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Electron Impact Excitation Cross Sections for B III*

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Abstract

A realistic analytical central potential with two adjustable parameters is used to generate wavefunctions for the ground and excited states of doubly ionized boron. Generalized oscillator strengths and integrated cross sections from threshold up to 5 keV are calculated in the Born approximation for 2s–*n*s, 2s–*n*p and 2s–*n*d excitations. Convenient analytic formulae for the cross sections are presented.

1. Introduction

Atomic excitation cross sections are useful in probing the details of atomic structure. It is important for the atomic theorist to be able to make accurate calculations of atomic excitation cross sections. When accurate experimental data exist, the calculations serve as a test of atomic theories and methods of calculation.

Electron impact excitation of positive ions plays an important role in many astrophysical phenomena (Seaton 1975) and in the analysis of impurities in controlled thermonuclear devices (McDowell and Ferendeci 1980). Direct measurement of the cross sections is extremely difficult, and theory must be relied upon to provide the vast majority of required data. In this study we calculate generalized oscillator strengths (GOS) and integrated cross sections for the electron impact excitation of B III in the Born approximation. We consider transitions involving the promotion of the valence electron into various s, p, d excited states.

The potential for the valence electron in B III is assumed to have the form

$$V(r) = -(2/r)[2\{H(e^{r/d}-1)+1\}^{-1}+3], \tag{1}$$

where r is the electron–nucleus distance, and d and H are adjustable parameters. This potential is inserted into the radial Schrödinger equation

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V(r)+E_{nl}\right)P_{nl}(r) = 0, \tag{2}$$

which is solved numerically by a Noumerov method to obtain the energy eigenvalues E_{nl} and wavefunctions $P_{nl}(r)/r$ of the active electron. In a previous article (Ganas 1979) it was shown that if the potential parameters are chosen to be $d = 0{\cdot}1885$ and

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$H = 0\cdot5819$, then the potential given by equation (1) reproduces the observed energy levels of B III very accurately, and gives optical oscillator strengths (OOS) which are in good agreement with experiment and other methods of calculation. The OOS are reproduced in Table 1. The importance of obtaining good agreement with experiment for the OOS lies in the fact that the accuracy of the cross sections is determined mainly by the accuracy of the OOS. This is discussed in Section 3.

Table 1. OOS values for the transitions $1s^2 2s(^2S) \rightarrow 1s^2 np(^2P)$ **in B III**

2s to	Ganas (1979)	Other calculations	Experiment
2p	0·3663	0·366[A]	0·43[C]
		0·3664[B]	0·342[D]
		0·3630[E]	
3p	0·1535	0·151[A]	
		0·1509[B]	
4p	0·0498	0·0486[A]	
5p	0·0225	0·0241[A]	

[A] Martin and Wiese (1976). [B] Weiss (1963).
[C] Bromander (1971). [D] Andersen *et al.* (1969).
[E] Onello *et al.* (1974).

2. Generalized Oscillator Strengths

We give a brief description of the general formulae used in this work. Derivations may be found in a previous article (Kazaks *et al.* 1972). We consider the transition of an atom from its ground state with momentum transfer $\boldsymbol{K}$. We define $x = K^2 a_0^2$, where a_0 is the Bohr radius; $x_t = W/R$, where W is the transition energy and R the Rydberg energy; and $\xi = x/x_t$. We suppose that the atom is initially in a state characterized by quantum numbers L_i, S_i, J_i, M_i. After the active electron has been promoted from an $n_0 l_0$ orbital to an nl orbital, the atom is in a final state which has quantum numbers L_f, S_f, J_f, M_f. Only transitions with $S_f = S_i$ are considered.

By using the first Born approximation and assuming LS coupling for the initial and final states, it can be shown that the GOS is given by

$$f_{L_f J_f}(\xi) = \sum_L C_L(2l_0+1)(2l+1)(2L+1)\begin{pmatrix} l_0 & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 S_L^2, \tag{3}$$

where

$$S_L = \xi^{-\frac{1}{2}} \int_0^\infty \mathrm{P}_{n_0 l_0}(r)\,\mathrm{j}_L(Kr)\,\mathrm{P}_{nl}(r)\,\mathrm{d}r, \tag{4}$$

$$C_L = N_0 F^2(2L_i+1)(2L_f+1)(2J_f+1)\begin{Bmatrix} L_f & L & L_i \\ l_0 & L_c & l \end{Bmatrix}^2 \begin{Bmatrix} J_i & L & J_f \\ L_f & S_i & L_i \end{Bmatrix}^2. \tag{5}$$

The array in the large parentheses in equation (3) is a $3j$ symbol, and the arrays in the braces in equation (5) are $6j$ symbols. The quantities $\mathrm{P}_{n_0 l_0}(r)/r$ and $\mathrm{P}_{nl}(r)/r$ are the radial wavefunctions for the single-particle excitations, and $\mathrm{j}_L(Kr)$ is a spherical Bessel function. The quantity N_0 in equation (5) is the number of electrons in the active subshell, and F is the coefficient of fractional parentage for constructing the initial state $(n_0 l_0)^{N_0} S_i L_i$ from the core state $(n_0 l_0)^{N_0-1} S_c L_c$ and an $n_0 l_0$ electron.

We are interested in the total GOS for a given single-particle excitation:

$$f(\xi) = \sum_{L_f J_f} f_{L_f J_f}(\xi)\,. \tag{6}$$

The final expression for the total GOS is

$$f(\xi) = N_0 F^2 \sum_L (2l+1)(2L+1) \begin{pmatrix} l_0 & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 S_L^2\,. \tag{7}$$

Using equation (7) we have computed the GOS for various excitations from the 2s ground state. The results are typical of those obtained in similar studies (Ganas 1981), and are not shown here. Essentially, as $\xi \to 0$, we have

$$\text{the GOS} \to \text{the OOS for 2s–}n\text{p} \tag{8a}$$

$$\to 0 \text{ for 2s–}n\text{s and 2s–}n\text{d}\,. \tag{8b}$$

As ξ increases from zero, the GOS pass through the usual series of minima. To facilitate use of the GOS in applications, we have parametrized all the GOS with simple analytical forms which are accurate in the region in which the GOS is significantly large. For the optically allowed transitions 2s–np, we use the form

$$f(\xi) = A(\mathrm{e}^{-\alpha\xi} + \beta\xi\mathrm{e}^{-\gamma\xi})^2\,, \tag{9}$$

and for the optically forbidden transitions 2s–ns and 2s–nd, we use

$$f(\xi) = \xi A(\mathrm{e}^{-\alpha\xi} + \beta\xi\mathrm{e}^{-\gamma\xi})^2\,. \tag{10}$$

In equations (9) and (10), the quantities A, α, β, γ are adjustable parameters. For 2s–np we set A equal to the OOS values, which were found in previous work (Ganas 1979) and which are reproduced in Table 1, and vary the three parameters α, β, γ so as to obtain the best fit to the numerical GOS. For 2s–ns and 2s–nd, all four parameters A, α, β, γ are varied. The final values of these parameters are given in Table 2.

Table 2. Values of A, α, β, γ in equations (9) and (10)

2s to	A	α	β	γ
2p	0·3663	0·2551	0·0681	0·1777
3p	0·1535	2·2701	−0·7838	0·7720
4p	0·0498	0·4822	−1·9601	0·8483
5p	0·0225	0·3712	−1·9238	0·7780
3s	0·3515	1·1361	1·1816	10·11
4s	0·0664	1·2547	1·3135	2·4269
3d	0·9829	1·3793	0·1559	0·8549
4d	0·1387	0·8681	1·1088	2·6286

3. Cross Sections

The integrated cross section is defined by

$$\sigma = \frac{q_0}{WE} \int_{\xi_1}^{\xi_u} \frac{f(\xi)}{\xi}\,\mathrm{d}\xi\,, \tag{11}$$

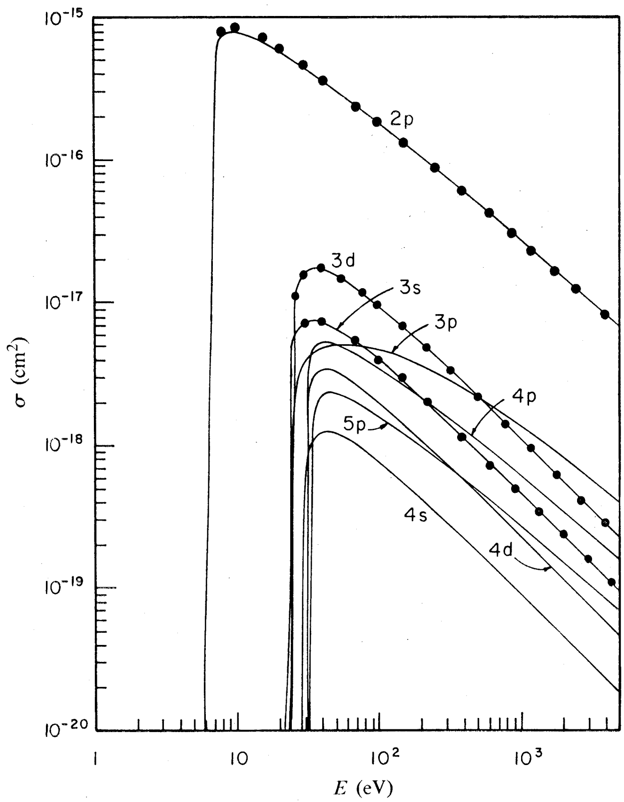

Fig. 1. Integrated cross sections for 2s–*n*s, 2s–*n*p and 2s–*n*d excitations in B III. The points are representative analytic fits using equation (15) with the parameter values of Table 3.

where W is the transition energy in eV, E is the incident electron energy in eV, $q_0 = 6{\cdot}514 \times 10^{-14}\,\text{cm}^2\,\text{eV}^2$, and

$$\xi_{\text{u,l}} = (2E/W)\{1 \pm (1 - W/E)^{\frac{1}{2}} - W/2E\}. \tag{12}$$

Equations (9) and (10) correspond, respectively, to the first three terms and the first four terms of the general form

$$f(\xi) = \sum_{s=0}^{\infty} f_s \xi^s \exp(-\alpha_s \xi). \tag{13}$$

On substituting equation (13) into (11), the integrated cross section is obtained in closed form:

$$\sigma(E) = \frac{q_0}{WE}\left(f_0\{\text{E}_1(\alpha_0 \xi_1) - \text{E}_1(\alpha_0 \xi_u)\} + \sum_{s=1}^{\infty} \frac{f_s}{\alpha_s^s}\{\gamma(s, \alpha_s \xi_u) - \gamma(s, \alpha_s \xi_1)\}\right). \tag{14}$$

Here E_1 is the first exponential integral function and $\gamma(s, y)$ is the incomplete gamma function. The computed integrated cross sections for various excitations of the valence electron, for incident electron energies ranging from threshold to 5 keV, are displayed in Fig. 1. We see that the 2s–2p transition is a resonance. No experimental cross sections are available, so that a direct comparison of the present results with experiment is not possible. However, the accuracy of the present cross sections for the allowed transitions may be inferred from the accuracy of the OOS, since the Born cross section is proportional to the OOS (Inokuti 1971; Kim and Bagus 1973; Heddle 1979). Since the present values of the OOS for these transitions are within 7% of experimental and theoretical data (see Table 1), this suggests that the present cross sections have an accuracy of 7% or better at those energies at which the plane-wave Born approximation is valid.

For problems such as electron-energy deposition in plasmas, atomic excitation cross sections are needed as input data. For this purpose it is useful to have analytic representations of the cross sections. For all the transitions we find that the cross sections at different energies can be represented by the formula (Peterson *et al.* 1973)

$$\sigma = cq_0 \frac{f}{W^2}\left(\frac{W}{E}\right)^s\left(1-\frac{W}{E}\right)^t, \tag{15}$$

where q_0, W and E have their usual meaning (see equation 11) and the quantities c, f, s, t are adjustable parameters. We set f equal to A as given in Table 2. After some experimentation it was found that we could set $s = 0\cdot847$ and $t = 0\cdot5$ for the transitions 2s–np, and $s = 1$ and $t = 0\cdot528$ for the transitions 2s–ns and 2s–nd. We then have only the one parameter c to vary. The final values of all the parameters are given in Table 3. Some representative fits are shown in Fig. 1.

Table 3. Values of c, f and W in equation (15)

For the transitions 2s–np: $s = 0\cdot847$, $t = 0\cdot5$.
For the transitions 2s–ns and 2s–nd: $s = 1$, $t = 0\cdot528$

2s to	c	f	W (eV)
2p	3·1235	0·3663	6·0
3p	1·0398	0·1535	23·92
4p	3·3655	0·0498	30·11
5p	3·6436	0·0225	32·95
3s	0·4583	0·3515	22·34
4s	0·6264	0·0664	29·47
3d	0·4339	0·9829	24·31
4d	0·7825	0·1387	30·27

4. Conclusions

The purpose of this work has been to generate electron impact excitation cross sections for B III which may be useful for practical applications of atomic theory. Using a semiempirical analytic central potential and the Born approximation, we have calculated cross sections for 2s–ns, 2s–np and 2s–nd excitations.

The present approach is directed towards practical applications of atomic theory. By adjusting the two potential parameters to reproduce the experimental energy levels, it is assured that the present model provides a realistic representation of the B III ion.

In this work we have obtained a number of useful phenomenological relationships. Equation (15) is a formula for all the cross sections which may be useful for providing input data for electron-energy deposition problems, and for other problems of applied physics.

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