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space Multiconfiguration Hartree-fock Method

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access to the work immediately and investigate your claim.
Lifetimes and transition probabilities of the boron atom calculated with the active-space multiconfiguration Hartree-Fock method

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Systematic multiconfiguration Hartree-Fock results are presented for the transition probabilities and excited-state lifetimes in the term system of the boron atom. Particularly, the interaction between the 1s22s2p2 configuration and the 1s22s2ns2S and 1s22s2nd2D Rydberg series is considered. Term energies and transition-matrix elements are calculated to convergence using increasing active sets of s, p, d, f, and g orbitals.

PACS number(s): 31.20.Tz, 32.70.Cs, 32.70.Fw

I. INTRODUCTION

It is desirable to perform ab initio atomic-structure calculations in a systematic way. For variational calculations this can be done with the active-space method [1,2] so that the convergence of individual properties of the atom can be studied as the active space is being built up.

Systematic calculations using the multiconfiguration Hartree-Fock (MCHF) method have in many cases been performed for the study of hyperfine structures [3–9], but only few systematic active-space calculations exist for lifetimes [8,10]. Also, these calculations have only been performed for ground states or other states lowest of their symmetry. Here, the applicability of active-space MCHF for the study of lifetimes of states in Rydberg series is demonstrated.

The boron atom, with the ground state 1s22s22p2P3/2, has an energy level structure similar to that of a one-electron system, formed by the excitation of the 2p electron. In addition to this, bound states are also formed by exciting one of the 2s electrons to a 2p orbital. The lowest term thus formed is 1s22s2p4P, which is of little importance to the doublet states studied here. Also, three doublet terms are formed: 2D which lies below 1s22s23d2D, 2P which lies above the ionization limit, and 2S which lies between 1s22s26s2S and 1s22s27s2S. Since 1s22s2p2P and 1s22s2np2P have opposite parity these do not interact. 1s22s2p2S and 1s22s2p2D, however, interact with the Rydberg series of the same symmetry. Particularly 1s22s2p2S, which lies in the middle of the 2S series, can be expected to have a strong influence, something which is evident already from the irregular energies of the 1s22s2ns2S states close to 1s22s2p2S.

Several of the previous theoretical studies of transition probabilities in the boron atom do not include the interaction between the 2s2nl and 2s2p2 configurations and must therefore be disregarded. Most of the remaining calculations were performed using different multiconfiguration self-consistent-field (MCSCF) or configuration-interaction (CI) procedures with expansions in the order of 10 or 20 configuration-state functions (CSF’s) [11–17]. Only the CI calculation of [18] is considerably larger. The hyperfine structure of the ground state has recently been determined by systematic MCHF calculations [4,9] similar to those performed for the present lifetime study.

The lifetimes of some of the lower excited states of boron atom have been studied using different experimental techniques: beam-foil spectroscopy [19–24], the phase-shift method with electron-beam excitation [25,26], level-crossing spectroscopy [27], and laser-induced fluorescence [17,28,29].

II. METHOD OF CALCULATION

The wave functions were generated with the MCHF atomic-structure package of Froese Fischer [30].

A complete active space is not used, for two reasons. First, with five electrons, the wave function expansion would grow unmanageable large. Secondly, the existing programs for calculating transition moments [31,32] can only handle a limited degree of the nonorthogonality that arises from optimizing the orbitals of the different states separately. It has been suggested how this limitation could be overcome, using a biorthogonal transformation [33] and a new transition program is now being developed [34]. The restriction that is made in this study is that the 1s shell is kept closed and the 1s orbital, obtained from a Hartree-Fock calculation for the 1s22s21S state of BII, is not varied during the optimization.

Calculations have been performed for the 1s22s2ns2S, n = 3 to 6, 1s22s2np2P, n = 2 to 6, 1s22s2nd2D, n = 3 to 5, 1s22s2p2F, 1s22s2p2D. For each term calculation were performed with an increasing active set of orbitals, the smallest calculation in each case a Hartree-Fock calculation, the largest one in each case with the active set 7s6p5d4f3g which means seven s orbitals, six p orbitals, etc. Starting with the Hartree-Fock calculation, orbitals were added to the active set.
one of each symmetry at a time, in the same way as orbitals appear in the shells in an atom. In each calculation all CSF's possible to form using the orbitals in the active set outside the 1s² core and which have the correct parity and LS term were included. The lists of configurations were generated using the generation program of the MCHF package [35]. These CSF's are called the active space. In each calculation all orbitals except 1s were optimized. The active set was increased until a satisfactory convergence of the energy and transition-matrix elements was obtained. The largest active space, for the 4f²F states, consisted of 4538 CSF's.

This type of calculation has previously been performed for states lowest of their symmetry. In such cases, the wave function is optimized for the lowest eigenvalue. For higher-lying states the eigenfunction must be orthogonal to all eigenfunctions belonging to lower states. In this study CSF's representing lower states were included in the expansions and by diagonalizing the interaction matrix the eigenvalue on which to optimize could be determined. For example, in the expansion of the 2s³3d²D state, the second of its symmetry, the CSF representing the lowest state 2s2p²2D was also included. After the diagonalization of the interaction matrix the orbitals were optimized on the second eigenvalue.

For the next state above those included in the study, 2s2p²2S, the attempted calculations were unstable when all orbitals were varied in the self-consistent-field procedure.

### III. RESULTS AND DISCUSSION

Table I shows the convergence of the calculated term energies for increasing active sets. From the calculated

#### TABLE II. Convergence of the reduced electric dipole transition-matrix elements in the length (l) and velocity (v) forms for transitions to the ground state, for increasing active sets of orbitals, in atomic units.

<table>
<thead>
<tr>
<th>Upper term</th>
<th>HF</th>
<th>3s2p1d</th>
<th>4s3p2d1f</th>
<th>5s4p3d2f1g</th>
<th>6s5p4d3f2g</th>
<th>7s6p5d4f3g</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s²2s³3s²⁵S</td>
<td>l</td>
<td>1.1292</td>
<td>1.3438</td>
<td>1.3785</td>
<td>1.3953</td>
<td>1.4002</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>1.2862</td>
<td>1.5169</td>
<td>1.4547</td>
<td>1.4317</td>
<td>1.4288</td>
</tr>
<tr>
<td>1s²2s³4s²⁵S</td>
<td>l</td>
<td>0.3941</td>
<td>0.4958</td>
<td>0.5109</td>
<td>0.5221</td>
<td>0.5371</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>0.4361</td>
<td>0.5358</td>
<td>0.5315</td>
<td>0.5310</td>
<td>0.5476</td>
</tr>
<tr>
<td>1s²2s³5s²⁵S</td>
<td>l</td>
<td>0.2266</td>
<td>0.3102</td>
<td>0.3414</td>
<td>0.3879</td>
<td>0.3980</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>0.2488</td>
<td>0.3294</td>
<td>0.3521</td>
<td>0.3956</td>
<td>0.4058</td>
</tr>
<tr>
<td>1s²2s³6s²⁵S</td>
<td>l</td>
<td>0.1541</td>
<td>0.2314</td>
<td>0.3354</td>
<td>0.3914</td>
<td>0.4074</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>0.1687</td>
<td>0.2427</td>
<td>0.3438</td>
<td>0.3986</td>
<td>0.4154</td>
</tr>
<tr>
<td>1s²2s²2p³2⁵D</td>
<td>l</td>
<td>-2.6468</td>
<td>-1.4650</td>
<td>-0.9027</td>
<td>-0.9146</td>
<td>-0.9139</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>-2.6529</td>
<td>-1.6128</td>
<td>-0.9465</td>
<td>-0.9709</td>
<td>-0.9697</td>
</tr>
<tr>
<td>1s²2s³3d²⁵D</td>
<td>l</td>
<td>-1.3993</td>
<td>-1.6550*</td>
<td>-1.7523</td>
<td>-1.7641</td>
<td>-1.7683</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>-1.3681</td>
<td>-1.6778*</td>
<td>-1.7648</td>
<td>-1.7750</td>
<td>-1.7816</td>
</tr>
<tr>
<td>1s²2s³4d²⁵D</td>
<td>l</td>
<td>-0.8827</td>
<td>-1.0669*</td>
<td>-1.1022</td>
<td>-1.0903</td>
<td>-1.0889</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>-0.8529</td>
<td>-1.0577*</td>
<td>-1.1040</td>
<td>-1.0907</td>
<td>-1.0930</td>
</tr>
<tr>
<td>1s²2s³5d²⁵D</td>
<td>l</td>
<td>-0.6171</td>
<td>-0.7460*</td>
<td>-0.7477</td>
<td>-0.7553</td>
<td>-0.7515</td>
</tr>
<tr>
<td>v/ΔE</td>
<td></td>
<td>-0.5934</td>
<td>-0.7330*</td>
<td>-0.7409</td>
<td>-0.7526</td>
<td>-0.7530</td>
</tr>
</tbody>
</table>

* Active set 3s2p2d for the 2D state.
wave functions transition-matrix elements were calculated. Table II shows, as an example, the convergence of the reduced transition-matrix elements for transitions to the ground state. Calculated values are given using both the length and velocity forms of the electric dipole operator. The velocity form values have been divided by the transition energy. In atomic units they should then, for the correct wave functions, equal the length form values. For the largest active sets the velocity values are on average 2% larger than the length values, with a larger difference for the transition from the $2s2p^22D$ states and a smaller difference for the transitions from the $2s^3nd^2D$ states. For the $2S$ series the difference approaches a constant for the higher members, whereas for the $2D$ series, the difference appears to be approaching zero. That it is the transition involving the $2s2p^22D$ states for which the velocity value differs the most from the length value is probably due to the single 2e electron of this configuration. This electron can be expected to cause a much stronger polarization of the 1s shell than any other single electron with higher $n$ or $l$ quantum numbers. This may also be the reason why the calculated energy of this term is too high compared with that of any other term, as can be seen in Table III, where the final values for the ionization energies can be compared with the experimental values. Table IV gives the final values for all electric dipole transition probabilities between the investigated states, calculated using either the length or velocity form of the electric dipole operator and using the calculated transition energies. The values of the length and velocity forms typically agree to within a few percent. The exception to this is the transitions with very small transition probabilities, for which the difference tends to be larger, and also most of the transitions involving the $2s2p^22D$ states. The velocity form, which depends more than the length form on the wave function close to the nucleus, may have been more affected by the closed 1s shell. The length form is therefore the more trusted one.

To some extent the difference between the length and velocity values is due to their different dependence on the transition energy. With the velocity form the transition probability is proportional to the transition energy, with the length form it is proportional to the transition energy to the third. This may affect the results particularly for transitions between very near-lying states for which cases the relative error of the calculated transition energy may be large. These transition probabilities are small and have no appreciable effect on the calculated lifetimes. The oscillator strengths for transitions from the $2s2p^2P$ ground state to the excited $2S$ and $2D$ states are given in Tables V and VI. These tables also include values obtained in previous calculations and experiments. On the whole, the agreement between the length and velocity forms is considerably improved in the present calculation.

Table VII gives the lifetime values, calculated from

### Table III

<table>
<thead>
<tr>
<th>Term</th>
<th>Calculated</th>
<th>Experimental*</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s^22s^3s^2S$</td>
<td>26856</td>
<td>26888.45</td>
<td>33</td>
</tr>
<tr>
<td>$1s^22s^4s^2S$</td>
<td>11900</td>
<td>11917.92</td>
<td>18</td>
</tr>
<tr>
<td>$1s^22s5s^2S$</td>
<td>6760</td>
<td>6781.65</td>
<td>22</td>
</tr>
<tr>
<td>$1s2s6s^2S$</td>
<td>4391</td>
<td>4445.87</td>
<td>55</td>
</tr>
<tr>
<td>$1s^22s2p^2P$</td>
<td>66542</td>
<td>66917.93</td>
<td>376</td>
</tr>
<tr>
<td>$1s^22s3p^2P$</td>
<td>18264</td>
<td>18315.09</td>
<td>51</td>
</tr>
<tr>
<td>$1s2s4p^2P$</td>
<td>9119</td>
<td>9141.30</td>
<td>22</td>
</tr>
<tr>
<td>$1s^22s5p^2P$</td>
<td>5480</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1s^2s6p^2P$</td>
<td>3657</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1s^22s2p^2D$</td>
<td>18593</td>
<td>19070.98</td>
<td>478</td>
</tr>
<tr>
<td>$1s^22s3d^2D$</td>
<td>12093</td>
<td>12160.36</td>
<td>67</td>
</tr>
<tr>
<td>$1s2s4d^2D$</td>
<td>6914</td>
<td>6934.67</td>
<td>20</td>
</tr>
<tr>
<td>$1s^22s5d^2D$</td>
<td>4430</td>
<td>4442.63</td>
<td>13</td>
</tr>
<tr>
<td>$1s^2s4f^2F$</td>
<td>6894</td>
<td>6897.07</td>
<td>3</td>
</tr>
</tbody>
</table>

* Reference [37].
LIFETIMES AND TRANSITION PROBABILITIES OF THE . . . 3429

TABLE V. Weighted multiplet oscillator strengths, $gf$, for transitions between the ground state and excited $^{2}S$ states of boron.

<table>
<thead>
<tr>
<th>Upper term</th>
<th>$1s^22s^23s,^2S$</th>
<th>$1s^22s^24s,^2S$</th>
<th>$1s^22s^25s,^2S$</th>
<th>$1s^22s^26s,^2S$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Calculations</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>This work, length</td>
<td>0.474</td>
<td>0.0963</td>
<td>0.0583</td>
<td>0.0645</td>
</tr>
<tr>
<td>This work, velocity</td>
<td>0.492</td>
<td>0.100</td>
<td>0.0660</td>
<td>0.0670</td>
</tr>
<tr>
<td>Ref. [11], length</td>
<td>0.402</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [11], velocity</td>
<td>0.444</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [12], length</td>
<td>0.372</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [12], velocity</td>
<td>0.408</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [13], length</td>
<td>0.216</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [18], length</td>
<td>0.417</td>
<td>0.188</td>
<td>0.0230</td>
<td>0.0533</td>
</tr>
<tr>
<td>Ref. [16], length</td>
<td>0.444</td>
<td>0.102</td>
<td>0.072</td>
<td>0.102</td>
</tr>
<tr>
<td>Ref. [16], velocity</td>
<td>0.540</td>
<td>0.108</td>
<td>0.078</td>
<td>0.114</td>
</tr>
<tr>
<td><strong>Experiments</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [19], beam foil</td>
<td>0.48 (0.03)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [21], beam foil</td>
<td>0.33 (0.01)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [26], phase shift</td>
<td>0.72 (0.15)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [23], beam foil</td>
<td>0.54 (0.06)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [24], beam foil</td>
<td>0.52 (0.03)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [28], laser-induced fluorescence</td>
<td>0.47 (0.03)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

detailed. It shows the cancellation in the matrix element for the transition to $2s2p\,^2\!2D$, explaining the large variation in the theoretical $gf$ values for this transition reported in Table VI.

In Table VII the lifetimes calculated in this study can be compared with those obtained in experiments. Without even being impartial one can say that a large part of the experimentally obtained values are either wrong or have too small error bars, not because they disagree with theory but because they disagree with each other.

Many of the experiments have been performed using

TABLE VI. Weighted multiplet oscillator strengths, $gf$, for transitions between the ground state and excited $^{2}D$ states of boron.

<table>
<thead>
<tr>
<th>Upper term</th>
<th>$1s^22s^22p,^2!2D$</th>
<th>$1s^22s^23d,^2!2D$</th>
<th>$1s^22s^24d,^2!2D$</th>
<th>$1s^22s^25d,^2!2D$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Calculations</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>This work, length</td>
<td>0.243</td>
<td>1.035</td>
<td>0.428</td>
<td>0.213</td>
</tr>
<tr>
<td>This work, velocity</td>
<td>0.274</td>
<td>1.051</td>
<td>0.432</td>
<td>0.214</td>
</tr>
<tr>
<td>Ref. [11], length</td>
<td>0.402</td>
<td>1.182</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [11], velocity</td>
<td>0.504</td>
<td>1.134</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [12], length</td>
<td>0.690</td>
<td></td>
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<tr>
<td>Ref. [12], velocity</td>
<td>0.942</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [14], length</td>
<td>0.216</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [16], length</td>
<td>0.174</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [15], velocity</td>
<td>0.210</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [18], length</td>
<td>0.292</td>
<td>0.998</td>
<td>0.367</td>
<td>0.187</td>
</tr>
<tr>
<td><strong>Experiments</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [25], phase shift</td>
<td>0.28 (0.09)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [19], beam foil</td>
<td>0.24 (0.01)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [20], beam foil</td>
<td>0.30 (0.05)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [21], beam foil</td>
<td>0.36 (0.02)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [23], beam foil</td>
<td>0.30 (0.02)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [24], beam foil</td>
<td>0.27 (0.02)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [27], level crossing</td>
<td>0.28 (0.03)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ref. [28], laser-induced fluorescence</td>
<td>0.28 (0.02)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
the beam-foil technique and these were all done before
the necessity of a careful cascade analysis was fully
understood. The same problem, repopulation from higher
states due to the nonselective excitation, appears using
electron-beam excitation.

Table of the experiments have been performed using
pulsed laser excitation, two of them for $2P$ states. Un-
fortunately these two studies give lifetime values for the
$4p^2P$ states which differ by a factor of 1.65. In one of
these experiments [17] two states were studied and for
both the result agrees very well with that of the present
publication. In the second experiment [29] only one life-
time was measured. This experiment was performed at

\begin{table}
\centering
\caption{Calculated and experimental lifetimes, in ns. The calculated lifetimes were ob-
tained using the length form of the electric dipole operator and the calculated energies.}
\begin{tabular}{lcc}
\hline
Term & Calculated & Experimental \\
\hline
$1s^22s^23s^2S$ & 4.02 & $3.8(0.2)^a$, 5.7(0.3)$b$, 3.4(0.4)$c$ \\
$1s^22s^24s^2S$ & 8.90 & $3.57(0.20)^d$, 2.5(0.5)$e$, 4.0(0.2)$f$ \\
$1s^22s^25s^2S$ & 12.7 & \\
$1s^22s^26s^2S$ & 11.4 & \\
$1s^22s^22p^23P$ & 57.7 & $3.6(0.3)^g$ \\
$1s^22s^23p^2P$ & 219 & $32(5)^h$ \\
$1s^22s^24p^2P$ & 450 & \\
$1s^22s^25p^2P$ & 757 & \\
$1s^22s^26p^2P$ & 26.8 & 26.4(1.0)$a$, 18.4(0.8)$b$, 21.8(0.5)$c$ \\
$1s^22s^23d^2D$ & 46.0 & 24.4(1.5)$d$, 23.1(1.2)$e$, 21.8(1.1)$f$, \\
$1s^22s^24d^2D$ & 9.61 & 23.0(2.0)$g$, 23.1(2.5)$h$ \\
$1s^22s^25d^2D$ & 17.9 & \\
$1s^22s^24f^2P$ & 66.9 & \\
\hline
\end{tabular}

\begin{tablenotes}
\item[a] Reference [19], beam foil.
\item[b] Reference [21], beam foil.
\item[c] Reference [23], beam foil.
\item[d] Reference [24], beam foil.
\item[e] Reference [26], phase shift with electron-beam excitation.
\item[f] Reference [28], laser-induced fluorescence.
\item[g] Reference [22], beam foil.
\item[h] Reference [17], laser-induced fluorescence.
\item[i] Reference [29], laser-induced fluorescence.
\item[j] Reference [20], beam foil.
\item[k] Reference [25], phase shift with electron-beam excitation.
\item[l] Reference [27], level crossing.
\end{tablenotes}
\end{table}

The most extensive experimental study of the boron

\begin{table}
\centering
\caption{2s2p$^2$ admixture to the $2S$ and $2D$ states.}
\begin{tabular}{lcc}
\hline
Term & Eigenvector coefficient \\
\hline
$1s^22s^23s^2S$ & -0.108 \\
$1s^22s^24s^2S$ & -0.109 \\
$1s^22s^25s^2S$ & -0.136 \\
$1s^22s^26s^2S$ & -0.203 \\
$1s^22s^22p^2D$ & 0.891 \\
$1s^22s^23d^2D$ & 0.255 \\
$1s^22s^24d^2D$ & 0.107 \\
$1s^22s^25d^2D$ & 0.066 \\
\hline
\end{tabular}
\end{table}

high pressure in a cell and the lifetime value was extrapo-
lated after having performed the experiment at different
pressures. This was a more complicated procedure than
the one used in [17] and, it seems, one which did not work.

The most extensive experimental study of the boron
lifetimes is one of the five lowest even parity doublet terms using pulsed laser excitation [28]. For four of these five terms our calculated lifetimes are well within the 5% error bars of the experiment, the only term for which it is not is $2s2p^2 D$. As discussed above, the discrepancy for this particular term could be explained by the neglected polarization of the 1s shell.

Finally, one of the measurements of the $1s^22s2p^2 D$ states [27] was performed using level-crossing spectroscopy.

What has not been included in this study is the polarization of the 1s shell and the core-core correlation. This is expected to affect the transition energies more than the transition-matrix elements, as has been seen in a similar system in CIII [36]. Since the calculated transition energies are correct typically to within 1% the neglected effects of the 1s shell should, for most of the states, be small, at least for the length form operator.

**IV. CONCLUSION**

The active-space multiconfiguration Hartree-Fock method has been extended to the study of Rydberg series. This has been done for boron, an atom in which two of the Rydberg series exhibit a strong configuration interaction due to the near degeneracy with states formed by excitation from an inner subshell.

The accuracy of the calculated transition probabilities is difficult to estimate. The convergence procedure, the accuracy of the transition energies, and the agreement between the length and velocity forms of the electric dipole operator indicate that the length form values may be accurate to within a few percent. Comparison with the most reliable experimental lifetime values [17,27,28] seems to indicate that the calculated values are at least accurate to within 5% or 10%, that is, as accurate as the experiments.

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[34] M. Godefroid and J. Olsen (private communication).