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Lifetimes of Doubly-Excited 2p3*l* Levels in Singly Ionized Boron, B II

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Abstract

Lifetimes of several 2p3s, 2p3p and 2p3d levels in singly ionized boron, B II, have been determined by means of beam–foil spectroscopy and theoretical calculations, using the superposition-of-configurations (SOC) program of Cowan. These doubly-excited terms which lie close to the first ionization limit of B II make radiative transitions to the singly excited system. For a few autoionizing 2p3*l* levels we have calculated excitation energies and decay rates. The theoretical and experimental data are generally in very good agreement.

1. Introduction

The present paper is part of a systematic study of the structure of levels belonging to the doubly-excited 2p*nl* system in Be-like ions. These levels – which may perturb the various 2s*nl* spectral series – frequently have radiative as well as non-radiative (autoionization) decay channels.

In a previous paper Ellis *et al.* [1] reported experimental and theoretical studies of lifetimes of three doubly-excited levels in Be I. The terms studied, 2p3p ^{3}P, 2p3d ^{1}D and 2p3d ^{3}D lie energetically above the first ionization limit of Be I, but they are stable against the fast (10^{13}–$10^{15}\,\mathrm{s}^{-1}$) autoionization via the Coulomb interaction which has the selection rules $\Delta L = 0$ and no parity change. For 2p*nl* levels with $l = L$ there are no final states which fulfill these selection rules, and the levels preferentially decay by transitions to the Be I singly-excited system. However, early beam–foil work [2, 3] had yielded lifetimes for these levels which were drastically shorter than the available theoretical values [4]. Although autoionization through spin–orbit mixing with rapidly decaying 2p3*l* levels (with *l* differing from *L*) was considered, it was believed that this effect was not sufficiently strong in a neutral atom to account for the large difference between theory and experiment. It took more than 20 years before detailed calculations of this process could explain the previous discrepancy. By combining the calculated autoionization rates with the theoretical radiative transition probabilities, theoretical level lifetimes were obtained which agreed with the experimentally determined data [1].

In view of the theoretical and experimental difficulties in accurately determining rates of the relativistic spin–orbit autoionization process as well as those of radiative decay modes, the agreement in the Be I case could perhaps be somewhat fortuitous. To further understand such mechanisms we have now performed experimental and theoretical studies of the 2p3*l* levels in B II. One difference between these two spectra is that for B II a larger number of 2p3*l* levels lie below the first ionization limit and they have only radiative decay channels. In the B II case lifetime measurements provide information about the accuracy of theoretical calculations of radiative transition probabilities. If theory and experiment agree in this case, reliable data on weak autoionization can be extracted whenever this additional decay mode occurs.

In addition to the basic atomic physics interest, detailed knowledge of the structure and spectra of neutral and ionized boron is now needed in astrophysics and fusion plasma physics. While the cosmic abundance of B is extremely low, it plays an important role in testing models of Big Bang Nucleosynthesis [5]. Optical spectroscopy is the only method for determining B abundances in stellar objects. A good knowledge of energy structures and transition probabilities is required for this purpose [6]. In thermonuclear fusion research boron is one of the most abundant light impurities in the plasmas of several presently operating tokamaks. Thus, being a constituent in carbon-based wall materials, boron can enter the plasma by various plasma-wall interaction mechanisms, sputtering, erosion, etc. [7]. Fusion plasma diagnostics thus utilize experimental and theoretical data on the structure and interaction of boron in various stages of ionization.

2. Survey of previous work in B II

The 2p3*l* configurations in B II include 2p3s, 2p3p and 2p3d singlet and triplet terms. In a thorough spectroscopic investigation Ölme [8], who used a sliding-spark light source, provided accurate excitation energies for the 2p3s ^{3}P, 2p3p ^{1}P and 2p3d ^{1}D and ^{3}D terms. On the basis of beam–foil studies [9] the energies of 2p3p ^{1}S, ^{3}S, ^{3}P and ^{3}D were also proposed [8, 9]. However, due to the modest wavelength accuracy in the early beam–foil spectra the estimated energy uncertainties varied from ±25 to $\pm 250\,\mathrm{cm}^{-1}$. The accuracy was subsequently improved, by more than an order of magnitude, in later beam–foil work [10–13] which also led to the identifications of the 2p3s ^{1}P and 2p3d ^{3}F levels. Furthermore, Berry and Subtil [10] identified some non-autoionizing 2p4*l* levels in B II as well. An extended lifetime study, which also included some of the 2p3*l* levels in B II, was reported by Kernahan *et al.* [13]. Absorption spectroscopy for B II has been performed by Esteva *et al.* [14]

Jannitti *et al.* [15]. In the latter work some new assignments are given, including some autoionizing studies.

Very little theoretical work has until now been reported concerning the energies and transition probabilities for the 2p*nl* system in B II. The only exception is the paper by Fawcett [16] who applied the Cowan code [17]. Moreover, the previous studies [8–16] have also established that 10 of the 14 possible *LS*-terms of the 2p3*l* configurations lie below the 2s ^{2}S ionization limit of B II, whereas 2p3p ^{1}S, 2p3d ^{1}P, ^{1}F and ^{3}P are located above it.

3. Experiment

The experimental work was carried out in the University of Toledo Heavy Ion Accelerator laboratory. The experimental facilities, including the Danfysik 330 kV accelerator and the on-line data analysis systems have been described earlier [18, 19]. The accelerator produced stable beams of B$^+$ ions with energies ranging from 240 keV to 270 keV. The ions were directed through a thin carbon foil of a prescribed thickness that ranged from 2.1 to 2.4 μg/cm^2. In this energy range about 55% of the ions after the foil are singly-charged [20]. The energy loss of the ions in the foil was typically 5 keV, while the relative velocity uncertainty of the ions after the foil was estimated to be 1.5%. The radiation emitted by the foil-excited ions was analyzed with an Acton 1 m normal incidence vacuum ultraviolet spectrometer equipped with a 2400 lines/mm concave grating, blazed at 800 Å. The photons were detected with a channeltron detector.

Spectra were registered in the region 400–2000 Å. The lifetimes were measured by recording the intensity of a given line as a function of the distance (downstream) from the foil. The decay curves were analyzed using the program DISCRETE [21] which fits the data to a sum of exponentials, representing the lifetime of the level under study and those of the levels feeding it.

4. Theoretical calculations

The calculations of radiative transitions were carried out using the SOC code of Cowan [17] which employs the Blume–Watson method [22] for spin–orbit integrals. In this calculation the even configurations 2s^2, 2p^2, 2s3s, 2p3p, 2s3d, 2s4s, 2p4p, 2s4d, 2p4f, 2s5s, 2p5p, 2s5d, 2p5f, 2s5g and the odd ones 2s2p, 2p3s, 2s3p, 2p3d, 2p4s, 2s4p, 2p4d, 2s4f, 2p5s, 2s5p, 2p5d, 2s5f, 2p5g were included. The spin–orbit integrals were reduced to 95% of the *ab initio* values. The electrostatic integrals between equivalent electrons and non-equivalent electrons and the configuration interaction integrals were all reduced to 70% to compensate for the interaction from more distant configurations.

In computing the autoionization rates we used the same method which gave the best results for the Be I case [1]. For the 2p3p ^{1}S calculation we used 16 bound and 6 continuum configurations for the odd parity cases and 15 bound and 7 continuum ones for the even parity cases. We used the "standard" scaling of 85% for the electrostatic integrals and no empirical adjustments.

5. Results and discussion

The results of our measurements and calculations are given in Tables I (lifetimes) and II (excitation energies and autoionization rates) where they are compared with previous experimental and theoretical results. Table I shows that we have measured the lifetimes of 4 singlet terms, 2p3s ^{1}P, 2p3p ^{1}P, ^{1}D and 2p3d ^{1}D as well as of 5 triplet ones, 2p3s ^{3}P, 2p3p ^{3}S, ^{3}P, ^{3}D and 2p3d ^{3}D. For all these terms and for the 2p3d ^{3}F we also report new theoretical lifetime data.

Table I. *Lifetimes of 2p3s, 2p3p and 2p3d terms in B II*

Term	Energy (cm^{-1})	Wavelength (Å)	Lifetime (ns)	
			Experiment	Theory
2p3s ^{1}P	186 636	1695.7	2.17 ± 0.15[b]	4.97[a] 2.24[b]
2p3p ^{1}P	189 128	864.1	1.4 ± 0.2[c] 1.30 ± 0.03[b]	0.472[a] 1.16[b]
2p3p ^{1}D	196 978	809.2	2.05 ± 0.06[b]	0.765[a] 2.18[b]
2p3d ^{1}D	197 720	1048.7	0.79 ± 0.08[c] 0.67 ± 0.04[b]	1.08[a] 0.68[b]
2p3s ^{3}P	181 667	1208.3	1.4 ± 0.1[c] 1.15 ± 0.06[d]	1.80[a] 1.15[b]
2p3p ^{3}S	193 216	641.6	2.2 ± 0.1[b]	0.49[a] 1.99[b]
2p3p ^{3}P	195 630	631.9	2.4 ± 0.2[c] 2.18 ± 0.12[d] 2.14 ± 0.05[b]	1.17[a] 2.17[b]
2p3p ^{3}D	191 071	650.5	5.64 ± 0.22[b]	1.25[a] 3.1[b]
2p3d ^{3}D	200 484	984.7	0.41 ± 0.04[c] 0.35 ± 0.02[d] 0.35 ± 0.01[b]	0.334[a] 0.31[b]
2p3d ^{3}F	197 709	2123.9	6 ± 1[c] 5.36 ± 0.32[d]	10.8[a] 3.8[b]

[a] Fawcett [16].
[b] This work.
[c] Martinson *et al.* [9].
[d] Kernahan *et al.* [13].

As pointed out above the terms 2p3p ^{1}S, 2p3d ^{1}P, ^{1}F and 2p3d ^{3}P lie well above the B II ionization limit, 202 887 cm^{-1} [5] and they can therefore autoionize via the Coulomb interaction. The corresponding lifetimes are very short, and this fact together with low branching ratios rules out the observation of transitions from these terms in photon spectra. Our theoretical results for these terms are given in Table II.

In Table I we also include the "best" experimental excitation energies of the various terms. These values originate mainly from the work by Ölme [8], but also from the more recent studies, by Berry and Subtil [10], Bashkin *et al.* [11] and Dumont *et al.* [12]. For details concerning, e.g. uncer-

Table II. *Energies and autoionization rates for terms in B II*[a]

Term	Energy (cm^{-1})		Autoionization rate[b] (10^{13} s^{-1})
	Theory[b]	Experiment[c]	
2p3p ^{1}S	205 000		37
2p3d ^{1}P	207 870	205 120	3.9
2p3d ^{1}F	206 890		58
2p3d ^{3}P	203 950		6.7

[a] Ionization energy 202 887 cm^{-1}.
[b] This work.
[c] Jannitti *et al.* [15].

tainties, we refer to these papers. Furthermore, in Table I the present experimental and theoretical lifetime values are compared with each other and with previous experimental [9, 13] and theoretical [16] results.

5.1. *B II singlet system*

In the singlet system our lifetime values for 2p3p ^{1}P, ^{1}D and 2p3d ^{1}D are in excellent agreement with the new calculated values, whereas the difference is much larger when compared with previous theoretical predictions [16]. Within the mutual error limits our experimental lifetimes also agree with the early results [9] although the latter tend to be slightly longer.

We also measured the decay time of a line at 770.3 Å, assigned to the 2s2p ^{1}P–2p3p ^{1}S combination [5, 6]. The value, $\tau = 0.72 \pm 0.06$ ns, is much shorter than the theoretical values 3.89 ns [16] and 2.10 ns (present calculation) for the radiative lifetime implied by this assignment. Furthermore this places the 2p3p ^{1}S well into the continuum, with an autoionization rate of order $10^{14}\,\mathrm{s}^{-1}$. It is thus clear that the 770.3 Å line is of a different origin than previously assumed. We have considered various other assignments for this line but have not been able to find a conclusive answer.

We have now also determined the lifetime of the 2p3s ^{1}P level, the energy of which was suggested by Bashkin *et al.* [11], on the basis of unpublished calculations by Weiss [23]. In beam–foil spectra this level was determined from the two lines 1186.1 (to 2p^2 ^{1}D) and 1694.8 (to 2p^2 ^{1}S). Our lifetime value, 2.17 ± 0.15 ns is in very good agreement with the result of the present calculation, 2.24 ns, whereas it differs markedly from the previous prediction, 4.97 ns [16].

The identification of the 2p3p ^{1}D level was initially based on one transition only, the 809.2 Å line to 2s2p ^{1}P. Later also the decay to 2s3p ^{1}P, at 1891.4 Å was reported [12]. The good agreement between our experimental and theoretical values for the 2p3p ^{1}D lifetime provides additional confirmation of the spectral assignment.

5.2. *B II triplet system*

Here, also, our experimental results are in quite satisfactory agreement with earlier such data [9, 13]. Similarly, we agree with the newly calculated theoretical data, whereas larger deviations can be noted from the previous theoretical predictions [16]. The difference between these two calculations is probably due to the inclusion of about 50% more configurations in the present work, as compared to Ref. [16].

The energy of the 2p3p ^{3}S term, initially derived from only one line at 641.5 Å, in beam–foil spectra [9], has later been determined more accurately. Not only has the wavelength of this line been remeasured, with an uncertainty as low as ±0.06 [12], but the transition from 2p3p ^{3}S to 2s4p ^{3}P has also been observed [10]. Our experimental lifetime agrees with the recent theoretical result. However the decay curves also exhibit a prompt component of unknown origin (decay time 0.22 ns).

The new experimental 2p3p ^{3}P lifetime nearly coincides with that found by Kernahan *et al.* [13] and agrees, within error limits, also with older data [9]. In the early work [8, 9] the 2s2p ^{3}P–2p3p ^{3}D wavelength was given as 652.0 Å. The value has now been corrected to 650.53 Å by Dumont *et al.* [12] and to 650.7 Å by Jannitti *et al.* [15]. These authors also point out that the 652.0 line in Refs [8, 9] is an unresolved blend between the transition from the 2p3p ^{3}D level and a line at 653.8 which is the 2s2p ^{3}P–2s6d ^{3}D combination. The latter transition, first observed by Esteva *et al.* [14], is in our present beam foil spectra well resolved from the 650.53 Å line. We have here determined the decay times of these neighboring lines. For the 2p3p ^{3}D level we obtain $\tau = 5.64 \pm 0.20$ ns which does not agree too well with our calcuated 3.1 ns and deviates even more from the earlier theoretical result of 1.25 ns [16]. However, the lifetime of the 2s6d ^{3}D level now obtained $\tau = 2.9 \pm 0.2$ ns agrees reasonably well with the previous theoretical value 3.72 ns, of Markiewicz *et al.* [24]. It is thus obvious that the two lines are correctly identified and we may speculate that the difference between theory and experiment in the 2p3p ^{3}D case is due to shortcomings on the theoretical side.

The 2p3d ^{3}D level, on the other hand, belongs to those accurately determined by Ölme [8], and the transitions from it are free from blends. There also exists an early experimental lifetime value, 0.41 ± 0.04 ns [9]. Our remeasurement showed a 2-component decay with a primary lifetime of 0.35 ± 0.03 ns. Agreement is here very satisfactory with the experimental value of Kernahan *et al.* [13] and the theoretical values, Ref. [16] and the present work.

The 2p3d ^{3}F term, finally, has only one allowed decay mode, to 2s3d ^{3}D, at 2124.3 Å. Its lifetime was determined by Martinson *et al.* [9], and by Kernahan *et al.* [13] whose values are in satisfactory agreement with each other, whereas they differ from our recent theoretical result. However, it is possible that the 2124.3 Å line is blended by another B II transition, 2s3p ^{3}P–2p3p ^{3}D, the calculated wavelength of which is 2123.3 Å. High-resolution studies, using a Fourier Transform Spectrometer, are scheduled to study this problem.

5.3. *Autoionizing levels*

Table II includes our calculated excitation energies and autoionization rates for the four terms lying in the B II continuum. In the case of 2p3d ^{1}P there is also an experimental energy value, from the photoabsorption measurement of Jannitti *et al.* [15]. We make no claim for the precision of autoionization decay rates, but it is clear that they are 3–4 orders of magnitude larger than typical radiative transition probabilities, as expected for Coulomb-allowed transitions. Thus there is no prospect of studying these levels by means of photon spectroscopy, as was done for the Coulomb-forbidden autoionizing levels in Be I.

6. Concluding remarks

The present study of the decays of 2p3s, 2p3p, 2p3d configurations in Be-like B II has generally demonstrated very satisfactory agreement between experimental and theoretical results. This holds, in particular, for the 2p3p ^{3}P, 2p3d ^{1}D and ^{3}D terms which were studied in the Be I paper [1]. Since the radiative decays of these terms can be accurately calculated for Be-like light ions, a conclusion is that the experimental data for Be I [1] also yield important information about the fairly weak relativistic (spin–orbit) ionization rates in this case.

Our future work will deal with 2p4*l* configurations in Be I and B II. However we also plan to extend similar work to

C III and perhaps N IV. It is well known that isoelectronic comparisons are very valuable in systematic studies of atomic structure. This is definitely true in the present case, in particular because the rates of the competing processes, i.e. radiative and non-radiative decay modes, scale differently with the nuclear charge Z. For an illustration of the Z-dependence of the energies of the 2p3l levels in Be-like ions we finally refer to a figure by Edlén [25], which nicely illustrates both the irregularities at low values of Z, caused by series perturbations between 2p3l levels and 2snl series, and the smooth variation of the energies with Z for highly charged four-electron ions.

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