$1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ transition in B II

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An experimental and theoretical study has been made of the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ transition in B II. The experimental wavelength and lifetime (1323.92±0.07 Å and 0.65±0.01 ns), determined by beam-foil spectroscopy, are more than five times more accurate than previous experimental results. Our theoretical data, from multiconfiguration Hartree-Fock calculations, 1311.6 Å and 0.601 ns, are in excellent agreement with previous theoretical predictions of Beck and Nicolaides [Phys. Lett. **61A**, 227 (1977)]. We have also observed the $1s2p^3\,{}^5S$—$1s2p^23s\,{}^5P$ transition, at 857.7±0.2 Å, in accord with the theoretical value 859.1 Å.

The most thoroughly investigated terms in Be I and Be-like ions are singlet and triplet terms of the $1s^22snl$ and $1s^22pnl$ configurations. By exciting one of the $1s$ electrons, quintet terms can also be formed. In a beam-foil electron-spectroscopy experiment, Bruch *et al.*[1] observed the decay of the lowest quintet term, $1s2s2p^2\,{}^5P$, in Be I by spin-orbit-induced autoionization and they also discussed the possibility of studying photon emission from higher quintet levels to $1s2s2p^2\,{}^5P$. (Because of well-known angular-momentum and parity-selection rules such quintet states can be stable against Coulomb autoionization.) Somewhat later, Bruch, Schneider, and collaborators[2–4] extended their electron-spectroscopic studies to Be-like B and C.

In a theoretical investigation, using the first-order theory of oscillator strengths (FOTOS), Beck and Nicolaides[5] calculated energies and transition rates for a number of high-lying states of high multiplicities in light atoms and ions. They found that the wavelength of the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ combination in B II should lie close to 1310 Å, while the predicted oscillator strengths were $f=0.143$ (length) and $f=0.149$ (velocity). The authors also noted that these values were consistent with beam-foil data (1324.5±0.5 Å, lifetime 0.75±0.08 ns) reported in 1970 by Martinson *et al.*[6] and 0.65±0.04 ns subsequently obtained by Kernahan *et al.*[7] When these two experiments were carried out, the 1324.5-Å line was tentatively identified as the $2p^2\,{}^1D$—$2p3s\,{}^1P$ transition in B II. However, the results of Beck and Nicolaides[5] supported a reclassification in favor of the B II inner-shell excited quintet system. Recently, the B II $2p^2\,{}^1D$—$2p3s\,{}^1P$ transition has been established[8] from a line at 1186.1 Å, an identification supported by observed transitions from $2p3s\,{}^1P$ to the singlet terms $2p^2\,{}^1S$ and $2s3s\,{}^1S$.

Experimental photon spectroscopy of the quintet states was greatly stimulated in 1980 when Bunge[9] theoretically explained the origin of a spectral line at 3489 Å, known to be persistent in the beam-foil spectra of lithium,[10,11] as the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ combination in the negative Li ion, Li^-. This prediction was soon verified by experimental beam-foil work, using electrostatic fields, first carried out by Mannervik *et al.*[12] and Brooks *et al.*[13] The latter authors also suggested the wavelength of the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ multiplet in Be I—F VI. While they apparently overlooked the B II results of Beck and Nicolaides,[5] they reached the same conclusion concerning the line at 1324.5 Å, mentioned above. In recent years there have appeared reliable experimental data[14] for the quintets in Be I and C III—Ne VII, whereas no reexamination of B II has been reported. Such an investigation, aiming at improved experimental and theoretical energies and transition probabilities, is now also motivated because the identification of the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ transition is certain. We have therefore undertaken a new study of the B II transition.

The experimental work was carried out at the Research Institute of Physics, Stockholm. Boron ions ($^{11}B^+$), obtained from the ion source of the 400-kV heavy-ion accelerator, were accelerated to 200—250 keV and sent through a thin carbon foil. The light emitted by the foil-excited species was analyzed with a Minuteman 310 NIV 1-m normal-incidence monochromator, equipped with a EMR 541-F photomultiplier or a Channeltron detector. Spectra were taken over a wide wavelength range and the 1324-Å quintet line was measured in first, second, and third order. By using a large number of B II and B III transitions with accurately known wavelengths as references, we were able to determine the center-of-gravity wavelength of the $1s2s2p^2\,{}^5P_{1,2,3}$—$1s2p^3\,{}^5S_2$ multiplet to 1323.92±0.07 Å, an improvement by about an order of magnitude of the previous value. It can be noted that the ^5P fine structure, which has been measured for C III and higher ions,[14] is too small to be resolved in the present study of B II. For theoretical values of this fine structure, we refer to the accurate relativistic calculations of Hata and Grant.[15]

The lifetime of the $^5S_2$ level was measured in the usual way by recording the intensity of the 1324-Å line as the function of the distance from the foil. The velocity of the foil-excited ions was accurately determined using a 90°, 50-cm-radius electrostatic analyzer. A number of decay curves were recorded and analyzed using the multiexponential curve-fitting program DISCRETE.[16] We found that the decay curves were best approximated by a single exponential, indicating that cascading into the $1s2p^3\,^5S_2$ term from higher quintets was not severe. The final analysis yielded a lifetime of 0.65 ± 0.01 ns.

The theoretical work was carried out at the Argonne National Laboratory. The multiconfiguration Hartree-Fock (MCHF) procedure[17] was used with the inclusion of some nonorthogonality between orbitals of the same quantum number l. Eight configurations were included in the expansion for ^5P and five for ^5S. The $1s$ orbital was taken from a Hartree-Fock calculation and kept fixed during the MCHF procedure. Thus, mainly correlations between the three outer electrons are included. A test calculation was performed, with relativistic shifts—in the form of mass-correction, Darwin, and spin-spin—contact terms—included as perturbations after the optimization of the orbitals. These effects, which are J independent, were found to only have a minor effect on the transition probabilities.

Our experimental and theoretical results are included in Table I, together with previous data. Both nonrelativistic and relativistic energies are given for the two terms. Using the relativistic value, we find that the $1s2s2p^2\,^5P$ term lies 168.854 eV above the $1s^22s\,^2S$ ground state of B III, in good agreement with the value 169.0 ± 0.3 eV, obtained by electron spectroscopy.[2–4] The theoretical ^5P-^5S transition wavelength of 1311.6 Å is close to the experimental value, and also to the result of Beck and Nicolaides.[5] In contrast, the wavelength obtained from the relativistic Dirac-Fock calculation[13] differs notably from these results.

Our experimental value for the $^5S_2$ lifetime confirms the result of Kernahan *et al.*,[7] but the uncertainty has been reduced significantly. The earlier experimental value[6] is somewhat longer, possibly because of a systematic uncertainty.

A necessary, but not sufficient, condition for obtaining a good representation of the wave functions is the agreement between the length and velocity form of the oscillator strength. In the present case we obtain $f_l=0.143$ and $f_v=0.142$, i.e., agreement within less than 1%. These results agree quite well with the data of Beck and Nicolaides.[5] Our theoretical lifetime of the $1s2p^3\,^5S$ term, as obtained by only taking the radiative decay channel $1s2s2p^2\,^5P-1s2p^3\,^5S$ into account, is 0.601 ns, a value consistent with the experimental decay time and the previous theoretical result.[5]

Beck and Nicolaides[5] further discuss the possibility of spin-orbit-induced mixing between the $1s2p^3\,^5S_2$ and $1s2p^3\,^3P_2$ levels. Since the latter level autoionizes to the $1s^22p\varepsilon d(\varepsilon s)$ continua, such a mixing would result in a shortening of the $^5S_2$ lifetime. This effect has been quantitatively studied by Chen,[18] who presents theoretical $^5S_2$ autoionization rates for $Z=6$–26. These data can be fitted to a formula

$$A=210Z^{7.5}\,, \qquad (1)$$

where A is the autoionization rate (in s^{-1}) and Z the nuclear charge. An extrapolation to B II yields $A=3.7\times10^7$ s^{-1}, which is only 2% of the radiative deexcitation rate of the $^5S_2$ level.

This result is consistent with the fact that our experimental lifetime for $^5S_2$ is close to the theoretical values which only consider radiative decay. There is thus no indication of significant contributions to the $^5S_2$ decay rate from relativistic autoionization. Chen[18] also discusses the decay of the $^5S_2$ term by K x-ray transitions, but concludes that this process is negligible for $Z\le8$. It is interesting to note, however, that Huddle and Mowat[19] have observed x-ray decay of the metastable $1s2s2p^2\,^5P$ term in C III.

We have also calculated the locations of levels that may decay to $1s2p^3\,^5S$, i.e., ^5P terms of even parity. The energetically lowest of these cascading levels was found to be $1s2s2p3p\,^5P$, followed by $1s2p^23s\,^5P$ and $1s2p^23d\,^5P$. This ordering is consistent with theoretical results for the quintets in C III, reported by Schneider *et al.*[20] From our theoretical energies we obtain the transition wavelengths 1413 Å ($1s2p^3\,^5S-1s2s2p3p\,^5P$), 859.1 Å ($1s2p^3\,^5S-1s2p^23s\,^5P$), and 707.0 Å ($1s2p^3\,^5S-1s2p^23d\,^5P$). In the beam-foil spectrum we find an unidentified line at 857.7 ± 0.2 Å, whereas the two other transitions are ab-

TABLE I. Experimental and theoretical data for the $1s2s2p^2\,^5P-1s2p^3\,^5S$ transition in B II.

Energy (a.u.)[a]		Wavelength (Å)		Lifetime (ns)	
^5P	^5S	Expt.	Theor.	Expt.	Theor.
−17.213 540[a,b]	−16.866 147[a,b]	1324.5±0.5[d]	1310[e]	0.75±0.08[d]	0.616[e]
−17.218 608[a,c]	−16.870 761[a,c]	1323.92±0.07[a]	1279[f]	0.65±0.04[g]	0.601[a]
			1311.6[a]	0.65±0.01[a]	

[a]This work.
[b]Nonrelativistic calculation.
[c]Relativistic calculation.
[d]Martinson *et al.* (Ref. 6).
[e]Beck and Nicolaides (Ref. 5).
[f]Brooks *et al.* (Ref. 13).
[g]Kernahan *et al.* (Ref. 7).

sent. However, the 1413-Å line arises from a two-electron jump (in the single-configuration approximation) and our calculations here predict a radiative decay rate of 1.7×10^5 s^{-1}, to be compared to that of 5.6×10^8 s^{-1} for the $1s2p^3\,{}^5S$—$1s2p^23s\,{}^5P$ transition. We have thus found reasonable evidence for assigning the observed 857.7-Å line to the latter transition. The $1s2p^23d\,{}^5P$ term, finally, is found to lie energetically above the $1s2s2p\,{}^4P$ threshold in B III and it can thus autoionize to the $1s2s2p\epsilon p\,{}^5P$ continuum.

In summary, we have obtained accurate experimental and theoretical data for the $1s2s2p^2\,{}^5P$—$1s2p^3\,{}^5S$ multiplet in B II. The $1s2p^3\,{}^5S$—$1s2p^23s\,{}^5P$ transition has also been identified. Our future work will be extended to other bound quintet terms in B II.

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