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Accurate transition probabilities in ions obtained by isoelectronic smoothing of line strengths

N. Reistad and I. Martinson
Department of Physics, University of Lund, S-223 62 Lund, Sweden
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Lifetime measurements, based on the method of beam-foil spectroscopy, together with careful corrections for cascade effects, have in recent years yielded the line strength of the $2s^2\,{}^1S-2s2p\,{}^1P^{\circ}$ transition in Be-like ions with uncertainties ranging from 3.4% to 8.1% in Be I–O V. By applying a method of isoelectronic smoothing of line strengths, similar to those earlier used for excitation energies and transition wavelengths, we have reduced the experimental uncertainties by about a factor of 2, to 1.9–3.6% for these transitions. The fitted results are in excellent agreement with the best theoretical data. The applicability of this method to other isoelectronic sequences is briefly discussed.

I. INTRODUCTION

A variety of experimental methods has been developed for the determination of lifetimes and transition probabilities in atoms and ions.[1,2] The experimental uncertainties are typically in the 5–20% range. In recent years new techniques have been introduced which allow more accurate measurements. In particular, the fast beam laser technique (FBL), developed by Andrä *et al.*[3] has made it possible to measure lifetimes with errors as low as 0.1–0.2% in favorable cases, see e.g., Gaupp *et al.*[4] and Hartmetz and Schmoranzer.[5] There is also one beam-foil measurement[6] of a comparable accuracy, 0.26%.

Although it can provide highly accurate results for neutral and singly ionized atoms, the FBL method usually cannot be extended to multiply charged species. In the latter the transition wavelengths, particularly of the resonance lines, are normally too short in comparison with the radiation available from a tunable dye laser. Practically all experimental lifetimes for multiply charged atoms are instead based on beam-foil measurements. In most cases such data have quoted errors of around 10%. However, several investigators[7–9] have critically evaluated beam-foil results and thereby questioned the reported uncertainties. In contrast to optical excitation, used in FBL experiments, the beam-foil interaction is not selective. A large number of levels in an atom or ion can consequently be populated. This may lead to chain decays and cascading processes. Hence, the decay curves obtained in beam-foil measurements represent superpositions of several exponentials. Partly because of numerical problems, standard curve-fitting methods may not provide the correct lifetime values.

Fortunately, efficient techniques for cascade corrections have been developed, which remove many problems. The most successful approach, usually called ANDC (arbitrarily normalized decay curves) was introduced by Curtis *et al.*[10] in 1971. It requires measurement of the decay curves of the levels directly combining with the so-called primary level, the lifetime of which is under study. By inserting all the measured data into a population equation, the lifetime of the primary level can be extracted, free from systematic errors caused by cascading. Such analyses are facilitated by the computer program CANDY, developed by Engström.[11] We have successfully applied the ANDC/CANDY method to rather complicated decay processes in, e.g., Be-like,[12–14] Na-like,[15–17] and Mg-like[17,18] ions, and thereby determined lifetimes with typical uncertainties of 3–7%. In all cases the data were in excellent agreement with the results of elaborate theoretical investigations. Similar work has also been carried out by other beam-foil groups, references being found in the review of Pinnington.[19]

If the experimental accuracy could be improved even further, a more detailed comparison with theoretical data would be possible. It was concluded by Ekberg *et al.*[15] in their study of lifetimes for S VI, that significant reductions of the error limits, e.g. by further improving the statistics, did not appear to be straightforward or easy. In this paper we therefore propose a different approach, which takes advantage of some well-known regularities for oscillator strengths (f) and line strengths (S) for transitions in isoelectronic sequences. The method will be tested for the $2s^2\,{}^1S-2s2p\,{}^1P^{\circ}$ resonance transition in the Be I isoelectronic sequence, for which many experimental and theoretical results can be found in the literature.

II. ISOELECTRONIC SMOOTHING OF LINE STRENGTHS

The excitation energies and transition wavelengths along isoelectronic sequences show well-known regularities, as discussed, e.g., by Edlén.[20] In a number of recent articles Edlén[21] has reported detailed investigations of such Z dependent regularities for the $n=2$ complex in ions isoelectronic with Li–F. Such analyses test the experimental identifications, reveal incorrect assignments, and provide simple numerical relations, which are suitable for interpolation and extrapolation purposes.

Similar regularities also exist for oscillator strengths (f) and line strengths (S). A Z^{-1} perturbation expansion leads to the following well-known expressions

$$f = f_0 + f_1 Z^{-1} + f_2 Z^{-2} + \cdots , \tag{1}$$

$$Z^2 S = S_0 + S_1 Z^{-1} + S_2 Z^{-2} + \cdots , \tag{2}$$

see, e.g., Wiese and Weiss,[22] Dalgarno[23] and Hibbert.[24] These relations are used to investigate systematic trends and regularities for transition probabilities, often by graphically displaying f versus $1/Z$, see, e.g., Smith and Wiese.[25] Another way of expressing the line strength S is

$$S = S_0/(Z-s)^2 , \tag{3}$$

where S_0 is a parameter which depends on the transition and s is a measure of the screening.[26,27] This expression is essentially equivalent with Eq. (2). However, since the Z^{-1} expression does not work very well at the low-Z end of an isoelectronic sequence, alternative expressions have been introduced. Thus Laughlin[28,29] has suggested a $(Z-s)^{-1}$ expansion in the form

$$S = [I_0(Z-s)^{-1} + (I_1 - I_0)(Z-s)^{-2}]^2 . \tag{4}$$

Here I_0 and I_1 are the zero- and first-order terms of the transition matrix element. This expression has been shown to work well for the He I and Li I sequences.[28,29]

A "continued screening approximation", in which the Z dependence of the screening parameter is taken into account in a detailed way, has been introduced by Froese Fischer.[30] This approach has also been extended to forbidden transitions.[31]

In a semiempirical study of f value regularities Mewe[32] used a relation of the type

$$f = A(Z+B)^{-1} + C(Z+D)^{-2} \tag{5}$$

to describe the Z dependence of oscillator strengths for $\Delta n = 0$ resonance transitions. Here A, B, C, and D were treated as adjustable parameters.

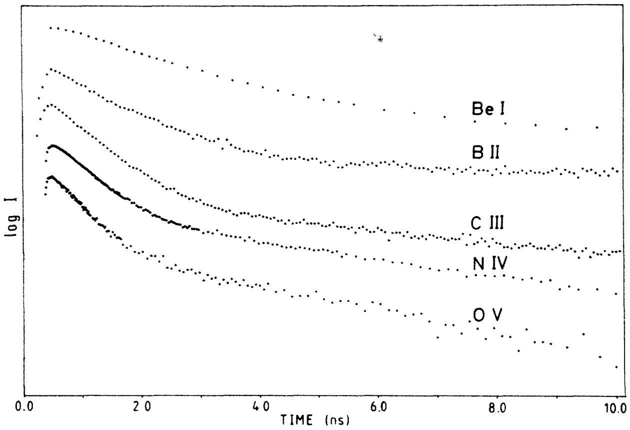

FIG. 1. Some representative decay curves of the $2s2p\ ^1P^{\circ}$ level in Be I–O V, determined in Refs. 12–14 and 35. The graphs show only the first 10 ns of the decays and the curves have been shifted vertically for the purpose of illustration. The differences in slope and cascading effects are clearly visible.

In connection with Hartree-Fock calculations of line strenghts for the resonance lines in the Li I, Na I, and Cu I isoelectronic sequences, Weiss[33] used the relation given in Eq. (2) and presented the results in the form of Z^2S versus $1/Z$. Subsequently Edlén[34] pointed out that the line strengths could be expressed by the relation

$$Z^2 S = S_0 + a(Z-s_1)^{-1} + b(Z-s_2)^{-2} . \tag{6}$$

For example, in the case of the $3s\ ^2S_{1/2}$–$3p\ ^2P^{\circ}_{1/2}$ line in Na-like ions, the fitted constants were $S_0 = 101.9$ $a = 1588$, $b = -0.0044$, $s_1 = 9.9$, and $s_2 = 10$. The main advantage of Edlén's modification was the increased linearity, useful for interpolations and extrapolations.

It is thus obvious that there exist several relations which describe the Z dependence of line strengths. Such relations are useful when fitting the experimental data along isoelectronic sequences. The results could then form a set of smoothed experimental values which show smaller uncertainties than those of the individual measurements.

In our first analysis along these lines we have used as input data the experimentally determined lifetimes of the first excited term, $2s2p\ ^1P^{\circ}$ in the important four-electron systems Be I–O V. This material originates from beam-foil measurements. The results for B II–O V (Refs. 12–14), were obtained by applying the ANDC/CANDY analysis technique for cascade corrections, whereas multiexponential fitting was used in the case of Be I.[35] In the latter case cascading is much less severe, because the im-

TABLE I. Experimental data for the $2s^2\ ^1S$–$2s2p\ ^1P^{\circ}$ transition in Be I–O V.

Spectrum	Z	Wavelength (Å)	Lifetime (ns)	Oscillator strength	Line strength
Be I	4	2 348.610[a]	1.85±0.07[d]	1.341±0.051	10.37±0.39
B II	5	1 362.461[b]	0.86±0.07[e]	0.971±0.079	4.35±0.35
C III	6	977.026[c]	0.57±0.02[f]	0.753±0.026	2.422±0.085
N IV	7	765.144[c]	0.425±0.015[g]	0.619±0.022	1.560±0.055
O V	8	629.730[c]	0.338±0.015[g]	0.528±0.023	1.094±0.049

[a] Johansson (Ref. 38). [b] Ölme (Ref. 39). [c] Edlén (Ref. 37). [d] Martinson *et al.* (Ref. 35). [e] Bashkin *et al.* (Ref. 13). [f] Reistad *et al.* (Ref 14). [g] Engström *et al.* (Ref. 12).

portant $2p^2\,{}^1S$ level lies above the ionization limit and mainly decays by autoionization,[36] whereas the other cascading levels all have much longer lifetimes than $2s2p\,{}^1P^o$. To illustrate the quality of the data Fig. 1 displays some decay curves, recorded in Refs. 12—14 and 35.

The experimental lifetimes are quoted in Table I. It can be noted that the errors range from 3% to 8%. Using tabulated wavelengths for the $2s^2\,{}^1S$–$2s2p\,{}^1P^o$ resonance transition[37–39] we have also computed experimental oscillator strengths and line strengths.

In trying to find a suitable expression for fitting the experimental material it is important to have as few adjustable parameters as possible. Furthermore, the expression should vary smoothly with Z and not be unphysical. A fit of S (and not f) appears as preferable. Indeed it turns out that a simplified version of the relation provided by Edlén,[34] viz.,

$$Z^2S = S_0 + a(Z-s)^{-1} \tag{7}$$

is well suited for the present purpose.

Using the method of least squares[40] we fitted to Eq. (7) the experimental line strengths (Table I), with their individual weights determined by the quoted experimental uncertainties. The following linear relation was thereby obtained:

$$Z^2S = 42.54 + 140.62/(Z-2.86)\ . \tag{8}$$

(Also see Fig. 2).

It is worth noting that when Eq. (3) is applied to the resonance line in Be-like ions, the calculations of Cohen and Dalgarno[26] gave $S_0 = 41.06$ and $s = 1.93$, whereas the corresponding values of Viktorov and Safronova[27] were $S_0 = 48$ and $s = 1.9122$.

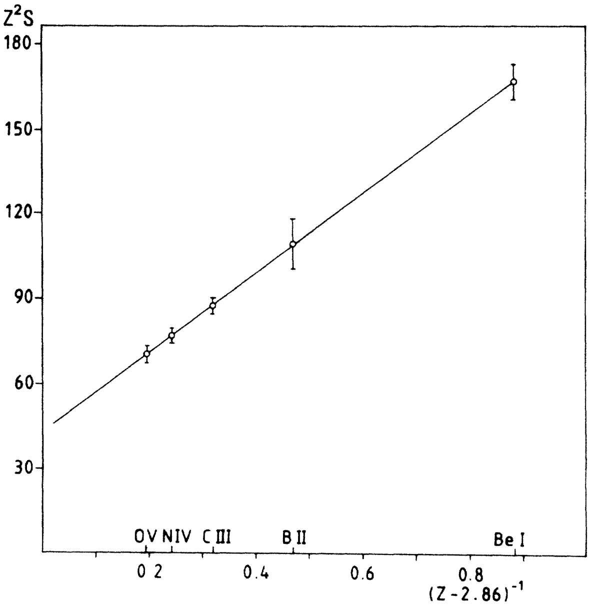

FIG. 2. Graphic presentation of the fitted polynomial given in Eqs. (7) and (8), for the $2s^2\,{}^1S$–$2s2p\,{}^1P^o$ transition in the Be I isoelectronic sequence. The experimental points used in the fit are marked with circles and error bars.

It is interesting to compare the value $s = 2.86$, which represents the best fit to our experimental line strengths, with the data obtained from spectroscopic term values T for the $2s^2\,{}^1S$ and $2s2p\,{}^1P^o$ levels in Be I—O V. Using the well-known relation $T = R(Z-s)^2/n^2$ we find that s varies from 2.34 to 2.21 for the ground state and from 2.91 to 2.74 for the excited state in the range $Z = 4$–8. These experimental numbers are rather close to our fitted value, $s = 2.86$.

The line strengths and oscillator strengths computed with Eq. (8) are given in Table II. Using the method of error propagation[40] we have calculated the internal errors which are also included in the table. A comparison of Tables I and II shows that all the smoothed line strengths remain close to the input data whereas the uncertainties have decreased. While there is not much change in the case of Be I, the B II uncertainty has been reduced by about a factor of 3. Also for C III—O V there are significant changes. We can conclude that the isoelectronically fitted line strengths have uncertainties as low as 1.9—3.6%. The external errors, originating from the spread of the input data were found to be 0.1—0.2% and thus much smaller than the internal errors, quoted here. This fact indicates that the error estimates in the literature (Table I) may be too large.

In his semiempirical studies of energy levels Edlén[21] has frequently taken advantage of a consistent set of theoretical data, the multiconfiguration Dirac-Fock (MCDF) calculations of Cheng *et al.*[41] The Z dependence of the difference between experimental and theoretical excitation energies was used by Edlén for extrapolation and interpolation purposes.

We have also tried a similar approach in the present analysis of f values. For theoretical data we used the model-potential results of Laughlin *et al.*[42] We formed the differences between experimental and theoretical line strengths and tried to fit them to a linear relation. This approach also worked well and it gave results very close to those obtained using Eq. (8). However, no improvement in accuracy was obtained. The first method used ought therefore to be preferred from the experimental point of view, because knowledge of theoretical line strengths is not required.

The smoothing procedure would only work well when the data are free from major systematic errors. If one or more of the values used as inputs were of lower quality, they might influence the other data in a nondesired way. We have tested such possibilities, using early beam-foil data for B II and O V, determined from multiexponential

TABLE II. Results of isoelectronic smoothing of the $2s^2\,{}^1S$–$2s2p\,{}^1P^o$ line strengths in Be I—O V.

Spectrum	Oscillator strength	Line strength
Be I	1.341±0.047	10.37±0.37
B II	0.965±0.020	4.330±0.092
C III	0.754±0.014	2.426±0.045
N IV	0.620±0.014	1.561±0.035
O V	0.527±0.014	1.092±0.030

fitting of decay curves.[43,44] However, the use of one or both of these data points resulted in totally erroneous fits for the whole sequence and such effects could be easily spotted.

III. DISCUSSION

We have introduced a method of isoelectronic smoothing of line strengths and applied it to the resonance transition in Be I—O V. In this way it has been possible to significantly lower the experimental uncertainties. The improvement is graphically shown in Fig. 3 where we compare our final data with the important theoretical results of Sims and Whitten[45] who performed very elaborate configuration-interaction calculations of f values for Be I, C III, and O V. Using a procedure introduced by Weinhold,[46] Sims and Whitten were able to provide rigorous theoretical upper and lower bounds, typically 7—10%, while their estimated uncertainties were as low as 2%. Figure 3 makes clear that the experimental data are in perfect agreement with these theoretical results. The estimated theoretical uncertainties of 2% appear as realistic.

There exist many additional experimental lifetime results for the $2s2p\,^1P^{\circ}$ level in Be-like ions, up to Fe XXIII. However, we have not included them in the present analysis, mainly because most of the published data for F VI—Fe XXIII are based on multiexponential fitting of decay curves, and they may not be entirely free from systematic errors caused by cascading. Furthermore, several of the spectra beyond F VI are not sufficiently well investigated. There are thus possibilities of line blends in the beam-foil spectra which may complicate lifetime determinations. For example, Engström[47] has recently found that the $2s^2\,^1S$—$2s2p\,^1P^{\circ}$ resonance line in F VI (535.207 Å) is severely blended by another F VI transition ($2p3d\,^1F_3$—$2p4f\,^1G_4$). This fact was not known when the beam-foil lifetime determinations[48,49] were carried out. Both for F VI and Ne VII, an extrapolation based on our data for Be I—O V is probably more accurate than the results of earlier, direct measurements. To further test the extrapolation procedure, we have compared our values, based on Eq. (8) with the results of the MCDF calculations of Cheng *et al.*,[41] as shown in Fig. 4. At low Z, where the MCDF method is not expected to be very accurate, the smoothed f values are lower than the theoretical results. The agreement tends to improve when Z increases and there is a region in which the extrapolated and calculated f values are very close (see Fig. 4). Furthermore, by including the second-degree term in the formula provided by Edlén, i.e., Eq. (6), the data of Cheng *et al.*[41] could be reproduced for very high values of Z. This fact should provide additional support of the validity of the simple formula used in our smoothing procedure. However, additional ANDC/CANDY measurements of the $2s^2\,^1S$—$2s2p\,^1P^{\circ}$ transition probability in Be-like ions, preferably for high values of Z, appear as desirable to further test the present conclusions and reduce the experimental uncertainties. We have recently been informed that such studies are in progress.[50]

In this paper we have only discussed the resonance transition in the Be I sequence. However, the same method of reducing the uncertainties can be applied to other transitions, both in the Be I and other sequences.

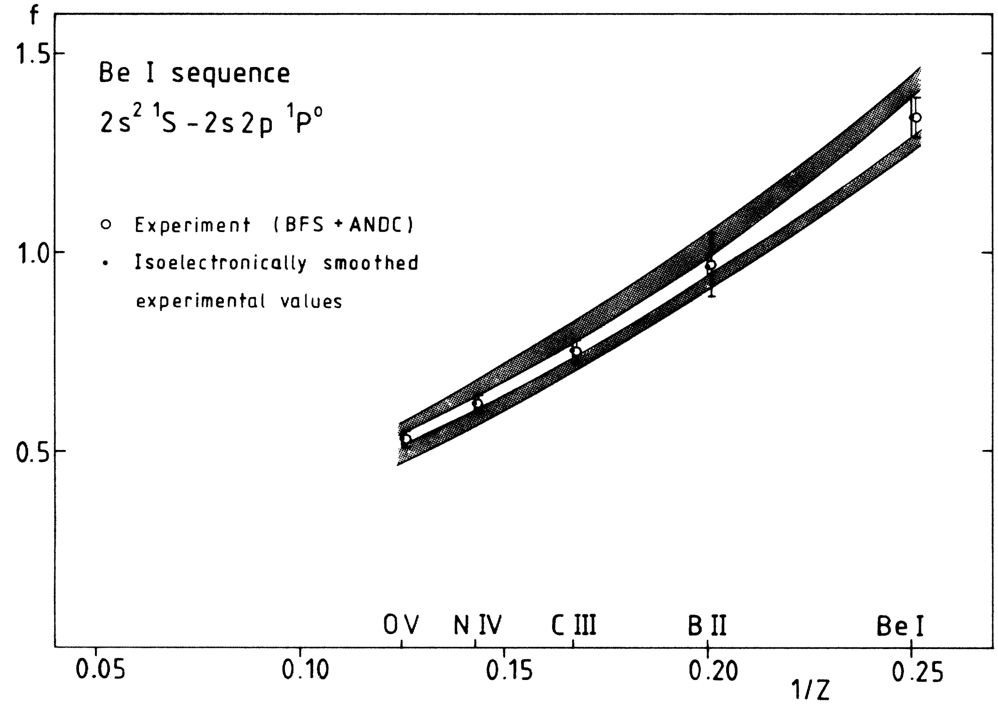

FIG. 3. Isoelectronic plot of the oscillator strengths for the $2s^2\,^1S$—$2s2p\,^1P^{\circ}$ transition in the Be I sequence. The shaded area represents the theoretical limits given by Sims and Whitten (Ref. 45), while the white area inside it is the limit obtained in the present work by means of isoelectronic smoothing.

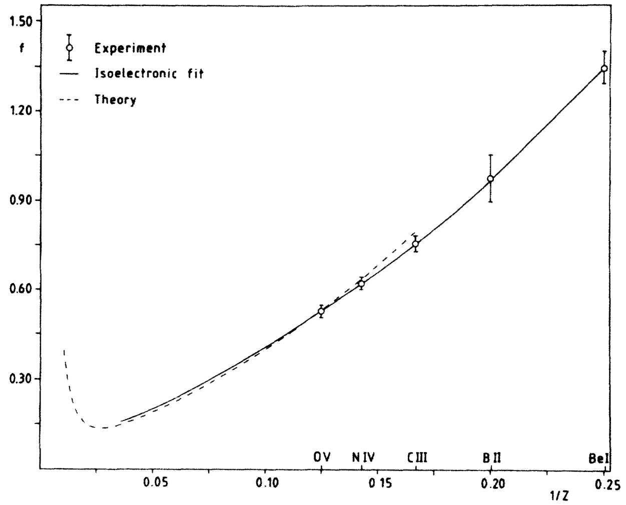

FIG. 4. Systematics of the f values for the $2s^2\,{}^1S$—$2s\,2p\,{}^1P^\circ$ transition in Be I sequence. The data points, indicated with circles and error bars, are from Refs. 12—14 and 35. The dashed line represents the MCDF calculations by Cheng *et al.* (Ref. 41). The f values obtained when combining experimental wavelengths (Refs. 37—39) and the oscillator strengths calculated from the fitted polynomial are displayed with the solid line. Note that for F VI—Ni XXV this graph represents an extrapolation (see discussion in the text).

We have made preliminary analyses for the resonance lines in the Na I and Mg I sequences. Here, also, the accuracy can be significantly improved by the smoothing procedure. Some difficulties are encountered in these cases, however, mainly because the amount of data based on accurate cascade corrections is not sufficiently high. Additional experiments are therefore urgently needed.

It should perhaps be pointed out that the simple method applied in the present paper has some limitations. For example, there may occur f value anomalies along isoelectronic sequences, a well-known case being the extremely low f value for the $2s^2 2p\,{}^2P^\circ$—$2s^2 3s\,{}^2S$ multiplet in B-like C II, see, e.g., Reistad *et al.*[14] and Weiss.[51] In such cases the simple equations used here would not hold. However, somewhat more complicated sums of terms could be tried to describe the Z dependence of the f values,[52] which may make it possible to extend the method even to those cases.

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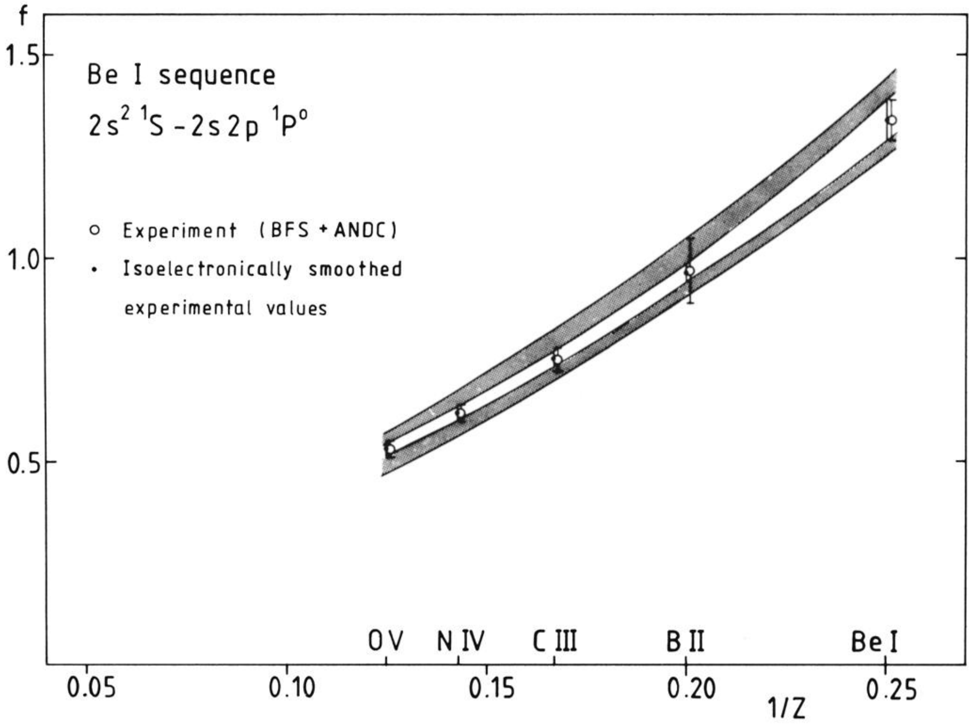

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