

### The Spin-Orbit effects on the CB, SiB and GeB molecules

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#### INTRODUCTION

Boron is used as *p*-type dopant in carbon, silicon and/or germanium semiconductor devices. The description of CB, SiB and GeB diatomic molecules has previously been performed.<sup>1-4</sup> However, in this work, we present a systematic comparison of the lowest quartet electronic states of these borides using state-of-art CASSCF/MRCI methodology with extensive basis sets, and including spin-orbit effects

#### METHODS

In the present work, we have performed CASSCF/MRCI calculations for the low-lying quartet states of CB, SiB and GeB. The spin-orbit states ( $\Omega$ ) step were carried out within Breit-Pauli approximation using the aug-cc-pV5Z-DK basis set, relativistic effects were included. All the steps were carried out as implemented in MOLPRO code, while the molecular constants were evaluated using the INTENSITY software.

#### RESULTS AND DISCUSSION

In order to complement the electronic description of these species, this work presents the spin-orbit

states for the first time. As far as we know, there is no data to the CB and SiB<sup>1-3</sup> at this level of theory. Our main results for to the (X)<sup>4</sup> $\Sigma^-$ , (1)<sup>4</sup> $\Pi$  and  $\Omega$  states are collected in Table 1. The ground spin-orbit state splitting, in cm<sup>-1</sup>, is 0.004 and 0.009, 0.022 and 0.154, 0.658 and 6.145 for CB, SiB and GeB, respectively. The avoided crossing gives rise to disturbances in the curvature of the spin-orbit states, it is detected by the minimum shift of the equilibrium distances, vibrational frequencies and dissociation energy.

#### CONCLUSIONS

Here we report, a complete description of some low-lying electronic quartet states related to the first dissociation channel of CB, SiB and GeB molecules. We also provided the molecular constants for these electronic and spin-orbit states. The main behavior shows the increasing of atomic number decrease the dissociation energy for ground state, while the excitation energy for the first excited quartet increases.

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Table 1. Molecular constants of the BC, SiB and GeB electronic and  $\Omega$  states.  $R_e$  in Å,  $T_e$  and  $\omega_e$  in cm<sup>-1</sup> and  $D_e$  in eV.

State	$R_e$	$T_e$	$\omega_e$	$D_e$	$R_e$	$T_e$	$\omega_e$	$D_e$	$R_e$	$T_e$	$\omega_e$	$D_e$
	CB				SiB				GeB			
(X <sub>1</sub> ) <sup>4</sup> $\Sigma^-_{1/2}$	1.498	0	1173	4.40	1.920	0	745	3.27	1.999	0	632	2.87
(X <sub>2</sub> ) <sup>4</sup> $\Sigma^-_{3/2}$	1.498	0.004	1173	4.40	1.918	0.022	745	3.27	1.999	0.658	632	2.87
(X) <sup>4</sup> $\Sigma^-$	<b>1.498</b>	<b>0.009</b>	<b>1164</b>	<b>4.41</b>	<b>1.918</b>	<b>0.154</b>	<b>746</b>	<b>3.28</b>	<b>1.999</b>	<b>6.145</b>	<b>632</b>	<b>2.97</b>
(1) <sup>4</sup> $\Pi$	<b>1.366</b>	<b>9050</b>	<b>1557</b>	<b>3.28</b>	<b>1.809</b>	<b>18672</b>	<b>860</b>	<b>0.97</b>	<b>1.900</b>	<b>20495</b>	<b>390</b>	<b>0.43</b>
(1) <sup>4</sup> $\Pi_{-1/2}$	1.366	9065	1549	3.28	1.809	18552	867	0.97	1.892	20342	438	0.40
(1) <sup>4</sup> $\Pi_{1/2}$	1.366	9072	1495	3.28	1.809	18574	865	0.97	1.905	20447	402	0.39
(1) <sup>4</sup> $\Pi_{3/2}$	1.367	9081	1506	3.28	1.809	18595	865	0.97	1.902	20527	361	0.38
(1) <sup>4</sup> $\Pi_{5/2}$	1.367	9089	1506	3.27	1.810	18616	875	0.96	1.918	20619	385	0.37

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