# Electron collisional excitation of beryllium-like ions: $C^{2+}$ , $N^{3+}$ , $O^{4+}$ and $Ne^{6+}$

Shinobu Nakazaki and Tasuke Hashino

Department of Applied Physics, Faculty of Engineering, Miyazaki University, Miyazaki 880, Japan

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**Abstract.** The Coulomb-Born and Coulomb-Born-Bely approximations have been used to calculate the cross sections of electron impact excitation for six allowed transitions in the beryllium-like ions C<sup>2+</sup>, N<sup>3+</sup>, O<sup>4+</sup> and Ne<sup>6+</sup>. The cross sections have been obtained for electron impact energies from threshold to the high-energy region. We find that the Coulomb-Born-Bely calculation gives good results comparable with the distorted-wave calculation.

#### 1. Introduction

Electron impact excitation cross sections are required for various applications in fusion research, ion laser studies, astrophysics and atmospheric physics. In particular, the data for impurity ions in fusion plasmas are important in the study of the radiative power loss and the diagnostic problem. An accuracy of the cross section better than 20% is desired.

Seaton (1975) has reviewed theories for excitation of positive ions by electron impact to 1975. Recently, Henry (1981) has published a comprehensive review article to 1980 on theoretical methods and results. He has attempted to assess the reliability of collision strengths to  $\pm 20\%$ . For beryllium-like ions, he has concluded that it is necessary to use accurate configuration-mixed wavefunctions in order to obtain collision strengths accurate to 20%, and that the choice of scattering approximation is not as important as target wavefunctions, provided allowance is made for correlation terms.

So far, the cross sections for beryllium-like ions, by using the distorted-wave (DW) and close-coupling (CC) approximations, have been calculated by many theoreticians (Eissner 1971, Flower and Launay 1973, Malinovsky 1975, Norcross 1977, Younger 1980, Mann (quoted in Merts et al 1980), Peek (quoted in Merts et al 1980), Berrington et al 1977, 1979, Robb (quoted in Merts et al 1980)). The DW and CC approximations are available to obtain the cross sections for low incident electron energy. On the other hand, the Coulomb-Born (CB) and Coulomb-Born-Oppenheimer (CBO) approximations, which are simple methods, are useful to calculate the cross sections for high incident energies. The cross sections for beryllium-like ions have been calculated by a few theoreticians for various transitions by using the CB or CBO approximations. In particular, for allowed transitions there are a few data obtained by the CB and CBO approximations. Nakazaki and Hashino (1977) have made calculations in the CB approximation for  $C^{2+}$ ,  $N^{3+}$ ,  $O^{4+}$  and  $Ne^{6+}$  ions for the  $2s^2 \cdot S \rightarrow 2s2p \cdot P$ 

transition. Younger (1980) has studied  $O^{4+}$  for the same transition using the CB and CBO approximations and also the DW approximation. Mann (quoted in Magee et al 1977) has calculated the collision strengths in  $C^{2+}$  for some transitions by using the CB and CBO approximations. Sampson et al (1980) and Clark et al (1980) have calculated the collision strengths for fine-structure transitions between states of the  $2s^2$ ,  $2p^2$  and 2s2p configurations in ions with nuclear charge number Z in the range  $14 \le Z \le 74$ . They have used the CBO approximation in the limit  $Z \to \infty$ . An inclusion of electron exchange is found to be important at low incident energies.

Bely (1966, 1967) has generalised the Ochkur-Rudge approximation for the exchange amplitude in the neutral atom to the electron-ion collision. His approximation for the exchange amplitude, which we shall call the Coulomb-Born-Bely (CBB) approximation, has the advantage of being simpler to apply than the CBO approximation. Few applications of the CBB approximation have been made. Bely (1967) has calculated excitation cross sections for the  $^3P \rightarrow ^1D$  transition in the ground configuration of several silicon- and carbon-like ions at threshold energy. Tully (1980) has applied it to obtain the cross sections for some  $1^1S \rightarrow n^3L$  transitions in helium-like ions. Nakazaki and Hashino (1982) have calculated the cross sections for  $1^1S \rightarrow 2^1S$  and  $1^1S \rightarrow 2^1P$  transitions in helium-like ions.

The purpose of this investigation is to obtain the electron impact cross sections for six allowed transitions in beryllium-like ions by using the CB and CBB approximations. The present results are compared with the previous DW and CC results. Relativistic effects have been neglected in this paper. Atomic units are used unless otherwise stated.

## 2. Target wavefunctions

We have used 2s<sup>2</sup> <sup>1</sup>S, 2s2p <sup>3</sup>P, <sup>1</sup>P, 2p<sup>2</sup> <sup>3</sup>P, <sup>1</sup>D, <sup>1</sup>S, 2s3p <sup>1</sup>P and 2s3s <sup>3</sup>S target wavefunctions in our calculation. The wavefunctions of the initial and final states are represented as configuration interaction (CI) expansions in terms of orthogonal basis orbitals (1s, 2s, 2p, 3s, 3p and 3d). The radial part of each orbital is expanded in the form

$$P_{n_a l_a}(r) = \sum_{i} C_{i} r^{I_i} \exp(-\xi_{i} r).$$
 (1)

The values we used for  $C_i$  and  $\xi_i$  were provided by Burke *et al* (1972) and Hibbert (1974, 1976, 1977). The energy differences ( $\Delta E$ ) and oscillator strengths ( $f_i$  (length),  $f_v$  (velocity)) used in the present calculation have been obtained for several interacting configurations using the program CIV3 of Hibbert (1975). The configurations  $m \times n$  used to obtain the cross sections in the present paper have been chosen so that the values  $4\omega_a f_i/\Delta E$  (given in equation (9)) agree to within 5% with the best values given by Hibbert (1974, 1976). The notation  $m \times n$  implies that there are m(n) configurations in the initial (final) state. The theoretical energy differences and oscillator strengths used in the present calculation are given in table 1. The configurations, CI coefficients, and term energies for each state have been given by Nakazaki (1982).

### 3. The Coulomb-Born-Bely approximation

Bely (1966, 1967) has given a simple expression for approximating the exchange amplitude in the CBO formulation of the collision problem. The Coulomb-Born-Bely

			Energy	Oscilla	tor strength
Transition	Configuration	Ion	difference $\Delta E$ (Ryd)	Length	Velocity
$2s^2 {}^1S \rightarrow 2s2p {}^1P$	2×2	C <sup>2+</sup> N <sup>3+</sup> O <sup>4+</sup> Ne <sup>6+</sup>	0.953 80 1.195 8 1.448 6 1.951 2	0.784 1 0.636 1 0.529 4 0.396 9	0.821 4 0.554 0 0.453 5 0.334 3
$2s^2 {}^1S \rightarrow 2s3p {}^1P$	3×3	$C^{2+}$ $N^{3+}$ $O^{4+}$ $Ne^{6+}$	2.360 1 3.691 1 5.297 3 9.346 7	0.208 4 0.280 3 0.334 9 0.470 5	0.218 2 0.321 7 0.380 4 0.494 8
$2s2p^{3}P \rightarrow 2p^{2}^{3}P$	2×2	$C^{2+}$ $N^{3+}$ $O^{4+}$ $Ne^{6+}$	0.786 96 0.998 66 1.208 6 1.624 4	0.278 0 0.229 1 0.193 8 0.148 0	0.290 0 0.239 7 0.204 3 0.156 9
$2s2p ^3P \rightarrow 2s3s ^3S$	3×2	C <sup>2+</sup> N <sup>3+</sup> O <sup>4+</sup> Ne <sup>6+</sup>	1.692 8 2.830 7 4.238 5 7.890 4	0.050 57 0.043 42 0.041 25 0.036 46	0.058 76 0.045 65 0.045 26 0.039 42
$2s2p ^{1}P \rightarrow 2p^{2} ^{1}D$	2×2	$C^{2+}$ $N^{3+}$ $O^{4+}$ $Ne^{6+}$	0.403 71 0.541 78 0.677 84 0.945 47	0.182 1 0.171 9 0.156 9 0.129 9	0.118 8 0.101 7 0.089 09 0.071 64
$2s2p^{-1}P \rightarrow 2p^{2-1}S$	7×7	C <sup>2+</sup> N <sup>3+</sup> O <sup>4+</sup> Ne <sup>6+</sup>	0.735 32 0.962 48 1.184 0 1.623 1	0.169 2 0.139 8 0.118 9 0.091 95	0.166 5 0.138 0 0.116 8 0.089 10

Table 1. Energy differences and oscillator strengths for the transitions.

(CBB) approximation extends the Ochkur-Rudge method to electron-ion collisions. We use the LS-coupled representation of the ion plus electron system and use the following notations:  $k_a$  and  $k_{q'}$  are the wavenumber vectors of incident and scattered electrons, respectively; l and l' are the angular momenta of the incident and scattered electrons, respectively;  $L_a$  and  $L'_a$  are the angular momenta of the initial and final states of the ion, respectively. The total cross section for electron impact excitation of a final state  $q'(=\alpha'_aS'_aL'_a)$  of the beryllium-like ion from an initial state  $q(=\alpha_aS_aL_a)$  in the CBB approximation is given by

$$Q(q \to q') = \frac{2\pi}{k_q^2 \omega_q} \sum_{SLll'} (2S + 1)(2L + 1) |R_{\Gamma'\Gamma}|^2$$
 (2)

where

$$R_{\Gamma'\Gamma} = R_{\Gamma'\Gamma}^d - R_{\Gamma'\Gamma}^e \tag{3}$$

$$R_{\Gamma\Gamma}^{d(e)} = \sum_{M_{S_{a}}'m_{s}M_{s}}^{S_{a}'} C_{M_{S_{a}}'m_{s}M_{s}}^{S_{a}} C_{M_{S_{a}}'m_{s}M_{s}}^{S_{a}} C_{M_{a}'m'M}^{L'l'} C_{M_{a}mM}^{L} R_{\gamma'\gamma}^{d(e)}$$

$$\tag{4}$$

$$R_{\gamma'\gamma}^{d} = -2 \int d\mathbf{r}_{5} d\mathbf{R} \ \Psi_{q'}^{*}(\mathbf{R}) u_{k_{q}'l'm'}(\mathbf{r}_{5}) \left( \sum_{p \neq 5} \frac{1}{r_{p5}} - \frac{4}{r_{5}} \right) \Psi_{q}(\mathbf{R}) u_{k_{q}lm}(\mathbf{r}_{5}) \delta_{m_{s}'m_{s}}$$
 (5)

$$R_{\gamma'\gamma}^{e} = \frac{-32\pi}{k_{q}^{2} + U_{q'}} \int d\mathbf{R} d\sigma_{5} \Psi_{q'}^{*}(\mathbf{R}) u_{k_{q}'l'm'}(\mathbf{r}_{4}) \Psi_{q}(\mathbf{R}^{5}) u_{k_{q}lm}(\mathbf{r}_{4}) \delta(m_{s}|\sigma_{4}) \delta(m'_{s}|\sigma_{5})$$
(6)

and the C's are Clebsch-Gordan coefficients.  $u_{k_qlm}(\mathbf{r})$  are partial-wave Coulomb functions,  $\delta(m_s|\sigma)$  the spin function,  $U_{q'}$  the ionisation potential of the final state q',  $\omega_q$  the statistical weight for the initial state, and  $\Psi_q(\mathbf{R})$  the target wavefunction represented by a CI expansion as described in the previous section. The space  $(r_i)$  and spin  $(\sigma_i)$  coordinates of the *i*th electron are denoted by  $x_i$ , and  $\mathbf{R} = (x_1, x_2, x_3, x_4)$  and  $\mathbf{R}^5 = (x_1, x_2, x_3, r_4\sigma_5)$ . The summation  $\Sigma$  is taken over all magnetic quantum numbers except  $M_s$  and M. Using the target CI wavefunctions in the previous section and expressing the Coulomb function as

$$u_{k_{q}lm}(\mathbf{r}) = F_{k_{q}l}(z|r) Y_{lm}(\hat{\mathbf{r}})/r$$
  $z = Z - 4$ 

we need to carry out angular momentum calculations including the Wigner 3-j and 6-j symbols and the following radial integrals to obtain the total cross section:

(i) for the direct amplitude

$$D_{\lambda} = \int dr_1 dr_2 F_{k_a'l'}(z|r_2) P_{n_a'l_a'}(r_1) \left(\frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} - \frac{\delta_{\lambda 0}}{r_2}\right) F_{k_a l}(z|r_2) P_{n_a l_a}(r_1)$$
(7)

(ii) for the exchange amplitude

$$E = \int dr F_{k_a'l'}(z|r) P_{n_a'l_a'}(r) F_{k_al}(z|r) P_{n_al_a}(r) r^{-2}.$$
 (8)

The radial integrals,  $D_{\lambda}$ , for the monopole  $(\lambda = 0)$  and dipole  $(\lambda = 1)$  cases, and E are expressed in terms of the Gauss hypergeometric functions by the method of Nakazaki (1978). Thus, the CBB calculation is much easier than the usual CBO calculation in which the exchange amplitude must be obtained from the prestored Coulomb functions and atomic radial functions by double numerical quadrature.

For large values of the angular momentum l at high incident energies the Coulomb-Bethe approximation has been used. The total contribution to the cross section from all l has been obtained by using the sum rule given by Burgess (1974) and Burgess and Sheorey (1974). For the transitions  $2s2p \ ^3P \rightarrow 2p^2 \ ^3P$  and  $2s2p \ ^1P \rightarrow 2p^2 \ ^1D$  for which the sum rule cannot be employed, the cross sections have been obtained from the calculations for partial waves  $0 \le l \le l_{\text{max}}$  with  $l_{\text{max}}$  chosen so that

$$(Q_l - Q_{l+10}) \left(\sum_{l=0}^{l_{\text{max}}} Q_l\right)^{-1} \le 10^{-6}$$

for large enough l ( $Q_l$  are the partial cross sections).

#### 4. Results and discussions

We have carried out calculations for the allowed transitions  $2s^2$   $^1S \rightarrow 2s2p$   $^1P$ ,  $2s^2$   $^1S \rightarrow 2s3p$   $^1P$ , 2s2p  $^3P \rightarrow 2p^2$   $^3P$ , 2s2p  $^3P \rightarrow 2s3s$   $^3S$ , 2s2p  $^1P \rightarrow 2p^2$   $^1D$  and 2s2p  $^1P \rightarrow 2p^2$   $^1S$  in  $C^{2+}$ ,  $N^{3+}$ ,  $O^{4+}$  and  $Ne^{6+}$  by using of the CB and CBB approximations. In tables 2–7 the resulting CBB cross sections are given for each transition.

4.1. The 
$$2s^2$$
  $^1S \rightarrow 2s2p$   $^1P$  transition

There are many calculations for the  $2s^2$  <sup>1</sup>S  $\rightarrow 2s2p$  <sup>1</sup>P transition. Figure 1 gives the collision strength as a function of X, the incident energy in threshold units, for  $O^{4+}$ 

	C <sup>2+</sup>	N <sup>3+</sup>	O <sup>4+</sup>	Ne <sup>6+</sup>
$k^2(eV)$	(12.976) <sup>a</sup>	(16.269)	(19.708)	(26.546)
$\Delta E$	4.870 + 2 <sup>b</sup>	2.994+2	1.903+2	9.054+1
20	3.616 + 2	2.547 + 2	1.879 + 2	_
30	2.764 + 2	1.874 + 2	1.348 + 2	8.129 + 1
40	2.291 + 2	1.520 + 2	1.075 + 2	6.341 + 1
60	1.759 + 2	1.140 + 2	7.900 + 1	4.525 + 1
80	1.454 + 2	9.323 + 1	6.391 + 1	3.593 + 1
100	1.251 + 2	7.979 + 1	5.435 + 1	3.017 + 1
150	9.448 + 1	5.998 + 1	4.057 + 1	2.216 + 1
200	7.692 + 1	4.882 + 1	3.295 + 1	1.787 + 1
300	5.702 + 1	3.626 + 1	2.448 + 1	1.322 + 1
400	4.582 + 1	2.920 + 1	1.974 + 1	1.066 + 1
500	3.855 + 1	2.461 + 1	1.666 + 1	9.011 + 0
600	3.340 + 1	2.136 + 1	1.448 + 1	7.843 + 0
1000	2.216 + 1	1.423 + 1	9.679 + 0	5.274 + 0
1500	1.589 + 1	1.022 + 1	6.970 + 0	3.815 + 0
2000	1.250 + 1	8.051 + 0	$5.499 \pm 0$	3.020 + 0

**Table 2.** Cross sections for the  $2s^2$  <sup>1</sup>S  $\rightarrow 2s2p$  <sup>1</sup>P transition (in units of  $10^{-18}$  cm<sup>2</sup>).

**Table 3.** Cross sections for the  $2s^2$  <sup>1</sup>S  $\rightarrow$  2s3p <sup>1</sup>P transition (in units of  $10^{-18}$  cm<sup>2</sup>). The same notation is used as in table 2.

	C <sup>2+</sup>	N <sup>3+</sup>	O <sup>4+</sup>	Ne <sup>6+</sup>
$k^2(eV)$	(32.109)	(50.218)	(72.072)	(127.17)
$\Delta E$	4.942 – 1	5.288-1	4.865-1	3.246 – 1
50	1.308 + 0		_	
75	1.971 + 0	9.962 - 1	5.124 - 1	_
100	2.239 + 0	1.246 + 0	6.857 - 1	
150	2.331 + 0	1.425 + 0	8.521 - 1	3.588 - 1
200	2.243 + 0	1.438 + 0	9.017 - 1	4.074 - 1
300	1.993 + 0	1.345 + 0	8.879 - 1	4.410 - 1
400	1.772 + 0	1.230 + 0	8.355 - 1	4.394 - 1
500	1.594 + 0	1.127 + 0	7.798 - 1	4.264 - 1
600	1.450 + 0	1.038 + 0	7.285 - 1	4.094 – 1
1000	1.079 + 0	7.959 - 1	5.757 - 1	3.449 - 1
1500	8.319 - 1	6.248 - 1	4.603 - 1	2.869 - 1
2000	6.844 - 1	5.194 - 1	3.869 - 1	2.468 - 1
2500	5.852 - 1	4.473 - 1	3.357 - 1	2.175 - 1
3000	5.135 - 1	3.945 - 1	2.977 - 1	1.951 - 1

with various calculations. Berrington  $et\,al\,(1977)$  have calculated the collision strength using the R-matrix (six-state calculation) method. They used the CI target wavefunctions which have high accuracy for energy differences and oscillator strengths. Furthermore, Berrington  $et\,al\,(1979)$  have obtained the collision strength using the R-matrix method with twelve states. The DW results of Peek and of Mann (both quoted in

<sup>&</sup>lt;sup>a</sup> Number in parentheses denotes the threshold energy,  $\Delta E$ , in units of electron volts. <sup>b</sup>  $4.870 + 2 = 4.870 \times 10^2$ .

This notation is similarly used for tables 3-7.

	$C^{2+}$	N <sup>3+</sup>	O <sup>4+</sup>	Ne <sup>6+</sup>
$k^2(eV)$	(10.707)	(13.587)	(16.443)	(22.101)
$\Delta E$	3.069+2	1.819+2	1.154+2	5.461+1
15	2.365 + 2	1.672 + 2	_	_
25	1.620 + 2	1.097 + 2	8.009 + 1	4.881 + 1
50	9.915 + 1	6.418 + 1	4.533 + 1	2.652 + 1
75	7.468 + 1	4.757 + 1	3.309 + 1	1.891 + 1
100	6.096 + 1	3.858 + 1	2.663 + 1	1.500 + 1
150	4.553 + 1	2.870 + 1	1.968 + 1	1.093 + 1
200	3.681 + 1	2.321 + 1	1.589 + 1	8.767 + 0
300	2.707 + 1	1.711 + 1	1.172 + 1	6.443 + 0
400	2.164 + 1	1.372 + 1	9.410 + 0	5.175 + 0
500	1.813 + 1	1.152 + 1	7.916 + 0	4.360 + 0
600	$1.567 \pm 1$	9.973 + 0	6.862 + 0	3.786 + 0
1000	1.033 + 1	6.600 + 0	4.559 + 0	2.530 + 0

**Table 4.** Cross sections for the  $2s2p^{3}P \rightarrow 2p^{2}^{3}P$  transition (in units of  $10^{-18}$  cm<sup>2</sup>). The same notation is used as in table 2.

**Table 5.** Cross sections for the  $2s2p ^3P \rightarrow 2s3s ^3S$  transition (in units of  $10^{-18} \text{ cm}^2$ ). The same notation is used as in table 2.

	$C^{2+}$	$N^{3+}$	O <sup>4+</sup>	Ne <sup>6+</sup>	
$k^2(eV)$	(23.031)	(38.513)	(57.666)	(107.35)	
$\Delta E$	1.612+0	6.108 – 1	3.063-1	8.470 – 2	
25	1.635 + 0	_		_	
50	1.677 + 0	5.439 - 1	_		
75	1.598 + 0	4.972 - 1	2.503 - 1		
100	1.499 + 0	4.786 - 1	2.211 - 1		
150	1.314 + 0	4.462 - 1	2.030 - 1	6.178 - 2	
200	1.165 + 0	4.138 - 1	1.926 - 1	5.406 - 2	
300	9.539 - 1	3.580 - 1	1.739 - 1	4.954 - 2	
400	8.127 - 1	3.151 - 2	1.576 - 1	4.693 - 2	
500	7.115 - 1	2.820 - 1	1.439 - 1	4.451 - 2	
600	6.351 - 1	2.558 - 1	1.324 - 1	4.222 - 2	
1000	4.528 - 1	1.893 - 1	1.014 - 1	3.477 - 2	
1500	3.402 - 1	1.455 - 1	7.963 - 2	2.856 - 2	
2000	2.756 - 1	1.195 - 1	6.623 - 2	2.439 - 2	
2500	2.332 - 1	1.021 - 1	5.706 - 2	2.139 - 2	
3000	2.030 - 1	8.952 - 2	5.033 - 2	1.911 - 2	

Merts et al 1980) lie about 9% higher than those of Berrington et al (1979) for X < 2. We have not compared our results with calculations that have used single-configuration target wavefunctions since these are known to give very poor results. The CB results of Nakazaki and Hashino (1977) are larger than the R-matrix results by 25% at X = 2. The present CBB results lie about 10% lower than the CB results and lie about 15% higher than the R-matrix (six state) results at X = 2. The CBB results lie about 8% higher than the DW results of Peek and Mann at X = 1. As the incident energy

<b>Table 6.</b> Cross sections for the $2s2p ^{1}P \rightarrow 2p^{2} ^{1}D$ transition (in units of $10^{-18} \text{ cm}^{2}$ ).	The
same notation is used as in table 2.	

	$C^{2+}$	$N^{3+}$	O <sup>4+</sup>	Ne <sup>6+</sup>
$k^2(eV)$	(5.4926)	(7.3711)	(9.2223)	(12.864)
$\Delta E$	9.436+2	5.397+2	3.355+2	1.556+2
10	5.745 + 2	4.131 + 2	3.118 + 2	_
15	4.181 + 2	2.934 + 2	2.178 + 2	1.350 + 2
20	3.362 + 2	2.322 + 2	1.703 + 2	1.040 + 2
30	2.490 + 2	1.689 + 2	1.218 + 2	7.275 + 1
40	2.019 + 2	1.356 + 2	9.685 + 1	5.692 + 1
60	1.501 + 2	1.000 + 2	7.073 + 1	4.076 + 1
80	1.214 + 2	8.073 + 1	5.683 + 1	3.240 + 1
.00	1.027 + 2	6.834 + 1	4.802 + 1	2.720 + 1
.50	7.536 + 1	5.031 + 1	3.534 + 1	1.990 + 1
200	6.017 + 1	4.032 + 1	2.838 + 1	1.596 + 1
250	5.038 + 1	3.388 + 1	2.389 + 1	1.345 + 1
300	4.350 + 1	2.933 + 1	2.072 + 1	1.169 + 1
00	3.439 + 1	2.329 + 1	1.650 + 1	9.345 + 0
00	2.859 + 1	1.942 + 1	1.380 + 1	7.840 + 0

**Table 7.** Cross sections for the  $2s2p ^{1}P \rightarrow 2p^{2} ^{1}S$  transition (in units of  $10^{-18} \text{ cm}^{2}$ ). The same notation is used as in table 2.

	$C^{2+}$	N <sup>3+</sup>	O <sup>4+</sup>	Ne <sup>6+</sup>
$k^2(eV)$	(10.004)	(13.095)	(16.109)	(22.083)
$\Delta E$	1.886+2	1.077+2	6.751+1	3.172+1
25	9.969 + 1	6.486 + 1	4.674 + 1	2.840 + 1
50	6.274 + 1	3.907 + 1	2.712 + 1	1.567 + 1
75	4.767 + 1	2.930 + 1	2.005 + 1	1.129 + 1
100	3.905 + 1	2.390 + 1	1.624 + 1	9.015 + 0
150	2.924 + 1	1.788 + 1	1.209 + 1	6.618 + 0
200	2.366 + 1	1.449 + 1	9.792 + 0	5.333 + 0
300	1.741 + 1	1.070 + 1	7.242 + 0	3.937 + 0
400	1.392 + 1	8.583 + 0	5.821 + 0	3.169 + 0
500	1.167 + 1	7.211 + 0	4.900 + 0	2.672 + 0

increases, the CBB results merge with the DW results  $(X \ge 5)$ . The present CBB values are in close accord with the DW values of Younger (1980) for all X. Younger has also obtained CBO results that lie about 2% lower than the present CBB results for low energies.

For  $C^{2+}$  the present CBB results lie about 30% higher than the DW results of Peek and Mann at X=1 and lie about 26% higher than the 5CC results of Robb (quoted in Magee *et al* 1977) and the R-matrix results of Berrington *et al* (1977) at X=1.5. For Ne<sup>6+</sup> the present CBB results agree within 10% with the DW results of Norcross (1977) for X>1.3. Note that Norcross used a revised version of the distorted-wave

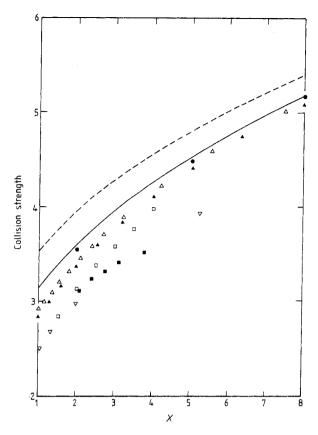


Figure 1. The collision strength for the  $2s^2$  <sup>1</sup>S  $\rightarrow$  2s2p <sup>1</sup>P transition in  $O^{4+}$  as a function of X (the incident energy in threshold units): ---, present CB results; — present CBB results; •, DW results of Younger (1980);  $\triangle$ , DW results of Mann (quoted in Merts *et al.* 1980);  $\triangle$ , DW results of Peek (quoted in Merts *et al.* 1980);  $\nabla$ , DW results of Malinovsky (1975); •, R-matrix (six state) results of Berrington *et al.* (quoted in Merts *et al.* 1980);  $\square$ , R-matrix (twelve state) results of Berrington *et al.* (1979).

program of Eissner and Seaton (1972) together with the CI target wavefunctions described by Hummer and Norcross (1974).

# 4.2. The $2s^2$ $^1S \rightarrow 2s3p$ $^1P$ transition

There are only a few calculations for the  $2s^2$   $^1S \rightarrow 2s3p$   $^1P$  transition. Mann (quoted in Magee *et al* 1977) has obtained the collision strength for  $C^{2+}$  using the CBO approximation in which the CI target wavefunctions  $(2\times4)$  have been used. The present CBB results agree within 10% with his results for X>1.5. At X=30 the difference between our CBB results and his are 10%. Note that our CB and CBB results differ by less than 1% for  $X \ge 30$ . Thus, it seems that this difference between the present CBB results and Mann's CBO results for  $X \ge 30$  is due to a different choice of target wavefunctions. For  $O^{4+}$  the present CBB results lie about 20% higher than the DW results of Malinovsky (1975) at X=1.5. For  $Ne^{6+}$  the present CBB results agree within 10% with the DW results of Norcross (1977) for  $X \ge 4$  where comparisons can be made.

## 4.3. The $2s2p^{3}P \rightarrow 2p^{2}^{3}P$ transition

Figure 2 compares the present CBB calculations for  $O^{4+}$  with various calculations. The DW results of Mann (quoted in Merts et al 1980) agree to within 6% with the present CBB results for all X. The CBB calculation gives collision strengths larger by 10 to 16% than the R-matrix calculation of Berrington et al (quoted in Merts et al 1980) for 1.9 < X < 4.0.

For  $C^{2+}$  the DW results of Mann (quoted in Merts *et al* 1980) and Eissner (1971) are smaller by 20% than the present CBB results at  $X \approx 1.5$ , but for X > 3 the DW results are within 6% of the CBB results. The CBB results are about 40% larger than the 5CC results of Robb (quoted in Merts *et al* 1980) at  $X \approx 1.3$ . For Ne<sup>6+</sup> the CBB results agree within 2% with the DW results of Norcross (1977) for 1.6 < X < 45.

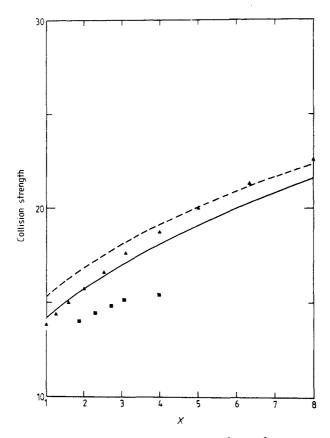


Figure 2. The collision strength for the  $2s2p^3P \rightarrow 2p^3P$  transition in  $O^{4+}$  as a function of X: ---, present CB results; —, present CBB results;  $\triangle$ , DW results of Mann (quoted in Merts et al 1980);  $\square$ , R-matrix (six state) results of Berrington et al (quoted in Merts et al 1980).

# 4.4. The $2s2p ^3P \rightarrow 2s3s ^3S$ transition

The only previous calculation we are aware of for this transition is that carried out by Norcross (1977) for  $Ne^{6+}$ . Norcross used the Dw approximation and the results he obtained at X = 4.5 and 9.1 agree to better than 8% with the present CBB results.

# 4.5. The $2s2p ^{1}P \rightarrow 2p^{2} ^{1}D$ transition

Figure 3 shows collision strengths for  $C^{2^+}$  for  $X \le 8$ . The 5CC results of Robb (quoted in Merts *et al* 1980) lie about 6% lower than the present CBB results for X = 1.4, while at X = 20 the 5CC results are about 9% larger than the CBB results. The present energy difference is 1.8% greater than the experimental threshold energy, while that of Robb is 10.6% less than experiment. Therefore, it seems that the difference between the 5CC results and the present CBB results for  $X \ge 20$  is due to a different choice of target wavefunction. The DW results of Eissner (1971) lie about 20% higher than the CBB results for 1.2 < X < 3.8. For  $N^{3^+}$  and  $O^{4^+}$  there are no calculations which may be compared with the present CB and CBB results. For  $Ne^{6^+}$  the DW results of Norcross (1977) agree within 5% with the CBB results for 1.7 < X < 40.

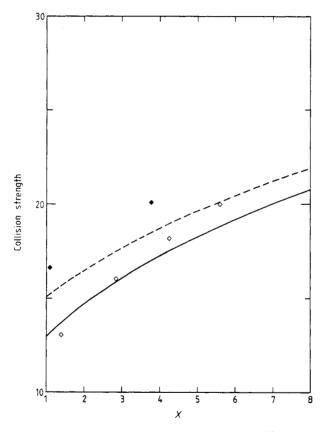


Figure 3. The collision strength for the  $2s2p \, ^1P \rightarrow 2p^2 \, ^1D$  transition in  $C^{2+}$  as a function of X: ---, present CB results; —, present CBB results;  $\spadesuit$ , DW results of Eissner (1971);  $\diamondsuit$ , 5CC results of Robb (quoted in Merts *et al* 1980).

# 4.6. The $2s2p ^{1}P \rightarrow 2p^{2} ^{1}S$ transition

There exist two independent calculations for this transition. For  $C^{2^+}$  the present CBB results lie about 2% lower than the DW results of Eissner (1971) at  $X \simeq 2$ . For Ne<sup>6+</sup> the present CBB results agree within 2% with the DW results of Norcross (1977) for 1 < X < 44.

## 4.7. The excitation rate coefficients

The collision strengths obtained in the CBB calculations are fitted to the following form

$$\Omega = d_1 + \frac{d_2}{X} + \frac{d_3}{X^2} + d_4 \ln X \tag{9}$$

where the coefficient  $d_4$  is fixed by using the Bethe approximation  $(d_4 = 4\omega_q f_l/\Delta E)$ . The other coefficients  $d_i$  (i = 1-3) are determined by the least-squares method. These coefficients are given in table 8. This fit proves to be accurate to better than a few per cent for all X and Z in six transitions. The excitation rate coefficients are given as a function of electron temperature T by

$$R = D\left[\frac{d_1 \exp(-\alpha)}{\alpha} + d_3 \exp(-\alpha) + \left(d_2 - d_3\alpha + \frac{d_4}{\alpha}\right) \int_1^\infty dy \frac{\exp(-\alpha y)}{y}\right] \text{cm}^3 \text{ s}^{-1}$$
 (10)

where

$$D = 8.010 \times 10^{-8} \frac{\alpha}{(kT)^{1/2} \omega_a} \tag{11}$$

and  $\alpha = 13.605 \Delta E/kT$ , with kT in electron volts, and  $\Delta E$  in rydbergs as given in table 1.

Table 8.	Coefficients for	r equation	(9) for	collision	strengths in	the CBB	calculation.
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Transition	Ion	$d_1$	$d_2$	$d_3$	$d_4$
$2s^2 S \rightarrow 2s2p P$	C <sup>2+</sup>	4.065+0	-1.112 + 0	2.503+0	3.288+0
•	$N^{3+}$	2.980 + 0	-4.463 - 1	1.694 + 0	2.128 + 0
	O <sup>4+</sup>	2.236 + 0	-5.803 - 2	1.024 + 0	1.461 + 0
	Ne <sup>6+</sup>	1.357 + 0	3.404 - 1	3.575 - 1	8.136 - 1
$2s^2 S \rightarrow 2s3p P$	$C^{2+}$	-3.236 - 1	3.420 - 1	-3.580 - 3	3.532 - 1
•	· N <sup>3+</sup>	-2.603 - 1	3.343 - 1	-5.175 - 2	3.038 - 1
	O <sup>4+</sup>	-2.041 - 1	2.867 - 1	-5.346 - 2	2.529 - 1
	Ne <sup>6+</sup>	-1.578 - 1	2.495 - 1	-5.775-2	2.014 - 1
$2s2p^{3}P \rightarrow 2p^{2}^{3}P$	$C^{2+}$	1.870 + 1	-2.396+0	9.004 + 0	1.272 + 1
•	$N^{3+}$	1.313 + 1	4.108 - 1	5.487 + 0	8.259 + 0
	O <sup>4+</sup>	9.795 + 0	9.885 - 1	3.852 + 0	5.773 + 0
	Ne <sup>6+</sup>	6.047 + 0	1.506 + 0	1.644 + 0	3.280 + 0
$2s2p ^3P \rightarrow 2s3s ^3S$	$C^{2+}$	-6.762 - 1	1.014 + 0	-5.109 - 2	1.075 + 0
•	$N^{3+}$	-3.991 - 1	6.132 - 1	-3.255-2	5.522 - 1
	O <sup>4+</sup>	-2.599 - 1	4.035 - 1	-8.083 - 3	3.504 - 1
	Ne <sup>6+</sup>	-1.310 - 1	2.021 - 1	-1.982 - 3	1.663 - 1
$2s2p^{-1}P \rightarrow 2p^{2-1}D$	$C^{2+}$	1.064 + 1	-4.888 + 0	7.508 + 0	5.413+0
•	$N^{3+}$	7.660 + 0	-1.581+0	4.199 + 0	3.807 + 0
	O <sup>4+</sup>	5.720 + 0	-1.571 - 1	2.354 + 0	2.778 + 0
	Ne <sup>6+</sup>	3.494 + 0	8.434 - 1	7.776 - 1	1.649 + 0
$2s2p^{1}P \rightarrow 2p^{2} S$	$C^{2+}$	3.682 + 0	-1.327 + 0	2.397 + 0	2.761 + 0
•	$N^{3+}$	2.525 + 0	1.399 - 1	9.297 - 1	1.743 + 0
	O <sup>4+</sup>	1.877 + 0	3.476 - 1	5.584 - 1	1.205 + 0
	Ne <sup>6+</sup>	1.195 + 0	2.489 - 1	3.462 - 1	6.798 - 1

#### 5. Conclusions

The CBB calculation, which takes into account the electron exchange, have been performed using the closed-form method given by Nakazaki (1978). This calculation is much easier than the usual CBO calculation. The CB and CBB cross sections of electron impact excitation for six allowed transitions in beryllium-like ions  $(C^{2+}, N^{3+}, O^{4+}, Ne^{6+})$  have been calculated for impact energies from threshold to the high-energy region. A simple fitting formula (9) for reproducing the present CBB results has been used. The CBB method may be not as accurate at near-threshold energies as the CC or R-matrix method which includes channel coupling and resonance effects explicitly. However, the CBB calculation may be accurate with an increase of the incident electron energy.

The difference between the CBB results and the DW or CC results for ions with low Z is larger than for ions with high Z at low incident energies. It is seen that for  $C^{2+}$  the present CBB results agree within 30% with the DW results which have been published until now and for  $Ne^{6+}$  the CBB results agree within 10% with the DW results of Norcross (1977). Thus, we find that the CBB calculation which is a simple method gives an improvement over the CB approximation and good results comparable with the DW calculation for the present six allowed transitions. Therefore, we consider that the simple fitting formula (9) is useful for applications to astrophysics and plasma physics. Calculations using the CBB approximation for other transitions are desirable to study its usefulness.

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#### References

Bely O 1966 Proc. Phys. Soc. 87 1010-1

---- 1967 Nuovo Cim. B 49 66-86

Berrington K A, Burke P G, Dufton P L and Kingston A E 1977 J. Phys. B: At. Mol. Phys. 10 1465-75 Berrington K A, Burke P G, Dufton P L, Kingston A E and Sinfailam A L 1979 J. Phys. B: At. Mol. Phys. 12 L275-8

Burgess A 1974 J. Phys. B: At. Mol. Phys. 7 L364-7

Burgess A and Sheorey V B 1974 J. Phys. B: At. Mol. Phys. 7 2403-16

Burke P G, Hibbert A and Robb W D 1972 J. Phys. B: At. Mol. Phys. 5 37-43

Clark R E H, Sampson D H and Parks A D 1980 Astrophys. J. Suppl. 44 215-22

Eissner W 1971 Proc. 7th Int. Conf. on Physics of Electronic and Atomic Collisons (Amsterdam: North-Holland) p 460

Eissner W and Seaton M J 1972 J. Phys. B: At. Mol. Phys. 5 2187-98

Flower D R and Launay J M 1973 Astron. Astrophys. 29 321-6

Henry R J W 1981 Phys. Rep. 68 3-91

Hibbert A 1974 J. Phys. B: At. Mol. Phys. 7 1417-34

- ---- 1975 Comput. Phys. Commun. 9 141-72
- 1976 J. Phys. B: At. Mol. Phys. 9 2805-13
- --- 1977 private communication

Hummer D G and Norcross D W 1974 Mon. Not. R. Astron. Soc. 168 263-72

Magee N H, Mann J B, Merts A L and Robb W D 1977 Los Alamos Scientific Laboratory Report LA-6691-MS

Malinovsky M 1975 Astron. Astrophys. 43 101-10

Merts A L, Mann J B, Robb W D and Magee N H 1980 Los Alamos Scientific Laboratory Report LA-8267-MS

Nakazaki S 1978 J. Phys. Soc. Japan 45 225-9

---- 1982 to be published

Nakazaki S and Hashino T 1977 J. Phys. Soc. Japan 43 281-6

---- 1982 J. Phys. B: At. Mol. Phys. 15 2295-305

Norcross D W 1977 private communication

Sampson D H, Clark R E H and Golden L B 1980 Astrophys. J. Suppl. 44 193-213

Seaton M J 1975 Adv. At. Mol. Phys. 11 83-142

Tully J A 1980 J. Phys. B: At. Mol. Phys. 13 3023-34

Younger S M 1980 J. Quant. Spectrosc. Radiat. Transfer 23 489-98