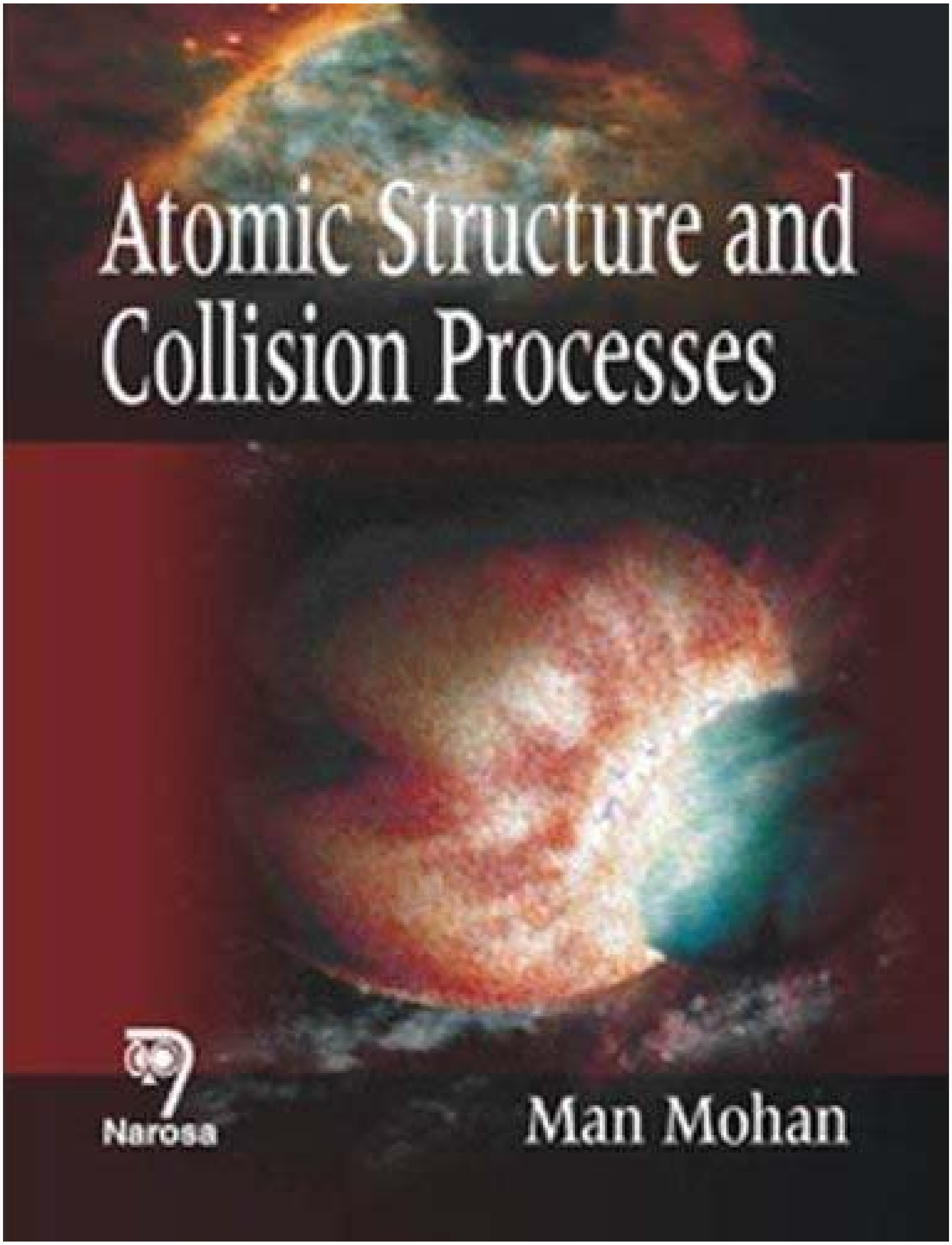

Atomic Structure and Collision Processes

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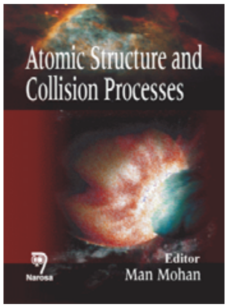

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About the book

Atomic and Molecular physics play a central role in many other fields such as analytical techniques, biophysics, and chemical & condensed matter physics. Accurate atomic and molecular data is required for understanding Earth, Sun, other's Astrophysical objects (like Stars, Nebulae, Novae, Supernovae) atmospheres and high temperature plasma coming from fusion type of reaction in (ITER) future Tokomak-machines. The main processes of direct interests are data for collisional processes involving electron, proton & photon resulting excitation, ionization, dissociation and recombination. In addition, collision processes is central to the understanding of phenomena such as global warming, and air and water pollution. Not only this branch impacts numerous branches of engineering, from information technology and nanotechnology to bioengineering.

Key Features

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Additions to the spectra and energy levels of ionized boron, B II – B V

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Abstract. We have undertaken a number of studies of the spectra of ionized boron, B II - B V. The spectroscopic data, collected by us over several years, originate from experiments with beam-foil spectroscopy and high-resolution spark spectroscopy, together with *ab initio* and semi-empirical calculations. The present work follows a recent study of B II [A.N. Ryabtsev *et al.*, Physica Scripta **71**, 489 (2005)]. A significant amount of new transitions and new levels has been found for B II - B V, and we have critically evaluated all previous and new data for these spectra. We believe that these four spectra are now quite satisfactorily known.

1. Introduction

Neutral and ionized boron are of considerable interest from the basic atomic physics points of view. Comparison of experimental data for wavelengths, energies and oscillator strengths with results of sophisticated theoretical calculations can provide valuable information about the accuracy of various theoretical models. Detailed knowledge of the structure and spectra of boron is also needed in astrophysics and fusion plasma physics. The cosmic abundance of boron is extremely low, but it is important for testing models of Big Bang nucleosynthesis. In fusion research boron is an important material in thermonuclear fusion devices such as tokamaks. As a light element boron is used as a plasma facing material for the reactor walls, and because of sputtering boron ions enter the hot plasma and emit line radiation from it. Thus, plasma diagnostics need reliable values for wavelengths and oscillator strengths for transitions in neutral and ionized boron.

About 10 years ago, one of us (A. N. Ryabtsev) made extensive compilations of the energy levels for neutral and ionized boron. The results have not been formally published, however. In recent years we started detailed investigations of the spectra of singly ionized boron, B II, as well as of multiply ionized boron, B III, B IV and B V.

As will be mentioned below, most of the data for B II have been published recently, whereas the results for B III - B V, are still being analyzed. In the present article we shall briefly summarize the results for B II, together with some more recent data, and discuss the progress for more highly ionized boron.

The spectra B II – B IV were already studied in the 1930's by Edlén in Uppsala, and the results are given in his thesis [1]. In the "Atomic Energy Levels, Vol. I" [2], the situation of 1949 is given. The data were largely based on early work by Edlén [1]. Later Ölme reinvestigated B II [3] and B III [4], whereas Eidelsberg [5] analyzed B IV. These studies provided many additional levels and it was generally believed that all three spectra were quite satisfactorily known. However, as will be discussed below, additional studies began to appear in the 1970's and later. In several cases the technique of beam-foil spectroscopy, BFS, was applied. This method was often directed toward measurement of lifetimes of various excited states, but frequently also new transitions were observed in beam-foil spectra. This fact could also be useful for the identification of new energy levels, despite the fact the wavelength accuracy was fairly modest in the early BFS work.

2. Doubly excited states

In atomic spectroscopy one usually studies singly excited states. In neutral lithium, Li I, for instance, such states are doublets, 1s2nl ^{2}L, and the ionization energy is about 5.39 eV. However, inner-shell excited or doubly-excited states are also possible. These can be either doublets or quartets, the latter 1s2snl or 1s^{2}pnl ^{4}L, and they lie in the continuum. Thus, the lowest quartet term 1s2s2p ^{4}P lies at 57.42 eV, and thus more than 50 eV above the Li II ground state. In general, such levels should autoionize via the Coulomb interaction, with typical decay constants of 1013 s^{-1} or higher. However, this electrostatic interaction has selection rules $\Delta J = 0$ (also $\Delta L = 0$ and $\Delta S = 0$ in LS-coupling) and no parity change. This fact rules out autoionization whereas radiative transitions between quartet states are possible. However, there can also be inner-shell excited doublet states, *e.g.* 1s^{2}p^2 ^{2}D, and these can decay by autoionization. Such transitions (photons, or electrons, from ionization) are often observed in beam-foil experiments. In the case of the Li sequence, such data have been found for many systems, from Li I to Ar XIV, see the review by Mannervik [6]. The multiply excited states are also of considerable theoretical interest, because they constitute challenges for modern computational methods.

3. B II

After the high-resolution study by Ölme [3] and a BFS investigation by Martinson *et al.* [7] it indeed appeared that B II was quite satisfactorily known. However, in 1973 we heard from Dr. A. W. Weiss that he had made *ab initio* calculations (unpublished) of the structure of B II, using the SOC (superposition of configurations) method.

The calculations of level energies, were very accurate, and in good agreement with the experimental results [3, 7], typically within 100-200 cm^{-1}. However, there was a large discrepancy for the 2s3s ^{1}S level, about 2 700 cm^{-1}. This particular level was experimentally found from the transition to 2s2p ^{1}P, at 1607.76 Å [3], a wavelength much longer than the theoretical value proposed by Weiss, 1573 Å. This puzzling fact motivated us and other colleagues to make theoretical calculations and new experiments, by means of BFS and high-resolution spark spectroscopy. It was soon realized that the theoretical f-value (oscillator strength) for the 2s2p ^{1}P – 2s3s ^{1}S transition obtained by Weiss was 0.002, whereas the lifetime measurement for the 1607.76 Å line [7] would yield $f = 0.048$, a very puzzling difference. It became obvious that the 1607.76 Å line was misidentified. It was indeed later shown that it really belonged to the B I quartet system. However, experimental searches for the correct 2s2p ^{1}P – 2s3s ^{1}S combination continued for several years.

In 1999 we performed a new beam-foil experiment, using the 3 MV Pelletron tandem accelerator at Lund. Positive ions of atomic B were accelerated to 1.4 MeV or 2 MeV energy and sent through a thin carbon foil. The light emitted by the foil-excited ions was dispersed with a Minuteman 1 m VUV monochromator, equipped with a CCD detector. This modern equipment largely increased the recording efficiency and thus the effective sensitivity, as compared to previous experiments. Spectra were observed in the interval 1100 – 6000 Å, and the linewidths were about 0.5 Å. After time-consuming analyses we observed a very weak line, at 1557.03 Å, which could be explained as the elusive 2s2p ^{1}P – 2s3s ^{1}S transition. This wavelength is in satisfactory agreement with 1 557.5 Å, from a later calculation by Weiss [8]. The experimental line was very weak, but the result was supported by previously unobserved transitions to 2s3s ^{1}S from the well-established 2s4p and 2s5p ^{1}P terms in B II [9].

As a spin-off of the long-lasting search for only one hidden transition in B II, we had a obtained a wealth of experimental and theoretical spectroscopic data for ionized boron. Furthermore, we also had access to experimental data obtained by other groups as well as results of theoretical calculations. It was therefore motivated to use all this data in order to complement and improve the available knowledge about the structures of ionized boron, initially B II and B III.

The extensive results for B II have already been published [10]. The new material contains more than 80 newly classified (or revised) spectral lines. It also originated from spectroscopy in Lund with a sliding spark light source and a high-resolution 3 m normal incidence spectrograph (300 – 2 500 Å), beam-foil spectroscopy with a 380 kV heavy-ion accelerator in Stockholm (450 – 6 000 Å), and with a 300 kV heavy-ion accelerator in Toledo, Ohio (500 – 1 200 Å) in addition to the data with the 3 MV tandem accelerator in Lund, mentioned above. The data analysis was followed by a critical compilation of all known levels and lines of B II. The work by Ölme [4] essentially included singly excited states. However, in the Be I sequence, there are of course also inner-shell excited states [10]. For instance, Mannervik *et al.* [11] observed the 1s2s2p^2 ^{5}P – 1s2p^3 ^{5}S combination at 1323.92 Å, and some other transition from the 1s2p^3 ^{5}S term.

4. B III

In the case of B III, Ölme [4] measured the wavelengths of 31 lines in the doublet system and provided accurate energies for many levels up to $n = 5$ and 6. Additional data for levels in the $1s2nl\ ^2L$ system were presented in some beam-foil articles [7,12-14]. As in the case of B II we have used all this published material and combined it with the new and unpublished results from beam-foil experiments in Stockholm, Toledo and Lund, and high-resolution spectra from Lund, as listed above.

We have now a list of 121 B III lines in the region 350 – 7 850 Å, out of which 15 are new, and we have also improved the wavelengths for 40 lines which had been observed earlier. Thus, for the energy levels in the doublet system of B III there are now experimental data up to $n = 10$. The energies of even higher levels can be calculated with high accuracy.

Doubly-ionized boron, B III, belongs to the Li I isoelectronic sequence, and we can there expect doubly-excited quartet states. Indeed, several beam-foil experiments and theoretical studies have been carried out to search for such levels and transitions between them. In one of the latest beam-foil studies Baudinet-Robinet *et al.* [15] list 28 lines, transitions in the B III quartet system, in the wavelength region 360- 2000 Å. In the present experiment we observed 16 new lines belonging to this system and we also have improved the wavelengths of 23 such lines which have been observed previously. There are now nearly 70 lines and 40 energy levels (all experimentally observed) in this interesting quartet system.

5. B IV and B V

Triply ionized boron, B IV, belongs to the He isoelectronic system. Edlén [16] mentioned that already in the late 1920's he had observed radiative transitions in He-like Li, using a spark light source. At that time the Norwegian theorist Hylleraas tried to apply quantum-mechanical calculations to such systems. The two young Scandinavians presented their independent results - which were in perfect agreement - at a conference in Copenhagen in 1929. This made a great impression on Niels Bohr, who attended the conference, because these early results showed that quantum mechanics also worked for a system containing more than one electron. Thus, for many years, theory and experiment have been collaborating as well as competing, while the He-like ions were investigated carefully.

As mentioned, the B IV system was studied by Eidelsberg [5] who used a laser-produced plasma as light source. She observed about 30 lines and could report energies for several terms, up to $2s5g\ ^{3,1}G$. Also, some lines of B IV were observed in beam-foil studies by Berry and Subtil [12] and Dumont *et al.* [13].

There are of course also doubly-excited levels in He and He-like ions. A famous photoabsorption experiment for He was done by Madden and Codling with synchrotron radiation [17], in which they observed autoionizing, doubly excited states. This early experiment showed that synchrotron radiation could be successfully applied to atomic physics research and it also inspired much theoretical work. From experiments with laser-produced plasmas, Kennedy and Carroll [18] reported doubly-excited states in B IV, and such states were also investigated by To and Drouin, who used beam-foil spectroscopy [19]. In the B IV spectrum we have observed 5 new lines and improved the wavelengths of 17 previously observed transitions. Experimental energies up to 1s8p ^{3}P are now known.

The one-electron system B V has been very precisely computed by Garcia and Mack, who covered H I – Ca XX and even included QED corrections to the Dirac values [20]. Thus, ordinary experimental values should not bring any new information in such cases. However, we have observed four B V transitions which have not been reported earlier.

6. Lifetimes and transition probabilities

We have here concentrated on radiative transitions and excitation energies in ionized boron, but will here briefly discuss the equally important quantities, *e.g.* lifetimes of excited states and radiative transition probabilities. These can provide valuable information about the effects of electron correlation, relativity, nuclear structure and quantum electrodynamics (QED) in atomic systems. Furthermore, transition probabilities have important applications in astrophysics (interpretation of spectra from space, the modeling of stellar atmospheres, *etc.*), fusion plasma physics (*e.g.* diagnostics of plasma impurities, studies of transport mechanisms) as well as in the development of new laser systems. These quantities can be can be calculated but also measured. For calculating atomic structure powerful nonrelativistic codes, such as the multiconfiguration Hartree-Fock (MCHF), configuration interaction (CI), superposition of configurations (SOC), and many-body perturbation theory (MBPT) are widely used. For highly charged ions, relativistic programs, *e.g.* multiconfiguration Dirac-Fock (MCDF) are very popular and useful. On the experimental side, beam-foil spectroscopy (BFS), introduced more than 40 years ago, has made it possible to extend lifetime measurements to singly and multiply ionized atoms and also to investigate transitions at very short wavelengths. The BFS method has been applied to a large number of atomic species, including U^{90+} and U^{91+} . Many such investigations have been carried out for boron, some early references are [7] and [21]. As a more recent example we mention a study of the resonance line of B II, $2s^2\ ^1S$ – $2s2p\ ^1P$, at 1362.4 Å. An elaborate beam-foil experiment, using the 300 kV heavy ion accelerator in Toledo [22], gave here a lifetime of 0.85 (7) ns, in excellent agreement with the theoretical value of Weiss, 0.999 ns [8]. This particular transition has been seen in solar and stellar spectra, and the transition probability is important for the determination of the abundance of boron in astrophysics.

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