule ScBr.



**Figure 4.** Potential energy curves of the lowest electronic states  $\Omega = 2$  of the molecule ScBr.



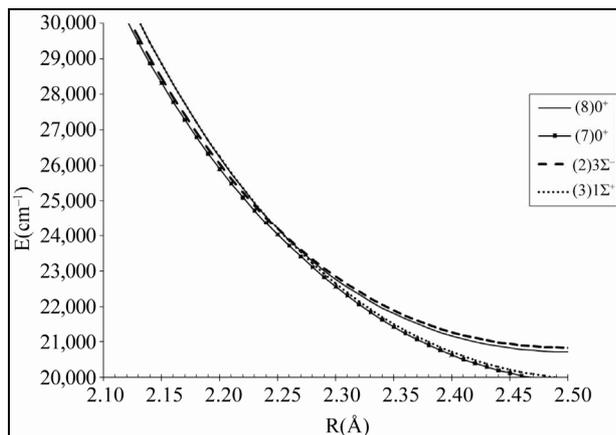
**Figure 5.** Potential energy curves of the lowest electronic states  $\Omega = 3, 4$  of the molecule ScBr.

In the range of  $R$  considered, the avoided crossings that appear between the investigated  $\Omega$ -states are displayed in **Table 1** together with their positions  $R_{AC}$ , the corresponding parent states and the energy difference between two states  $(n+1)\Omega/(n)\Omega$  at these points.

This is illustrated by the avoided crossing at  $R_{AC} = 2.26\text{\AA}$  for the states  $(8)0^+/(7)0^+$  in **Figure 6** where the parent states are respectively  $(3)^1\Sigma^+$  and  $(2)^3\Sigma^-$ .

**Table 1. Positions of the avoided crossing  $R_{AC}$  and the energy difference  $E_{AC}$  at these points with the corresponding crossing of  $\Lambda$  states for  $\Omega$  states of ScBr.**

$\Omega$	$(n+1)\Omega/n\Omega$	$R_{AC}$ (Å)	$\Delta E_{AC}$ (cm <sup>-1</sup> )	Crossing of $\Lambda$ states
0 <sup>+</sup>	2/1	2.9	18	(1) <sup>3</sup> Π/ X <sup>1</sup> Σ <sup>+</sup>
	8/7	2.26	154	(3) <sup>1</sup> Σ <sup>+</sup> /(2) <sup>3</sup> Σ <sup>-</sup>
1	9/8	2.19	107	(3) <sup>3</sup> Π/(2) <sup>1</sup> Π
	10/9	2.99	154	(2) <sup>3</sup> Σ <sup>-</sup> /(3) <sup>3</sup> Π
2	3/2	2.85	64	(1) <sup>3</sup> Π/(1) <sup>1</sup> Δ

**Figure 6. The avoided crossings between the electronic states (7)0<sup>+</sup> and (8)0<sup>+</sup> with the corresponding crossing between the parent states (3)<sup>1</sup>Σ<sup>+</sup> and (2)<sup>3</sup>Σ<sup>-</sup> of the molecule ScBr.**

The composition in percentage of the  $\Omega$  state wave functions in terms of the  $\Lambda$  states, calculated at  $R = 2.4\text{Å}$ , is presented in **Table 2**.

For each state  $\Omega$  there is a predominant component  $\Lambda$  with a contribution larger than 57.54% so that a main parent SA may be identified. Nevertheless, the states where the contribution of the other  $\Lambda$  is smaller than the dominant also have been obtained. For instance, the wave functions for the states (1) $\Omega = 0^+$  and (2) $\Omega = 0^+$  are mixing of the two crossing states X<sup>1</sup>Σ<sup>+</sup> and (1)<sup>3</sup>Π, and the states (7) $\Omega = 0^+$  and (8) $\Omega = 0^+$  are mixing of the two states (2)<sup>3</sup>Σ<sup>-</sup> and (3)<sup>1</sup>Σ<sup>+</sup>. The wave functions for the states (8) $\Omega = 1$  and (9) $\Omega = 1$  are mixing of the two closest states (2)<sup>1</sup>Π and (3)<sup>3</sup>Π, while those for the states (9) $\Omega = 1$  and (10) $\Omega = 1$  are mixing of the two closest states (3)<sup>3</sup>Π and (2)<sup>3</sup>Σ<sup>-</sup>. The wave functions for the states (2) $\Omega = 2$  and (3) $\Omega = 2$  are mixing of the two closest states (1)<sup>1</sup>Δ and (1)<sup>3</sup>Π. These results are consistent with the avoided crossings and crossings reported in **Table 2**.

The spectroscopic constants such as the vibrational harmonic constant  $\omega_e$ , the internuclear distance at equilibrium  $R_e$ , the rotation constant  $B_e$ , and the electronic transition energy with respect to the ground state  $T_e$  have been calculated by fitting the energy values around the equilibrium position to a polynomial in terms of the in-

**Table 2. Composition of  $\Omega$ -states wave functions of the molecule ScBr in terms of  $\Lambda$ -states (in percentage) at  $R = 2.4\text{Å}$ .**

$n\Omega$	% $\Lambda$ -parents	$n\Omega$	% $\Lambda$ -parents
(1)0 <sup>+</sup>	99.72 X <sup>1</sup> Σ <sup>+</sup> , 0.28 (1) <sup>3</sup> Π	(4)0 <sup>+</sup>	77.98(2) <sup>3</sup> Π, 21.97(1) <sup>3</sup> Σ <sup>-</sup> , 0.02(3) <sup>1</sup> Σ <sup>+</sup> , 0.03(2) <sup>1</sup> Σ <sup>+</sup>
(1)3	100(1) <sup>3</sup> Δ	(3)0 <sup>-</sup>	100(2) <sup>3</sup> Π
(1)2	99.49(1) <sup>3</sup> Δ, 0.33(1) <sup>1</sup> Δ, 0.08(1) <sup>3</sup> Π	(7)1	88.78(1) <sup>3</sup> Σ <sup>-</sup> , 11.08(2) <sup>3</sup> Π, 0.09(2) <sup>3</sup> Δ, 0.02(2) <sup>1</sup> Π, 0.01(3) <sup>3</sup> Π, 0.01(1) <sup>1</sup> Π, 0.01(3) <sup>3</sup> Π
(1)1	99.72(1) <sup>3</sup> Δ, 0.07(1) <sup>1</sup> Π, 0.21(1) <sup>3</sup> Π	(5)0 <sup>+</sup>	77.88(1) <sup>3</sup> Σ <sup>-</sup> , 21.88(2) <sup>3</sup> Π, 0.12(2) <sup>1</sup> Σ <sup>+</sup> , 0.03(3) <sup>1</sup> Σ <sup>+</sup> , 0.03(4) <sup>1</sup> Σ <sup>+</sup> , 0.06(3) <sup>3</sup> Π
(2)2	57.88(1) <sup>3</sup> Π, 42.12(1) <sup>1</sup> Δ	(7)2	98.40(2) <sup>1</sup> Δ, 1.4(3) <sup>3</sup> Π, 0.09(1) <sup>3</sup> Φ, 0.11(2) <sup>3</sup> Δ
(2)1	99.34(1) <sup>3</sup> Π, 0.02(1) <sup>1</sup> Π, 0.42(1) <sup>3</sup> Σ <sup>+</sup> , 0.22(1) <sup>3</sup> Δ	(8)1	97.11(2) <sup>1</sup> Π, 2.44(3) <sup>3</sup> Π, 0.29(2) <sup>3</sup> Σ <sup>-</sup> , 0.16(2) <sup>3</sup> Π
(1)0 <sup>-</sup>	99.08(1) <sup>3</sup> Π, 0.90(1) <sup>3</sup> Σ <sup>+</sup> , 0.02(1) <sup>1</sup> Π	(8)2	98.55(3) <sup>3</sup> Π, 1.39(2) <sup>1</sup> Δ, 0.02(2) <sup>3</sup> Δ, 0.04(3) <sup>1</sup> Δ
(3)2	57.54(1) <sup>1</sup> Δ, 31.47(1) <sup>3</sup> Π, 0.50(1) <sup>3</sup> Δ	(9)1	97.27(3) <sup>3</sup> Π, 2.49(2) <sup>1</sup> Π, 0.19(3) <sup>1</sup> Π, 0.05(2) <sup>3</sup> Σ <sup>-</sup>
(2)0 <sup>+</sup>	99.72(1) <sup>3</sup> Π, 0.27 X <sup>1</sup> Σ <sup>+</sup>	(6)0 <sup>+</sup>	99.73(3) <sup>3</sup> Π, 0.17(2) <sup>3</sup> Σ <sup>-</sup> , 0.04(5) <sup>1</sup> Σ <sup>+</sup> , 0.03(2) <sup>1</sup> Σ <sup>+</sup> , 0.02(1) <sup>3</sup> Σ <sup>-</sup> , 0.01(4) <sup>1</sup> Σ <sup>+</sup>
(3)1	99.08(1) <sup>3</sup> Σ <sup>+</sup> , 0.92(1) <sup>3</sup> Π	(4)0 <sup>-</sup>	99.99(3) <sup>3</sup> Π, 0.01(2) <sup>3</sup> Σ <sup>+</sup>
(2)0 <sup>-</sup>	98.45(1) <sup>3</sup> Σ <sup>+</sup> , 1.15(1) <sup>1</sup> Π, 0.39(1) <sup>3</sup> Π	(7)0 <sup>+</sup>	97.05(2) <sup>3</sup> Σ <sup>-</sup> , 1.82(3) <sup>1</sup> Σ <sup>+</sup> , 0.88(4) <sup>1</sup> Σ <sup>+</sup> , 0.16(3) <sup>3</sup> Π, 0.08(5) <sup>1</sup> Σ <sup>+</sup> , 0.01(2) <sup>1</sup> Σ <sup>+</sup>
(4)1	98.74(1) <sup>1</sup> Π, 0.09(1) <sup>3</sup> Δ, 1.12(1) <sup>3</sup> Σ <sup>+</sup> , 0.05(1) <sup>3</sup> Π,	(10)1	95.11(2) <sup>3</sup> Σ <sup>-</sup> , 4.51(3) <sup>1</sup> Π, 0.23(2) <sup>1</sup> Π, 0.15(3) <sup>3</sup> Π
(3)0 <sup>+</sup>	99.81(2) <sup>1</sup> Σ <sup>+</sup> , 0.09(2) <sup>3</sup> Π, 0.04(3) <sup>3</sup> Π, 0.05(1) <sup>3</sup> Σ <sup>-</sup> , 0.01(2) <sup>3</sup> Σ <sup>-</sup>	(11)1	95.27(3) <sup>1</sup> Π, 4.56(2) <sup>3</sup> Σ <sup>-</sup> , 0.12(3) <sup>3</sup> Π, 0.04(2) <sup>3</sup> Δ, 0.01(2) <sup>1</sup> Π
(2)3	97.96(2) <sup>3</sup> Δ, 1.99(2) <sup>3</sup> Π, 0.03(3) <sup>1</sup> Π, 0.02(1) <sup>3</sup> Σ <sup>-</sup>	(8)0 <sup>+</sup>	98.12(3) <sup>1</sup> Σ <sup>+</sup> , 1.79(2) <sup>3</sup> Σ <sup>-</sup> , 0.04(1)3Σ <sup>-</sup> , 0.05(4) <sup>1</sup> Σ <sup>+</sup>
(4)2	97.47(2) <sup>3</sup> Δ, 0.82(1) <sup>3</sup> Φ, 1.6(2) <sup>3</sup> Π, 0.10(2) <sup>1</sup> Δ, 0.01(3) <sup>1</sup> Δ	(9)2	99.91(3) <sup>1</sup> Δ, 0.045(3) <sup>3</sup> Π, 0.045(1) <sup>3</sup> Φ
(5)1	98.84(2) <sup>3</sup> Δ, 1.15(1) <sup>3</sup> Φ, 0.01(1) <sup>1</sup> Φ	(4)3	99.975(1) <sup>1</sup> Φ, 0.025(1) <sup>3</sup> Φ
(1)4	98.92(1) <sup>3</sup> Φ, 0.74(2) <sup>3</sup> Δ, 0.11(2) <sup>1</sup> Δ, 0.19(2) <sup>3</sup> Π, 0.04(3) <sup>1</sup> Δ	(2)4	99.965(1) <sup>1</sup> Γ, 0.035(1) <sup>3</sup> Φ
(3)3	98.82(1) <sup>3</sup> Φ, 1.15(2) <sup>3</sup> Δ, 0.01(1) <sup>3</sup> Φ, 0.02(1) <sup>1</sup> Φ	(9)0 <sup>+</sup>	99.03(4) <sup>1</sup> Σ <sup>+</sup> , 0.05(3) <sup>3</sup> Π, 0.90(2) <sup>3</sup> Σ <sup>-</sup> , 0.02(1) <sup>3</sup> Σ <sup>-</sup>
(5)2	99.97(1) <sup>3</sup> Φ, 0.03(1) <sup>1</sup> Γ	(10)0 <sup>+</sup>	99.875(5) <sup>1</sup> Σ <sup>+</sup> , 0.05(1) <sup>3</sup> Φ, 0.075(2) <sup>3</sup> Σ <sup>-</sup>
(6)2	98.22(2) <sup>3</sup> Π, 0.11(1) <sup>3</sup> Φ, 1.67(2) <sup>3</sup> Δ	(5)0 <sup>-</sup>	99.99(2) <sup>3</sup> Σ <sup>+</sup>
(6)1	86.76(2) <sup>3</sup> Π, 11.16(1) <sup>3</sup> Σ <sup>-</sup> , 1.94(2) <sup>3</sup> Δ, 0.14(2) <sup>1</sup> Π	(12)1	100(2) <sup>3</sup> Σ <sup>+</sup>

ternuclear distance. These data are given in **Table 3**. The only available data in literature concerning the electronic states of the molecule ScBr in the representation  $\Omega^{(\pm)}$  are the transition energy with respect to the ground state  $T_e$  of Bencheikh (Bencheikh 1997) calculated by ligand field theory. The comparison of these values to those of the present work showed a good agreement with the relative difference  $0.8\% \leq \Delta T_e/T_e \leq 11.7$  for the states (2, 4) $\Omega = 1$  and (2, 3) $\Omega = 2$ . This relative difference becomes moderate with  $12.8\% \leq \Delta T_e/T_e \leq 17.5$  for the states (1, 2) $\Omega = 0^+$ , (1, 3) $\Omega = 1$ , and (1) $\Omega = 3$ . The agreement deteriorates for the states (1) $\Omega = 1$ , (1) $\Omega = 2$  where  $\Delta T_e/T_e$  are respectively 33.1% and 24.1%. The calculated values of the splitting of the present work and those of three states investigated by Bencheikh (Bencheikh 1997) are given in **Table 4**. The comparison between our values and the limited number of data of Bencheikh (Bencheikh 1997) shows an over all acceptable agreement. We are not aiming in the present work to show the advantage of one of the theoretical technique on the other, but the investigation of new valid excited electronic states with spin orbit effect in order to lead the investigation of new experimental works on this molecule.

The useful information about the degree of ionic and covalent character in the bonding can be investigated by using an *ab initio* calculation of the dipole moment operator

A best accuracy may be obtained by constructing a multireference configuration interaction (MRCI) wave functions using multi configuration Self-consistent field (MCSCF) active space. By taking the Sc atom as an origin in our calculation, the permanent dipole moments have been investigated for the considered electronic states of the molecule ScBr, the calculated values (in Debye) in terms of the internuclear distance R are plotted in **Figures 7 and 8** where these curves tend to zero when R tends to infinity

All these calculations have been performed by using the MOLPRO [6] program. One can notice the agreement between the position of the avoided crossing of the potential energy curves (**Figure 1** and **Table 1**) of the (7) $0^+$  and (8) $0^+$  and the crossings of dipole moment curves of these states in **Figure 8** which confirm the validity and the accuracy of our results.

### 3. Conclusions

In the present work, *ab initio* investigations for 42 low-lying electronic states of ScBr molecule (including spin-orbit effects) have been performed via CAS-SCF/MRCI method. Multireference CI calculations (single and double excitations + Davidson corrections) in which the entire CAS-SCF configuration space was used as

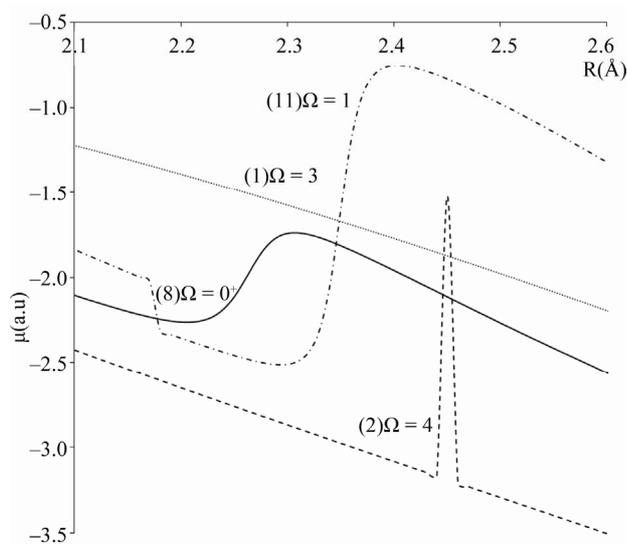
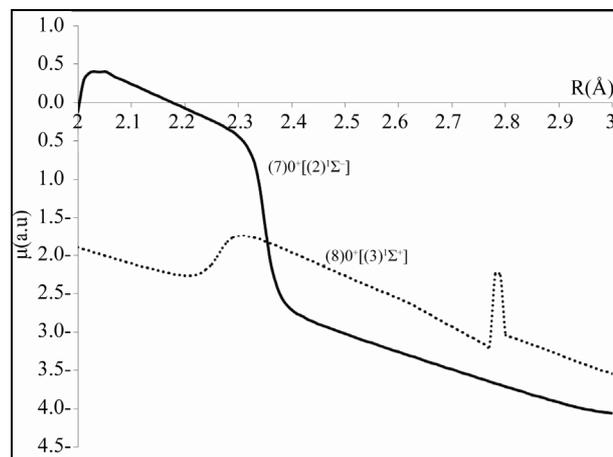
**Table 3. The values of transition energy  $T_e$ , the equilibrium internuclear distance  $R_e$ , the rotational constant  $B_e$  and the harmonic frequency  $\omega_e$  for  $\Omega$ -states of the molecule ScBr.**

Sym.	n $\Omega$	state	$T_e$ (cm <sup>-1</sup> )	$\delta T_e/T_e$ %	$\omega_e$ (cm <sup>-1</sup> )	$B_e \times 10^2$ (cm <sup>-1</sup> )	$R_e$ (Å)
$\Omega = 0^+$	1	$X^1\Sigma^+$	0 <sup>a</sup>		342.4	10.1845	2.3987
	2	(1) $^3\Pi$	2860 <sup>a</sup> 2518 <sup>b</sup>	13.58	297.1	9.2098	2.5225
	3	(2) $^1\Sigma^+$	12129 <sup>a</sup>		297.1	9.2098	2.5224
	4	(2) $^3\Pi$	14041 <sup>a</sup>		279.4	9.0191	2.5490
	5	(1) $^3\Sigma^-$	14453 <sup>a</sup>		280.2	8.9655	2.5566
	6	(3) $^3\Pi$	18748 <sup>a</sup>		300.8	9.3664	2.5013
	7	(2) $^3\Sigma^-$	19789 <sup>a</sup>		288.3	9.0699	2.5418
	8	(3) $^1\Sigma^+$	20704 <sup>a</sup>		279.5	9.3146	2.5082
	9	(4) $^1\Sigma^+$	21152 <sup>a</sup>		367.8	8.9610	2.5573
	10	(5) $^1\Sigma^+$	26031 <sup>a</sup>		306.3	9.2458	2.5176
$\Omega = 0^-$	1	(1) $^3\Pi$	2827 <sup>a</sup> 2507 <sup>b</sup>	12.76	295.6	9.1998	2.5239
	2	(1) $^3\Sigma^+$	4284 <sup>a</sup> 3567 <sup>b</sup>	16.7	287.8	9.2056	2.5231
	3	(2) $^3\Pi$	14050 <sup>a</sup>		283.4	9.0057	2.5509
	4	(3) $^3\Pi$	18809 <sup>a</sup>		300.9	9.3665	2.5013
	5	(2) $^3\Sigma^+$	35358 <sup>a</sup>		269	9.62	2.5687
$\Omega = 1$	1	(1) $^3\Delta$	414 <sup>a</sup> 626 <sup>b</sup>	33.9	305.2	9.3298	2.5062
	2	(1) $^3\Pi$	2787 <sup>a</sup> 2569 <sup>b</sup>	8.49	295.5	9.1971	2.5242
	3	(1) $^3\Sigma^+$	4307 <sup>a</sup> 3553 <sup>b</sup>	17.5	288.2	9.2124	2.5221
	4	(1) $^1\Pi$	4866 <sup>a</sup> 4826 <sup>b</sup>	0.8	296.4	9.1468	2.5311
	5	(2) $^3\Delta$	13213 <sup>a</sup>		286.3	9.1448	2.5314
	6	(2) $^3\Pi$	14055 <sup>a</sup>		278.9	8.9829	2.5541
	7	(1) $^3\Sigma^-$	14530 <sup>a</sup>		280.7	8.9779	2.5549
	8	(2) $^1\Pi$	18104 <sup>a</sup>		296.9	9.2389	2.5185
	9	(3) $^3\Pi$	18862 <sup>a</sup>		300.5	9.3664	2.5013
	10	(2) $^3\Sigma^-$	19820 <sup>a</sup>		287.9	9.0738	2.5413
	11	(3) $^1\Pi$	20987 <sup>a</sup>		297.6	9.3161	2.5080
	12	(2) $^3\Sigma^+$	35358.9 <sup>a</sup>		269.6	9.6138	2.4689
$\Omega = 2$	1	(1) $^3\Delta$	553 <sup>a</sup> 729 <sup>b</sup>	24.1	305.2	9.3304	2.5061
	2	(1) $^1\Delta$	2686 <sup>a</sup> 3260 <sup>b</sup>	11.7	302.7	9.2399	2.5184
	3	(1) $^3\Pi$	2686 <sup>a</sup> 2619 <sup>b</sup>	2.56	296.5	9.2075	2.5228
	4	(2) $^3\Delta$	13343 <sup>a</sup>		286.0	9.1417	2.5319
	5	(1) $^3\Phi$	13502 <sup>a</sup>		302.9	9.1417	2.5318
	6	(2) $^3\Pi$	14193 <sup>a</sup>		280.8	9.0113	2.5501
	7	(2) $^1\Delta$	17628 <sup>a</sup>		296.1	9.3533	2.5031
	8	(3) $^3\Pi$	18867 <sup>a</sup>		300.8	9.3684	2.5010
	9	(3) $^1\Delta$	21479 <sup>a</sup>		290.8	9.1328	2.5331
$\Omega = 3$	1	(1) $^3\Delta$	710 <sup>a</sup> 845 <sup>b</sup>	15.98	305.2	9.3323	2.5059
	2	(2) $^3\Delta$	13438 <sup>a</sup>		273.3	9.0039	2.5512
	3	(1) $^3\Phi$	13660 <sup>a</sup>		281.9	9.0281	2.5477
	4	(1) $^1\Phi$	20574 <sup>a</sup>		301.6	9.4411	2.4914
$\Omega = 4$	1	(1) $^3\Phi$	13859 <sup>a</sup>		281.3	9.0306	2.5474
	2	(1) $^1\Gamma$	20840 <sup>a</sup>		302.3	9.3204	2.5075

<sup>a</sup>Present work, <sup>b</sup>Ref. [4].

**Table 4. Calculation of the splitting of the  $\Omega$ -states of the molecule ScBr.**

Parent State $^{2S+1}\Lambda$	$\Omega$ state	$\Omega$ state	$\Delta E = E(\Omega) - E(\Omega')$ ( $\text{cm}^{-1}$ )		$\Delta E_{\text{tot}} = \sum \Delta E$ ( $\text{cm}^{-1}$ )	
			Present work	Ref.[4]	Present work	Ref.[4]
$(1)^3\Pi$	$0^+$	$0^-$	33	11		
	$0^-$	1	40	62	174	112
	1	2	101	50		
$(2)^3\Pi$	$0^+$	$0^-$	9			
	$0^-$	1	5		152	
	1	2	138			
$(1)^3\Sigma^-$	$0^+$	1	77		77	
	$0^+$	$0^-$	61			
$(3)^3\Pi$	$0^-$	1	53		119	
	1	2	5			
$(2)^3\Sigma^-$	$0^+$	1	31		31	
$(1)^3\Sigma^+$	$0^-$	1	23	14	23	14
$(2)^3\Sigma^+$	$0^-$	1	0.1		0.1	
	1	2	157	103		
$(1)^3\Delta$	2	3	139	106	296	219
	1	2	95			
$(2)^3\Delta$	2	3	130		225	
	2	3	199			
$(1)^3\Phi$	3	4	158		357	

**Figure 7. Calculated dipole moment curves of the  $\Omega$ -states of the molecule ScBr.****Figure 8. Calculated dipole moment curves for the  $(7)0^+$  and  $(8)0^+$  states showing the crossing at the position of the avoided crossing of the corresponding potential energy curves of the molecule ScBr.**

reference were performed in order to obtain the correlation effects. The potential energy curves and the permanent dipole moment along with the spectroscopic constants  $T_e$ ,  $R_e$ ,  $\omega_e$  and the rotational constant  $B_e$ , have been investigated for the lowest-lying electronic states of ScBr including the spin orbit effect. Thirty states have been investigated here for the first time. The comparison of the present results with the few available data in literature for the molecule ScBr has demonstrated a good accuracy. To the best of our knowledge no *ab initio* study of this molecule including spin orbit effect in literature.

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