Accurate transition probabilities for the $2s^2\ ^1S - 2s2p\ ^1P$ transition in Be I and B II

R.E. Irving, M. Henderson, L.J. Curtis, I. Martinson, and P. Bengtsson

Abstract: Transition probability determinations are reported for the $2s^2\ ^1S-2s2p\ ^1P$ transition in Be I and B II, based on lifetime measurements made by beam-foil excitation. The lifetimes were extracted by the ANDC method, which incorporates cascade-related decay curves into the analysis of the primary decay curve, thus accounting for the effects of cascade repopulation. The results are of higher precision than earlier measurements and improve the agreement with recent theoretical calculations.

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Résumé: Des mesures de demi-vies par méthode faisceau-lame permettent de déterminer la probabilité de transition $2s^2\ ^1S - 2s2p\ ^1P$ dans le Be I et le Be II. Les demi-vies sont obtenues par la méthode ANDC qui incorpore des courbes de désintégration en cascade dans l'analyse des courbes primaires de désintégration, tenant ainsi compte des effets de repopulation par cascade. Ceci mène à une précision accrue des résultats par rapport à des mesures antérieures et améliore l'accord avec les récents résultats théoriques.
[Traduit par la rédaction]

1. Introduction

The Be-like ions have for many years been test cases for elaborate calculations of atomic structure. They provide interesting examples of electron correlation, core polarization, and relativistic effects. In particular, the transition probability of the $2s^2\ ^1S - 2s2p\ ^1P$ resonance line in this sequence has been investigated by many authors, both experimentally and theoretically. Practically all experimental data originate from beam-foil studies, i.e., determination of the lifetime of the $2s2p\ ^1P$ level. On the theoretical side, however, a wide variety of approaches have been employed.

In 1980 it could be noted that, while the most recent experimental f-value for neutral Be I [1] was in excellent agreement, the results of large-scale theoretical calculations (see, for example, ref.2), for its isoelectronic ions B II – O V (as well as for some higher members of the sequence) the experimental f-values were markedly lower (typically 20%) than the most reliable theoretical predictions. In the

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case of Be I the cascades have lifetimes much longer than that of the primary, and the experiment [1] sought to specify cascading accurately by following the primary decay curve far out on the tails with high statistical accuracy. Since the lifetimes of the primary and cascade levels are closer to each other for the Be-like ions, it was assumed that discrepancies there were due largely to shortcomings on the experimental side, viz. insufficient correction for cascading in the analyses of multiexponential beam–foil data.

In subsequent beam–foil studies of these ions the method of Arbitrarily Normalized Decay Curves (ANDC) [3], which is able to correct for cascading in a rigorous way, was therefore applied. The new values thereby obtained for B II [4], C III [5], N IV, and O V [6] were all in satisfactory agreement with theory. To further refine the experimental f-values and to reduce the effect of statistical uncertainty, a method of isoelectronic smoothing of line strengths was applied to Be I - O V [7] (and later extended to other ions [8]). More recently, a detailed investigation of line strengths in the Be sequence ($Z = 4$–54) has appeared [9], which also relates this resonance transition probability to that of the $2s^2\,{}^1S - 2s2p\,{}^3P$ intercombination line through intermediate coupling relationships that can be specified from measured spectroscopic data [9,10].

In recent years a number of elaborate large-scale calculations have been undertaken for neutral Be and Be-like ions, using techniques such as SOC, MCHF, and CI [11]- [20]. For the resonance lines in Be I and B II, the new theoretical f-values have estimated uncertainties as low as 0.5–1%. A comparison of these results with the experimental data for Be and B seems to indicate that the latter are 1–2% lower than the theoretical values. While this might still appear to be very good agreement, concern has been expressed in refs.11–20 that uncertainties in the experimental work for Be I and B II [1,4,7] might have been too optimistic. A recent paper by Jönsson et al. [20] provides a thorough discussion of the oscillator strengths in the Be isoelectronic sequence, and emphasizes these concerns. These authors point out that parametrizations of isoelectronic trends are more robust than individual data and provide better templates for theoretical comparison, but the validity of the method is particularly sensitive to the ions near the data-limiting neutral end, where the smoothing procedure using a low-order polynomial in the reciprocal screened charge may break down.

These lines also have astrophysical applications that motivate their accurate specification. For example, the B II resonance line has been used extensively to determine stellar boron abundances, and the abundance of boron and the $^{11}B/^{10}B$ abundance ratio are crucial for testing various models for cosmic production of the light elements (cf. ref.15 and references therein). In addition, this 1362 Å line is also important because it coincides with and masks lines in Hg II and Hg III that have been observed in chemically peculiar stars.

For these reasons, we conclude that small differences among theoretical, experimental, and smoothed data for Be I and B II are of particular concern, and that confirmation (or correction) of existing measurements at the same or slightly improved precision is desirable. We have therefore undertaken a new study of the experimental lifetimes of the $2s2p\,{}^1P$ level in Be I and B II, using beam–foil spectroscopy (BFS) and ANDC analyses.

2. Experiment

Standard BFS techniques were used in the present experiment, which was carried out in the University of Toledo Heavy Ion Laboratory. The facilities, including a Danfysik 300 kV accelerator and the on-line data analysis system have been described earlier [21,22]. Singly charged ions of energies 170 keV (Be^+) and 240–270 keV (B^+) were directed through thin foils of carbon of a prescribed thickness that ranged from 2.1 to 2.4 μ g/cm^2. The energy loss in the foils was about 5 keV and the relative velocity uncertainty of the excited species of Be and B^+ was estimated to be below 1.5%, using tabulated energy-loss data [23]. Spectra were registered with an Acton 1-m normal incidence vacuum monochromator, which can be equipped with a number of concave gratings, depending on the wavelength range of interest. In the present case a 2400 lines/mm (blazed at 800 Å), a 1200 l/mm (1500 Å), and a 600 l/mm

(3000 Å) grating were used.

Prior to lifetime measurements, spectra were registered in the regions of the $2s^2\ ^1S - 2s2p\ ^1P$ resonance lines, as well as those where the singlet transitions that feed the $2s2p\ ^1P$ levels were expected to lie. The term systems Be I and B II are well known and the transitions of interest are all free from blends .

The lifetimes were measured in the usual way, by recording the intensity decay of a given spectral line as a function of the distance from the foil. In the Be experiment the decays of the $2s2p\ ^1P$ level were measured as well as of those levels primarily feeding it, viz. $2s3d\ ^1D$ and $2s4d\ ^1D$. These are the only significant cascades, as already discussed in ref.1. The $2s2p\ ^1P - 2s3s\ ^1S$ transition (8254 Å) lies outside our experimental range, while the $2s3s\ ^1S$ lifetime is quite long, 87.5 ns (according to Weiss' calculations [12]. Cascading from $2p^2\ ^1S$ and $2p^2\ ^1D$ into $2s2p\ ^1P$ plays an important role for Be-like systems except Be I. In the neutral atom the $2p^2\ ^1S$ level lies above the first ionization limit and is autoionizing [24], whereas the $2s2p\ ^1P - 2p^2\ ^1D$ transition is extremely weak, because of cancellation [12].

For B II the situation is somewhat different, and here the decays of the $2s2p\ ^1P$ level and the primary cascades $2s3d\ ^1D$, $2p^2\ ^1S$ and $2p^2\ ^1D$ were investigated, as was done in the earlier experimental study [4] of this system. In contrast to the Be I case, the $2s2p\ ^1P - 2s3s\ ^1S$ line is extremely weak [12] due to cancellations, and the position of the $2s3s\ ^1S$ has only been tentatively proposed [4].

The decay curves were first analyzed using the multiexponential fitting program DISCRETE [25], and then by the ANDC [3] method, which corrects for cascading in a rigorous way. In this procedure the ANDC computer program CANDY [26] and a similar code developed specifically for this set of transitions were both used.

3. Results and discussion

The use of the ANDC method to extract lifetime data from cascade-correlated decay curves is illustrated in Fig. 1 for the $2s2p\ ^1P$ level in B II. The measured decay curves for a primary transition $I_p(t_i)$ and three dominant cascades $I_{c1}(t_i)$, $I_{c2}(t_i)$, $I_{c3}(t_i)$ that repopulate can be related by the equation

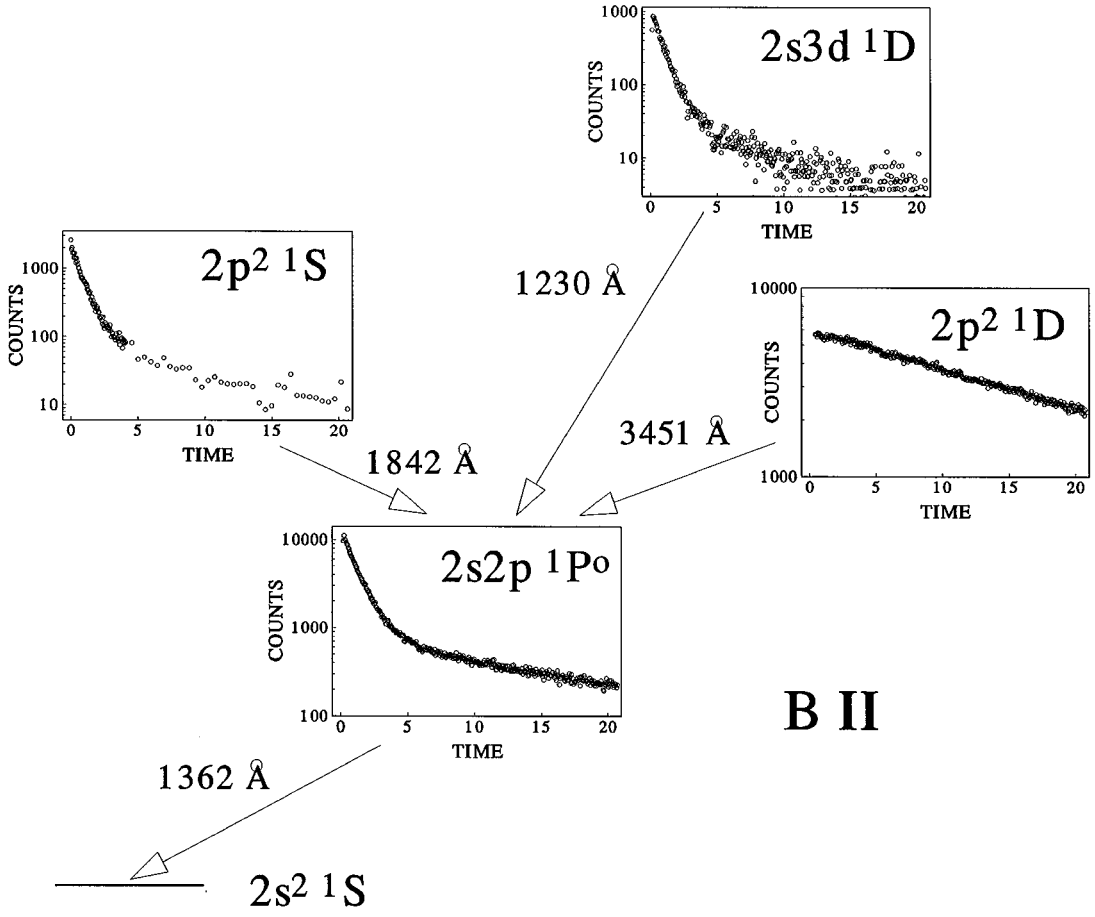
$$\frac{\mathrm{d}I_p}{\mathrm{d}t}(t_i) = \xi_1 I_{c1}(t_i) + \xi_2 I_{c2}(t_i) + \xi_3 I_{c3}(t_i) - \frac{I_p(t_i)}{\tau_p} \tag{1}$$

Here τ_p is the primary lifetime and the ξ_k are the undetermined normalizations of the cascade and primary decay curves. Thus, for each measured point (or panel of points used to compute the numerical derivative) t_i on the decay curves shown in Fig. 1, (1) provides a separate independent linear relationship connecting τ_p, ξ_1, ξ_2, and ξ_3. In the cases of both Be I and B II this ANDC analysis was able to reliably extract the lifetimes despite the fact that the multiexponential fits yielded only uncertain upper limits on the lifetimes.

In the case of Be I, the results of multiexponential fitting were approximately 1.80–1.85 ns, and thus close to the value given in ref. 1, 1.85±0.07 ns. However, the ANDC analysis resulted in a lifetime that is shorter by 4%, 1.77±0.05 ns. As can be noted, the difference between the lifetimes obtained by curve fit and by ANDC are within the uncertainties in this case. The reason that this agreement is achieved was pointed out already in ref. 1, i.e., the $2s2p\ ^1P$ lifetime is much shorter than the $2s3d\ ^1D$ and $2s4d\ ^1D$ ones and in such a case multiexponential fitting yields satisfactory results.

The situation is quite different for B II and other ions in the Be-sequence. In the present study, we obtained a $2s2p\ ^1P$ lifetime of about 0.96 ns when using a multiexponential DISCRETE fit, whereas the ANDC analysis yielded a lifetime 0.85±0.05 ns. This value is shorter by 11% (and outside of the uncertainties), and in excellent agreement with an earlier ANDC measurement by Bashkin et al. [4]. The difference in values between the multiexponential fit and the ANDC values is due to cascading from the $2p^2\ ^1S$, $2s3d\ ^1D$, and $2p^2\ ^1D$ level into $2s2p\ ^1P$. For B II and other Be-like ions the $2p^2\ ^1S$ and

Fig. 1. Schematic plot for B II of the decay curves of the primary level and its principal cascades, juxtaposed on a Grotrian diagram to illustrate their joint analysis by the ANDC method.



$2s2p\ ^1P$ levels have very similar lifetimes and this fact practically rules out obtaining reliable lifetime data from multiexponential fitting.

The ANDC analysis in this B II case was complicated by a strong sensitivity to the number of cascade decay curves included. We began by including only a single cascade in the analysis, but when each of the three cascades was used alone, it yielded nonphysical results (either negative values for τ_p and ξ, or a variation in the fit that was sensitive to the time region included). Similarly, when all three cascades were included a nonphysical negative value for ξ_2 resulted that produced a sensitivity in the fit to the time region included. A study of these results indicated that the decay curves of the $2p^2\ ^1S$ and $2s3d\ ^1D$ are very similar in shape, which causes the ANDC amplitudes (the ξ's in (1)) to be poorly determined. We found that by reducing the number of fitting parameters by including only the two $2p^2$ levels and not the $2s3d$ level in the ANDC analysis, the contribution of the $2s3d\ ^1D$ was effectively included, as evidenced by a constancy in the fit over a wide range of time regions. However, because of the similarity of the $2p^2\ ^1S$ and $2s3d\ ^1D$ decay curves, these results do not rule out the possibility that the $2s3d\ ^1D$ contributes significantly to the repopulation of the $2s2p\ ^1P$ level.

Table 1. Oscillator strengths of the $2s^2\ ^1S - 2s2p\ ^1P$ transition in Be I and B II.

		Oscillator strength			
Spectrum	Wavelength (Å)	Lifetime (ns)	Experiment	Semiempirical	Theory
Be I	2348.6	1.85±0.07[a]	1.34±0.05[a]	1.34±0.05[d]	1.374[f], 1.38[g]
		1.77±0.05[b]	1.40±0.04[b]	1.34[e]	1.375[h] 1.375[k]
B II	1362.4	0.86±0.07[c]	0.97±0.08[c]	0.97±0.02[d]	1.000[g], 0.998[i]
		0.85±0.05[b]	0.98±0.06[b]	0.97[e]	0.999[j]

[a] Martinson et al. [1].
[b] This work.
[c] Bashkin et al. [4].
[d] Reistad and Martinson. [7].
[e] Curtis and Ellis. [9].
[f] Chung and Zhu. [11].
[g] Weiss. [12].
[h] Fleming et al. [16].
[i] Fleming et al. [17].
[j] Godefroid et al. [14].
[k] Chen. [19].

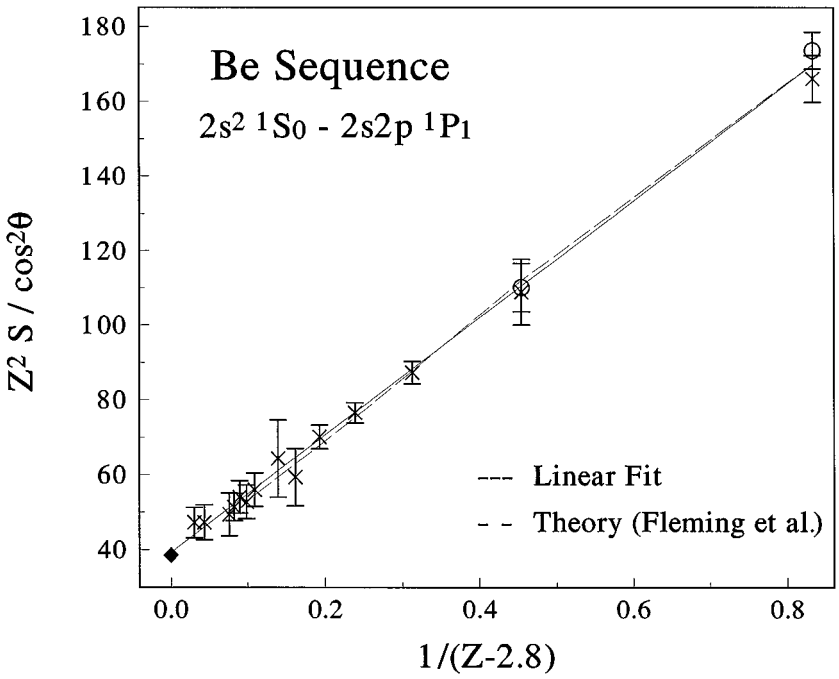
This result demonstrates that the inclusion of an inappropriate decay curve in the ANDC analysis can cause a linear least-squares fitting program to yield a nonphysical minimum. Thus, in cases where there are constraints on the allowable values for the fitting parameters, a nonlinear least-squares fitting program may have advantages. The nonlinear algorithm can search for a local minimum in the allowed region, whereas the linear fit obtains the absolute minimum regardless of the region. This tendency should be considered when the ANDC method is applied to cases that show this sensitivity.

The f-values computed from our new lifetime data are given in Table 1 together with some previous experimental values and with the results of recent elaborate theoretical studies, see refs. 11–20. Our ANDC determinations are of slightly higher precision than earlier measurements, and are in excellent agreement with these theoretical predictions. Our results also confirm the suggestion by Fleming et al. [16] that the earlier variational calculation of Sims and Whitten [2] slightly underestimated the f-value in Be I, and that the isoelectronic extrapolation [7] that seemed to confirm that result similarly underestimated the uncertainties in that procedure.

It has been demonstrated earlier [7–9] that the quantity $Z^2S/\cos^2\theta$ (where S is the line strength and θ is the singlet–triplet mixing angle determined from energy level data) can be represented as a nearly linear function of the reciprocal screened charge, and fitted to the form $A+B/(Z\text{-}C)$. This has been exploited to produce smoothed values that are more robust than individual data, which are valuable for comparison with isoelectronic trends of theoretical calculations. We have updated the exposition of this quantity that was presented in ref. 9 so as to include our new measurements, and the result is shown in Fig. 2. The symbols denote the measured data with error bars indicating quoted uncertainties. A linear fit to this exposition was made using the screening constant $C = 2.8$, which yielded fitting constants $A = 39.28$ and $B = 156.6$, and is indicated on the plot by a continuous line. The theoretical calculations of ref. 17 are indicated by a broken line.

While the experimental accuracies might be improved further through cascade-free selective excitation methods, these short wavelengths and lifetimes (particularly for B II) challenge existing laser methods. The agreement between recent calculations and our measurements, and the close agreement between theoretical and experimental isoelectronic behavior demonstrated in Fig.2, indicates that theoretical calculations for the Be sequence are now reliable to within 3% or better.

Fig. 2. Plot of the charge-scaled reduced line strength versus the reciprocal screened charge. The symbols (O) denote the measured data reported here, the symbols (X) denote the measured data obtained from the critical compilation reported in ref. 9, and the error bars represent their quoted uncertainties. The continuous line traces a linear fit to the data in this space, the broken line traces the theoretical calculations of ref. 17, and the diamond indicates the hydrogenic limit [9].



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