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Electron Impact Excitation of Carbon and Oxygen Ions

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ELECTRON IMPACT EXCITATION OF CARBON AND OXYGEN IONS

by

N. H. Magee, Jr., J. B. Mann, A. L. Merts, and W. D. Robb

ABSTRACT

This report is an attempt at a comprehensive compilation of currently available theoretical data on electron impact excitation of carbon and oxygen ions. It is designed to be of use primarily to theoretical atomic physicists, allowing them a broader than usual view of how various approximations compare. We do not attempt to place an estimate on the accuracy to which any of the collision strengths are known. The reader may obtain some idea of the accuracy from the spread in the calculations. Further, we do not evaluate rate coefficients, or make any comparison with observed results. We do provide simple analytic fits to the data, where possible, thus allowing the reader to make comparison with observation or evaluate rate coefficients if he desires. The present data contains little about resonance effects, due to the difficulty of their presentation. It is possible that resonances could make a considerable change in the average collision strength near threshold, and this topic requires further study.

1. INTRODUCTION

The need for electron-ion impact excitation rate coefficients in many physical applications is quite obvious. The cross sections needed for the calculation of these rates have always been scarce. We, like other people, were unable to collect enough cross sections to decide on the reliability of numbers calculated by a given theoretical method. We therefore decided to settle on some important low-Z elements and invite those people who were active in calculations of collisional excitation cross sections to send us their data for comparison. The ions of carbon and oxygen were chosen, since they are sufficiently complicated to show resonance and configuration interaction effects, yet they are light enough so that the computational load was not unusually burdensome. Furthermore,

these ions are of importance both in laboratory and astrophysical plasmas; they can also serve as the low-Z limit for isoelectronic scaling to higher Z elements.

The numbers presented in this report are those sent to us by various people mentioned in the acknowledgments, together with some numbers from the literature and numbers calculated by the authors. They are available on punched cards, by application to the authors. These numbers should not be considered as the final word on any of the transitions. However, the general trend and the spread of the numbers can be taken as an indication of the possible reliability of the cross sections. It is our feeling that this is certainly the least assemblage of data required for a realistic assessment of the performance of various methods. We have not attempted to give any of the details of the theory for any of the methods used in calculation of the cross sections. References to the literature should give the interested reader these details.

In one case the method for obtaining the numbers appearing in this report deviated sufficiently from that published, that it was thought advisable to include an Appendix for the presentation of the method.

Rate coefficients can be calculated from the fits given in this report. These fits, to dimensionless collision strengths, are given in terms of the scaled energies $X = \frac{E}{\Delta E_0}$, where E is the kinetic energy of the incident electron energy in rydbergs and ΔE_0 is the threshold energy (in rydbergs) for excitation of the transition under consideration. The fitting formulae were chosen so that one may carry out rate coefficient integration easily for the important transitions. For spin-allowed transitions and a Maxwellian energy distribution for the electrons, one needs only a table of exponential integrals to evaluate the rate coefficients.

With the assumption of a Maxwellian electron energy distribution, the rate coefficient (in units $\text{cm}^3 \text{s}^{-1}$) for the transition from an initial state αSL is:

$$R(\alpha SL \rightarrow \alpha' S' L') = \frac{c \Delta E_0}{(2S + 1)(2L + 1)(kT)^{3/2}} \int_1^{\infty} \Omega(X) e^{-\frac{\Delta E_0}{kT} X} dX, \quad (1)$$

where $\Omega(X)$ is the collision strength, defined as

$$\Omega(X) = (2S + 1)(2L + 1) E Q(E). \quad (2)$$

$Q(E)$ is the cross section in units of πa_0^2 . In Eq. (1) c is a constant which depends on the units used for kT . If kT is in electron volts then $c = 8.010 \times 10^{-8}$. For Fe plasmas of density $\sim 10^{12} \text{ cm}^{-3}$ and temperatures (kT) of about 1 keV, the $\Delta n = 0$ transitions are of particular importance. For these transitions the temperature may be large compared to the excitation energy. For example, in the case of Fe XXIV, the 2s - 2p transition energy is approximately 60 eV, giving $u_0 = \frac{\Delta E_0}{kT} = 0.06$. Hence at 100 times threshold (i.e., $X = 100$) the exponential factor is $e^{-6.0} = 2.48 \cdot 10^{-3}$, while in the same ion the 2s - 3p has $u_0 = 1.16$, giving an equivalent exponential factor of $e^{-5.8} = 3.03 \times 10^{-3}$ at only 5 times threshold. It is clear that the cross-section calculations must be carried out to much higher values of X for the $\Delta n = 0$ than for the $\Delta n \neq 0$ transitions.

2. DATA PRESENTATION AND FORMAT

The data presented in Sec. 6 can be divided into two main parts. First there are the transitions for which we could make meaningful comparisons between two or more calculations. In this case we present two graphs per transition, one for X between one and five on a linear scale, and one showing the complete range of X on a log scale. In front of the graphs is the data in numerical form and some brief description of the calculations. Second, there are data for which meaningful comparison is not possible, and these are presented in numerical form with comments.

To facilitate the computer plotting of the data, each author, or group of authors, was assigned a number and symbol. These are listed in the table at the beginning of Sec. 6. Following this table are two indexes to the data.

We received data in a variety of forms. The most desirable form was a table of the incident energies, collision strengths, and the threshold energy used, all to three or more significant figures. Some data were sent on log/linear graphs, other data were given numerically in terms of Z^4 times the cross section, but with only one significant figure accuracy. Consequently when this data is plotted on the present scale it shows a certain amount of noise.

In listing the data in the tables in Sec. 6, it was decided not to differentiate between X values which were less than 0.01 apart. Thus all values of X lying within 0.01 of each other were given a single value -- that value being the first number encountered. The error produced by doing this is insignificant, since all the collision strengths presented are nonresonant and slowly varying.

3. GENERAL THEORETICAL COMMENTS ON THE DATA

3.1. Energy Ranges and Angular Momentum Contributions

Excitation rate coefficient data is required over a wide range of temperatures in many applications. This requires a knowledge of the collision strength from threshold up to asymptotic energies. Most calculations cover only a narrow and completely inadequate range of energies. In the present work we show where possible the asymptotic form of the collision strengths in the Coulomb-Born (CB) approximation, which we assume to be correct. Comparison with the asymptotic CB results revealed many errors in the initial data. Most of the errors were due to incorrect treatment of the higher L partial contributions to the collision strength. Some people use a formula $\ln \Omega_L = A L + B^*$ to extrapolate to higher L partial collision strengths Ω_L for optically allowed transitions. This is in general inadequate, and caution should be exercised in using extrapolation formulae. Coulomb-Born or Coulomb-Bethe estimates of the high- L contribution are much preferable. Even in optically forbidden (but not spin-forbidden) transitions (e.g., $1s^2 2s - 1s^2 3d$) there can be significant contributions from high L (say $L \geq 80$) at high energies. Here simple closure formulae do not exist. However, comparison can be made with the first Born approximation limit.

3.2. Oscillator Strengths and Target State Wave Functions

Some of the optically allowed transition data indicate different asymptotic trends in the collision strengths, even when the above-mentioned problems are known not to occur. This is a direct result of the difference in oscillator strengths obtained from the various target state wave functions used. In hydrogen-, helium-, and lithium-like ions this is not a severe problem. However with more complex target structures more serious differences will be produced. The use of target wave functions giving different oscillator strengths not only affects the asymptotic behavior of the collision strength, it may also produce large differences in magnitude at all energies. This latter difference has often been attributed to differences in theoretical methods, instead of wave function differences.

* We use the total angular momentum L of the target and incident electrons in the present discussion and formulae. In doing so we actually lump together contributions from several incident electron partial waves ℓ . It is probably more convenient and common for users of the Coulomb-Born and Distorted Wave approximations to deal in terms of ℓ rather than L .

To illustrate this point more vividly, two of the authors, Mann and Robb, compared unitarized Coulomb-Born Exchange (CBXII) and five-state Close-Coupling (CC) results for $e^- + \text{C II}$ scattering, with a variety of target state wave functions. The CC method is widely regarded as the most accurate theoretical method available, while the CBXII method is relatively poorly rated, especially for singly ionized targets, as in this instance. We use two sets of bound-state wave functions. The first set are Hartree-Fock (HF) wave functions for the ground and excited states. The second set allow for interaction of the configurations $1s^2 2s^2 2p^2 P$ and $1s^2 2p^3^2 P$ in the ground state, and have single configurations for the excited states. Since Mann used the HF code of Cowan¹ and Robb used the code of Hibbert² to produce their target state wave functions, small differences in oscillator strengths remain. In Fig. 1 we show three transitions from the ground state. These are $\Delta n = 0$ spin and dipole-allowed transitions. The two sets of wave functions yield entirely different behaviors in the collision strength, and thus entirely different rate coefficients. The difference between the CC and CBXII collision strengths, for either set of wave functions, is significant near threshold energies, however the difference that this would produce in rate coefficients, especially at higher temperatures, would be insignificant.

We conclude from these results that the CBXII results show the same trends as the CC results in the case of C^+ , provided that approximately the same target state wave functions are used in each calculation. Further, the agreement in magnitude is good (i.e., better than 20%) for $X > 3$, and the difference in the rates predicted by the calculations for use in high-temperature plasma applications is on the order of 5-7%. For example, in the transition $2s^2 2p^2 P - 2s 2p^2^2 S$ for C II at an electron temperature of 50 eV the rates given by the various calculations are presented in Table I. The notation 5 x 4 means five configurations in the ground state and four configurations in the excited state. Table I

TABLE I

	<u>Mann</u>	<u>Robb</u>
1 x 1 Configuration	6.75×10^{-9}	6.29×10^{-9}
2 x 1 Configuration	9.75×10^{-9}	9.22×10^{-9}
5 x 4 Configuration	1.12×10^{-8}	---

Fig. 1. Comparison of Coulomb-Born (CB) and Close-Coupling (CC) calculations for dipole-allowed transitions in C II. The CB calculations are shown as the numbers 1, 2, 3, and the CC calculations as the letters A and B. They correspond to the calculations of Table I.

shows the importance of target configuration interaction (CI) effects on the excitation rate coefficient.

3.3. Deviations from LS Coupling

All of the data presented in Sec. 6 are for transitions between LS-coupled target ion states. For C and O ions this is fine, since relativistic components of the Hamiltonian usually give negligible mixing of LS terms. For heavier ions this mixing of levels is nonnegligible and produces interesting effects on the collision strength, in some cases drastically changing the familiar forms of the collision strength assumed in Sec. 5.

As an example of what may happen, even for carbon ions, we show the $1s^2 2s^2 \ ^1S - 1s^2 2s 3p \ ^3P$ transition for C III in Fig. 2. This is a unitarized Coulomb-Born calculation with and without exchange. The direct contribution arises because of configuration mixing of various LS terms through the spin-orbit interaction. Specifically, the ground state includes 6.7% (eigenvector 0.259) of $1s^2 2p^2 \ ^1S$, and the excited state includes 0.9% of $1s^2 2p 3d \ ^3P$, and 0.03% of the configuration $1s^2 2s 3p \ ^1P_1$. The threshold energy for the transition is 2.366831 rydbergs. This is the only example of mixing of a spin-allowed with a spin-non-allowed transition in this compilation. Without the mixing, the direct curve would be absent, and the exchange curve would be close to $\Omega = AX^{-2}$ for large X.

3.4. Effect of Nonorthogonality of Target State Orbitals

With a few exceptions all wave functions used by Mann for the Coulomb-Born calculations were obtained from a single-configuration Hartree-Fock code developed by R. D. Cowan.¹ The transition C V $1s^2$ to $1s 2s \ ^1S$ showed extraordinary sensitivity to the nonorthogonality of the 2s function to the 1s function of the ground state. Wave functions obtained by minimizing the $1s 2s$ configuration average energy gave collision strength results well above the data from other methods; on the other hand, functions obtained by minimizing the energy of the 1S term produced results lower than all other data. The wave functions finally used were from the code of Hibbert,² and were orthogonal to about 1.2×10^{-9} .

3.5 Resonances

The simple forms for the collision strength which we present in this paper are, in reality, greatly complicated by resonant scattering processes. To illustrate their effect we have calculated the $^2P^o - ^4P$ for C II at near threshold energies, showing the lowest few resonances in Fig. 3. It is a tedious, expensive, and complicated matter to calculate resonances in such a point-by-point manner. Seaton³ has discussed a quantum defect theory method for the calculation of

Fig. 2. Unitarized Coulomb-Born calculations, with and without exchange, and with intermediate coupling. In LS-coupling there would only be an exchange curve, a straight line plot ($\ln \Omega = a - 2 \ln X$) except near threshold. In intermediate-coupling, the configurations $1s^2 2s 3p 3p$ and $1s^2 2s 3p 1p$ mix, and this gives rise to the direct contribution (lower curve), which dominates at high energies.

Fig. 3. Resonance structure in the $2p^o - 4p^e$ collision strength just above threshold.

collision strengths in resonant regions just below threshold. This procedure should have great applicability in the near future, however, to date, it has not been applied in sufficiently many cases to allow us to make any definitive comment on the effect of resonances on the average collision strength and on low-temperature rate coefficients. Presnyakov and Urnov⁴ have derived an expression for the resonance contribution to the collision strength in terms of autoionization and radiative decay probabilities. They have made a calculation for the $1s^2 2p^2 P - 1s^2 3s^2 S$ transition in O VI, which indicates that the resonance contribution increases the near threshold collision strength thirty-fold. However, they emphasize that for heavier highly stripped ions, dielectronic recombination seriously reduces the resonance contribution to more like a 30% increase.

4. DESCRIPTION OF THEORETICAL METHODS AND CONTRIBUTED DATA

Since our primary objective is to afford an overall comparison of the performance of the main theoretical methods in use, we start by giving a brief description of each of these; they are

- 4.1 The Close-Coupling Method
- 4.2 The Distorted Wave Method
- 4.3 The Coulomb-Born Method
- 4.4 The Infinite-Z Hydrogenic Method
- 4.5 The Impact Parameter Method
- 4.6 The Second-Order Potential Method .

4.1. The Close-Coupling Method

The formulation of the close-coupling equations is now standard, however their numerical solution may be accomplished by several independent techniques -- these differ only in their computational efficiency and give identical results. Several recent reviews of the method exist.^{3,5,6,7} The close-coupling method does take full account of exchange, coupling, and distortion associated with the states included in the calculation, and properly includes resonance states.

4.2. The Distorted Wave Method

There is no standard formulation of the Distorted Wave equations. Indeed the method has as many formulations as it has proponents. The formulations for which results are presented here, may briefly be described as follows:

4.2.1. Bhatia-Temkin Formulation:⁸ This is presented here only for two-electron targets, using the target state wave functions of Morse, Young, and

Haurwitz.⁹ A static-exchange incoming wave solution is used, with an unsymmetrized Coulomb outgoing wave solution. The S-matrix is not constructed to be unitary.

4.2.2. Davis-Kepple-Blaha Formulation:¹⁰ This has been developed for arbitrarily complex targets, using the ground-state wave functions of Clementi,¹¹ augmented with semi-empirical excited-state orbitals. The incoming and outgoing waves are static potential solutions, and the S-matrix is unitary. Exchange matrix elements may or may not be evaluated (see individual calculations in Sec. 6). Only single-configuration wave functions are used.

4.2.3. Peek Formulation:¹² This is similar to (4.2.2) with the Hartree-Fock wave functions of Cowan¹ used for the target states. A local exchange potential¹³ is added to the static potential in determining the continuum wave functions. Exchange matrix elements are evaluated, but the S-matrix is not constructed to be unitary.

4.2.4. The University College Formulation:³ This has been developed for and applied to arbitrarily complex targets, but differs considerably from the previous approaches. It is based on the use of scaled Thomas-Fermi potentials¹⁴ to obtain both bound and continuum orbitals. These orbitals are then used to construct antisymmetric trial wave functions for the initial and final $e^- + \text{ion}$ states, and the reactance matrix elements are evaluated by application of the Kohn variational principle (see Ref. 3, pp. 98-100, 103-4). The resulting S-matrix is unitary. In general, configuration interaction target state wave functions are used and a large number of closed-channel functions are added, thus giving this method potentially greater power than the previous methods.

4.3. The Coulomb-Born Method

The Coulomb-Born calculations presented here are mostly those of Mann¹⁵ and are based on the formulation of Burgess, et al.¹⁶ The target states are represented by the Hartree-Fock wave functions of Cowan,¹ but superposition of configuration wave functions may be used. Exchange matrix elements are included in the post approximation, and the S-matrix may or may not be unitarized.

4.4. The Infinite-Z Hydrogenic Method

This is the work of D. H. Sampson, A. D. Parks, L. B. Golden, and R. E. H. Clark. However, the results for He-like ions which they present here differ considerably from those which would be obtained from the original prescription of Sampson and Parks.^{17,18} The authors' description of their present work is given in Appendix I.

4.5. The Impact Parameter Method

This method applies only to optically allowed transitions.¹⁹ It has relatively few applications in electron-ion collisions, indeed there are results²⁰ for only four of the transitions presented here. The advantages of the method are its simplicity of application (the only target data required being the transition probability), and that it offers some improvement over the Born approximation.

4.6. The Second-Order Potential Method

This method has been developed and applied by Bransden and coworkers.²¹ It is an impact parameter treatment of the collision problem, with a local approximation for exchange potentials and the variation of constants taken to second order in the potential. It has been applied to scattering by hydrogenic targets.

Some additional comments are required about the first three methods described. These are all partial wave methods. The Coulomb-Born is the simplest and least expensive of these to apply. For most transitions the Coulomb-Born partial cross sections are in excellent agreement with the Close-Coupling and Distorted Wave results for $L \geq 10$. We therefore accept it as common practice to calculate the higher partial wave contributions using the Coulomb-Born method. For optically allowed transitions the high partial wave contributions are often obtained using the Coulomb-Bethe approximation¹⁶ -- this is also satisfactory.

5. FITTING OF COLLISION STRENGTH DATA

Any of the collision strengths presented here may be fit by one of the following forms:

a) The Inverse-Power Fit:

$$\Omega(X) = c_0 + \frac{c_1}{X} + \frac{c_2}{X^2} + c_3 \ln X .$$

This is used for spin-allowed transitions. The parameter c_3 is zero for all but dipole-allowed transitions.

b) The Exponential Fit:

$$\Omega(X) = \frac{c_0}{X^2} + \sum_{n=1}^4 c_n e^{-n\alpha X} .$$

This is used for spin-forbidden transitions. For certain other transitions, which do not involve change of spin, parity, or configuration, it is also appropriate.

c) The Logarithmic Fit:

$$\ln \Omega(X) = c_0 + \frac{c_1}{X} + \frac{c_2}{X^2} + c_3 \ln X .$$

This is also used for spin-forbidden transitions.

All of the fitting was done by a fractional least squares procedure. Since in most cases four parameters must be determined, we did not attempt to fit those calculations for which there were less than eight data points available. Further we did not fit calculations for which values of X less than ten were not provided. Examples of the fits to the three major types of transitions are given in Fig. 4(a)-(c).

General cross-section forms have been given by Sobel'man,²² which differ from the forms chosen here. His form was deduced from Coulomb-Born and Born calculations without exchange. The form given for a dipole-forbidden transition is illustrated in Fig. 4d. The Sobel'man form is satisfactory for those cases in which $\Omega(X)$, with or without exchange, is a monotonic increasing function of X .

Fig. 4. Fits to collision strengths. Figures a), b), and c) are for the first three forms of Sec. 5, and figure d) is for the Sobel'man form.

6. DATA

6.1. List of Authors, their Plotting Symbols and Identification Numbers

1. + MANN CBX
2. * MANN CB
3. □ ROBB CC
4. ○ NORCROSS
5. Δ DAVIS
6. ∇ PEEK
7. ◆ BHATIA
8. ∩ SEATON (UCL)
9. ≠ HENRY
10. ∥ FLOWER + LAUNAY
11. \$ NUSSBAUMER
12. U BURKE (QUB)
13. θ SAMPSON
14. I COOPER
15. 8 TULLY
16. H OSTERBROCK
18. W BRANDSDEN + NOBLE
19. X MERTS FITTED CURVE
20. 1 MANN SC
21. 2 MANN 2P3 MIX
22. 3 MANN FULL MIX
23. A ROBB SC
24. B ROBB 2P3 MIX

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... DATA SETS

23	C II 152 252 2P = 152 25 2P2(4P)	MANN CBX , SEATON , ROBB CC , MANN CBXCI II C II 252 2P TO 25 2P2(4P) MIX JACKSON SCCX C II 25(2)2P(2P0) = 252P(2)(4PE) ROBB SCCX C II 25(2)2P(2P0)=252P(2)(4PE)	
25	C II 152 252 2P = 152 25 2P2(2S)	MANN CB , MANN CBX , ROBB CC , MANN CBXCI II C II 252 2P TO 25 2P2(2S) FULL MIX MANN CBXCI II C II 252 2P TO 25 2P2(2S) FULL MIX ROBB CII SCCX 25(2)2P=252P(2)2S CI	
27	C II 152 252 2P = 152 25 2P2(2P)	MANN CB , MANN CRX , ROBB CC , DAVIS , MANN CBXCI II C II 252 2P TO 25 2P2(2P) FULL MIX MANN CBXCI II C II 252 2P TO 25 2P2(2P) FULL MIX ROBB CII SCCX 25(2)2P=252P(2)2P CI DAVIS UDNNX C II 25(2)2P = 252P(2)(2P)	
29	C II 152 252 2P = 152 25 2P2(2D)	ROBB CC , MANN CB , MANN CRX , ROBB CII SCCX 25(2)2P=252P(2)2D CI MANN CBXCI II C II 252 2P TO 25 2P2(2D) FULL MIX MANN CBXCI II C II 252 2P TO 25 2P2(2D) FULL MIX	
113,114	C II 25 2P2(4P) = 25 2P2(2S)	ROBB CC , ROBB SCCX C II 252P(2)(4P)=252P(2)(2S)	SC
113,114	C II 25 2P2(4P) = 25 2P2(2P)	ROBB CC , ROBB SCCX C II 252P(2)(4P)=252P(2)(2P)	SC
113,114	C II 25 2P2(4P) = 25 2P2(2D)	ROBB CC , ROBB SCCX C II 252P(2)(4P)=252P(2)(2D)	SC
113,114	C II 25 2P2(2S) = 25 2P2(2P)	ROBB CC , ROBB SCCX C II 252P(2)(2S)=252P(2)(2P)	SC
113,114	C II 25 2P2(2D) = 25 2P2(2S)	ROBB CC , ROBB SCCX C II 252P(2)(2D)=252P(2)(2S)	SC
113,114	C II 25 2P2(2D) = 25 2P2(2P)	ROBB CC , ROBB SCCX C II 252P(2)(2D)=252P(2)(2P)	SC

6.2. Listing of all Calculations for Carbon Ions

PAGE NO.

ELEMENT AND ION

... DATA SETS

107,110 C II
192 292 2P = 192 292 39

MANN CBX , MANN CBX ,
MANN CBX II C II 292 2P TO 292 39(29) UNITARIZED
MANN CBXCI II C II 292 2P TO 292 39(29) MIX

107,110 C II
192 292 2P = 192 292 3P

MANN CBX , MANN CBX ,
MANN CBX II C II 292 2P TO 292 3P(2P) UNITARIZED
MANN CBXCI II C II 292 2P TO 292 3P(2P) MIX

108,110 C II
192 292 2P = 192 292 3D

MANN CBX , MANN CBX ,
MANN CBX II C II 292 2P TO 292 3D(2D) UNITARIZED
MANN CBXCI II C II 292 2P TO 292 3D(2D) MIX

31 C III
192 292 = 192 29 2P(1P)

OSTERBROCK , MANN CB , MANN CBX , ROBB CC , NUSSBAUMER ,
NUSSBAUMER , FLOWER , FLOWER , DAVIS ,
OSTERBROCK 3CCX C III 192 292 = 192 29 2P(1P)
MANN CBXCI II C III 292(19) TO 29 2P(1P) MIX+UNITARY
MANN CBXCI II C III 292(19) TO 29 2P(1P) MIX+UNITARY
ROBB 5CCX C III 29(2) = 292P(1P)
NUSSBAUMER DMX C III 29(2)=292P(1P)
NUSSBAUMER IP C III 29(2)=292P(1P)
FLOWER/LAUNAY DMX C III 29(2)=292P(1P)
FLOWER/LAUNAY 6CCX C III 29(2)=292P(1P)
DAVIS UD-MX C III 29(2)(19) = 292P(1P)

34 C III
192 292 = 192 29 2P(3P)

MANN CBX , OSTERBROCK , BURKE , SEATON , FLOWER ,
FLOWER , ROBB CC ,
MANN CBXCI II C III 292(19) TO 29 2P(3P) MIX+UNITARY
OSTERBROCK 3CCX C III 192 292 = 192 29 2P(3P)
BURKE 6CCXCI C III 292 = 292P(3P)
EISSNER C III 292 = 292P(3P)
FLOWER/LAUNAY 6CCX C III 29(2)=292P(3P)
FLOWER/LAUNAY DMX C III 29(2)=292P(3P)
ROBB 5CCX C III 29(2) = 292P(3P)

118 C II:
192 292 = 192 2P2(19)

FLOWER , FLOWER ,
FLOWER/LAUNAY 6CCX C III 29(2)=2P(2)(19)
FLOWER/LAUNAY UD-MX C III 29(2)=2P(2)(19)

37	C III 1S2 2S2 - 1S2 2P2 (3P)	FLOWER , FLOWER , ROBB CC FLOWER/LAUNAY DMX C III 2S(2)-2P(2)(3P) FLOWER/LAUNAY 6CCX C III 2S(2)-2P(2)(3P) ROBB 5CCX C III 2S(2) - 2P(2)(3P)
39	C III 1S2 2S2 - 1S2 2P2 (1D)	FLOWER , FLOWER , ROBB CC FLOWER/LAUNAY SCCX C III 2S(2)-2P(2)(1D) FLOWER/LAUNAY DMX C III 2S(2)-2P(2)(1D) ROBB 5CCX C III 2S(2) - 2P(2)(1D)
113,115	C III 2S 2P(3P) - 2S 2P(1P)	ROBB CC , ROBB 5CCX C III 2S2P(3P)-2S2P(1P) CI
113,115	C III 2S 2P(3P) - 2P2(1D)	ROBB CC , ROBB 5CCX C III 2S2P(3P)-2P(2)(1D) CI
113,115	C III 2S 2P(1P) - 2P2(3P)	ROBB CC , ROBB 5CCX C III 2S2P(1P)-2P(2)(3P) CI
118	C III 2S 2P(3P) - 2P2(3P)	NUSSBAUMER , NUSSBAUMER , NUSSBAUMER DM C III 2S2P(3P)-2P(2)(3P) NUSSBAUMER IP C III 2S2P(3P)-2P(2)(3P)
113,115	C III 2S 2P(3P) - 2P2(3P)	ROBB CC , ROBB 5CCX C III 2S2P(3P)-2P(2)(3P) CI
118	C III 2S 2P(1P) - 2P2(1D)	NUSSBAUMER , NUSSBAUMER , NUSSBAUMER DM C III 2S2P(1P)-2P(2)(1D) NUSSBAUMER IP C III 2S2P(1P)-2P(2)(1D)
113,115	C III 2S 2P(1P) - 2P2(1D)	ROBB CC , ROBB 5CCX C III 2S2P(1P)-2P(2)(1D) CI
118	C III 2S 2P(1P) - 2P2(1S)	NUSSBAUMER , NUSSBAUMER , NUSSBAUMER DM C III 2S2P(1P)-2P(2)(1S) NUSSBAUMER IP C III 2S2P(1P)-2P(2)(1S)

PAGE NO.	ELEMENT AND ION	...	DATA SETS
113,115	C III 192 292(3P) - 192 2P2(1D)		ROBB CC , ROBB SCCX C III 2P(2)(3P)-2P(2)(1D) CI
108,110	C III 192 292 - 192 2S 3S(1S)		MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3S(1S) WITH 2S2,2P2
108,110	C III 192 292 - 192 2S 3S(3S)		MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3S(3S) MIX+UNITARY
108,111	C III 192 292 - 192 2S 3P(1P)		MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3P(1P) MIX+UNITARY
108,111	C III 192 292 - 192 2S 3P(3P)		MANN CB , MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3P(3P) MIX+UNITARY MANN CBX C III 2S2(1S) TO 2S 3P(3P) UNITARIZED
108,111	C III 192 292 - 192 2S 3D(1D)		MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3D(1D) MIX+UNITARY
109,111	C III 192 292 - 192 2S 3D(3D)		MANN CBX , MANN CBXCI II C III 2S2(1S) TO 2S 3D(3D) MIX+UNITARY
41	C IV 192 2S - 192 2P		MANN CB , MANN CBX , ROBB CC , DAVIS , HENRY
44	C IV 192 2S - 192 3S		MANN CB II , CARBON IV 2S TO 2P CB II RUN MANN CBX II , CARBON IV 2S TO 2P CB II RUN ROBB SCCX C IV 2S - 2P DAVIS UD-MX C IV 2S - 2P HENRY SCCX C IV 2S - 2P
46	C IV 192 2S - 192 3P		MANN CB , MANN CBX , HENRY MANN CB II , CARBON IV 2S TO 3S , CB II RUN MANN CBX II , CARBON IV 2S TO 3S CB II RUN HENRY SCCX C IV 2S - 3S
			MANN CB , MANN CBX , HENRY MANN CB II , CARBON IV 2S TO 3P , CB II RUN MANN CBX II , CARBON IV 2S TO 3P CB II RUN HENRY SCCX C IV 2S - 3P

109,111	C IV 152 2S - 152 3D	WANN CB , MANN CBX , HENRY WANN CR CARBON IV 2S TO 3D WANN CBX CARBON IV 2S TO 3D HENRY SCCX C IV 2S - 3D
109,111	C IV 152 2S - 1S 252	WANN CBX , WANN CBX CARBON IV 152 2S TO 1S 252
109,112	C IV 152 2S - 1S 2S 2P(4P)	WANN CBX , WANN CBX II CARBON IV 152 2S TO 1S 2S(3S) 2P(4P)
109,112	C IV 152 2S - 1S 2S(1S) 2P(2P)	WANN CBX , WANN CBX II C IV 152 2S TO 1S 2S(1S) 2P(2P)
109,112	C IV 152 2S - 1S 2S(3S) 2P(2P)	WANN CBX , WANN CBX II C IV 152 2S TO 1S 2S(3S) 2P(2P)
109,112	C IV 152 2S - 1S 2S 2P(2P)	WANN CBX , MANN CBX , WANN CBX II C IV 152 2S TO 1S 2S 2P(2P) AT 22,03887 WANN CBX II C IV 152 2S TO 1S 2S 2P(2P) AT 22,34022
118,119	C IV 152 2P - 152 3S	HENRY HENRY SCCX C IV 2P - 2S
118,119	C IV 152 2P - 152 3P	HENRY HENRY SCCX C IV 2P - 3P
118,119	C IV 152 2P - 152 3D	HENRY HENRY SCCX C IV 2P - 3D

PAGE NO.

ELEMENT AND ION

... DATA SETS

50

C V
1S2 = 1S 2S(1S)

MANN CB , MANN CBX , ROBB CC , PEEK , SAMPSON ,
COOPER , BHATIA , BHATIA , NORCROSS ,
MANN CB C V 1S2 TO 1S 2S(1S)
MANN CBX C V 1S2 TO 1S 2S(1S)
ROBB SCCX C V 1S2 - 1S 2S(1S)
PEEK DMX C V 1S(2)(1S)-1S2S(1S)
CARBON V 2 SINGLET S SAMPSON
COOPER SCCX C V 2 SINGLET S
BHATIA CR C V 1S2 = 1S 2S(1S)
BHATIA DM C V 1S2 = 1S 2S(1S)
NORCROSS C V 2 SINGLET S

54

C V
1S2 = 1S 2S(3S)

MANN CBX , MANN CBX , ROBB CC , SAMPSON , PEEK ,
COOPER , BHATIA , NORCROSS ,
MANN CBX C V 1S2 TO 1S 2S(3S)
MANN CBX C V 1S2 TO 1S 2S(3S)
ROBB SCCX C V 1S2 = 1S 2S(3S)
CARBON V 2 TRIPLET S SAMPSON
PEEK DMX C V 1S(2)(1S)-1S2S(3S)
COOPER SCCX C V 2 TRIPLET S
BHATIA DM C V 1S2 = 1S 2S(3S)
NORCROSS C V 2 TRIPLET S

57

C V
1S2 = 1S 2P(1P)

MANN CB , MANN CBX , SAMPSON , PEEK , DAVIS ,
ROBB CC , COOPER , BHATIA , BHATIA , NORCROSS ,
MANN CB C V 1S2 TO 1S 2P(1P)
MANN CBX C V 1S2 TO 1S 2P(1P)
CARBON V 2 SINGLET P SAMPSON
PEEK DMX C V 1S(2)(1S)-1S2P(1P)
DAVIS DMX C V 1S(2)(1S) - 1S2P(1P)
ROBB SCCX C V 2 SINGLET P
COOPER SCCX C V 2 SINGLET P
BHATIA CR C V 1S2 = 1S 2P(1P)
BHATIA DM C V 1S2 = 1S 2P(1P)
NORCROSS C V 2 SINGLET P

61

C V
1S2 = 1S 2P(3P)

MANN CBX , ROBB CC , PEEK , SAMPSON , COOPER
 BHATIA , NORCROSS
 MANN CBX C V 1S2 TO 1S 2P(3P)
 ROBB SCCXCI C V 1S2 = 1S2P(3P)
 PEEK DMX C V 1S(2)(1S) = 1S2P(3P)
 CARBON V 2 TRIPLET P SAMPSON
 COOPER SCCX C V 2THIRPLET P
 BHATIA DM C V 1S2 = 1S 2P(3P)
 NORCROSS C V 2 TRIPLET P

64

C V
1S 2S(3S) = 1S 2P(1P)

MANN CBX , SAMPSON , NORCROSS , ROBB CC ,
 MANN CBX C V 1S 2S(3S) TO 1S 2P(1P)
 SAMPSON C V 1S 2S(3S) = 1S 2P(1P)
 NORCROSS DM C V 1S2S(3S) TO 1S2P(1P)
 ROBB SCCXCI C V 1S2S(3S) = 1S2P(1P)

67

C V
1S 2S(1S) = 1S 2P(1P)

MANN CB , MANN CBX , ROBB CC , NORCROSS ,
 MANN CB C V 1S 2S(1S) TO 1S 2P(1P)
 MANN CBX C V 1S 2S(1S) TO 1S 2P(1P)
 ROBB SCCXCI C V 1S2S(1S) = 1S2P(1P)
 NORCROSS DM C V 1S2S(1S) TO 1S2P(1P)

69

C V
1S 2S(3S) = 1S 2P(3P)

MANN CB , MANN CBX , ROBB CC , NORCROSS ,
 MANN CB C V 1S 2S(3S) TO 1S 2P(3P)
 MANN CBX C V 1S 2S(3S) TO 1S 2P(3P)
 ROBB SCCX C V 1S 2S(3S) = 1S 2P(3P)
 NORCROSS DM C V 1S2S(3S) TO 1S2P(3P)

71

C V
1S 2S(3S) = 1S 2S(1S)

MANN CBX , NORCROSS , SAMPSON , ROBB CC ,
 MANN CBX CARBON V 1S 2S(3S) TO 1S 2S(1S)
 NORCROSS DMX C V 1S 2S(3S) = 1S 2S(1S)
 SAMPSON C V 1S 2S(3S) = 1S 2S(1S)
 ROBB SCCXCI C V 1S2S(3S) = 1S2S(1S)

113,115

C V
1S 2S(1S) = 1S 2P(3P)

ROBB CC ,
 ROBB SCCXCI C V 1S 2S(1S) = 1S 2P(3P)

73

C V
1S 2P(3P) = 1S 2P(1P)

NORCROSS , SAMPSON , ROBB CC ,
 NORCROSS DMX C V 1S 2P(3P) = 1S 2P(1P)
 SAMPSON C V 1S 2P(3P) = 1S 2P(1P)
 ROBB SCCXCI C V 1S 2P(3P) = 1S2P(1P)

75

C VI
IS - 2S

MANN CB , MANN CBX , BRANDSEN , PEEK , SAMPSON ,
 MANN CB C VI IS TO 2S
 MANN CBX C VI IS TO 2S
 BRANDSEN SOP C VI IS - 2S
 PEEK DMX C VI IS - 2S
 CARBON VI IS-2S SAMPSON

77

C VI
IS - 2P

MANN CB , MANN CBX , BRANDSEN , PEEK , ROBB CC ,
 SAMPSON
 MANN CB C VI IS TO 2P
 MANN CBX C VI IS TO 2P
 BRANDSEN SOP C VI IS - 2P
 PEEK DMX C VI IS - 2P
 ROBB 3CCX C VI IS - 2P
 CARBON VI IS-2P SAMPSON

79

C VI
IS - 3S

MANN CB , PEEK , MANN CBX ,
 MANN CB C VI IS TO 3S
 PEEK DMX C VI IS - 3S
 SAMPSON C VI IS - 3S
 MANN CBX C VI IS TO 3S

81

C VI
IS - 3P

MANN CB , PEEK , MANN CBX ,
 MANN CB C VI IS TO 3P
 PEEK DMX C VI IS - 3P
 SAMPSON C VI IS - 3P
 MANN CBX C VI IS TO 3P

83

C VI
IS - 3D

MANN CB , PEEK , MANN CBX ,
 MANN CB C VI IS TO 3D
 PEEK DMX C VI IS - 3D
 SAMPSON C VI IS - 3D
 MANN CBX C VI IS TO 3D

109,112

C VI
IS - 4S

MANN CBX , C VI IS TO 4S

109,112

C VI
IS - 4P

MANN CBX , C VI IS TO 4P

109,112

C VI
IS - 5P

MANN CBX , C VI IS TO 5P

6.3. Comparative Data in Graphical and Numerical Form for Carbon Ions

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange and the following wave functions: single-configuration excited state, two-configuration ground state $2s^2 2p + 2p^3$. HF orbitals; threshold energy (expt) is 0.391611 Ry. All C II results are unitarized.
3. Five-state Close-Coupling with single-configuration excited state and two-configuration ground state $c_1 1s^2 2s^2 2p + c_2 1s^2 2p^3 \text{ } ^2P$. Clementi¹¹ $1s, 2s, 2p \text{ } ^2P$ orbitals; calculated threshold energy is 0.3467891 Ry.
8. Five-state Close-Coupling by A. R. G. Jackson²³ -- identical to calculation 3. However, calculations here were done in resonant region just below 2D threshold. Two arbitrary points chosen from graph. Threshold energy is 0.3463 Ry.

C II
1S2 2S2 2P - 1S2 2S 2P2(4P)

1	2	3	4
SYMBOL	1	3	8
	MANN	CHX	ROBB CC SEAYON
1.00	.	.	3.250E+00
1.01	3.976E+00	3.330E+00	.
1.04	3.806E+00	.	.
2.00	.	.	3.150E+00
2.04	3.007E+00	.	.
2.16	.	2.000E+00	.
2.01	3.647E+00	.	.
3.46	.	2.430E+00	.
4.10	3.273E+00	.	.
4.33	.	2.254E+00	.
5.19	.	2.002E+00	.
5.89	2.604E+00	.	.
6.06	.	1.919E+00	.
6.92	.	1.761E+00	.
7.79	.	1.611E+00	.
8.3A	1.875E+00	.	.
8.65	.	1.472E+00	.
11.53	.	1.091E+00	.
11.92	1.165E+00	.	.
14.02	.	6.236E-01	.
16.75	6.484E-01	.	.
17.30	.	6.292E-01	.
20.19	.	4.947E-01	.
23.07	.	3.973E-01	.
24.12	3.368E-01	.	.
25.95	.	3.245E-01	.
28.04	.	2.693E-01	.
34.31	1.702E-01	.	.
48.82	8.588E-02	.	.
69.45	4.355E-02	.	.
98.81	2.209E-02	.	.
140.58	1.115E-02	.	.
200.00	5.590E-03	.	.

$C II$
1S2 2S2 2P - 1S2 2S 2P2(4P)

C II $1s^2 2s^2 2p^2 P - 1s^2 2s 2p^2 {}^2S$

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange. Ground state includes $2p^3 {}^2P$ (3.2%) plus smaller amounts of $2s2p({}^3P)3s {}^2P$, $2s2p({}^1P)3d {}^2P$, and $2s2p({}^3P)3d {}^2P$; excited state includes $2s^2 3s$ (2.85%) plus smaller amounts of $2s2p({}^3P)3p {}^2S$ and $2s2p({}^1P)3p {}^2S$. Threshold energy (expt) is 0.878778 Ry.
2. As for calculation No. 1, but without exchange.
3. Five-state Close-Coupling as described on page 23. Threshold energy is 0.9489358 Ry.

C II
 $1S2\ 2S2\ 2P + 1S2\ 2S\ 2P2(2S)$

X SYMBOL	1		2		3	
	MANN	CBX	MANN	CB	ROBB	CC
1.01	3.187E+00		4.211E+00		-	
1.26					2.398E+00	
1.37	3.936E+00		4.981E+00			
1.58					3.235E+00	
1.86	4.826E+00		5.825E+00			
1.90					3.863E+00	
2.21					4.397E+00	
2.53	5.824E+00		6.732E+00		4.850E+00	
2.85					5.228E+00	
3.16					5.641E+00	
3.44	6.897E+00		7.694E+00			
4.22					6.715E+00	
4.67	8.022E+00		8.701E+00			
5.27					7.599E+00	
6.32					8.324E+00	
6.35	9.182E+00		9.742E+00			
7.38					8.948E+00	
8.43					9.480E+00	
8.62	1.036E+01		1.081E+01			
9.48					9.949E+00	
10.54					1.036E+01	
11.71	1.154E+01		1.189E+01			
15.91	1.272E+01		1.298E+01			
21.62	1.388E+01		1.408E+01			
29.36	1.502E+01		1.518E+01			
39.89	1.616E+01		1.627E+01			
54.19	1.727E+01		1.736E+01			
73.61	1.838E+01		1.845E+01			
100.00	1.948E+01		1.953E+01

C II. $1s^2 2s^2 2p^2 P - 1s^2 2s 2p^2 \ ^2P$

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange. Ground state includes $2p^3$ plus small amount of $2s2p(^3P)3p^2P$ and $2s2p(^1P)3p^2P$. Threshold energy (expt) is 1.007801 Ry.
2. As for calculation No. 1, but without exchange.
3. Five-state Close-Coupling as described on page 23. Threshold energy is 1.114771 Ry.
5. Unitarized Distorted Wave without exchange. Clementi¹¹ $1s$, $2s$ and $2p$ from $^2P^0$ wave function; threshold energy is 0.992 Ry.

C II
 $1S2\ 2S2\ 2P - 1S2\ 2S\ 2P2(^2P)$

1	2	3	5
SYMBOL	MANN CBX	MANN CB	ROBR CC DAVIS
1.00	.	.	1.690E+01
1.01	7.822E+00	1.070E+01	.
1.08	.	.	4.632E+00
1.35	.	.	7.555E+00
1.37	1.047E+01	1.362E+01	.
1.50	.	.	2.480E+01
1.61	.	.	9.900E+00
1.86	1.376E+01	1.700E+01	.
1.88	.	.	1.190E+01
2.00	.	.	3.100E+01
2.13	.	.	1.366E+01
2.42	.	.	1.525E+01
2.53	1.765E+01	2.078E+01	.
2.69	.	.	1.671E+01
3.00	.	.	3.850E+01
3.44	2.203E+01	2.480E+01	.
3.59	.	.	2.076E+01
4.00	.	.	4.400E+01
4.49	.	.	2.396E+01
4.67	2.674E+01	2.920E+01	.
5.00	.	.	4.800E+01
5.38	.	.	2.660E+01
6.28	.	.	2.884E+01
6.35	3.161E+01	3.365E+01	.
7.18	.	.	3.074E+01
8.07	.	.	3.242E+01
8.62	3.651E+01	3.814E+01	.
8.97	.	.	3.392E+01
11.71	4.136E+01	4.263E+01	.
15.91	4.611E+01	4.728E+01	.
21.62	5.073E+01	5.147E+01	.
29.36	5.524E+01	5.579E+01	.
39.89	5.963E+01	6.005E+01	.
54.19	6.393E+01	6.425E+01	.
73.61	6.815E+01	6.839E+01	.
100.00	7.231E+01	7.249E+01	.

1S2 2S2 2P - 1S2 2S 2P2(2P) C II

C II $1s^2 2s^2 2p^2 \ ^2P - 1s^2 2s 2p^2 \ ^2D$

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange. Ground state same as on page 25; excited states include small amounts of $2s^2 3d$, $2p^2 ({}^3P) 3d \ ^2D$, and $2s 2p ({}^3P) 3p \ ^2D$. Threshold energy (expt) is 0.682276 Ry.
2. As for calculation No. 1, but without exchange.
3. Five-state close-coupling as described on page 23. Threshold energy is 0.741244 Ry.

C II
 $1s^2 2s^2 2p^2 \ ^2P - 1s^2 2s 2p^2 ({}^2D)$

X, SYMBOL	1		2		3	
	MANN	CBX	MANN	CB	ROBB	CC
1.01	9.403E+00		1.002E+01		-	
1.37	1.078E+01		1.155E+01		-	
1.62					8.923E+00	
1.86	1.244E+01		1.328E+01			
2.02					1.032E+01	
2.43					1.144E+01	
2.53	1.433E+01		1.522E+01			
2.83					1.231E+01	
3.24					1.328E+01	
3.44	1.637E+01		1.732E+01			
3.64					1.403E+01	
4.05					1.465E+01	
4.67	1.855E+01		1.955E+01			
5.40					1.663E+01	
6.35	2.088E+01		2.189E+01			
6.75					1.824E+01	
8.09					1.954E+01	
8.62	2.334E+01		2.428E+01			
9.44					2.067E+01	
10.79					2.165E+01	
11.71	2.588E+01		2.670E+01			
12.10					2.252E+01	
13.49					2.331E+01	
15.91	2.844E+01		2.913E+01			
21.62	3.130E+01		3.154E+01			
29.36	3.351E+01		3.393E+01			
39.89	3.598E+01		3.630E+01			
54.19	3.839E+01		3.864E+01			
73.61	4.077E+01		4.095E+01			
100.00	4.310E+01		4.324E+01

C III $1s^2 2s^2 \ ^1S - 1s^2 2s 2p \ ^1P$

Calculation No.	Description
1.	Coulomb-Born Unitarized with exchange. Includes mixing of same functions as in calculation 3 below. Threshold energy (expt) is 0.932743 Ry. The single-configuration calculation (not shown) with exchange gave 6.023 at $X = 1.01$, 11.38 at $X = 4.19$, and 33.28 at $X = 300$.
2.	As for calculation No. 1, but without exchange.
3.	Five-state Close-Coupling with ground-state wave function $c_1 1s^2 2s^2 + c_2 1s^2 2p^2 \ ^1S$ and excited-state wave function $c_1 1s^2 2s 2p + c_2 1s^2 2p 3d \ ^1P$. Calculated threshold energy is 0.995377 Ryds.
5.	Unitarized Distorted Wave with exchange. Single-configuration ground- and excited-state wave functions, with 1s and 2s orbitals of Clementi and a semi-empirical 2p orbital. Threshold energy is 0.933 Ry.
10.	The two calculations of Flower and Launay ²⁴ in the six-state Close-Coupling and unitarized Distorted Wave (UCL) approximations are so close that they cannot be distinguished. Threshold energy is 1.033 Ry.
11.	The two calculations of Nussbaumer ²⁰ are in the Impact Parameter (upper points) and Distorted Wave (lower points) approximations. They use CI wave functions. The Distorted Wave calculations are due to Eissner.
16.	Three-state Close-Coupling by D. E. Osterbrock ²⁵ using single-configuration wave functions in ground and excited states.

C III
152 252 = 152 28 2P(1P)

X. SYMBOL	1 MANN CBX	2 MANN CB	3 ROBB CC	5 DAVIS	10 FLOWER	10 FLOWER	11 NUSSBAUMER	11 NUSSBAUMER	16 OSTERBROCK
1.00	.	.	.	5.820E+00	.	.	.	.	.
1.01	5.724E+00	7.256E+00	.	.	.	.	.	.	.
1.06	.	.	.	.	.	.	.	.	5.870E+00
1.16	.	.	.	.	.	.	4.570E+00	3.580E+00	.
1.17	.	.	.	.	.	.	.	.	6.220E+00
1.34	6.490E+00	7.952E+00	.	.	.	.	.	.	.
1.45	.	.	.	.	3.667E+00	3.625E+00	.	.	.
1.46	.	.	.	.	.	.	4.780E+00	3.660E+00	.
1.51	.	.	4.410E+00	7.320E+00	.	.	.	.	6.780E+00
1.78	7.389E+00	8.758E+00	.	.	.	.	.	.	.
1.94	.	.	.	.	4.409E+00	4.420E+00	.	.	.
2.01	.	.	5.150E+00	8.400E+00	.	.	.	.	.
2.37	8.419E+00	9.674E+00	.	.	.	.	.	.	.
2.42	.	.	.	.	5.034E+00	4.997E+00	.	.	.
2.47	.	.	.	.	.	.	5.730E+00	5.120E+00	.
2.51	.	.	5.770E+00	.	.	.	.	.	.
3.00	.	.	.	1.020E+01	.	.	.	.	.
3.15	9.574E+00	1.070E+01	.	.	.	.	.	.	.
4.00	.	.	.	1.175E+01	.	.	.	.	.
4.02	.	.	7.400E+00	.	.	.	.	.	.
4.19	1.084E+01	1.182E+01	.	.	.	.	.	.	.
5.00	.	.	.	1.270E+01	.	.	.	.	.
5.57	1.218E+01	1.303E+01	.	.	.	.	.	.	.
6.03	.	.	8.810E+00	.	.	.	.	.	.
7.41	1.359E+01	1.430E+01	.	.	.	.	.	.	.
9.05	1.504E+01	1.562E+01	.	.	.	.	.	.	.
12.06	.	.	1.114E+01	.	.	.	.	.	.
13.09	1.651E+01	1.698E+01	.	.	.	.	.	.	.
14.06	.	.	1.170E+01	.	.	.	.	.	.
16.07	.	.	1.218E+01	.	.	.	.	.	.
17.41	1.797E+01	1.835E+01	.	.	.	.	.	.	.
18.08	.	.	1.262E+01	.	.	.	.	.	.
20.09	.	.	1.300E+01	.	.	.	.	.	.
22.10	.	.	1.335E+01	.	.	.	.	.	.
23.14	1.943E+01	1.973E+01	.	.	.	.	.	.	.
24.11	.	.	1.366E+01	.	.	.	.	.	.
26.12	.	.	1.396E+01	.	.	.	.	.	.
30.76	2.087E+01	2.111E+01	.	.	.	.	.	.	.
40.89	2.230E+01	2.248E+01	.	.	.	.	.	.	.
54.36	2.370E+01	2.384E+01	.	.	.	.	.	.	.
72.26	2.508E+01	2.519E+01	.	.	.	.	.	.	.
96.06	2.644E+01	2.652E+01	.	.	.	.	.	.	.
127.70	2.778E+01	2.785E+01	.	.	.	.	.	.	.
169.76	2.912E+01	2.916E+01	.	.	.	.	.	.	.
225.67	3.043E+01	3.047E+01	.	.	.	.	.	.	.
300.00	3.174E+01	3.177E+01	.	.	.	.	.	.	.

IS2 2S2 - 1S2 2S 2P(1P)
C III

C III $1s^2 2s^2 1S - 1s^2 2s2p^3 P$

Calculation No.	Description
1.	Coulomb-Born Unitarized with exchange; same configurations as in No. 3. Threshold energy is 0.477703 Ry. A single-configuration run gave results approximately 7% higher.
3.	Five-state Close-Coupling as described on page 31. Calculated threshold energy used is 0.4522424 Ry.
8.	Distorted Wave calculations by Eissner ²⁶ using CI target state wave functions with Thomas-Fermi orbitals.
10.	Distorted Wave (upper points) and Close-Coupling (lower points), both six-state, ²⁴ with CI ground-state wave function (single-configuration excited-state wave function) and Thomas-Fermi orbitals. Threshold energy is 0.485 Ry.
12.	Six-state Close-Coupling ²⁷ with considerable CI in both initial- and final-state wave functions to give experimental oscillator strengths and threshold energies.
16.	Three-state Close-Coupling ²⁵ using single-configuration wave functions.

C III
182 282 - 182 25 2P(3P)

X.SYMBOL	1 MANN	3 CBX	3 ROBB	CC	8 SEATON	10 FLOWER	10 FLOWER	12 BURKE	16 OSTERBROCK
1.01	1.426E+00		9.580E-01						
1.05									
1.33			7.720E-01					1.210E+00	
1.39	1.273E+00								
1.47								9.400E-01	
1.68			7.000E-01						
1.91	1.094E+00								
2.48				6.900E-01					
2.63	8.956E-01								
2.71									6.690E-01
3.00									6.450E-01
3.09						6.890E-01	6.190E-01		
3.11				6.170E-01					
3.14								5.120E-01	
3.32		6.140E-01							
3.62	6.934E-01								
3.67								4.690E-01	
3.86									5.940E-01
4.12						5.640E-01	5.270E-01		
4.19								4.350E-01	
4.43		5.500E-01							5.620E-01
4.72								4.020E-01	
4.79	5.053E-01								
5.15						4.930E-01	4.470E-01		
5.21				4.490E-01					
5.24								3.750E-01	
5.53		4.740E-01							
5.77								3.450E-01	
6.63		4.100E-01							
6.86	3.472E-01								
8.84		3.100E-01							
9.44	2.760E-01								
11.06		2.560E-01							
13.00	1.420E-01								
13.27		2.100E-01							
15.48		1.670E-01							
17.69		1.340E-01							
17.89	8.773E-02								
19.90		1.140E-01							
22.11		9.800E-02							
24.62	5.295E-02								
26.53		7.300E-02							
30.96		5.670E-02							
33.88	3.141E-02								
35.38		4.510E-02							
39.80		3.672E-02							
44.22		3.056E-02							
46.63	1.829E-02								
48.65		2.585E-02							
53.07		2.203E-02							
57.49		1.901E-02							
64.17	1.044E-02								
88.31	5.843E-03								
121.53	3.218E-03								
167.26	1.750E-03								
230.18	9.433E-04								
316.79	5.050E-04								
435.97	2.601E-04								
600.00	1.429E-04

C III $1s^2 2s^2 \ ^1S - 1s^2 2p^2 \ ^3P$

Calculation No.	Description
3.	Five-state Close-Coupling with two-configuration ground- and excited-state wave functions, $c_1 1s^2 2s^2 \ ^1S$ and $c_2 1s^2 2p^2 \ ^1S$ and $c_1 1s^2 2p^2 \ ^3P$ + $c_2 1s^2 3d^2 \ ^3P$. Threshold energy is 1.2626512 Ry.
10.	Distorted Wave (lower points) and Close-Coupling (upper points) calculations as described on page 31. Threshold energy is 1.266 Ry.

C III
 $1S^2 \ 2S^2 - 1S^2 \ 2P^2 \ (3P)$

X.SYMBOL	3 ROBB CC	10 FLOWER	10 FLOWER
1.18	1.160E-02	1.800E-02	1.320E-02
1.58	1.040E-02	1.700E-02	1.200E-02
1.97	9.300E-03	1.500E-02	1.100E-02
2.38	8.400E-03	-	-
3.17	6.700E-03	-	-
3.96	5.300E-03	-	-
4.75	4.200E-03	-	-
5.54	3.200E-03	-	-
6.34	2.500E-03	-	-
7.13	2.000E-03	-	-
7.92	1.600E-03	-	-
9.50	1.090E-03	-	-
11.09	7.839E-04	-	-
12.67	5.782E-04	-	-
14.26	4.379E-04	-	-
15.84	3.408E-04	-	-
17.42	2.737E-04	-	-
19.01	2.161E-04	-	-
20.59	1.721E-04	-	-

C_{II}^{II}
1S2 2S2 - 1S2 2P2 (3P)

C III $1s^2 2s^2 \ ^1S - 1s^2 2p^2 \ ^1D$

Calculation
No.

Description

3. Five-state Close-Coupling with two-configuration ground-state wave function (see p. 37) and three-configuration excited-state function $c_1 1s^2 2p^2 + c_2 1s^2 2s3d + c_3 1s^2 3d^2 \ ^1D$. Threshold energy is 1.349947 Ry.
10. Distorted Wave (upper points) and Close-Coupling (lower points) as described on page 31. Threshold energy is 1.418 Ry.

C III
 $1S2 \ 2S2 - 1S2 \ 2P2 \ (^1D)$

X.SYMBOL	3 ROBB CC	10 FLOWER	10 FLOWER
1.06	-	4.120E-01	2.600E-01
1.11	4.250E-01	-	-
1.41	-	3.690E-01	-
1.48	4.050E-01	-	-
1.58	-	-	2.540E-01
1.76	-	3.430E-01	-
1.85	3.880E-01	-	-
1.97	-	-	2.470E-01
2.22	3.750E-01	-	-
2.96	3.534E-01	-	-
3.70	3.420E-01	-	-
4.44	3.344E-01	-	-
5.19	3.259E-01	-	-
5.93	3.192E-01	-	-
6.67	3.116E-01	-	-
7.41	3.054E-01	-	-
8.89	2.965E-01	-	-
10.37	2.905E-01	-	-
11.85	2.872E-01	-	-
13.33	2.843E-01	-	-
14.81	2.837E-01	-	-
16.30	2.832E-01	-	-
17.78	2.830E-01	-	-
19.26	2.830E-01	-	-

1S2 2S2 - 1S2 2P2 (1D) C_{II}^I

C IV $1s^2 2s^2 S - 1s^2 2p^2 P$

Calculation No.	Description
1.	Unitarized Coulomb-Born with exchange and Hartree-Fock ¹ target wave functions. Threshold energy is 0.588303 Ry.
2.	As for calculation No. 1, but without exchange.
3.	Two-state Close-Coupling with Hartree-Fock ²⁸ target state wave functions. Threshold energy is 0.5924 Ry.
5.	Unitarized Distorted Wave without exchange. Clementi ¹¹ ground-state 1s and 2s orbitals and a semiempirical 2p orbital. Threshold energy is 0.5883 Ry.
9.	Five-state Close-Coupling calculation by Gau and Henry (unpublished) using Hartree-Fock ²⁸ wave functions and threshold energies.

C IV
192 2S • 192 2P

X SYMBOL	1	2	3	5	9
	MANN CBX	MANN CB	ROBB CC	DAVIS	HENRY
1.00	-	-	-	1.100E+01	-
1.01	9.297E+00	9.987E+00	8.850E+00	-	-
1.23	9.560E+00	1.026E+01	-	-	-
1.35	-	-	9.330E+00	-	-
1.50	9.867E+00	1.057E+01	-	1.150E+01	-
1.69	-	-	9.810E+00	-	-
1.84	1.022E+01	1.093E+01	-	-	-
2.00	-	-	-	1.200E+01	-
2.03	-	-	1.016E+01	-	-
2.24	1.063E+01	1.134E+01	-	-	-
2.36	-	-	1.054E+01	-	-
2.70	-	-	1.089E+01	-	-
2.74	1.109E+01	1.180E+01	-	-	-
3.00	-	-	-	1.300E+01	-
3.04	-	-	1.121E+01	-	-
3.34	1.161E+01	1.231E+01	-	-	-
3.38	-	-	1.153E+01	-	-
4.00	-	-	-	1.370E+01	-
4.08	1.219E+01	1.287E+01	-	-	-
4.98	1.283E+01	1.349E+01	-	-	-
5.00	-	-	-	1.430E+01	-
6.08	1.352E+01	1.415E+01	-	-	-
6.75	-	-	1.417E+01	-	-
6.81	-	-	-	-	1.354E+01
7.42	1.427E+01	1.486E+01	-	-	-
9.05	1.506E+01	1.561E+01	-	-	-
10.13	-	-	1.554E+01	-	-
10.21	-	-	-	-	1.520E+01
11.05	1.588E+01	1.640E+01	-	-	-
13.49	1.674E+01	1.721E+01	-	-	-
13.50	-	-	1.668E+01	-	-
13.61	-	-	-	-	1.659E+01
16.47	1.762E+01	1.805E+01	-	-	-
20.10	1.852E+01	1.890E+01	-	-	-
24.53	1.942E+01	1.977E+01	-	-	-
27.01	-	-	1.962E+01	-	-
27.22	-	-	-	-	2.007E+01
29.95	2.034E+01	2.064E+01	-	-	-
36.56	2.125E+01	2.151E+01	-	-	-
44.62	2.216E+01	2.239E+01	-	-	-
54.47	2.306E+01	2.326E+01	-	-	-
66.49	2.395E+01	2.412E+01	-	-	-
81.16	2.484E+01	2.498E+01	-	-	-
99.07	2.571E+01	2.583E+01	-	-	-
120.92	2.658E+01	2.668E+01	-	-	-
147.61	2.743E+01	2.752E+01	-	-	-
180.18	2.828E+01	2.835E+01	-	-	-
219.93	2.911E+01	2.917E+01	-	-	-
268.46	2.995E+01	2.999E+01	-	-	-
327.69	3.077E+01	3.081E+01	-	-	-
400.00	3.159E+01	3.162E+01	-	-	-

$1S2\ 2S^C\ 1V - 1S2\ 2P$

C IV $1s^2 2s^2 S - 1s^2 3s^2 S$

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange and Hartree-Fock target state wave functions. Threshold energy is 2.759889 Ry.
2. As for calculation No. 1, but without exchange.
9. Five-state Close-Coupling as described on page 41.

C IV
1S2 2S - 1S2 3S

X	SYMBOL	1	2	9
		MANN CBX	MANN CB	HENRY
1.01	4.411E-01	4.287E-01	"	
1.10	4.318E-01	4.366E-01	"	
1.37	4.268E-01	4.438E-01	"	
1.45	"	"		3.920E-01
1.60	4.251E-01	4.502E-01	"	
1.86	4.257E-01	4.559E-01	"	
2.17	4.280E-01	4.609E-01	4.200E-01	
2.53	4.314E-01	4.651E-01	"	
2.90	"	"		4.320E-01
2.95	4.355E-01	4.688E-01	"	
3.44	4.399E-01	4.719E-01	"	
4.01	4.444E-01	4.745E-01	"	
4.67	4.487E-01	4.766E-01	"	
5.45	4.528E-01	4.783E-01	"	
5.80	"	"		4.480E-01
6.35	4.565E-01	4.797E-01	"	
7.40	4.599E-01	4.807E-01	"	
8.62	4.629E-01	4.816E-01	"	
10.05	4.656E-01	4.822E-01	"	
11.71	4.680E-01	4.826E-01	"	
13.65	4.701E-01	4.829E-01	"	
15.91	4.719E-01	4.832E-01	"	
18.55	4.735E-01	4.833E-01	"	
21.62	4.748E-01	4.834E-01	"	
25.19	4.760E-01	4.834E-01	"	
29.36	4.770E-01	4.834E-01	"	
34.22	4.778E-01	4.834E-01	"	
39.39	4.786E-01	4.835E-01	"	
46.49	4.793E-01	4.835E-01	"	
54.19	4.798E-01	4.834E-01	"	
63.16	4.803E-01	4.834E-01	"	
73.61	4.807E-01	4.833E-01	"	
85.80	4.810E-01	4.833E-01	"	
100.00	4.813E-01	4.833E-01	"	

$1S2\ 2S^C\ 1V - 1S2\ 3S$

C IV 1s²2s 2S - 1s²3p 2P

Calculation
No.

Description

1. Unitarized Coulomb-Born with exchange and Hartree-Fock target state wave functions. Threshold energy is 2.916836 Ry.
2. As for calculation No. 1, but without exchange.
9. Five-state Close-Coupling as described on page 41.

C IV
1S2 2S - 1S2 3P

X.SYMBOL	1	2	9
	MANN CBX	MANN CB	HENRY
1.01	1.018E-01	8.264E-02	.
1.18	1.076E-01	1.070E-01	.
1.37	1.232E-01	1.357E-01	2.530E-01
1.60	1.474E-01	1.688E-01	.
1.86	1.791E-01	2.060E-01	.
2.06	.	.	2.810E-01
2.17	2.173E-01	2.474E-01	.
2.53	2.612E-01	2.927E-01	.
2.74	.	.	3.270E-01
2.95	3.101E-01	3.417E-01	.
3.44	3.635E-01	3.943E-01	.
4.01	4.207E-01	4.500E-01	.
4.67	4.814E-01	5.089E-01	.
5.45	5.451E-01	5.705E-01	.
5.49	.	.	5.600E-01
6.35	6.116E-01	6.347E-01	.
7.40	6.804E-01	7.012E-01	.
8.62	7.513E-01	7.699E-01	.
10.05	8.239E-01	8.405E-01	.
11.71	8.982E-01	9.128E-01	.
13.65	9.739E-01	9.867E-01	.
15.91	1.051E+00	1.062E+00	.
18.55	1.129E+00	1.138E+00	.
21.62	1.200E+00	1.216E+00	.
25.19	1.287E+00	1.295E+00	.
29.36	1.368E+00	1.374E+00	.
34.22	1.448E+00	1.454E+00	.
39.89	1.530E+00	1.534E+00	.
46.49	1.612E+00	1.616E+00	.
54.19	1.694E+00	1.697E+00	.
63.16	1.776E+00	1.779E+00	.
73.61	1.859E+00	1.861E+00	.
85.80	1.941E+00	1.944E+00	.
100.00	2.024E+00	2.026E+00	.

$1S2\ 2S^C\ IV - 1S2\ 3P$

C IV $1s^2 2s^2 S - 1s^2 3d^2 D$

Calculation
No.

Description

1. Coulomb-Born with exchange and Hartree-Fock target state wave functions. The high-energy droop in the collision strength is caused by an inadequate closure formula. The constant asymptotic value which obtains from these wave functions via the Born approximation is 1.26. Threshold energy is 2.960715 Ry.
2. As for calculation No. 1, but without exchange.
9. Five-state Close-Coupling as described on page 41.

C IV
 $1s^2 2s^2 - 1s^2 3d$

X SYMBOL	1		2		9
	MANN	CBX	MANN	CB	HENRY
1.01	6.461E-01		6.860E-01		.
1.18	6.501E-01		7.304E-01		.
1.35	-		-		6.560E-01
1.37	6.674E-01		7.755E-01		.
1.60	6.953E-01		8.207E-01		.
1.86	7.308E-01		8.655E-01		.
2.03	-		-		7.800E-01
2.17	7.717E-01		9.092E-01		.
2.53	8.157E-01		9.511E-01		.
2.70	-		-		8.640E-01
2.95	8.610E-01		9.909E-01		.
3.44	9.059E-01		1.028E+00		.
4.01	9.492E-01		1.062E+00		.
4.67	9.899E-01		1.093E+00		.
5.41	-		-		1.024E+00
5.45	1.028E+00		1.120E+00		.
6.35	1.062E+00		1.144E+00		.
7.40	1.092E+00		1.165E+00		.
8.62	1.119E+00		1.184E+00		.
10.05	1.142E+00		1.199E+00		.
11.71	1.162E+00		1.212E+00		.
13.65	1.179E+00		1.222E+00		.
15.91	1.194E+00		1.231E+00		.
18.55	1.205E+00		1.237E+00		.
21.62	1.215E+00		1.243E+00		.
25.19	1.222E+00		1.246E+00		.
29.36	1.228E+00		1.249E+00		.
34.22	1.232E+00		1.249E+00		.
39.89	1.234E+00		1.249E+00		.
46.40	1.234E+00		1.247E+00		.
54.19	1.232E+00		1.243E+00		.
63.16	1.228E+00		1.237E+00		.
73.61	1.222E+00		1.230E+00		.
85.80	1.216E+00		1.223E+00		.
100.00	1.208E+00		1.214E+00		.

C_{IV}
1S2 2S - 1S2 3D

C V $1s^2\ ^1S - 1s2s\ ^1S$

Calculation No.	Description
1.	Coulomb-Born with exchange. Wavefunctions obtained from the code of Hibbert. ² This transition shows unusually large sensitivity to nonorthogonality of the 2s function to the 1s function of the ground state, as discussed in Sec. 3.4. Experimental threshold energy is 22.372848 Ry.
2.	Same as calculation No. 1, but without exchange.
3.	Five-state Close-Coupling with CI target states made up from all possible configurations from 1s, 2s, and 2p orbitals. Threshold energy is 22.140116 Ry.
4.	Unitarized Distorted Wave calculations of Norcross (unpublished) using sophisticated CI target state wave functions (with n = 1, 2 and 3s, 3p orbitals) in five states. Threshold energy is 22.3572 Ry.
6.	Distorted Wave with exchange by Peek (unpublished) using Hartree-Fock ¹ wave functions but with orbitals Schmidt-orthogonalized. The difference in curve shape between this calculation and calculations No. 1 shows the effect of distortion. Same threshold as No. 1.
7.	Distorted wave calculations (lower points) by Bhatia and Temkin ⁸ (see Sec. 4b). The upper points are Coulomb-Born calculations of Tully. ²⁹ Threshold energy is 22.247 Ry.
13.	Infinite-Z Hydrogenic approximation, as described in Appendix I.
14.	Five-state Close-Coupling calculations by J. W. Cooper (unpublished) using the target wave functions of Morse, Young, and Haurwitz. ⁹ Threshold energy is 22.3026 Ry.

X SYMBOL	1	2	3	4	6	7	7	13	14			
	MANN	CBX	MANN	CB	ROBR	CC	NORCROSS	PEEK	BHATIA	BHATIA	SAMPSON	COOPER
1.00	2.010E-02	2.450E-02	1.464E-02	6.431E-03	1.666E-02	-	-	-	-	-	1.632E-02	-
1.01	-	-	-	6.683E-03	-	-	-	-	-	-	-	-
1.05	-	-	-	-	-	-	-	-	-	-	-	-
1.07	-	-	-	-	-	-	-	-	-	-	1.698E-02	-
1.12	-	-	-	-	-	-	-	-	-	-	-	1.070E-02
1.13	1.988E-02	2.511E-02	1.555E-02	9.875E-03	-	-	-	-	0.330E-03	1.960E-02	-	-
1.15	-	-	-	-	-	-	-	-	-	-	-	-
1.20	-	-	-	-	-	-	-	-	-	-	-	-
1.21	-	-	-	-	-	-	-	-	-	-	-	-
1.24	-	-	-	-	-	-	-	-	-	-	-	-
1.31	1.985E-02	2.558E-02	1.628E-02	1.271E-02	-	-	-	-	0.990E-03	1.982E-02	-	-
1.33	-	-	-	1.302E-02	-	-	-	-	-	-	-	-
1.35	-	-	-	-	1.720E-02	-	-	-	-	-	-	-
1.37	-	-	-	1.810E-02	-	-	-	-	-	-	-	-
1.47	2.000E-02	2.597E-02	-	-	-	-	-	-	-	-	-	-
1.48	-	-	-	-	-	-	-	-	-	-	-	-
1.55	-	-	-	-	-	-	-	-	-	-	-	-
1.58	-	-	-	-	-	-	-	-	-	-	-	-
1.62	-	-	-	-	1.865E-02	-	-	-	-	-	-	-
1.69	2.027E-02	2.628E-02	-	1.553E-02	-	-	-	-	1.134E-02	2.040E-02	-	-
1.79	-	-	-	-	-	-	-	-	-	-	-	-
1.81	-	-	-	-	-	-	-	-	-	-	-	-
1.92	2.063E-02	2.653E-02	1.991E-02	1.662E-02	2.159E-02	-	-	-	-	-	-	2.320E-02
2.00	-	-	-	-	-	-	-	-	-	-	-	-
2.03	-	-	-	-	-	-	-	-	-	-	-	-
2.10	-	-	-	-	1.782E-02	-	-	-	-	-	-	-
2.18	2.104E-02	2.673E-02	-	-	-	-	-	-	-	-	-	-
2.24	-	-	-	-	-	-	-	-	-	-	-	-
2.40	-	-	-	-	-	-	-	-	1.370E-02	2.090E-02	-	-
2.48	2.104E-02	2.689E-02	-	-	-	-	-	-	-	-	-	-
2.67	-	-	-	-	-	-	-	-	-	-	-	-
2.70	-	-	-	-	-	-	-	-	-	-	-	-
2.71	-	-	-	-	-	-	-	-	-	-	-	-
2.82	2.193E-02	2.702E-02	2.299E-02	-	-	-	-	-	1.022E-02	2.106E-02	2.396E-02	-
3.04	2.238E-02	2.711E-02	-	-	-	-	-	-	-	-	-	-
3.21	-	-	-	-	-	-	-	-	-	-	-	-
3.59	-	-	-	-	-	-	-	-	-	-	-	-
3.61	-	-	-	-	-	-	-	-	-	-	-	-
3.65	2.202E-02	2.710E-02	2.446E-02	-	-	-	-	-	-	-	-	-
4.00	-	-	-	-	-	-	-	-	-	-	-	-
4.14	2.324E-02	2.724E-02	-	-	-	-	-	-	-	-	2.581E-02	-
4.20	-	-	-	-	-	-	-	-	-	-	-	-
4.49	-	-	-	-	-	-	-	-	-	-	-	-
4.52	-	-	-	-	-	-	-	-	-	-	-	-
4.71	2.364E-02	2.727E-02	2.538E-02	-	-	-	-	-	1.730E-02	2.120E-02	-	-

1S2 - 1S 2S(1S) C_V

C V $1s^2 1S - 1s2s^3S$

Calculation No.	Description
1.	Coulomb-Born with exchange. Threshold energy is 21.974044 Ry. Orthogonalization as described for $1s2s^1S$ brings about only minor changes (less than 10%) near threshold.
3.	Five-state Close-Coupling calculation as described on page 50. Threshold energy is 21.7675938 Ry.
4.	Five-state Distorted Wave calculation as described on page 50. Threshold energy is 21.9724 Ry.
6.	Distorted Wave calculation as described on page 50. Same threshold as No. 1.
7.	Distorted Wave calculation as described on page 50. Threshold energy is 21.849 Ry.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.
14.	Five-state Close-Coupling calculation as described on page 50. Threshold energy is 21.891 Ry.

C V
152 - 15 25(38)

1	2	3	4	5	6	7	8	9	10	11	12	13	14
X.SYMBOL	MANN	CRX	ROBB	CC	NORCROSS	PEEK	BHATIA	SAMPSON	COOPER				
1.00	.	.	.	.	.	7.837E-03	.	7.775E-03	.				
1.01	2.08AE-03	.	.	.	.	.	.	.	.				
1.03	.	8.003E-03	.	.	5.456E-03	.	.	.	.				
1.07	.	.	.	.	4.739E-03	.	.	7.267E-03	.				
1.13	.	.	.	.	5.631E-03	.	.	.	.	1.490E-02			
1.15	2.182E-03	6.427E-03	.	.	.	6.878E-03	4.875E-03	.	.				
1.28	.	.	.	.	.	.	.	6.379E-03	.				
1.24	.	.	.	.	.	.	4.887E-03	.	.				
1.26	.	5.442E-03	.	.	.	.	.	.	.				
1.31	2.270E-03	.	.	.	.	.	.	.	.				
1.33	.	.	.	4.953E-03	.	.	.	5.648E-03	.				
1.35	.	.	.	.	5.756E-03	.	.	.	.				
1.37	.	.	.	4.878E-03	.	.	.	.	.	1.060E-02			
1.38	.	4.838E-03	.	.	.	.	.	.	.				
1.40	2.306E-03	4.386E-03	.	.	.	.	.	.	.				
1.55	.	.	.	.	.	4.844E-03	.	.	.				
1.61	.	3.960E-03	.	.	.	.	.	.	.				
1.65	.	.	4.139E-03	.	.	.	4.392E-03	.	.				
1.69	2.276E-03	.	.	.	.	.	.	.	.				
1.80	.	.	.	.	.	3.968E-03	.	.	.				
1.82	.	.	3.739E-03	.	.	.	.	.	.	6.930E-03			
1.84	.	3.290E-03	.	.	.	.	.	.	.				
1.92	2.187E-03	.	.	.	.	.	.	.	.				
2.00	.	.	.	3.250E-03	.	.	.	3.378E-03	.				
2.06	.	.	.	.	.	.	.	.	.				
2.10	.	.	.	.	.	3.210E-03	.	.	.				
2.18	2.037E-03	.	.	.	.	.	.	.	.				
2.20	.	.	.	.	.	.	2.800E-03	.	.				
2.48	.	.	.	.	.	2.665E-03	.	.	.				
2.48	1.856E-03	.	.	.	.	.	.	.	.				
2.67	.	.	.	.	.	.	.	2.253E-03	.				
2.70	.	.	.	.	.	2.258E-03	.	.	.				
2.76	.	1.881E-03	.	.	.	.	2.640E-03	.	.				
2.82	1.657E-03	.	.	.	.	.	.	.	.				
3.09	.	.	1.908E-03	.	.	.	.	.	.				
3.21	1.452E-03	.	.	.	.	1.764E-03	.	.	.				
3.65	1.252E-03	.	.	.	.	.	.	.	.				
3.66	.	.	.	.	.	.	1.760E-03	.	.				
3.68	.	1.208E-03	.	.	.	.	.	.	.				
4.00	.	.	.	.	.	.	.	1.202E-03	.				
4.14	1.065E-03	.	.	.	.	.	.	.	.				
4.20	.	.	.	.	.	1.158E-03	.	.	.				
4.53	.	.	.	.	.	.	1.300E-03	.	.				
4.59	.	8.599E-04	.	.	.	.	.	.	.				
4.71	8.942E-04	.	.	.	.	.	.	.	.				
5.14	.	.	8.639E-04	.	.	.	.	.	.				
5.33	.	.	.	.	.	.	.	7.593E-04	.				
5.36	7.429E-04	.	.	.	.	.	.	.	.				
5.51	.	6.921E-04	.	.	.	.	.	.	.				
5.68	.	.	.	.	.	7.182E-04	.	.	.				
6.09	6.114E-04	.	.	.	.	.	.	.	.				
6.93	4.990E-04	.	.	.	.	.	.	.	.				
7.50	.	.	.	.	.	4.381E-04	.	.	.				
7.87	4.003E-04	.	.	.	.	.	.	.	.				
8.95	3.255E-04	.	.	.	.	.	.	.	.				
10.00	.	.	.	.	.	2.646E-04	.	.	.				
10.18	2.606E-04	.	.	.	.	.	.	.	.				
11.57	2.076E-04	.	.	.	.	.	.	.	.				
13.16	1.647E-04	.	.	.	.	.	.	.	.				
13.50	.	.	.	.	.	1.538E-04	.	.	.				
14.96	1.302E-04	.	.	.	.	.	.	.	.				
17.01	1.026E-04	.	.	.	.	.	.	.	.				
18.00	.	.	.	.	.	9.058E-05	.	.	.				
19.34	8.465E-05	.	.	.	.	.	.	.	.				
21.99	6.324E-05	.	.	.	.	.	.	.	.				
24.00	.	.	.	.	.	5.277E-05	.	.	.				
25.00	4.948E-05	.	.	.	.	.	.	.	.				
32.00	.	.	.	.	.	3.046E-05	.	.	.				
42.00	.	.	.	.	.	1.800E-05	.	.	.				
56.00	.	.	.	.	.	1.031E-05	.	.	.				
75.00	.	.	.	.	.	5.815E-06	.	.	.				
100.00	.	.	.	.	.	3.202E-06	.	.	.

$$\underline{C\ V\ 1s^2\ ^1S - 1s2p\ ^1P}$$

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy is 22.631176 Ry.
2. Same, without exchange.
3. Five-state Close-Coupling calculation as described on page 50. Threshold energy used is 22.3914612 Ry.
4. Five-state Distorted Wave calculation as described on page 50. Threshold energy is 22.6318 Ry.
5. Distorted Wave calculation with exchange and Clementi ground-state wave function and semiempirical 2p orbital in the excited-state wave function. Threshold energy is 22.631 Ry.
6. Distorted Wave calculation as described on page 50. Same threshold energy as in No. 1.
7. Distorted Wave⁵ (lower points) and Coulomb-Born²⁹ calculations. Threshold energy is 22.523 Ry.
13. Infinite-Z Hydrogenic approximation, as described in Appendix I.
14. Five-state Close-Coupling calculation as described on page 50. Threshold energy is 22.555 Ry.

[illegible]

X.SYMBOL	1	2	3	4	5	6	7	7	13	14			
	MANN	COX	MANN	CB	ROBB	CC	NORCROSS	DAVIS	PEEK	SHATIA	SHATIA	SAMPSON	COOPER
4.44	-	-	-	-	1.848E-01	-	-	-	-	1.895E-01	1.830E-01	-	-
4.47	-	-	-	-	-	-	-	-	-	-	-	-	-
4.71	2.070E-01	2.240E-01	-	-	-	-	-	-	-	-	-	-	-
5.00	-	-	-	-	-	-	2.001E-01	2.000E-01	-	-	-	-	-
5.33	-	-	-	-	-	-	-	-	-	-	-	2.712E-01	-
5.36	2.234E-01	2.340E-01	-	-	-	-	-	-	-	-	-	-	-
5.60	-	-	-	-	-	-	-	-	-	-	-	-	-
6.09	2.390E-01	2.534E-01	-	-	-	-	-	-	2.278E-01	-	-	-	-
6.93	2.563E-01	2.682E-01	-	-	-	-	-	-	-	-	-	-	-
7.50	-	-	-	-	-	-	-	-	2.645E-01	-	-	-	-
7.87	2.728E-01	2.832E-01	-	-	-	-	-	-	-	-	-	-	-
8.05	2.893E-01	2.905E-01	-	-	-	-	-	-	-	-	-	-	-
10.00	-	-	-	-	-	-	-	-	3.011E-01	-	-	-	-
10.18	3.058E-01	3.138E-01	-	-	-	-	-	-	-	-	-	-	-
11.57	3.240E-01	3.294E-01	-	-	-	-	-	-	-	-	-	-	-
13.16	3.389E-01	3.450E-01	-	-	-	-	-	-	-	-	-	-	-
13.50	-	-	-	-	-	-	-	-	-	-	-	-	-
14.96	3.554E-01	3.607E-01	-	-	-	-	-	-	3.398E-01	-	-	-	-
17.01	3.718E-01	3.765E-01	-	-	-	-	-	-	-	-	-	-	-
18.00	-	-	-	-	-	-	-	-	-	-	-	-	-
19.34	3.883E-01	3.924E-01	-	-	-	-	-	-	3.770E-01	-	-	-	-
21.99	4.048E-01	4.064E-01	-	-	-	-	-	-	-	-	-	-	-
24.00	-	-	-	-	-	-	-	-	-	-	-	-	-
25.00	4.212E-01	4.244E-01	-	-	-	-	-	-	4.123E-01	-	-	-	-
32.00	-	-	-	-	-	-	-	-	-	-	-	-	-
42.00	-	-	-	-	-	-	-	-	4.474E-01	-	-	-	-
56.00	-	-	-	-	-	-	-	-	4.810E-01	-	-	-	-
									5.121E-01	-	-	-	-

C V $1s^2 1S - 1s2p^3P$

Calculation No.	Description
1.	Coulomb-Born with exchange. Threshold energy is 22.374680 Ry.
3.	Five-state Close-Coupling calculation as described on page 50. Threshold energy is 22.1560958 Ry.
4.	Five-state Distorted Wave calculation as described on page 50. Threshold energy is 22.3573 Ry.
6.	Distorted Wave calculation using the same target state wave functions as in calculation No. 1. Same threshold energy as No. 1.
7.	Distorted Wave calculation ⁸ as described in Sec. 4.2.1. Thresh- old energy is 22.267 Ry.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.
14.	Five-state Close-Coupling as described on page 50. Threshold energy used is 22.299 Ry.

C V
152 - 13 2P(3P)

X SYMBOL	1 MANN	3 CRX	3 ROBB	4 CC	4 NORCROSS	6 PEEK	7 BHATIA	13 SAMPSON	14 COOPER
1.00	.	.	.	.	.	4.843E-02	.	4.384E-02	.
1.01	3.985E-02	.	3.118E-02	.	3.520E-02	.	.	.	.
1.05	.	.	.	.	3.222E-02	.	.	.	.
1.07	.	.	.	.	.	.	.	3.981E-02	.
1.11	.	.	.	.	3.631E-02	.	.	.	.
1.13	.	.	2.904E-02	.	.	2.800E-02	.	.	.
1.15	3.404E-02	.	.	.	3.441E-02	.	.	.	.
1.17	.	.	.	.	.	.	.	.	4.770E-02
1.20	.	.	.	.	.	.	.	3.327E-02	.
1.21	.	.	.	.	.	.	2.500E-02	.	.
1.24	.	.	2.587E-02	.	.	.	.	.	.
1.31	2.853E-02	.	.	.	2.428E-02	.	.	.	.
1.33	.	.	.	.	2.741E-02	.	.	2.812E-02	.
1.35	.	.	2.291E-02	.	.	2.894E-02	.	.	.
1.41	.	.	.	.	.	.	.	.	3.490E-02
1.47	.	.	2.022E-02	.	.	.	.	.	.
1.48	2.351E-02	.	.	.	.	.	.	.	.
1.55	.	.	.	.	.	2.240E-02	.	.	.
1.58	.	.	1.778E-02	.	.	.	.	.	.
1.62	.	.	.	.	2.017E-02	.	1.510E-02	.	.
1.69	1.910E-02	.	.	.	.	.	.	.	.
1.79	.	.	.	.	1.692E-02	.	.	.	.
1.81	.	.	1.392E-02	.	.	1.683E-02	.	.	.
1.88	.	.	.	.	.	.	.	.	2.050E-02
1.92	1.132E-02	.	.	.	.	.	.	.	.
2.00	.	.	.	.	.	.	.	1.406E-02	.
2.03	.	.	.	.	1.346E-02	.	.	.	.
2.10	.	.	.	.	.	1.246E-02	.	.	.
2.18	1.216E-02	.	.	.	.	.	.	.	.
2.25	.	.	.	.	.	.	7.600E-03	.	.
2.26	.	.	9.277E-03	.	.	.	.	.	.
2.40	.	.	.	.	.	9.565E-03	.	.	.
2.48	9.567E-03	.	.	.	.	.	.	.	.
2.67	.	.	.	.	.	.	.	8.265E-03	.
2.69	.	.	.	.	.	7.552E-03	4.900E-03	.	.
2.71	.	.	6.376E-03	.	.	.	.	.	.
2.82	7.467E-03	.	.	.	.	.	.	.	.
3.00	.	.	.	.	6.075E-03	.	.	.	.
3.16	.	.	4.770E-03	.	.	.	.	.	.
3.21	5.790E-03	.	.	.	.	5.347E-03	.	.	.
3.59	.	.	.	.	.	.	2.580E-03	.	.
3.61	.	.	3.498E-03	.	.	.	.	.	.
3.65	4.465E-03	.	.	.	.	.	.	.	.
4.00	.	.	.	.	.	.	.	3.743E-03	.
4.06	.	.	2.859E-03	.	.	.	.	.	.
4.14	3.426E-03	.	.	.	.	.	.	.	.
4.20	.	.	.	.	.	3.039E-03	.	.	.
4.49	.	.	.	.	.	.	1.380E-03	.	.
4.51	.	.	2.171E-03	.	.	.	.	.	.
4.71	2.622E-03	.	.	.	.	.	.	.	.
5.05	.	.	.	.	2.097E-03	.	.	.	.
5.33	.	.	.	.	.	.	.	2.096E-03	.
5.36	2.000E-03	.	.	.	.	.	.	.	.
5.80	.	.	.	.	.	1.654E-03	.	.	.
6.09	1.523E-03	.	.	.	.	.	.	.	.
6.93	1.157E-03	.	.	.	.	.	.	.	.
7.50	.	.	.	.	.	8.903E-04	.	.	.
7.87	8.790E-04	.	.	.	.	.	.	.	.
8.95	6.672E-04	.	.	.	.	.	.	.	.
10.00	.	.	.	.	.	4.838E-04	.	.	.
10.18	5.065E-04	.	.	.	.	.	.	.	.
11.57	3.846E-04	.	.	.	.	.	.	.	.
13.16	2.921E-04	.	.	.	.	.	.	.	.
13.50	.	.	.	.	.	2.567E-04	.	.	.
14.96	2.221E-04	.	.	.	.	.	.	.	.
17.01	1.690E-04	.	.	.	.	.	.	.	.
18.00	.	.	.	.	.	1.403E-04	.	.	.
19.34	1.287E-04	.	.	.	.	.	.	.	.
21.99	9.810E-05	.	.	.	.	.	.	.	.
24.00	.	.	.	.	.	7.706E-05	.	.	.
25.00	7.498E-05	.	.	.	.	.	.	.	.
32.00	.	.	.	.	.	2.249E-05	.	.	.
42.00	.	.	.	.	.	2.429E-05	.	.	.
56.00	.	.	.	.	.	1.348E-05	.	.	.

$C_V^{1S2-1S2P(3P)}$

C V 1s2s ³S - 1s2p ¹P

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy (expt) is 0.657136 Ry.
3. Five-state Close-Coupling calculation as described on page 50. Threshold energy is 0.6238674 Ry.
4. Five-state Distorted Wave calculation as described on page 50. Threshold energy is 0.6594 Ry.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C V
IS 2S(3S) - IS 2P(1P)

X.SYMBOL	1 MANN	3 CBX	3 ROBB	4 CC	4 NORCROSS	13 SAMPSON
1.00	-	-	-	-	-	1.171E-01
1.01	9.851E-02	-	-	-	-	-
1.10	-	-	-	-	1.168E-01	-
1.17	-	-	1.840E-01	-	-	-
1.29	9.510E-02	-	-	-	-	-
1.66	9.108E-02	-	-	-	-	-
2.13	8.638E-02	-	-	-	-	-
2.16	-	-	-	-	1.048E-01	-
2.73	8.894E-02	-	-	-	-	-
2.91	-	-	-	-	-	8.976E-02
3.49	7.478E-02	-	-	-	-	-
4.44	-	-	-	-	9.555E-02	-
4.48	6.789E-02	-	-	-	-	-
4.59	-	-	-	-	9.392E-02	-
5.18	-	-	1.125E-01	-	-	-
5.74	6.034E-02	-	-	-	-	-
6.72	-	-	-	-	-	5.648E-02
7.36	5.227E-02	-	-	-	-	-
9.19	-	-	7.240E-02	-	-	-
9.43	4.398E-02	-	-	-	-	-
10.52	-	-	-	-	-	3.856E-02
11.26	-	-	-	-	4.989E-02	-
12.08	3.588E-02	-	-	-	-	-
12.17	-	-	-	-	4.617E-02	-
13.20	-	-	4.974E-02	-	-	-
15.49	2.816E-02	-	-	-	-	-
17.28	-	-	3.601E-02	-	-	-
19.85	2.140E-02	-	-	-	-	-
21.21	-	-	2.714E-02	-	-	-
21.57	-	-	-	-	2.311E-02	-
25.44	1.572E-02	-	-	-	-	-
27.34	-	-	-	-	1.639E-02	-
29.23	-	-	1.690E-02	-	-	-
32.61	1.119E-02	-	-	-	-	-
35.37	-	-	-	-	1.107E-02	-
41.79	7.752E-03	-	-	-	-	-
45.26	-	-	8.305E-03	-	-	-
48.62	-	-	-	-	-	5.140E-03
53.57	5.238E-03	-	-	-	-	-
61.29	-	-	5.798E-03	-	-	-
68.66	3.467E-03	-	-	-	-	-
69.65	-	-	-	-	3.517E-03	-
77.32	-	-	3.847E-03	-	-	-
86.72	-	-	-	-	-	1.935E-03
88.00	2.256E-03	-	-	-	-	-
93.35	-	-	2.038E-03	-	-	-
109.38	-	-	1.434E-03	-	-	-
112.79	1.447E-03	-	-	-	-	-
124.82	-	-	-	-	-	1.003E-03
125.41	-	-	1.026E-03	-	-	-
138.04	-	-	-	-	1.000E-03	-
144.56	9.172E-04	-	-	-	-	-
185.28	5.763E-04	-	-	-	-	-
237.47	3.594E-04	-	-	-	-	-
304.37	2.229E-04	-	-	-	-	-
390.11	1.377E-04	-	-	-	-	-
500.00	8.471E-05	-	-	-	-	-
640.85	5.202E-05	-	-	-	-	-
821.37	3.187E-05	-	-	-	-	-
1052.75	1.950E-05	-	-	-	-	-
1340.31	1.192E-05	-	-	-	-	-
1729.40	7.275E-06	-	-	-	-	-

C V 1s2s ¹S - 1s2p ¹P

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy is 0.258328 Ry (expt).
2. As for calculation No. 1, but without exchange.
3. Five-state Close-Coupling as described on page 50. Threshold energy is 0.2513452 Ry.
4. Five-state Distorted Wave calculation as described on page 50. Threshold energy is 0.2746 Ry.

C V
1S 2S(1S) - 1S 2P(1P)

X, SYMBOL	1 MANN CBX	2 MANN CB	3 ROBB CC	4 NORCROSS
1.01	4.665E+00	4.888E+00	.	.
1.19	.	.	.	4.650E+00
1.33	4.746E+00	4.972E+00	.	.
1.43	.	.	4.802E+00	.
1.75	4.850E+00	5.079E+00	.	.
2.31	4.982E+00	5.215E+00	.	.
3.05	5.146E+00	5.383E+00	.	.
3.74	.	.	.	5.350E+00
4.01	5.347E+00	5.588E+00	.	.
5.29	5.597E+00	5.834E+00	.	.
6.97	5.876E+00	6.122E+00	.	.
9.18	6.207E+00	6.452E+00	.	.
9.20	.	.	.	6.367E+00
11.38	.	.	6.832E+00	.
12.10	6.581E+00	6.821E+00	.	.
15.94	6.991E+00	7.223E+00	.	.
21.01	7.433E+00	7.652E+00	.	.
21.34	.	.	7.868E+00	.
25.59	.	.	.	8.011E+00
27.69	7.898E+00	8.107E+00	.	.
31.29	.	.	8.559E+00	.
36.48	8.379E+00	8.560E+00	.	.
41.24	.	.	9.076E+00	.
48.07	8.866E+00	9.026E+00	.	.
50.35	.	.	.	9.220E+00
51.19	.	.	9.485E+00	.
63.35	9.354E+00	9.492E+00	.	.
71.10	.	.	1.011E+01	.
83.47	9.837E+00	9.953E+00	.	.
83.49	.	.	.	1.013E+01
110.00	1.031E+01	1.041E+01	.	.
110.01	.	.	1.097E+01	.
144.95	1.078E+01	1.085E+01	.	.
150.72	.	.	1.158E+01	.
165.79	.	.	.	1.132E+01
190.52	.	.	1.207E+01	.
191.00	1.123E+01	1.129E+01	.	.
230.33	.	.	1.247E+01	.
251.69	1.167E+01	1.172E+01	.	.
270.14	.	.	1.283E+01	.
309.95	.	.	1.314E+01	.
330.03	.	.	.	1.249E+01
331.66	1.210E+01	1.214E+01	.	.
437.04	1.252E+01	1.255E+01	.	.
575.90	1.293E+01	1.296E+01	.	.
758.88	1.334E+01	1.336E+01	.	.
1000.00	1.374E+01	1.375E+01	.	.

1S 2S(1S) - 1S 2P(1P) C_V

C V 1s2s ³S - 1s2p ³P

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy is 0.400639 Ry (expt).
2. As for calculation No. 1, but without exchange.
3. Five-state Close-Coupling calculation as described on page 50. Threshold energy is 0.3885 Ry.
4. Five-state Distorted Wave calculation as described on page 50. Threshold energy is 0.3854 Ry.

C V
1S 2S(3S) - 1S 2P(3P)

1. SYMBOL	1	2	3	4
	MANN CBX	MANN CB	ROBB CC	NORCROSS
1.01	1.291E+01	1.355E+01	"	"
1.33	1.318E+01	1.383E+01	"	"
1.75	1.352E+01	1.418E+01	"	"
1.89	"	"	1.652E+01	1.348E+01
2.31	1.395E+01	1.461E+01	"	"
3.05	1.448E+01	1.515E+01	"	"
3.70	"	"	"	1.494E+01
4.01	1.512E+01	1.579E+01	"	"
5.29	1.549E+01	1.655E+01	"	"
6.97	1.678E+01	1.743E+01	"	"
7.59	"	"	"	1.724E+01
8.32	"	"	2.011E+01	"
9.10	1.779E+01	1.843E+01	"	"
12.10	1.892E+01	1.952E+01	"	"
14.76	"	"	2.217E+01	"
15.94	2.013E+01	2.070E+01	"	"
19.27	"	"	"	2.124E+01
21.01	2.143E+01	2.195E+01	"	"
21.12	"	"	2.360E+01	"
27.63	"	"	2.470E+01	"
27.69	2.277E+01	2.324E+01	"	"
34.06	"	"	2.560E+01	"
36.48	2.414E+01	2.455E+01	"	"
36.91	"	"	"	2.444E+01
46.93	"	"	2.703E+01	"
48.07	2.553E+01	2.588E+01	"	"
60.52	"	"	"	2.691E+01
63.35	2.691E+01	2.721E+01	"	"
83.47	2.827E+01	2.852E+01	"	"
98.41	"	"	3.057E+01	"
110.00	2.961E+01	2.981E+01	"	"
119.16	"	"	"	3.022E+01
144.95	3.093E+01	3.100E+01	"	"
149.89	"	"	3.205E+01	"
191.00	3.221E+01	3.230E+01	"	"
201.37	"	"	3.463E+01	"
236.19	"	"	"	3.350E+01
251.69	3.348E+01	3.358E+01	"	"
252.85	"	"	3.610E+01	"
331.66	3.471E+01	3.480E+01	"	"
437.04	3.593E+01	3.600E+01	"	"
575.90	3.713E+01	3.718E+01	"	"
758.88	3.832E+01	3.836E+01	"	"
1000.00	3.949E+01	3.952E+01	"	"

C V 1s2s ³S - 1s2s ¹S

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy (expt) is 0.398807 Ry. The tail at high-X results from inner electron excitation.
3. Five-state Close-Coupling calculation as described on page 50. Threshold energy is 0.372522 Ry.
4. Five-state Distorted Wave calculation as described on page 50. Threshold energy is 0.3848 Ry.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C V
1S 2S(3S) - 1S 2S(1S)

X SYMBOL	1 MANN	3 CBX	3 ROBB	4 CC	4 NORCROSS	13 SAMPSON
1.00						7.220E-02
1.01	8.496E-02					
1.46	8.135E-02					
1.96			1.131E-01		1.036E-01	
2.11	7.659E-02					
3.04	7.055E-02					
3.83					8.458E-02	
4.13						5.700E-02
4.39	6.319E-02					
6.34	5.402E-02					
8.13					5.778E-02	
8.68			6.606E-02			
9.16	4.596E-02					
10.40						4.264E-02
13.22	3.736E-02					
15.38			4.738E-02			
16.67						3.564E-02
19.09	2.979E-02					
21.55					3.050E-02	
22.09			3.035E-02			
27.57	2.374E-02					
28.80			3.306E-02			
35.51			2.911E-02			
38.24					2.352E-02	
39.02	1.924E-02					
48.01						2.100E-02
48.39					2.125E-02	
48.93			2.431E-02			
57.50	1.587E-02					
62.59					1.900E-02	
75.77			1.059E-02			
79.35						1.450E-02
83.03	1.300E-02					
102.01			1.481E-02			
119.30					1.198E-02	
119.89	1.021E-02					
129.45			1.225E-02			
142.03						8.060E-03
156.29			9.547E-03			
173.13	7.471E-03					
183.13			8.571E-03			
204.71						5.116E-03
209.96			6.606E-03			
244.37					5.580E-03	
250.00	5.032E-03

C V 1s2p ³P - 1s2p ¹P

Calculation
No.

Description

3. Five-state Close-Coupling calculation as described on page 50.
Threshold energy is 0.235365 Ry.
4. Five-state Distorted Wave calculation as described on page 50.
Threshold energy is 0.2740 Ry.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C V
1S 2P(3P) - 1S 2P(1P)

X, SYMBOL	3 PORB CC	4 NORCROSS	13 SAMPSON
1.00	-	-	9.160E-01
1.46	7.412E-01	9.133E-01	-
4.43	-	7.922E-01	-
5.89	-	-	6.796E-01
11.23	-	6.228E-01	-
11.83	4.368E-01	-	-
15.68	-	-	4.304E-01
22.22	2.840E-01	-	-
25.46	-	-	3.064E-01
32.47	-	2.908E-01	-
32.60	2.022E-01	-	-
42.98	1.549E-01	-	-
53.36	1.244E-01	-	-
58.88	-	1.626E-01	-
74.13	8.881E-02	-	-
74.39	-	-	1.162E-01
74.96	-	1.266E-01	-
97.43	-	9.917E-02	-
115.65	5.692E-02	-	-
123.31	-	-	6.776E-02
157.18	4.193E-02	-	-
193.48	-	4.781E-02	-
198.71	3.238E-02	-	-
221.16	-	-	3.320E-02
240.24	2.497E-02	-	-
281.77	2.136E-02	-	-
319.01	-	-	2.002E-02
323.29	1.662E-02	-	-
385.13	-	2.000E-02	-

$C^V_{1S\ 2P(3P) - 1S\ 2P(1P)}$

C VI 1s - 2s

Calculation No.	Description
1.	Coulomb-Born with exchange. Threshold energy is 27.01036 Ry.
2.	Coulomb-Born without exchange.
6.	Distorted Wave calculation with exchange, and same threshold as in No. 1.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.
18.	Second-Order Potential calculations of Bransden and Noble. ²¹

C VI
1s - 2s

X SYMBOL	1 MANN CBX	2 MANN CB	6 PEEK	13 SAMPSON	18 BRANDSEN
1.00	.	.	2.115E-02	2.000E-02	.
1.01	1.029E-02	2.287E-02	.	.	.
1.07	.	.	.	2.020E-02	.
1.17	1.901E-02	2.334E-02	.	.	.
1.20	.	.	.	2.042E-02	.
1.33	.	.	.	2.060E-02	.
1.35	.	.	2.175E-02	.	.
1.36	1.960E-02	2.374E-02	.	.	.
1.50	2.010E-02	2.405E-02	.	.	.
1.80	.	.	2.214E-02	.	.
1.80	2.052E-02	2.431E-02	.	.	.
2.00	.	.	.	2.134E-02	.
2.13	2.089E-02	2.450E-02	.	.	.
2.45	.	.	.	.	1.991E-02
2.47	2.122E-02	2.464E-02	.	.	.
2.67	.	.	.	2.164E-02	.
2.67	2.151E-02	2.475E-02	.	.	.
3.20	.	.	2.286E-02	.	.
3.33	2.179E-02	2.482E-02	.	.	.
3.87	2.205E-02	2.487E-02	.	.	.
4.00	.	.	.	2.250E-02	.
4.49	2.230E-02	2.490E-02	.	.	.
4.90	.	.	.	.	2.080E-02
5.22	2.253E-02	2.491E-02	.	.	.
5.33	.	.	.	2.292E-02	.
5.60	.	.	2.345E-02	.	.
6.06	2.275E-02	2.491E-02	.	.	.
7.03	2.296E-02	2.491E-02	.	.	.
8.17	2.315E-02	2.489E-02	.	.	.
9.40	2.332E-02	2.480E-02	.	.	.
9.80	.	.	.	.	2.270E-02
10.00	.	.	2.390E-02	.	.
11.01	2.348E-02	2.486E-02	.	.	.
12.78	2.362E-02	2.485E-02	.	.	.
14.84	2.375E-02	2.483E-02	.	.	.
17.15	.	.	.	.	2.429E-02
17.23	2.386E-02	2.481E-02	.	.	.
18.00	.	.	2.421E-02	.	.
20.00	2.396E-02	2.480E-02	.	.	.
24.50	.	.	.	.	2.450E-02
32.00	.	.	2.438E-02	.	.

C_{VI}^{1S-2S}

C VI 1s - 2p

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy is 27.012964 Ry.
2. Coulomb-Born without exchange.
3. Three-state Close-Coupling calculation. Threshold energy is 27.0 Ry.
6. Distorted Wave calculation with exchange, and same threshold as No. 1.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.
18. Second-Order Potential calculation of Bransden and Noble.²¹

C VI 1s - 2p

X. SYMBOL	1 MANN	2 CBX	3 MANN	4 CB	5 ROBB	6 CC	7 PEEK	8 SAMPSON	9 BRANDEN
1.00	.	.	.	.	.	.	8.373E-02	8.212E-02	.
1.01	7.670E-02	8.429E-02	.	.	.	.	.	.	.
1.07	.	.	.	.	8.300E-02	.	.	8.412E-02	.
1.11	.	.	.	.	8.440E-02	.	.	.	.
1.15	.	.	.	.	8.600E-02	.	.	.	.
1.19	.	.	.	.	6.770E-02	.	.	.	.
1.20	.	.	.	.	.	.	.	8.884E-02	.
1.23	8.470E-02	1.021E-01	.	.	.	.	.	.	.
1.30	.	.	.	.	9.210E-02	.	.	.	.
1.33	.	.	.	.	.	.	.	9.428E-02	.
1.35	.	.	.	.	.	.	9.380E-02	.	.
1.50	9.646E-02	1.173E-01	.	.	.	.	.	.	.
1.67	.	.	.	.	1.081E-01	.	.	.	.
1.80	.	.	.	.	.	.	1.122E-01	.	.
1.84	1.115E-01	1.336E-01	.	.	.	.	.	.	.
2.00	.	.	.	.	.	.	.	1.239E-01	.
2.04	.	.	.	.	1.222E-01	.	.	.	.
2.24	1.293E-01	1.511E-01	.	.	.	.	.	.	.
2.41	.	.	.	.	1.361E-01	.	.	.	.
2.45	.	.	.	.	.	.	.	.	1.450E-01
2.67	.	.	.	.	.	.	.	1.506E-01	.
2.73	1.492E-01	1.697E-01	.	.	.	.	.	.	.
2.78	.	.	.	.	1.516E-01	.	.	.	.
3.20	.	.	.	.	.	.	1.663E-01	.	.
3.33	1.707E-01	1.892E-01	.	.	.	.	.	.	.
4.00	.	.	.	.	.	.	.	1.939E-01	.
4.07	1.934E-01	2.097E-01	.	.	.	.	.	.	.
4.90	.	.	.	.	.	.	.	.	2.450E-01
4.96	2.168E-01	2.309E-01	.	.	.	.	.	.	.
5.33	.	.	.	.	.	.	.	2.278E-01	.
5.60	.	.	.	.	.	.	2.301E-01	.	.
6.06	2.408E-01	2.528E-01	.	.	.	.	.	.	.
7.39	2.653E-01	2.753E-01	.	.	.	.	.	.	.
9.02	2.899E-01	2.983E-01	.	.	.	.	.	.	.
9.80	.	.	.	.	.	.	.	.	3.165E-01
10.00	.	.	.	.	.	.	3.003E-01	.	.
11.01	3.148E-01	3.217E-01	.	.	.	.	.	.	.
13.03	3.397E-01	3.454E-01	.	.	.	.	.	.	.
16.39	3.647E-01	3.694E-01	.	.	.	.	.	.	.
17.15	.	.	.	.	.	.	.	.	3.716E-01
18.00	.	.	.	.	.	.	3.745E-01	.	.
20.00	3.897E-01	3.935E-01	.	.	.	.	.	.	.
24.50	.	.	.	.	.	.	.	.	3.981E-01
32.00	.	.	.	.	.	.	4.477E-01	.	.

$1S - 2P$
 $C VI$

C VI 1s - 3s

Calculation
No.

Description

1. Coulomb-Born with exchange. Threshold energy is 32.013632 Ry.
2. Coulomb-Born without exchange.
6. Distorted Wave calculation with exchange, and same threshold as No. 1.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C VI
1s - 3s

X. SYMBOL	1	2	6	13
	MANN CBX	MANN CB	PEEK	SAMPSON
1.00	-	-	4.572E-03	4.258E-03
1.01	3.758E-03	4.692E-03	-	4.268E-03
1.13	-	-	-	4.286E-03
1.17	3.902E-03	4.783E-03	-	-
1.35	-	-	4.546E-03	-
1.36	4.009E-03	4.853E-03	-	-
1.50	-	-	-	4.260E-03
1.58	4.089E-03	4.905E-03	-	-
1.80	-	-	4.531E-03	-
1.84	4.152E-03	4.941E-03	-	-
2.13	4.205E-03	4.966E-03	-	-
2.25	-	-	-	4.350E-03
2.47	4.254E-03	4.982E-03	-	-
2.87	4.300E-03	4.991E-03	-	-
3.20	-	-	4.586E-03	-
3.33	4.345E-03	4.994E-03	-	-
3.38	-	-	-	4.450E-03
3.87	4.391E-03	4.994E-03	-	-
4.49	4.435E-03	4.991E-03	-	4.522E-03
5.22	4.478E-03	4.986E-03	-	-
5.60	-	-	4.671E-03	-
6.06	4.520E-03	4.981E-03	-	-
7.03	4.560E-03	4.974E-03	-	-
8.17	4.596E-03	4.968E-03	-	-
9.48	4.630E-03	4.961E-03	-	-
10.00	-	-	4.751E-03	-
11.01	4.662E-03	4.955E-03	-	-
12.78	4.690E-03	4.948E-03	-	-
14.84	4.715E-03	4.943E-03	-	-
17.23	4.738E-03	4.937E-03	-	-
18.00	-	-	4.809E-03	-
20.00	4.758E-03	4.933E-03	-	-
32.00	-	-	4.844E-03	-

C_{VI}^{1S-3S}

C VI 1s - 3p

Calculation
No.

Description

1. Coulomb-Born calculation with exchange. Threshold energy is 32.014416 Ry.
2. Coulomb-Born calculation without exchange.
6. Distorted Wave calculation with exchange, and same threshold as No. 1.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C VI 1s - 3p

X SYMBOL	1	2	6	13
	MANN CBX	MANN CB	PEEK	SAMPSON
1.00	.	.	1.893E-02	1.751E-02
1.01	1.654F-02	1.757E-02	.	1.758E-02
1.13	.	.	.	1.794E-02
1.17	1.710E-02	1.956E-02	.	.
1.35	.	.	1.984E-02	.
1.36	1.819E-02	2.165E-02	.	.
1.50	.	.	.	2.000E-02
1.58	1.976E-02	2.382E-02	.	.
1.80	.	.	2.282E-02	.
1.84	2.173E-02	2.608E-02	.	.
2.13	2.401E-02	2.841E-02	.	.
2.25	.	.	.	2.576E-02
2.47	2.655F-02	3.082E-02	.	.
2.87	2.927E-02	3.330E-02	.	.
3.20	.	.	3.216E-02	.
3.33	3.213E-02	3.586E-02	.	.
3.87	3.509E-02	3.847E-02	.	.
4.49	3.810F-02	4.115E-02	.	3.858E-02
5.22	4.117E-02	4.387E-02	.	.
5.60	.	.	4.295E-02	.
6.06	4.426E-02	4.665E-02	.	.
7.03	4.737E-02	4.946E-02	.	.
8.17	5.048E-02	5.230E-02	.	.
9.00	.	.	5.187E-02	.
9.48	5.359E-02	5.518E-02	.	.
11.01	5.671E-02	5.808E-02	.	.
12.75	5.981E-02	6.100E-02	.	.
14.84	6.291E-02	6.393E-02	.	.
17.23	6.600E-02	6.688E-02	.	.
18.00	.	.	6.678E-02	.
20.00	6.908E-02	6.984E-02	.	.
32.00	.	.	7.836E-02	.

$1S^C VI - 3P$

C VI 1s - 3d

Calculation
No.

Description

1. Coulomb-Born calculation with exchange. Threshold energy (expt) is 32.015097 Ry.
2. Coulomb-Born calculation without exchange.
6. Distorted Wave calculation with exchange, and same threshold as No. 1.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

C VI 1s - 3d

X. SYMBOL	1 MANN CBX	2 MANN CB	6 PEEK	13 SAMPSON
1.00	-	-	3.462E-03	2.978E-03
1.01	3.343E-03	1.266E-03	-	2.958E-03
1.13	-	-	-	2.550E-03
1.17	2.652E-03	1.471E-03	-	-
1.35	-	-	2.281E-03	-
1.36	2.249E-03	1.676E-03	-	-
1.50	-	-	-	2.002E-03
1.58	2.058E-03	1.877E-03	-	-
1.80	-	-	2.071E-03	-
1.84	2.014E-03	2.072E-03	-	-
2.13	2.064E-03	2.257E-03	-	-
2.25	-	-	-	2.112E-03
2.47	2.172E-03	2.431E-03	-	-
2.87	2.309E-03	2.593E-03	-	-
3.20	-	-	2.450E-03	-
3.33	2.459E-03	2.741E-03	-	-
3.87	2.609E-03	2.876E-03	-	-
4.49	2.752E-03	2.997E-03	-	2.814E-03
5.22	2.884E-03	3.105E-03	-	-
5.60	-	-	2.951E-03	-
6.06	3.004E-03	3.200E-03	-	-
7.03	3.111E-03	3.283E-03	-	-
8.17	3.205E-03	3.355E-03	-	-
9.48	3.287E-03	3.417E-03	-	-
10.00	-	-	3.276E-03	-
11.01	3.357E-03	3.470E-03	-	-
12.78	3.420E-03	3.517E-03	-	-
14.84	3.471E-03	3.556E-03	-	-
17.23	3.515E-03	3.588E-03	-	-
20.00	3.553E-03	3.615E-03	-	-

PAGE NO.

ELEMENT AND ION

... DATA SETS

113,115

O IV
152 252 2P = 152 25 2P2(4P)

ROBB CC ,
ROBB O IV SCCX 25(2)2P-252P(2)(4P) CI

113,115

O IV
152 252 2P = 152 25 2P2(2D)

ROBB CC ,
ROBB O IV SCCX 25(2)2P-252P(2)(2D) CI

113,116

O IV
152 252 2P = 152 25 2P2(2S)

ROBB CC ,
ROBB O IV SCCX 25(2)2P-252P(2)(2S) CI

89

O IV
152 252 2P = 152 25 2P2(2P)

DAVIS , ROBB CC ,
DAVIS UDMX O IV 25(2)2P(2P) = 252P(2)(2P)
ROBB SCCX O IV 25(2)2P-252P(2)(2P) CI

113,116

O IV
25 2P2(4P) = 25 2P2(2D)

ROBB CC ,
ROBB SCCX O IV 252P(2)(4P)-252P(2)(2D) CI

113,116

O IV
25 2P2(4P) = 25 2P2(2S)

ROBB CC ,
ROBB SCCX O IV 252P(2)(4P)-252P(2)(2S) CI

113,116

O IV
25 2P2(4P) = 25 2P2(2P)

ROBB CC ,
ROBB SCCX O IV 252P(2)(4P)-252P(2)(2P) CI

113,116

O IV
25 2P2(2D) = 25 2P2(2S)

ROBB CC ,
ROBB SCCX O IV 252P(2)(2D)-252P(2)(2S) CI

113,116

O IV
25 2P2(2D) = 25 2P2(2P)

ROBB CC ,
ROBB SCCX O IV 252P(2)(2D)-252P(2)(2P) CI

113,117

O IV
25 2P2(2S) = 25 2P2(2P)

ROBB CC ,
ROBB SCCX O IV 252P(2)(2S)-252P(2)(2P) CI

91

O V
152 252 = 152 25 2P(1P)

OSTERBROCK , DAVIS ,
OSTERBROCK SCCX O V 152 252 = 152 25 2P(1P)
DAVIS UDMX O V 25(2)(1S) = 252P(1P)

6.4. Listing of all Calculations for Oxygen Ions

93

O VI
1S2 2S - 1S2 2P

MANN CBX , ROBB CC , DAVIS
MANN CBX SCALED FIT O VI 1S2 2S - 1S2 2P
ROBB O VI 2CCX 2S - 2P
DAVIS UDAX O VI 2S - 2P

95

O VII
1S2 - 1S 2S(1S)

NORCROSS , TULLY , SAMPSON , BHATIA ,
ROBB CC ,
NORCROSS O VII 2 SINGLET S
TULLY CBX O VII 1S2 - 1S 2S(1S)
O VII 2 SINGLET S SAMPSON
BHATIA DW O VII 1S2 - 1S 2S(1S)
BHATIA CB O VII 1S2 - 1S 2S(1S)
ROBB 5CCX O VII 1S(2)-1S2S(1S)

97

O VII
1S2 - 1S 2S(3S)

ROBB CC , NORCROSS , BHATIA ,
ROBB 5CCX O VII 1S2 - 1S 2S(3S)
NORCROSS O VII 2 TRIPLET S
BHATIA DW O VII 1S2 - 1S 2S(3S)
VII 2 TRIPLET S SAMPSON

99

O VII
1S2 - 1S 2P(1P)

ROBB CC , TULLY , NORCROSS , SAMPSON , BHATIA ,
ROBB 5CCX O VII 1S(2)-1S2P(1P)
TULLY CBX O VII 1S2 - 1S 2P(1P)
NORCROSS O VII 2 SINGLET P
O VII 2 SINGLET P SAMPSON
BHATIA DW O VII 1S2 - 1S 2P(1P)

101

O VII
1S2 - 1S 2P(3P)

ROBB CC , NORCROSS , BHATIA ,
ROBB 5CCX O VII 1S2 - 1S 2P(3P)
NORCROSS O VII 2 TRIPLET P
BHATIA O VII 1S(2) - 1S2P(3P)
O VII 2 TRIPLET P SAMPSON

113,117

O VII
1S 2S(3S) - 1S 2P(3P)

ROBB CC ,
ROBB 5CCX O VII 1S2S(3S)-1S2P(3P)

PAGE NO.

ELEMENT AND ION

... DATA SETS

118,119	0 VII 1S 2S(3S) = 1S 2P(3P)	NORCROSS , NORCROSS UDMX 0 VII 1S2S(3S)-1S2P(3P)
113,117	0 VII 1S 2S(3S) = 1S 2S(1S)	ROBB CC , ROBB SCCX 0 VII 1S2S(3S)-1S2S(1S)
118,119	0 VII 1S 2S(3S) = 1S 2S(1S)	NORCROSS , NORCROSS UDMX 0 VII 1S2S(3S)-1S2S(1S)
113,117	0 VII 1S 2S(3S) = 1S 2P(1P)	ROBB CC , ROBB SCCX 0 VII 1S2S(3S)-1S2P(1P)
118,119	0 VII 1S 2S(3S) = 1S 2P(1P)	NORCROSS , NORCROSS UDMX 0 VII 1S2S(3S)-1S2P(1P)
113,117	0 VII 1S 2P(3P) = 1S 2S(1S)	ROBB CC , ROBB SCCX 0 VII 1S2P(3P)-1S2S(1S)
118,119	0 VII 1S 2S(1S) = 1S 2P(3P)	NORCROSS , NORCROSS UDMX 0 VII 1S2S(1S)-1S2P(3P)
113,117	0 VII 1S 2P(3P) = 1S 2P(1P)	ROBB CC , ROBB SCCX 0 VII 1S2P(3P)-1S2P(1P)
118,119	0 VII 1S 2P(3P) = 1S 2P(1P)	NORCROSS , NORCROSS UDMX 0 VII 1S2P(3P)-1S2P(1P)
113,117	0 VII 1S 2S(1S) = 1S 2P(1P)	ROBB CC , ROBB SCCX 0 VII 1S2S(1S)-1S2P(1P)
118,119	0 VII 1S 2S(1S) = 1S 2P(1P)	NORCROSS , NORCROSS UDMX 0 VII 1S2S(1S)-1S2P(1P)

PAGE NO.	ELEMENT AND ION	... DATA SETS
103	O VIII IS - 2S	BRANDEN , TULLY , SAMPSON BRANDEN SOP O VIII IS - 2S TULLY CBX O VIII IS - 2S O VIII IS-2S SAMPSON
105	O VIII IS - 2P	ROBR CC , BRANDEN , TULLY ROBR SCX O VIII IS - 2P BRANDEN SOP O VIII IS - 2P TULLY CBX O VIII IS - 2P O VIII IS-2P SAMPSON

6.5. Comparative Data in Graphical and Numerical Form for Oxygen Ions

$$0 \text{ IV } 1s^2 2s^2 2p^2 P - 1s^2 2s 2p^2 \text{ }^2 P$$

Calculation No.	Description
3.	Five-state Close-Coupling with single-configuration excited-state and two-configuration $c_1 1s^2 2s^2 2p + c_2 1s^2 2p^3 \text{ }^2 P$ ground-state wave functions. Clementi $1s, 2s, 2p \text{ }^2 P$ orbitals; calculated threshold energy is 1.75624 Ry.
5.	Unitarized Distorted Wave without exchange. Clementi target state wave functions. Threshold energy 1.6447 Ry.

$$0 \text{ IV } 1s^2 2s^2 2p^2 P - 1s^2 2s 2p^2 \text{ }^2 P$$

X.SYMBOL	3	5
.	ROBB CC	DAVIS
1.00	-	1.500E+01
1.02	6.804E+00	-
1.37	7.652E+00	-
1.50	-	1.680E+01
1.71	8.414E+00	-
2.00	-	1.810E+01
2.05	9.118E+00	-
2.39	9.760E+00	-
2.73	1.035E+01	-
3.00	-	2.080E+01
3.07	1.088E+01	-
3.42	1.137E+01	-
4.00	-	2.230E+01
4.56	1.202E+01	-
5.00	-	2.390E+01
5.69	1.399E+01	-
6.83	1.494E+01	-
7.97	1.581E+01	-
9.11	1.654E+01	-
11.39	1.776E+01	-
22.78	2.153E+01	-
34.16	2.371E+01	-

1S2 2S2 2P - 1S2 2S 2P2(2P) ^{0 IV}

$$\underline{0\ V\ 1s^2 2s^2\ ^1S - 1s^2 2s 2p\ ^1P}$$

Calculation
No.

Description

5. Unitarized Distorted Wave calculation with exchange. Single-configuration ground-and excited-state wave functions with Clementi 1s and 2s orbitals and a semiempirical 2p orbital. Threshold energy is 1.448 Ry.
12. Six-state Close-Coupling calculations for this and other transitions in 0 V have been performed by Berrington, et al.²⁷
16. Three-state Close-Coupling calculation by Osterbrock,²⁵ using single-configuration ground-and excited-state wave functions. Only one energy point which lies on top of the second point of calculation No. 5.

$$\begin{array}{c} 0\ V \\ 1S2\ 2S2 - 1S2\ 2S\ 2P(1P) \end{array}$$

X. SYMBOL	5	16
	DAVIS	OSTERBROCK
1.00	4.200E+00	-
1.50	4.550E+00	-
1.51	-	4.560E+00
2.00	4.950E+00	-
3.00	5.600E+00	-
4.00	6.000E+00	-
5.00	6.400E+00	-

1S2 2S2 - 1S2⁰ 2S 2P(1P)

O VI $1s^2 2s^2 S - 1s^2 2p^2 P$

Calculation
No.

Description

3. Two-state Close-Coupling calculation using Hartree-Fock orbitals of Weiss.²⁸ Threshold energy is 0.88315 Ry.
5. Unitarized Distorted Wave calculation without exchange, using $1s$ and $2s$ ground-state orbitals of Clementi¹¹ and a semiempirical $2p$ orbital. Threshold energy is 0.8819 Ry.
19. This is not a Coulomb-Born-Exchange calculation. Rather it is a fit to iso-electronic sequence CBX data for ions between C^{3+} and Fe^{23+} .

O VI
 $1S^2 2S - 1S^2 2P$

X.SYMBOL	3	5	19
	ROBB CC	DAVIS	MERTS FIT
1.00	-	5.750E+00	5.202E+00
1.02	5.124E+00	-	-
1.36	5.284E+00	-	-
1.50	-	5.900E+00	5.400E+00
1.70	5.446E+00	-	-
2.00	-	6.000E+00	5.583E+00
2.04	5.585E+00	-	-
2.38	5.697E+00	-	-
2.72	5.819E+00	-	-
3.00	-	6.400E+00	5.911E+00
3.40	6.070E+00	-	-
4.00	-	6.650E+00	6.192E+00
4.53	6.433E+00	-	-
5.00	-	7.000E+00	6.454E+00
5.66	6.751E+00	-	-
6.79	7.030E+00	-	-
7.93	7.308E+00	-	-
9.06	7.511E+00	-	-
10.19	7.720E+00	-	-
11.32	7.917E+00	-	-
22.65	9.291E+00	-	-
33.97	1.014E+01	-	-
45.29	1.076E+01	-	-
56.62	1.124E+01	-	-
67.94	1.163E+01	-	-
79.26	1.197E+01	-	-

0 VII $1s^2 1s - 1s2s 1s$

Calculation No.	Description
3.	Five-state Close-Coupling calculation with single-configuration ground-and excited-state wave functions using Clementi ¹¹ $1s$ orbital and $2s$ and $2p$ orbitals from the Hibbert ² code. Threshold energy is 41.9029 Ry.
4.	Five-state Distorted Wave calculation by Norcross (unpublished). Identical to the C V calculation described on page 50 . Low-energy resonance is observed. Threshold energy is 41.7824 Ry.
7.	Distorted Wave (lower points) and Coulomb-Born (upper points) calculations by Bhatia and Temkin, ⁸ using target state wave functions of Morse, Young, and Haurwitz. ⁹ Threshold energy is 41.671 Ry.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.
15.	Coulomb-Born calculation by Tully ²⁹ without exchange.

0 VII
 $1s2 - 1s 2s(1s)$

SYMBOL	3 ROBB	4 CC	7 NORCROSS	7 BHATIA	7 BHATIA	13 SAMPSON	15 TULLY
1.00	.	.	.	.	.	8.746E-03	1.273E-02
1.01	7.748E-03	4.855E-03	.	.	.	.	.
1.05	7.895E-03	4.633E-03	.	.	.	.	.
1.07	.	.	.	.	.	9.091E-03	.
1.11	8.292E-03	6.384E-03	.	.	.	.	.
1.20	8.907E-03	7.023E-03	1.195E-02	6.200E-03	9.704E-03	.	.
1.31	8.932E-03	7.759E-03	.	.	.	.	.
1.33	.	.	.	.	.	1.022E-02	.
1.53	9.216E-03	8.803E-03	1.222E-02	7.296E-03	.	.	.
1.62	.	9.117E-03	.	.	.	.	.
1.80	1.006E-02	9.683E-03	1.238E-02	7.950E-03	.	.	.
2.00	.	.	.	8.346E-03	1.191E-02	1.352E-02	.
2.02	1.069E-02	1.026E-02	.	.	.	.	.
2.16	.	.	1.251E-02	8.640E-03	.	.	.
2.52	.	.	1.260E-02	9.135E-03	.	.	.
2.67	.	.	.	.	1.284E-02	.	.
3.00	.	.	.	9.639E-03	.	1.377E-02	.
3.04	.	1.171E-02	.	.	.	.	.
4.00	.	.	.	.	1.382E-02	.	.
5.05	.	1.286E-02	.	.	.	.	.
5.33	.	.	.	.	1.432E-02	.	.

$O\ V II$
1S2 - 1S 2S(1S)

O VII $1s^2 1S - 1s2s^3S$

Calculation
No.

Description

3. Five-state Close-Coupling calculation as described on page 95.
Threshold energy is 41.223326 Ry.
4. Five-State Distorted Wave calculation as described on page 95.
Low-energy resonance is observed. Threshold energy is 41.2244 Ry.
7. Distorted Wave calculation as described on page 95. Threshold energy is 41.089 Ry.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.

O VII
1S2 - 1S 2S(3S)

X.SYMBOL	3	4	7	13
	ROBB CC	NORCROSS	RWATTA	SAMPSON
1.00	-	-	-	4.165E-03
1.03	4.856E-03	3.213E-03	-	-
1.06	4.636E-03	2.436E-03	-	3.893E-03
1.13	4.253E-03	3.270E-03	-	-
1.20	-	-	-	3.418E-03
1.21	3.911E-03	3.063E-03	2.900E-03	-
1.33	3.403E-03	2.836E-03	-	3.026E-03
1.55	2.647E-03	2.450E-03	2.432E-03	-
1.64	-	2.333E-03	-	-
1.82	2.236E-03	2.063E-03	2.100E-03	-
2.00	-	-	-	1.810E-03
2.04	1.904E-03	1.713E-03	-	-
2.19	-	-	1.800E-03	-
2.56	-	-	1.470E-03	-
2.67	-	-	-	1.208E-03
3.08	-	1.025E-03	-	-
4.00	-	-	-	6.440E-04
5.12	-	4.609E-04	-	-
5.33	-	-	-	4.068E-04

0V_{II}
1S2 - 1S 2S(3S)

0 VII $1s^2 1S - 1s2p 1P$

Calculation
No.

Description

3. Five-state Close Coupling calculation as described on page 95.
Threshold energy is 42.20669 Ry.
4. Five-state Distorted Wave calculation as described on page 95.
Threshold energy is 42.1700 Ry.
7. Distorted Wave calculation as described on page 95. Threshold
energy is 42.062 Ry.
13. Infinite-Z Hydrogenic approximation as described in Appendix I.
15. Coulomb-Born calculation²⁹ without exchange.

0 VII
1S2 - 1S 2P(1P)

X, SYMBOL	3 ROBB CC	4 NORCROSS	7 BHATIA	13 SAMPSON	15 TULLY
1.00	2.031E-02	1.514E-02	-	2.930E-02	4.416E-02
1.04	2.211E-02	1.633E-02	-	-	-
1.07	-	-	-	3.274E-02	-
1.10	2.504E-02	2.075E-02	-	-	-
1.18	2.841E-02	2.461E-02	3.425E-02	-	-
1.20	-	-	-	3.929E-02	-
1.30	5.279E-02	2.961E-02	-	-	-
1.33	-	-	-	4.554E-02	-
1.52	4.064E-02	3.847E-02	4.698E-02	-	-
1.60	-	4.161E-02	-	-	-
1.78	4.997E-02	4.797E-02	5.557E-02	-	-
2.00	5.635E-02	5.517E-02	6.188E-02	7.211E-02	7.307E-02
2.14	-	-	6.552E-02	-	-
2.50	-	-	7.644E-02	-	-
2.67	-	-	-	9.231E-02	-
3.00	-	-	8.233E-02	-	9.332E-02
3.01	-	8.172E-02	-	-	-
4.00	-	-	-	1.227E-01	-
5.00	-	1.159E-01	-	-	-
5.33	-	-	-	1.453E-01	-

$O\ V\ I\ I$
1S2 - 1S 2P(1P)

O VII $1s^2 1S - 1s2p\ 3P$

Calculation No.	Description
3.	Five-state Close-Coupling calculation as described on page 95. Threshold energy is 41.80598 Ry.
4.	Five-state Distorted Wave calculation as described on page 95. Threshold energy is 41.7606 Ry.
7.	Distorted Wave calculation as described on page 95. Threshold energy is 41.672 Ry.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.

O VII
1S2 - 1S 2P(3P)

X, SYMBOL	3 ROHR CC	4 NORCROSS	7 BHATIA	13 SAMPSON
1.00	-	-	-	2.348E-02
1.01	2.139E-02	2.088E-02	-	-
1.05	2.056E-02	1.836E-02	-	-
1.07	-	-	-	2.132E-02
1.11	1.929E-02	2.034E-02	-	-
1.20	1.735E-02	1.795E-02	1.350E-02	1.782E-02
1.31	1.475E-02	1.558E-02	-	-
1.33	-	-	-	1.506E-02
1.53	1.130E-02	1.208E-02	8.128E-03	-
1.62	-	1.103E-02	-	-
1.79	8.656E-03	9.163E-03	5.925E-03	-
2.00	-	-	-	7.532E-03
2.02	6.754E-03	7.430E-03	-	-
2.67	-	-	-	4.428E-03
3.04	-	3.333E-03	-	-
4.00	-	-	-	2.006E-03
5.05	-	1.169E-03	-	-
5.33	-	-	-	1.123E-03

$O\text{ VII}$
 $1S2 - 1S\ 2P(3P)$

0 VIII 1s - 2s

Calculation
No.

Description

- 13. Infinite-Z Hydrogenic approximation as described in Appendix I.
- 15. Coulomb-Born calculation of Tully³⁰ without exchange.
- 18. Second-Order Potential calculation by Bransden and Noble.²¹

0 VIII
1s - 2s

X SYMBOL	13 SAMPSON	15 TULLY	18 BRANDEN
1.00	1.130E-02	-	-
1.07	1.136E-02	-	-
1.20	1.148E-02	-	-
1.33	1.159E-02	-	-
2.00	1.200E-02	-	-
2.45	-	1.378E-02	1.321E-02
2.67	1.229E-02	-	-
4.00	1.266E-02	-	-
4.90	-	1.378E-02	-
5.33	1.289E-02	-	-
9.80	-	1.401E-02	1.309E-02
17.15	-	1.407E-02	-
24.50	-	1.378E-02	1.378E-02

O VIII 1S - 2S

O VIII 1s - 2p

Calculation No.	Description
3.	Three-state Close-Coupling calculation. Threshold energy is 48.0 Ry.
13.	Infinite-Z Hydrogenic approximation as described in Appendix I.
15.	Coulomb-Born calculation ³⁰ without exchange.
18.	Second-Order Potential calculation by Bransden and Noble. ²¹

O VIII
1S - 2P

X. SYMBOL	3 ROHR CC	13 SAMPSON	15 TULLY	18 BRANDEN
1.00	-	4.618E-02	-	-
1.04	4.662E-02	-	-	-
1.07	-	4.732E-02	-	-
1.20	-	4.996E-02	-	-
1.33	-	5.304E-02	-	-
1.56	5.876E-02	-	-	-
2.00	-	6.968E-02	-	-
2.08	7.097E-02	-	-	-
2.45	-	-	9.016E-02	8.155E-02
2.60	8.257E-02	-	-	-
2.67	-	8.468E-02	-	-
3.13	9.326E-02	-	-	-
3.65	1.028E-01	-	-	-
4.00	-	1.091E-01	-	-
4.17	1.115E-01	-	-	-
4.69	1.199E-01	-	-	-
4.90	-	-	1.286E-01	-
5.21	1.269E-01	-	-	-
5.33	-	1.281E-01	-	-
9.80	-	-	1.723E-01	1.792E-01
17.15	-	-	2.110E-01	-
24.50	-	-	2.354E-01	2.240E-01

O VII II
1S - 2P

6.6. Additional Data in Numerical Form

The following data are for transitions where no meaningful comparison could be made with other calculations. We divide the data up into three sections. The first section is for Coulomb-Born calculations of J. B. Mann, the second section is for Close-Coupling calculations of W. D. Robb, and the third section is for all other calculations. Both carbon and oxygen ion calculations are included in each section.

The currently available data for O II and O III is sparse and offers little meaningful comparison. We have therefore omitted it from this report. However, we did receive O II and O III data contributions from the following people -- J. Davis (private communication), W. D. Robb and S. P. Rountree (private communication) and M. J. Seaton.³¹⁻³⁵

The paper of Berrington, et al.²⁷ on C III and O V, contains much more data than presented here. However, this data is mostly in resonance regions and is presented in graphical form, and we did not feel competent to convert it to the basically numerical, nonresonant format of this report.

Other work³⁶⁻⁴³ exists on excitation of hydrogen, helium, and lithium-like ions which we do not present in this report. These calculations are mostly in the Born and Coulomb-Born approximations and do not provide any additional insight for the present transitions. However, they do provide information on exchange effects, correlation effects, and large Δn transitions which may interest the reader.

6.6.1. Additional Coulomb-Born Data of J. B. Mann:

$$\underline{\text{C II } 1s^2 2s^2 2p - 1s^2 2s^2 3s}$$

Unitarized Coulomb-Born with exchange, with and without CI. The larger valued data (at high X) are for single-configuration states. The lower includes four other configurations in the ground states (all small except for $2p^3$), and five additional configurations in the excited state, the largest components being 7.07% $2p^2 (1s) 3s^2 S$, 4.20% $2s^2 4s$, and 3.23% $2s 2p^2 (1s)^2 S$. Threshold energy is 1.061440 Ry.

$$\underline{\text{C II } 1s^2 2s^2 2p - 1s^2 2s^2 3p}$$

Unitarized Coulomb-Born with exchange, with and without CI. The larger valued result is single configuration. The lower includes four components in both ground and excited states. Threshold energy is 1.199905 Ry.

$$\underline{\text{C II } 1s^2 2s^2 2p - 1s^2 2s^2 3d}$$

Unitarized Coulomb-Born with exchange, with and without CI. The smaller valued result (at large X) is single configuration. The upper includes mixing of five components in the ground state and five in the excited. Threshold energy is 1.325833 Ry.

$$\underline{\text{C III } 1s^2 2s^2 - 1s^2 2s 3s \ ^1S}$$

Unitarized Coulomb-Born with exchange. Mixing of levels included. Ground state contains 6.66% $1s^2 2p^2 \ ^1S$; the excited state contains 4.16% $2p 3p \ ^1S$, 1.29% $1s^2 2p^2 \ ^1S$ and 0.18% $1s^2 2s^2$. Note that self-transitions ($2s^2$ to $2s^2$ and $2p^2$ to $2p^2$) are involved here. Threshold energy is 2.252484 Ry.

$$\underline{\text{C III } 1s^2 2s^2 - 1s^2 2s 3s \ ^3S}$$

Unitarized Coulomb-Born with exchange. Ground-state function $1s^2 2s^2$ and 6.7% $1s^2 2p^2 \ ^1S$, excited-state functions $1s^2 2s 3s \ ^3S$ and 1.87% $1s^2 2p 3p \ ^3S$. Threshold energy is 2.170856 Ry.

$$\underline{\text{C III } 1s^2 2s^2 - 1s^2 2s 3p \ ^1P}$$

Unitarized Coulomb-Born with CI, and with exchange. Ground state contains 6.7% $1s^2 2p^2 \ ^1S$; excited state has 8.07% $1s^2 2p 3s \ ^1P$ and small amounts of $2p 3d \ ^1P$ and $2s 2p \ ^1P$. Threshold energy is 2.359663 Ry.

$$\underline{\text{C III } 1s^2 2s^2 - 1s^2 2s 3p \ ^3P}$$

Unitarized Coulomb-Born, with and without exchange, as described in Sec. 3.3.

$$\underline{\text{C III } 1s^2 2s^2 - 1s^2 2s 3d \ ^1D}$$

Unitarized Coulomb-Born with CI, and with exchange. Ground state contains 6.7% $1s^2 2p^2 \ ^1S$; the excited level contains 1.98% of $1s^2 2p^2 \ ^1D$ and a small amount of $2p 3p \ ^1D$. Threshold energy is 2.519612 Ry. The collision strengths approach a value of approximately 0.94 and should then have zero slope. The fall-off observed is caused by the inadequacy of the simple closure formula derived from $\ln \Omega_L = a - bL$.

C III $1s^2 2s^2 - 1s^2 2s 3d \ ^3D$

Unitarized Coulomb-Born with CI and exchange. The ground state has a 6.7% component of $2p^2 \ ^1S$; the excited states contain 1.6% $2p 3p \ ^3D$. Threshold energy is 2.460652 Ry.

C IV $1s^2 2s - 1s 2s^2$

Coulomb-Born with exchange. Threshold energy is 21.612715 Ry.

C IV $1s^2 2s - 1s 2s 2p \ ^4P$

Unitarized Coulomb-Born with exchange. Threshold energy is 21.616440 Ry.

C IV $1s^2 2s - 1s 2s (\ ^1S) 2p \ ^2P$ and $1s 2s (\ ^3S) 2p \ ^2P$

The excited states here consist of two $\ ^2P$ terms, strongly mixed. The lower $\ ^2P$ at 22.03887 Ry is nominally called $1s 2s (\ ^1S) 2p$, but is only about 54% pure, and the upper $\ ^2P$ at 22.34022 Ry is nominally the $1s 2s (\ ^3S) 2p$ configuration. The tables show the unitarized Coulomb-Born (with exchange) results for the "pure" single-configuration transitions.

C IV $1s^2 2s - 1s 2s 2p \ ^2P$ at 22.03887 Ry and at 22.34022 Ry

Unitarized Coulomb-Born with exchange and configuration interaction. The collision strength to the lower lying $\ ^2P$ term is enhanced by constructive interference. The upper $\ ^2P$ term is much decreased in collision strength. A small component of $1s^2 2p \ ^2P$ was also included in the excited states.

C VI $1s - 4s, 1s - 4p, 1s - 5p$

Coulomb-Born with exchange. Threshold energies are 33.764631, 33.764962, and 34.575194 Ry, respectively.

C II
152 252 2P = 152 252 33

X.SYMBOL	1 MANN CBX	1 MANN CBX
1.01	0.007E-01	9.658E-01
1.37	9.498E-01	9.991E-01
1.86	1.052E+00	9.314E-01
2.53	1.166E+00	8.544E-01
3.44	1.343E+00	8.436E-01
4.67	1.594E+00	9.210E-01
6.35	1.905E+00	1.070E+00
8.62	2.254E+00	1.264E+00
11.71	2.622E+00	1.479E+00
15.91	3.002E+00	1.705E+00
21.62	3.383E+00	1.935E+00
29.36	3.768E+00	2.167E+00
39.89	4.154E+00	2.399E+00
54.19	4.542E+00	2.631E+00
73.61	4.931E+00	2.864E+00
100.00	5.319E+00	3.096E+00

C II
152 252 2P = 152 252 3P

X.SYMBOL	1 MANN CBX	1 MANN CBX
1.01	4.031E+00	4.213E+00
1.37	3.172E+00	2.611E+00
1.86	2.325E+00	1.805E+00
2.53	2.033E+00	1.521E+00
3.44	1.984E+00	1.454E+00
4.67	2.013E+00	1.460E+00
6.35	2.059E+00	1.494E+00
8.62	2.106E+00	1.519E+00
11.71	2.144E+00	1.543E+00
15.91	2.185E+00	1.571E+00
21.62	2.216E+00	1.588E+00
29.36	2.239E+00	1.602E+00
39.89	2.255E+00	1.617E+00
54.19	2.265E+00	1.615E+00
73.61	2.270E+00	1.619E+00
100.00	2.270E+00	1.611E+00

C II
152 252 2P = 152 252 3D

X.SYMBOL	1 MANN CBX	1 MANN CBX
1.01	2.136E+00	2.093E+00
1.37	2.768E+00	2.806E+00
1.86	3.528E+00	3.707E+00
2.53	4.522E+00	4.872E+00
3.44	5.728E+00	6.260E+00
4.67	7.082E+00	7.798E+00
6.35	8.529E+00	9.425E+00
8.62	1.003E+01	1.110E+01
11.71	1.156E+01	1.281E+01
15.91	1.311E+01	1.453E+01
21.62	1.464E+01	1.627E+01
29.36	1.623E+01	1.800E+01
39.89	1.779E+01	1.974E+01
54.19	1.936E+01	2.148E+01
73.61	2.092E+01	2.321E+01
100.00	2.247E+01	2.493E+01

C III
152 252 = 152 25 33(15)

X.SYMBOL	1 MANN CBX
1.01	4.158E-01
1.37	4.544E-01
1.86	4.872E-01
2.14	5.139E-01
2.75	5.351E-01
3.53	5.916E-01
4.53	5.643E-01
5.81	5.741E-01
7.46	5.817E-01
9.59	5.876E-01
12.31	5.922E-01
15.81	5.957E-01
20.29	5.985E-01
26.06	6.007E-01
33.46	6.024E-01
42.97	6.037E-01
55.17	6.048E-01
70.85	6.056E-01
90.97	6.062E-01
116.82	6.066E-01
150.00	6.069E-01

C III
152 252 = 152 25 33(33)

X.SYMBOL	1 MANN CBX
1.01	1.402E-01
1.37	9.224E-02
1.86	5.657E-02
2.14	3.429E-02
2.75	2.054E-02
3.53	1.213E-02
4.53	7.074E-03
5.81	4.007E-03
7.46	2.358E-03
9.59	1.371E-03
12.31	8.100E-04
15.81	4.879E-04
20.29	2.991E-04
26.06	1.857E-04
33.46	1.160E-04
42.97	7.208E-05
55.17	4.519E-05
70.85	2.772E-05
90.97	1.722E-05
116.82	1.046E-05
150.00	6.254E-06

C III
192 292 - 192 29 3P(1P)

X.SYMBOL MANN CBX
1

1,01 3.045E-02
1,30 0.032E-02
1,67 6.728E-02
2,14 1.090E-01
2,75 1.653E-01
3,53 2.311E-01
4,53 3.050E-01
5,01 3.800E-01
7,46 4.697E-01
9,59 5.582E-01
12,31 6.497E-01
15,81 7.434E-01
20,29 8.391E-01
26,06 9.361E-01
33,46 1.034E-00
42,97 1.133E-00
55,17 1.233E-00
70,85 1.333E-00
90,97 1.434E-00
116,82 1.532E-00
150,00 1.625E-00

C III
192 292 - 192 26 3P(3P)

X.SYMBOL MANN CBX
1 2
MANN CB

1,01 1.251E-01 1.336E-05
1,30 8.607E-02 3.120E-05
1,67 5.512E-02 3.241E-05
2,14 3.386E-02 4.675E-05
2,75 2.052E-02 6.348E-05
3,53 1.250E-02 8.348E-05
4,53 7.840E-03 1.052E-04
5,01 5.020E-03 1.288E-04
7,46 3.280E-03 1.539E-04
9,59 2.179E-03 1.803E-04
12,31 1.478E-03 2.078E-04
15,81 1.035E-03 2.362E-04
20,29 7.610E-04 2.653E-04
26,06 6.009E-04 2.950E-04
33,46 5.121E-04 3.252E-04
42,97 4.604E-04 3.558E-04
55,17 4.550E-04 3.866E-04
70,85 1.592E-04 4.177E-04
90,97 4.730E-04 4.488E-04
116,82 4.945E-04 4.794E-04
150,00 5.173E-04 5.083E-04

C III
192 292 - 192 29 3D(1D)

X.SYMBOL MANN CBX
1

1,01 1.542E-01
1,30 2.521E-01
1,67 3.573E-01
2,14 4.596E-01
2,75 5.531E-01
3,53 6.340E-01
4,53 7.037E-01
5,01 7.604E-01
7,46 8.057E-01
9,59 8.412E-01
12,31 8.688E-01
15,81 8.896E-01
20,29 9.048E-01
26,06 9.156E-01
33,46 9.210E-01
42,97 9.246E-01
55,17 9.244E-01
70,85 9.152E-01
90,97 9.064E-01
116,82 8.972E-01
150,00 8.906E-01

C III
192 292 - 192 29 3D(3D)

X.SYMBOL MANN CBX
1

1,01 4.000E-01
1,30 2.825E-01
1,67 1.606E-01
2,14 9.599E-02
2,75 5.624E-02
3,53 3.312E-02
4,53 1.058E-02
5,01 1.159E-02
7,46 6.072E-03
9,59 4.075E-03
12,31 2.410E-03
15,81 1.437E-03
20,29 2.504E-04
26,06 5.097E-04
33,46 3.006E-04
42,97 1.825E-04
55,17 1.095E-04
70,85 6.562E-05
90,97 3.922E-05
116,82 2.318E-05
150,00 1.345E-05

C IV
192 29 - 19 292

X.SYMBOL MANN CBX
1

1,01 4.654E-02
1,30 3.595E-02
1,67 2.968E-02
2,14 2.611E-02
2,75 2.417E-02
3,53 2.317E-02
4,53 2.272E-02
5,01 2.254E-02
7,46 2.262E-02
9,59 2.275E-02
12,31 2.294E-02
15,81 2.316E-02
20,29 2.339E-02
26,06 2.363E-02
33,46 2.385E-02
42,97 2.406E-02
55,17 2.426E-02
70,85 2.444E-02
90,97 2.460E-02
116,82 2.474E-02
150,00 2.487E-02

C IV
192 29 - 19 29 2P(4P)

X.SYMBOL MANN CBX
1

1,01 3.028E-02
1,30 3.611E-02
1,67 3.094E-02
2,14 2.522E-02
2,75 1.983E-02
3,53 1.515E-02
4,53 1.132E-02
5,01 8.320E-03
7,46 6.030E-03
9,59 4.325E-03
12,31 3.679E-03
15,81 2.100E-03
20,29 1.538E-03
26,06 1.083E-03
33,46 7.617E-04
42,97 5.360E-04
55,17 3.776E-04
70,85 2.664E-04
90,97 1.843E-04
116,82 1.334E-04
150,00 9.466E-05

C IV
152 25 - 18 25(15) 2P(2P)

X.SYMBOL I
MANN CBX

1,01	2.825E-02
1,19	3.194E-02
1,39	3.638E-02
1,63	4.173E-02
1,92	4.798E-02
2,25	5.525E-02
2,64	6.279E-02
3,11	7.126E-02
3,65	7.974E-02
4,28	8.872E-02
5,02	9.796E-02
5,90	1.072E-01
6,93	1.165E-01
8,13	1.268E-01
9,55	1.355E-01
11,21	1.449E-01
13,16	1.544E-01
15,45	1.639E-01
18,14	1.734E-01
21,29	1.829E-01
25.00	1.922E-01

C IV
152 25 - 13 25(35) 2P(2P)

X.SYMBOL I
MANN CBX

1,01	4.893E-02
1,19	5.914E-02
1,39	7.759E-02
1,63	9.924E-02
1,92	1.232E-01
2,25	1.489E-01
2,64	1.758E-01
3,11	2.035E-01
3,65	2.316E-01
4,28	2.601E-01
5,02	2.897E-01
5,90	3.174E-01
6,93	3.462E-01
8,13	3.749E-01
9,55	4.035E-01
11,21	4.322E-01
13,16	4.607E-01
15,45	4.892E-01
18,14	5.177E-01
21,29	5.461E-01
25.00	5.744E-01

C IV
152 25 - 13 25 2P(2P)

X.SYMBOL I
MANN CBX MANN CBX

1,01	5.284E-02	2.232E-02
1,19	7.113E-02	2.247E-02
1,39	9.519E-02	2.222E-02
1,63	1.236E-01	2.212E-02
1,92	1.551E-01	2.242E-02
2,25	1.899E-01	2.323E-02
2,64	2.245E-01	2.453E-02
3,11	2.611E-01	2.626E-02
3,65	2.985E-01	2.833E-02
4,28	3.363E-01	3.067E-02
5,02	3.745E-01	3.320E-02
5,90	4.129E-01	3.587E-02
6,93	4.515E-01	3.864E-02
8,13	4.901E-01	4.147E-02
9,55	5.287E-01	4.434E-02
11,21	5.674E-01	4.723E-02
13,16	6.061E-01	5.013E-02
15,45	6.447E-01	5.304E-02
18,14	6.834E-01	5.596E-02
21,29	7.220E-01	5.886E-02
25.00	7.606E-01	6.177E-02

C VI
15 - 43

X.SYMBOL I
MANN CBX

1,01	1.014E-03
1,17	1.468E-03
1,36	1.506E-03
1,58	1.532E-03
1,84	1.553E-03
2,13	1.579E-03
2,47	1.585E-03
2,87	1.601E-03
3,33	1.617E-03
3,87	1.633E-03
4,49	1.649E-03
5,22	1.665E-03
6,06	1.680E-03
7,03	1.695E-03
8,17	1.708E-03
9,48	1.721E-03
11,01	1.733E-03
12,78	1.743E-03
14,84	1.753E-03
17,23	1.761E-03
20.00	1.768E-03

C VI
15 - 4P

X.SYMBOL I
MANN CBX

1,01	6.349E-03
1,17	6.473E-03
1,36	6.812E-03
1,58	7.342E-03
1,84	8.028E-03
2,13	8.838E-03
2,47	9.742E-03
2,87	1.071E-02
3,33	1.174E-02
3,87	1.279E-02
4,49	1.387E-02
5,22	1.495E-02
6,06	1.605E-02
7,03	1.715E-02
8,17	1.825E-02
9,48	1.934E-02
11,01	2.044E-02
12,78	2.153E-02
14,84	2.262E-02
17,23	2.370E-02
20.00	2.478E-02

C VI
15 - 5P

X.SYMBOL I
MANN CBX

1,01	3.149E-03
1,17	3.168E-03
1,36	3.295E-03
1,58	3.543E-03
1,84	3.883E-03
2,13	4.252E-03
2,47	4.689E-03
2,87	5.148E-03
3,33	5.634E-03
3,87	6.135E-03
4,49	6.645E-03
5,22	7.161E-03
6,06	7.681E-03
7,03	8.200E-03
8,17	8.720E-03
9,48	9.238E-03
11,01	9.756E-03
12,78	1.027E-02
14,84	1.078E-02
17,23	1.129E-02
20.00	1.180E-02

6.6.2. Additional Close-Coupling Data of W. D. Robb:

C II Transitions between the $4P$, $2D$, $2S$ and $2P$ states of the $1s^2 2s 2p^2$ configuration

These results are from a five-state calculation using single-configuration wave functions and the $1s$, $2s$ and $2p$ $2P^0$ orbitals of Clementi,¹¹ for all states. The threshold energies are 0.39446 Ry ($4P - 2D$), 0.60215 Ry ($4P - 2S$), 0.76798 Ry ($4P - 2P$), 0.20769 Ry ($2D - 2S$), 0.37353 Ry ($2D - 2P$) and 0.16584 Ry ($2S - 2P$).

C III Transitions between the $3P^0$, $1P^0$, $3P$ and $1D$ states of the $1s^2 2s 2p$ and $1s^2 2p^2$ configurations

These results are from a five-state calculation. They use the same configuration interaction wave functions described on pages 31-39 for transitions out of the ground state. The threshold energies are 0.54313 Ry ($3P^0 - 1P^0$), 0.89770 Ry ($3P^0 - 1D$), 0.26727 Ry ($1P^0 - 3P$), 0.08730 Ry ($3P - 1D$), 0.81041 Ry ($3P^0 - 3P$), and 0.35457 Ry ($1P^0 - 1D$).

C V $1s 2s$ $1S - 1s 2p$ $3P^0$

These results are from the same five-state calculation as described on pages 50-74. The threshold energy is 0.015980 Ry.

O IV Transitions between the $2P^0$, $4P$, $2D$, $2S$ and $2P$ states of the $1s^2 2s^2 2p$ and $1s^2 2s 2p^2$ configurations

These results are from the same five-state calculation described on page 89 for the $2P^0 - 2P$ transition. The threshold energies are 0.59809 Ry ($2P^0 - 4P$), 1.21122 Ry ($2P^0 - 2D$), 1.55183 Ry ($2P^0 - 2S$), 0.61313 Ry ($4P - 2D$), 0.95375 Ry ($4P - 2S$), 1.15815 Ry ($4P - 2P$), 0.34062 Ry ($2D - 2S$), 0.54502 Ry ($2D - 2P$) and 0.20441 Ry ($2S - 2P$).

O VII Transitions between the $1S$, $3S$, $1P^0$ and $3P^0$ states of the $1s 2s$ and $1s 2p$ configurations

These results are from a five-state calculation using single-configuration wave functions, with the $1s$ orbital of Clementi¹¹ and $2s$ and $2p$ orbitals optimized on the singlet states from the Hibbert² code. The threshold energies are 0.58266

Ry ($^3S - ^3P^0$), 0.67957 Ry ($^3S - ^1S$), 0.98336 Ry ($^3S - ^1P^0$), 0.09692 Ry ($^3P^0 - ^1S$), 0.40071 Ry ($^3P^0 - ^1P^0$) and 0.30379 Ry ($^1S - ^1P^0$).

C II
2S 2P2(4P) = 2S 2P2(2S)

X.SYMBOL 3
ROBB CC

1,39	6.692E-01
1,88	7.271E-01
2,38	7.186E-01
2,88	6.727E-01
3,71	5.656E-01
4,54	4.573E-01
5,37	3.638E-01
6,20	2.881E-01
7,03	2.289E-01
7,86	1.834E-01
9,52	1.218E-01
12,84	5.935E-02
16,17	3.322E-02
19,49	2.044E-02
22,81	1.317E-02
26,13	9.446E-03
29,45	6.805E-03
32,77	4.882E-03

C II
2S 2P2(4P) = 2S 2P2(2P)

X.SYMBOL 3
ROBB CC

1,89	1.341E+00
1,48	1.252E+00
1,87	1.162E+00
2,26	1.049E+00
2,91	8.496E-01
3,56	6.732E-01
4,21	5.311E-01
4,86	4.218E-01
5,51	3.373E-01
6,16	2.739E-01
7,47	1.884E-01
10,07	1.013E-01
12,68	6.286E-02
15,28	4.243E-02
17,88	3.022E-02
20,49	2.326E-02
23,09	1.794E-02
25,70	1.397E-02

C II
2S 2P2(4P) = 2S 2P2(2D)

X.SYMBOL 3
ROBB CC

2,11	5.647E+00
2,68	5.688E+00
3,64	5.412E+00
4,48	5.006E+00
5,66	4.246E+00
6,93	3.529E+00
8,27	2.916E+00
9,47	2.415E+00
10,73	2.016E+00
12,02	1.698E+00
14,54	1.237E+00
19,61	7.160E-01
24,68	4.632E-01
29,75	3.180E-01
34,82	2.308E-01
39,89	1.777E-01
44,96	1.370E-01
50,03	1.077E-01

C II
2S 2P2(2S) = 2S 2P2(2P)

X.SYMBOL 3
ROBB CC

1,40	3.077E-01
3,21	3.756E-01
5,02	4.052E-01
6,83	4.080E-01
9,64	3.820E-01
12,86	3.421E-01
15,87	3.011E-01
18,89	2.640E-01
21,90	2.332E-01
24,92	2.081E-01
30,95	1.722E-01
43,01	1.319E-01
55,07	1.105E-01
67,13	9.730E-02
79,19	8.661E-02
91,25	7.879E-02
103,31	7.234E-02
115,37	6.652E-02

C II
2S 2P2(2D) = 2S 2P2(2S)

X.SYMBOL 3
ROBB CC

2,12	1.673E+00
3,56	1.979E+00
5,01	1.894E+00
6,45	1.881E+00
8,86	1.925E+00
11,27	1.996E+00
13,67	2.071E+00
16,08	2.138E+00
18,49	2.206E+00
20,89	2.264E+00
25,71	2.370E+00
35,34	2.520E+00
44,97	2.640E+00
54,60	2.720E+00
64,23	2.791E+00
73,86	2.856E+00
83,49	2.900E+00
93,12	2.925E+00

C II
2S 2P2(2D) = 2S 2P2(2P)

X.SYMBOL 3
ROBB CC

1,18	2.660E+00
1,98	3.006E+00
2,78	3.058E+00
3,59	2.952E+00
4,93	2.629E+00
6,26	2.273E+00
7,60	1.948E+00
8,94	1.670E+00
10,28	1.444E+00
11,62	1.260E+00
14,30	9.889E-01
19,65	6.690E-01
25,00	5.007E-01
30,36	3.967E-01
35,71	3.273E-01
41,07	2.798E-01
46,42	2.424E-01
51,78	2.124E-01

152 252 2P - 192 29 2P2(2D)
0 IV
X. SYMBOL 3
R088 CC

100.00
 80.65
 77.18
 65.72
 52.27
 42.81
 31.36
 19.17
 14.18
 5.45
 3.49
 2.72

192 2P2(3P) = 152 2P2(10)
C 111

2P(1P) - 2P(3P)
 C III
 3
 X.9YMBOL
 ROBB CC

1. 0.4703E-01
2. 0.2403E-01
3. 0.4701E-01
4. 0.2402E-01
5. 0.4701E-01
6. 0.2402E-01
7. 0.4698E-01
8. 0.2403E-01
9. 0.4701E-01
10. 0.2402E-01
11. 0.4703E-01
12. 0.2403E-01
13. 0.4701E-01
14. 0.2402E-01
15. 0.4703E-01
16. 0.2403E-01
17. 0.4701E-01
18. 0.2402E-01
19. 0.4703E-01
20. 0.2403E-01
21. 0.4701E-01
22. 0.2402E-01
23. 0.4703E-01
24. 0.2403E-01
25. 0.4701E-01
26. 0.2402E-01
27. 0.4703E-01
28. 0.2403E-01
29. 0.4701E-01
30. 0.2402E-01
31. 0.4703E-01
32. 0.2403E-01
33. 0.4701E-01
34. 0.2402E-01
35. 0.4703E-01
36. 0.2403E-01
37. 0.4701E-01
38. 0.2402E-01
39. 0.4703E-01
40. 0.2403E-01
41. 0.4701E-01
42. 0.2402E-01
43. 0.4703E-01
44. 0.2403E-01
45. 0.4701E-01
46. 0.2402E-01
47. 0.4703E-01
48. 0.2403E-01
49. 0.4701E-01
50. 0.2402E-01
51. 0.4703E-01
52. 0.2403E-01
53. 0.4701E-01
54. 0.2402E-01
55. 0.4703E-01
56. 0.2403E-01
57. 0.4701E-01
58. 0.2402E-01
59. 0.4703E-01
60. 0.2403E-01
61. 0.4701E-01
62. 0.2402E-01
63. 0.4703E-01
64. 0.2403E-01
65. 0.4701E-01
66. 0.2402E-01
67. 0.4703E-01
68. 0.2403E-01
69. 0.4701E-01
70. 0.2402E-01
71. 0.4703E-01
72. 0.2403E-01
73. 0.4701E-01
74. 0.2402E-01
75. 0.4703E-01
76. 0.2403E-01
77. 0.4701E-01
78. 0.2402E-01
79. 0.4703E-01
80. 0.2403E-01
81. 0.4701E-01
82. 0.2402E-01
83. 0.4703E-01
84. 0.2403E-01
85. 0.4701E-01
86. 0.2402E-01
87. 0.4703E-01
88. 0.2403E-01
89. 0.4701E-01
90. 0.2402E-01
91. 0.4703E-01
92. 0.2403E-01
93. 0.4701E-01
94. 0.2402E-01
95. 0.4703E-01
96. 0.2403E-01
97. 0.4701E-01
98. 0.2402E-01
99. 0.4703E-01
100. 0.2403E-01

0
192 262 2P = 192 2S 2P(4P)
X₂SYNBOL 3 RO88 CC

1. 42
 2. 34
 3. 28
 4. 56
 5. 47
 6. 27
 7. 53
 8. 41
 9. 11
 10. 93
 11. 76
 12. 22
 13. 48
 14. 3.09232340101

25 2P(1P) - 2P2(10)
111

$5 \text{ } 2P(3P) = 2P2(10)$
 $C \text{ } 111$
 $X.SYMBOL$
 3
 $ROBB \text{ } CC$

1.034E-01	30.60
1.097E-01	27.90
7.046E-02	55.37
4.840E-02	75.75
3.510E-02	99.64
2.650E-02	122.36
1.646E-02	171.77
4.231E-03	247.84
4.751E-03	360.27
3.021E-03	469.19
2.021E-03	565.04
1.420E-03	652.90
1.012E-03	748.67

19 28(19) - 19 2P(3P)
X.SYMBOL 3 ROBB 3 CC

1. 697E+01
2. 264E+01
2. 573E+01
2. 789E+01
3. 313E+01
3. 456E+01
3. 630E+01
4. 155E+01
4. 347E+01
4. 716E+01
4. 999E+01

22 20 (30) - 202 (30)
C.111

3 ROBB CC

0 IV
132 232 2P = 132 2S 2P2(2S)

X SYMBOL 3
ROBB CC

1,16	2.078E+00
1,55	2.279E+00
1,93	2.460E+00
2,32	2.628E+00
2,71	2.784E+00
3,09	2.930E+00
3,48	3.066E+00
3,87	3.193E+00
5,16	3.570E+00
6,44	3.879E+00
7,73	4.122E+00
9,02	4.360E+00
10,31	4.576E+00
12,09	4.867E+00
25,78	5.821E+00
38,66	6.367E+00

0 IV
25 2P2(4P) = 25 2P2(2D)

X SYMBOL 3
ROBB CC

1,96	2.835E+00
2,94	2.572E+00
3,92	2.314E+00
4,90	2.075E+00
5,87	1.859E+00
6,85	1.666E+00
7,83	1.497E+00
8,81	1.347E+00
12,07	9.668E-01
15,33	7.168E-01
18,60	5.406E-01
21,86	4.313E-01
25,12	3.462E-01
31,64	2.346E-01
64,26	6.367E-02
96,88	2.841E-02

0 IV
28 2P2(4P) = 28 2P2(2S)

X SYMBOL 3
ROBB CC

1,26	3.878E-01
1,89	3.520E-01
2,52	3.151E-01
3,15	2.787E-01
3,78	2.454E-01
4,41	2.158E-01
5,03	1.898E-01
5,66	1.672E-01
7,76	1.114E-01
9,86	7.653E-02
11,95	5.446E-02
14,05	4.011E-02
16,15	3.039E-02
20,34	1.848E-02
41,31	3.440E-03
62,20	1.220E-03

0 IV
25 2P2(4P) = 25 2P2(2P)

X SYMBOL 3
ROBB CC

1,24	5.363E-01
1,56	4.774E-01
2,07	4.202E-01
2,59	3.679E-01
3,11	3.219E-01
3,63	2.821E-01
4,15	2.480E-01
4,66	2.188E-01
6,39	1.486E-01
8,12	1.057E-01
9,84	7.853E-02
11,57	6.061E-02
13,30	4.812E-02
16,75	3.213E-02
30,02	8.780E-03
51,29	4.030E-03

0 IV
25 2P2(2D) = 25 2P2(2S)

X SYMBOL 3
ROBB CC

1,73	6.667E-01
3,49	5.834E-01
5,25	6.960E-01
7,01	7.118E-01
8,77	7.287E-01
10,54	7.460E-01
12,30	7.633E-01
14,06	7.798E-01
19,93	8.283E-01
25,80	8.720E-01
31,67	9.169E-01
37,55	9.542E-01
43,42	9.860E-01
55,16	1.020E+00
113,88	1.101E+00
172,59	1.153E+00

0 IV
25 2P2(2D) = 25 2P2(2P)

X SYMBOL 3
ROBB CC

1,08	1.553E+00
2,18	1.432E+00
3,28	1.302E+00
4,38	1.175E+00
5,48	1.058E+00
6,58	9.523E-01
7,69	8.581E-01
8,79	7.748E-01
12,46	5.617E-01
16,13	4.209E-01
19,80	3.261E-01
23,46	2.602E-01
27,13	2.123E-01
34,47	1.492E-01
71,17	4.890E-02
107,86	2.560E-02

0 IV
IS 2P2(2S) = 2S 2P2(2P)

X.SYMBOL 3
ROBB CC

1,21	2.462E-01
4,15	2.333E-01
7,08	2.164E-01
10,02	1.983E-01
12,96	1.825E-01
15,89	1.639E-01
18,83	1.489E-01
21,76	1.355E-01
31,55	1.012E-01
41,33	7.860E-02
51,11	6.360E-02
60,90	5.336E-02
70,68	4.598E-02
80,25	3.614E-02
100,10	1.834E-02
285.94	1.234E-02

0 VII
IS 2S(3S) = 1S 2P(3P)

X.SYMBOL 3
ROBB CC

1,85	8.591E+00
4,25	9.357E+00
8,88	1.051E+01
15,06	1.154E+01
23,30	1.246E+01
39,09	1.371E+01
57,97	1.466E+01
73.93	1.520E+01

0 VII
IS 2S(3S) = 1S 2S(1S)

X.SYMBOL 3
ROBB CC

1,58	5.062E-02
3,64	4.241E-02
7,62	3.269E-02
12,92	2.576E-02
19,98	2.040E-02
33,52	1.535E-02
49,70	1.195E-02
63.39	1.028E-02

0 VII
IS 2S(3S) = 1S 2P(1P)

X.SYMBOL 3
ROBB CC

1,09	8.907E-02
2,52	7.696E-02
5,26	5.822E-02
8,93	4.167E-02
13,81	2.816E-02
23,16	1.546E-02
34,35	8.923E-03
43.81	6.151E-03

0 VII
IS 2P(3P) = 1S 2S(1S)

X.SYMBOL 3
ROBB CC

5,18	8.164E-02
19,54	6.967E-02
47,40	5.362E-02
84,55	3.875E-02
134,17	2.652E-02
229,00	1.477E-02
342,50	8.637E-03
438.46	5.995E-03

0 VII
IS 2P(3P) = 1S 2P(1P)

X.SYMBOL 3
ROBB CC

1,23	3.702E-01
4,73	3.135E-01
11,46	2.295E-01
20,05	1.625E-01
32,43	1.128E-01
55,39	6.750E-02
82,84	4.495E-02
106.05	3.427E-02

0 VII
IS 2S(1S) = 1S 2P(1P)

X.SYMBOL 3
ROBB CC

1,31	2.694E+00
5,92	3.164E+00
14,80	3.756E+00
26,65	4.257E+00
42,45	4.696E+00
72,74	5.219E+00
108,95	5.612E+00
139.56	5.849E+00

6.6.3. Additional Data from Other Authors:

C III Calculations of H. Nussbaumer²⁰

These calculations are in the Distorted Wave and Impact Parameter approximations. They use CI wave functions in the target states. The Distorted Wave calculations are due to Eissner.

C III Calculations of Flower and Launay²⁴

These results are from six-state Close-Coupling and Distorted Wave calculations described earlier on pages 31-40. Flower and Launay present fits to their sparse data which should be cautiously applied for large values of X .

C IV Calculations of J. Gau and R. J. Henry

These results are from a five-state calculation described earlier on pages 41-49. The threshold energies and wave functions are those of Weiss.²⁸

O VII Calculations of D. W. Norcross

These results are from the five-state calculation described earlier on pages 95-102. They are transitions between all the $1s2s$ and $1s2p$ excited states. Configuration interaction target state wave functions were made up from the $1s^2$, $1s2s$, $2s^2$, $2p^2$, $1s2p$, $2s2p$, $1s3s$, and $1s3p$ configurations. The threshold energies are 0.5580 Ry ($^3S - ^1S$), 0.5362 Ry ($^3S - ^3P^0$), 0.9456 Ry ($^3S - ^1P^0$), 0.0218 ($^1S - ^3P^0$), 0.3876 Ry ($^1S - ^1P^0$), and 0.4094 Ry ($^3P^0 - ^1P^0$).

C III 2S 2P(3P) - 2P2(3P)			
X, SYMBOL	11 NUSSBAUMER	11 NUSSBAUMER	
1,29	2,230E+01	2,562E+01	
2,56	3,030E+01	3,102E+01	

C III 2S 2P(1P) - 2P2(1D)			
X, SYMBOL	11 NUSSBAUMER	11 NUSSBAUMER	
1,37	1,670E+01	1,600E+01	
2,74	2,400E+01	2,020E+01	

C III 2S 2P(1P) - 2P2(1S)			
X, SYMBOL	11 NUSSBAUMER	11 NUSSBAUMER	
2,11	5,040E+00	7,950E+00	

C III 1S2 2S2 - 1S2 2P2(1S)			
X, SYMBOL	10 FLOWER	10 FLOWER	
1,12	2,510E+02	1,000E+02	
1,40	2,740E+02	1,370E+02	

C IV
152 2P - 152 3S

X SYMBOL 9
HENRY

1.57 3.320E-01
2.49 3.300E-01
3.41 3.740E-01
7.10 5.660E-01

C IV
152 2P - 152 3P

X SYMBOL 9
HENRY

1.47 1.150E+00
2.33 1.120E+00
3.18 1.140E+00
6.62 1.200E+00

C IV
152 2P - 152 3D

X SYMBOL 9
HENRY

1.44 4.520E+00
2.28 6.030E+00
3.13 7.290E+00
6.50 1.091E+01

O VII
15 2S(3S) - 15 2P(3P)

X SYMBOL 4
NORCROSS

2.01 7.670E+00
4.62 8.550E+00
9.65 9.792E+00
25.32 1.203E+01
49.00 1.377E+01
80.33 1.526E+01
159.97 1.600E+01
316.63 1.859E+01

O VII
15 2S(3S) - 15 2S(1S)

X SYMBOL 4
NORCROSS

1.93 4.680E-02
4.44 3.905E-02
9.28 2.831E-02
15.73 2.145E-02
24.33 1.716E-02
43.82 1.368E-02
47.09 1.280E-02
67.53 1.131E-02
77.20 1.206E-02
153.72 8.210E-03
324.26 2.870E-03

O VII
15 2S(3S) - 15 2P(1P)

X SYMBOL 4
NORCROSS

1.14 5.994E-02
2.62 5.178E-02
5.47 4.680E-02
9.28 3.483E-02
14.36 2.444E-02
24.09 1.381E-02
27.79 1.147E-02
35.72 8.070E-03
45.55 2.445E-02
90.71 1.810E-03
179.54 5.300E-04

O VII
15 2S(1S) - 15 2P(3P)

X SYMBOL 4
NORCROSS

23.74 5.736E-02
87.96 4.955E-02
211.82 4.528E-02
376.95 3.361E-02
597.14 2.361E-02
1019.16 1.336E-02
1179.71 1.109E-02
1523.74 7.560E-03
1950.35 2.877E-02
3909.06 1.770E-03
7762.20 5.100E-04

O VII
15 2P(3P) - 15 2P(1P)

X SYMBOL 4
NORCROSS

1.32 4.896E-01
4.74 4.088E-01
11.33 3.241E-01
20.13 2.319E-01
31.85 1.625E-01
54.32 9.928E-02
67.87 8.592E-02
81.19 6.541E-02
103.91 7.222E-02
208.21 2.478E-02
413.38 1.031E-02

O VII
15 2S(1S) - 15 2P(1P)

X SYMBOL 4
NORCROSS

1.34 2.606E+00
4.95 3.020E+00
11.91 3.556E+00
33.59 4.438E+00
66.35 5.048E+00
100.70 5.539E+00
219.86 6.195E+00
436.58 6.773E+00

7. TABLES OF FITTING PARAMETERS FOR THE DATA

The tables of this section have some omissions and restrictions which need to be explained. First, the data of Sampson, et al. are not fitted, since they are essentially fits of Coulomb-Born data. Second, for O VII, the data of Norcross contain resonant structure, which for transitions between excited states does not allow us to make meaningful fits. Further we have omitted some spin-forbidden transitions because these fits give negative cross sections when extrapolated to large $X > 100$. Fits should not be extrapolated outside fit range.

In Table II we give the coefficients for the fits to calculated collision strengths. This table contains the spin-allowed transitions. The transition and the author are identified by the same procedure used in Sec. 6 for the plots and tables of data. Table III contains the spin-forbidden transitions, the coefficients being for the form b) of Sec. 5. Table IV is for the same type of transitions as Table III but using form c). The reader should note that rate coefficients using this form require a numerical integration. From form a) and formula (1), we can write for the rate coefficients

$$R(LS - L'S') = \frac{8.01 \times 10^{-8} y}{(2S + 1)(2L + 1)(kT)^{1/2}} \left[\frac{c_0 e^{-y}}{y} + \left(c_1 + \frac{c_3}{y} \right) E_1(y) + c_2 E_2(y) \right],$$

where $y = \Delta E_0/kT$, and kT is in electron volts. $E_n(y)$ is the exponential integral⁴⁴ of order n . For form b)

$$R(LS - L'S') = \frac{8.01 \times 10^{-8} y}{(2S + 1)(2L + 1)(kT)^{1/2}} \left[c_0 E_2(y) + \sum_{n=1}^4 \frac{c_n e^{-(n\alpha+y)}}{(n\alpha + y)} \right].$$

8. CONCLUSIONS

We have tried to assemble in this report a significant amount of theoretical electron-ion impact excitation data, in sufficient detail as to allow meaningful comparison of methods, and to be representative of the field. The various methods used have their own strong points: in some cases pure computational ease in usage.

Generally our faith in the Coulomb-Born method has been strengthened compared to what it was at the beginning of this work. Exchange should always be included

in Coulomb-Born or Distorted-Wave calculations for transitions without change of multiplicity. It produces significant improvement (in comparison with Close-Coupling) in the near threshold ($X = 1$) collision strength. From initial calculations on heavier ($Z = 26$) ions we conclude that this remains true. Although not shown by any of the previous graphs, unitarization of Coulomb-Born results is also necessary for ions which are only singly or doubly ionized, producing $> 10\%$ differences in the threshold collision strength. Even for more highly ionized ions, unitarization may be important if the excitation energy of the transition is small (e.g., $\Delta n = 0$), and the reactance matrix elements are larger than 0.1 in magnitude.

The comparison given in detail in Sec. 3.2 shows that considerable care must be exercised when comparing results from different methods, using different target state wave functions. Here it can be seen that differences in target state wave functions can easily obscure, or even be mistaken for, the difference in the calculation models.

It is important to use the best target state wave functions possible. Configuration mixing cannot be neglected in many instances -- even for heavy highly stripped ions. Very small mixing coefficients can often produce large effects (20%) on the collision strength. The changes which this in turn produces (through the rate coefficient) in predictions of electron density and temperature may be much more significant.

The question of the quantitative effect of resonances on the average collision strength and rate coefficient, has not been addressed here. Resonances certainly complicate the simple representation of collision strengths that we have presented, and may significantly alter them close to threshold.⁴ We hope to address this problem in future publications.

Finally, the collision strengths in the neighborhood of $X = 1$ show some rather wide disagreement, however, the agreement between the methods is almost always within 10% for $X > 5$. These differences may be taken as indicative of the uncertainty in the collision strengths. The development of new ion sources and high-resolution electron beams is encouraging, and offers new prospects for some accurate measurements of some of the collision strengths considered here. As theorists we feel most confident about the values obtained for the $2s - 2p$ collision strengths of Li-like ions. We look forward to experimental confirmation of these results.

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TABLE II

TRANSITION	DATA	THRESHOLD ENERGY	FIT	COEFFICIENTS		
				C2	C1	C3
152 252 2P - 152 2S 2P2(2S) C II	MANN CBX	8.788E-01	A	2.027E+00	-7.151E-01	1.405E+00
	ROBB CC	9.089E-01	A	-5.825E-01	3.076E+00	-1.005E+00
152 252 2P - 152 2S 2P2(2P) C II	MANN CBX	1.008E+00	A	6.673E+00	-1.013E+01	1.163E+01
	ROBB CC	1.115E+00	A	5.819E-01	3.591E+00	-4.111E-01
152 252 2P - 152 2S 2P2(2D) C II	ROBB CC	7.412E-01	A	1.722E+00	7.613E+00	-3.606E+00
	MANN CBX	6.823E-01	A	5.369E+00	2.609E+00	1.448E+00
152 252 2P - 152 2S 2P2(3S) C II	MANN CBX	1.001E+00	A	-9.843E-01	2.943E+00	-9.975E-01
	MANN CBX	1.202E+00	A	1.678E+00	-2.234E+00	4.829E+00
152 252 2P - 152 2S 2P2(3D) C II	MANN CBX	1.326E+00	A	-1.703E+00	2.675E+00	1.165E+00
	MANN CBX	9.327E-01	A	3.922E+00	-5.368E-01	2.450E+00
152 252 - 152 2S 2P(1P) C III	ROBB CC	9.934E-01	A	2.329E+00	-1.619E-02	1.413E+00
	ROBB CC	8.104E-01	A	1.358E+01	-5.321E+00	1.016E+01
2S 2P(3P) - 2P2(3P) C III	ROBB CC	3.546E-01	A	0.194E+00	1.020E+01	-2.127E+00
	MANN CBX	2.252E+00	A	6.084E-01	-2.076E-01	1.170E-02
152 252 - 152 2S 3S(1S) C III	MANN CBX	2.368E+00	A	-4.045E-01	0.423E-01	-5.987E-03
	MANN CBX	2.523E+00	A	9.433E-01	-1.186E+00	3.628E-01
152 252 - 152 2S 3P(1P) C III	MANN CBX	5.883E-01	A	4.616E+00	5.257E+00	-4.681E-01
	ROBB CC	5.924E-01	A	4.838E+00	4.856E+00	-8.373E-01
152 252 - 152 2S 3D(1D) C IV	MANN CBX	2.768E+00	A	-5.120E-01	6.935E-01	-8.351E-02
	MANN CBX	2.917E+00	A	1.264E+00	-1.432E+00	8.241E-01
152 25 - 152 3S C IV	MANN CBX	2.161E+01	A	2.639E+02	-2.927E-02	4.923E-02
	MANN CBX	2.204E+01	A	-3.651E-03	1.301E-02	1.936E-02
152 25 - 152 3P C IV	MANN CBX	2.234E+01	A	1.149E-02	-4.619E-02	7.931E-02
	MANN CBX	2.234E+01	A	-0.972E-03	-3.192E-02	4.411E-02
152 25 - 152 3D C IV	MANN CBX	2.234E+01	A	-6.274E-03	2.855E-02	7.981E-02
	MANN CBX	2.234E+01	A			

TABLE II (cont.)

TRANSITION	DATA	THRESHOLD ENERGY	FIT	C0	COEFFICIENTS		
					C1	C2	C3
1S2 - 1S 2S(1S) C V	MANN CBX	2.237E+01	A	2.717E+02	-1.892E+02	1.207E+02	0.
	ROBB CC	2.214E+01	A	3.192E+02	-2.402E+02	6.426E+03	0.
	PEEK	2.237E+01	A	2.799E+02	-1.158E+02	1.931E+00	0.
	NORCROSS	2.236E+01	A	2.494E+02	-9.196E+03	-9.405E+03	0.
1S2 - 1S 2P(1P) C V	MANN CBX	2.263E+01	A	8.077E+03	-7.314E+03	3.269E+02	1.285E+01
	ROBB CC	2.263E+01	A	1.795E+02	-1.920E+02	3.674E+02	1.238E+01
	PEEK	2.239E+01	A	-1.166E+01	2.029E+01	-5.665E+02	1.727E+01
	NORCROSS	2.263E+01	A	-2.973E+02	6.233E+02	-1.269E+02	1.356E+01
1S 2S(1S) - 1S 2P(1P) C V	MANN CBX	2.583E+01	A	2.134E+00	3.604E+00	-1.354E+00	1.704E+00
	ROBB CC	2.514E+01	A	1.131E+00	7.446E+00	-5.134E+00	2.041E+00
	PEEK	2.744E+01	A	2.006E+00	3.756E+00	-1.158E+00	1.815E+00
	NORCROSS	2.744E+01	A	2.006E+00	3.756E+00	-1.158E+00	1.815E+00
1S 2S(3S) - 1S 2P(3P) C V	MANN CBX	4.006E+01	A	6.334E+00	8.666E+00	-2.773E+00	4.865E+00
	ROBB CC	3.885E+01	A	6.535E+00	2.057E+01	-1.529E+01	5.262E+00
	PEEK	3.854E+01	A	5.829E+00	9.444E+00	-2.725E+00	5.074E+00
	NORCROSS	3.854E+01	A	5.829E+00	9.444E+00	-2.725E+00	5.074E+00
1S - 2S C VI	MANN CBX	2.721E+01	A	2.422E+02	-8.443E+03	2.713E+03	0.
	ROBB CC	2.701E+01	A	2.446E+02	-5.511E+03	2.264E+03	0.
	PEEK	2.701E+01	A	2.446E+02	-5.511E+03	2.264E+03	0.
	NORCROSS	2.701E+01	A	2.446E+02	-5.511E+03	2.264E+03	0.
1S - 2P C VI	MANN CBX	2.701E+01	A	-2.677E+03	4.501E+02	3.374E+02	1.303E+01
	ROBB CC	2.701E+01	A	-6.235E+03	5.704E+02	3.309E+02	1.305E+01
	PEEK	2.700E+01	A	-1.787E+01	3.615E+01	-1.044E+01	2.046E+01
	NORCROSS	2.700E+01	A	-1.787E+01	3.615E+01	-1.044E+01	2.046E+01
1S - 3S C VI	MANN CBX	3.201E+01	A	4.853E+03	-1.029E+03	7.455E+00	0.
	ROBB CC	3.201E+01	A	4.797E+03	-1.527E+03	5.553E+00	0.
	PEEK	3.201E+01	A	4.797E+03	-1.527E+03	5.553E+00	0.
	NORCROSS	3.201E+01	A	4.797E+03	-1.527E+03	5.553E+00	0.
1S - 3P C VI	MANN CBX	3.201E+01	A	6.023E+03	2.479E+03	1.742E+02	2.087E+02
	ROBB CC	3.201E+01	A	6.432E+03	-1.925E+03	1.219E+02	2.097E+02
	PEEK	3.201E+01	A	6.432E+03	-1.925E+03	1.219E+02	2.097E+02
	NORCROSS	3.201E+01	A	6.432E+03	-1.925E+03	1.219E+02	2.097E+02
1S - 3D C VI	MANN CBX	3.202E+01	A	3.938E+03	-6.922E+03	6.346E+03	0.
	ROBB CC	3.202E+01	A	3.938E+03	-6.922E+03	6.346E+03	0.
	PEEK	3.202E+01	A	3.938E+03	-6.922E+03	6.346E+03	0.
	NORCROSS	3.202E+01	A	3.938E+03	-6.922E+03	6.346E+03	0.
1S - 4S C VI	MANN CBX	3.377E+01	A	1.777E+03	-5.536E+04	2.135E+04	0.
	ROBB CC	3.377E+01	A	1.777E+03	-5.536E+04	2.135E+04	0.
	PEEK	3.377E+01	A	1.777E+03	-5.536E+04	2.135E+04	0.
	NORCROSS	3.377E+01	A	1.777E+03	-5.536E+04	2.135E+04	0.
1S - 4P C VI	MANN CBX	3.458E+01	A	1.697E+03	-1.319E+03	2.797E+03	3.307E+03
	ROBB CC	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	PEEK	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	NORCROSS	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
1S2 2S2 2P - 1S2 2S 2P2(2P) O IV	MANN CBX	3.458E+01	A	1.697E+03	-1.319E+03	2.797E+03	3.307E+03
	ROBB CC	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	PEEK	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	NORCROSS	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
1S2 2S2 2P - 1S2 2S 2P2(2S) O IV	MANN CBX	3.458E+01	A	1.697E+03	-1.319E+03	2.797E+03	3.307E+03
	ROBB CC	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	PEEK	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	NORCROSS	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
1S2 2S2 2P - 1S2 2S 2P2(2P) O VI	MANN CBX	3.458E+01	A	1.697E+03	-1.319E+03	2.797E+03	3.307E+03
	ROBB CC	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	PEEK	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	NORCROSS	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
1S2 2S - 1S2 2P O VI	MANN CBX	3.458E+01	A	1.697E+03	-1.319E+03	2.797E+03	3.307E+03
	ROBB CC	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	PEEK	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00
	NORCROSS	1.211E+00	A	2.097E+03	4.711E+00	-1.240E+00	3.241E+00

TABLE II (cont)

TRANSITION	DATA	THRESHOLD ENERGY	FIT	COEFFICIENTS				
				C0	C1	C2	C3	
O VII								
1S2 - 1S 2S(1S)	NORCROSS	4.178E+01	A	1.384E-02	-4.933E-03	-4.297E-03	0.	
	ROBB CC	4.190E+01	A	1.434E-02	-8.634E-03	2.293E-03	0.	
O VII								
1S2 - 1S 2P(1P)	ROBB CC	4.221E+01	A	-6.626E-02	1.164E-01	-2.779E-02	1.040E-01	
	NORCROSS	4.217E+01	A	-1.346E-02	3.527E-02	-6.847E-03	7.418E-02	
O VII								
1S 2S(3S) - 1S 2P(3P)	ROBB CC	5.827E-01	A	3.983E+00	7.944E+00	+4.389E+00	2.596E+00	
O VII								
1S 2S(3S) - 1S 2P(3P)	NORCROSS	5.362E-01	A	3.497E+00	6.396E+00	-2.212E+00	2.699E+00	
O VII								
1S 2S(1S) - 1S 2P(1P)	ROBB CC	3.038E-01	A	7.417E-01	3.433E+00	-1.896E+00	1.030E+00	
O VII								
1S 2S(1S) - 1S 2P(1P)	NORCROSS	3.876E-01	A	1.065E+00	2.284E+00	-7.873E-01	9.443E-01	
O VIII								
1S - 2P	ROBB CC	4.802E+01	A	-4.158E-02	1.048E-01	-1.743E-02	9.042E-02	

TABLE III

TRANSITION	DATA	THRESHOLD ENERGY	FIT	C0	C1	C2	C3	C4	ALPHA
C II									
1S2 2S2 2P - 1S2 2S 2P2(4P)	ROBB CC	3.468E-01	B	4.36PE-01	1.627E+00	-2.923E+00	1.094E+01	-6.58PE+00	5.769E-02
C III									
1S2 2S2 - 1S2 2S 2P(3P)	ROBB CC	4.522E-01	B	1.95PE-01	3.130E-01	-8.383E-01	2.360E+00	-1.247E+00	4.640E-02
C III									
1S2 2S2 - 1S2 2P2 (3P)	ROBB CC	1.263E+00	B	1.418E+03	4.628E+03	-1.119E-02	6.29PE-02	-4.588E-02	1.576E-01
C III									
2S 2P(3P) - 2P2(10)	ROBB CC	8.977E-01	B	1.933E+01	-1.739E+01	2.956E+00	-1.31PE+02	-3.797E+01	8.682E-01
C III									
1S2 2P2(3P) - 1S2 2P2(10)	ROBB CC	8.738E-02	B	1.079E+00	4.977E+00	-1.020E+01	2.319E+01	-1.438E+01	2.39PE-02
C III									
1S2 2S2 - 1S2 2S 3S(3S)	MANN CBX	2.171E+00	B	1.429E-01	-1.079E-03	6.051E-23	-2.712E-02	4.020E-02	1.418E-01
C III									
1S2 2S2 - 1S2 2S 3D(3D)	MANN CBX	2.461E+00	B	3.311E-01	1.529E-02	3.285E-02	-3.082E-01	9.196E-01	3.624E-01
C IV									
1S2 2S - 1S 2S 2P(4P)	MANN CBX	2.162E+01	B	6.169E-02	1.476E-02	-1.006E-01	6.024E-01	-1.011E+00	5.538E-01
C V									
1S2 - 1S 2S(3S)	ROBB CC	2.177E+01	B	3.079E-02	-1.071E-02	1.747E-03	-4.533E-02	-1.287E-01	6.334E-01
	PEEK	2.197E+01	B	3.055E-02	-5.645E-03	-1.845E-02	6.873E-02	-2.501E-01	5.603E-01
	NORCROSS	2.197E+01	B	2.382E-02	-2.366E-02	-1.000E-01	2.419E-01	-1.338E+00	1.237E+00
C V									
1S2 - 1S 2P(3P)	MANN CBX	2.237E+01	B	4.817E-02	6.669E-03	-3.952E-02	2.462E-01	-3.823E-01	5.088E-01
	ROBB CC	2.216E+01	B	4.172E-02	2.412E-02	-2.386E-01	1.483E+00	-3.579E+00	1.105E+00
	PEEK	2.237E+01	B	4.276E-02	3.473E-04	1.537E-03	-4.210E-03	1.822E-02	2.140E-01
	NORCROSS	2.236E+01	B	5.334E-02	7.836E-02	-2.906E+00	3.174E+01	-1.302E+02	1.793E+00
C V									
1S 2P(3P) - 1S 2P(1P)	NORCROSS	2.740E-01	B	3.463E-02	2.302E-01	4.419E-01	-1.978E+00	2.252E+00	8.726E-03
O IV									
2S 2P2(4P) - 2S 2P2(2D)	ROBB CC	6.131E-01	B	2.99PE-01	4.261E-01	-1.923E-01	-2.971E-01	3.472E+00	2.794E-02
O IV									
2S 2P2(4P) - 2S 2P2(2S)	ROBB CC	9.537E-01	B	4.727E-03	2.812E-02	1.875E-03	-5.547E-03	4.784E-01	5.129E-02
O IV									
2S 2P2(4P) - 2S 2P2(2P)	ROBB CC	1.158E+00	B	7.622E-02	7.117E-02	-5.254E-02	-9.925E-02	6.940E-01	5.625E-02
O VII									
1S2 - 1S 2S(3S)	NORCROSS	4.122E+01	B	1.188E-02	-7.662E-02	1.129E+00	-1.306E+01	4.430E+01	1.935E+00
O VII									
1S2 - 1S 2P(3P)	NORCROSS	4.176E+01	B	2.958E-02	1.770E-02	-4.352E-01	3.272E+00	-1.136E+01	1.495E+00
O VII									
1S 2S(3S) - 1S 2S(1S)	ROBB CC	6.796E-01	B	1.082E-02	4.627E-02	-3.523E-02	-3.404E-02	7.472E-02	1.946E-02
O VII									
1S 2S(3S) - 1S 2P(1P)	ROBB CC	9.834E-01	B	2.454E-04	2.660E-02	1.281E-03	4.645E-03	6.742E-02	3.452E-02
O VII									
1S 2S(3S) - 1S 2P(1P)	NORCROSS	9.456E-01	B	4.086E-03	4.306E-02	-1.298E-01	2.945E-01	-1.482E-01	3.341E-02
O VII									
1S 2P(3P) - 1S 2S(1S)	ROBB CC	9.692E-02	B	4.012E-02	2.372E-02	8.582E-04	4.333E-03	5.537E-02	3.254E-03

TABLE IV

TRANSITION	DATA	THRESHOLD ENERGY	FIT	C0	COEFFICIENTS C1 C2 C3		
1S2 2S2 2P - 1S2 2S 2P2(4P) C II	WANN CBX	3.916E-01	C	5.940E+02	-0.003E+00 3.469E+00 -2.103E+00		
2S 2P2(4P) - 2S 2P2(2S) C II	ROBB CC	6.022E-01	C	6.183E+00	-1.049E+01 3.892E+00 -3.228E+00		
2S 2P2(4P) - 2S 2P2(2P) C II	ROBB CC	7.689E-01	C	4.002E+00	-4.768E+00 1.019E+00 -2.522E+00		
2S 2P2(20) - 2S 2P2(2P) C III	ROBB CC	3.735E-01	C	4.246E+00	-5.205E+00 1.916E+00 -1.456E+00		
1S2 2S2 - 1S2 2S 2P(3P) C III	WANN CBX ROBB CC	4.777E-01 4.522E-01	C C	3.075E+02 3.755E+02	-4.312E+00 -7.721E+00 1.626E+00 3.998E+00 -1.826E+00 -1.863E+00		
1S2 2S2 - 1S2 2P2 (3P) C III	ROBB CC	1.263E+00	C	7.221E-01	-0.310E+02 3.297E+00 -2.968E+00		
1S2 2S2 - 1S2 2S 3S(3S) C III	WANN CBX	2.171E+00	C	-2.418E+00	1.591E+00 -1.102E+00 -1.906E+20		
1S2 2S2 - 1S2 2S 3D(3D) C IV	WANN CBX	2.461E+00	C	-0.694E-01	2.305E-01 -6.917E-02 -2.068E+00		
1S2 2S - 1S 2S 2P(4P) C V	WANN CBX	2.162E+01	C	-2.179E+02	-0.353E-02 -1.021E+02 -2.275E+20		
1S2 - 1S 2S(3S) C V	WANN CBX ROBB CC PEEK NORCROSS	2.197E+01 2.177E+01 2.197E+01 2.197E+01	C C C C	-3.094E+00 -3.963E+00 -3.542E+00 -4.872E+00	-3.363E+00 -1.758E+00 -1.771E+00 9.147E-01	2.595E-01 9.348E-01 4.843E-01 -1.362E+00	-2.079E+00 -1.748E+00 -1.965E+00 -1.408E+00
1S2 - 1S 2P(3P) C V	WANN CBX ROBB CC PEEK NORCROSS	2.237E+01 2.216E+01 2.237E+01 2.236E+01	C C C C	-2.516E+00 -3.230E+00 -2.852E+00 -4.466E+00	-2.127E-01 9.072E-01 2.250E-01 3.548E+00	-4.955E-01 -1.123E+00 -4.109E-01 -2.421E+00	-2.171E+00 -2.007E+00 -2.002E+00 -1.429E+00
1S 2S(3S) - 1S 2P(1P) C V	WANN CBX	6.571E-01	C	3.968E-01	-6.274E+02 3.204E+00 -1.520E+00		
1S 2S(3S) - 1S 2S(1S) O IV	WANN CBX ROBB CC	3.988E-01 3.725E-01	C C	-1.408E+00 -0.623E-01	-1.055E+00 -2.163E+00	4.801E-01 1.155E+00	-6.498E-01 -7.411E-01
2S 2P2(4P) - 2S 2P2(2P) O VII	ROBB CC	1.158E+00	C	2.591E+00	-4.048E+00 1.729E+00 -2.032E+00		
1S2 - 1S 2S(3S) O VII	NORCROSS	4.122E+01	C	-6.341E+00	2.607E+00 -2.172E+00 -1.093E+00		
1S2 - 1S 2P(3P) O VII	ROBB CC NORCROSS	4.181E+01 4.176E+01	C C	-4.040E+00 -4.314E+00	2.744E+00 2.221E+00	-1.254E+00 -1.593E+00	-1.519E+00 -1.710E+00
1S 2S(3S) - 1S 2S(1S) O VII	ROBB CC	6.796E-01	C	-1.842E+00	-2.070E+00 1.166E+00 -6.506E-01		

APPENDIX I

The results for collision strengths given here are based on scaled collision strengths $Z^2\Omega$ evaluated at $Z = \infty$. According to this approach results for a transition $q \rightarrow q'$ in a highly charged member of the same isoelectronic series with finite Z are obtained from those for $Z = \infty$ using the formula

$$\Omega(q \rightarrow q') = \frac{1}{Z_{\text{eff}}^2} \left[Z^2\Omega(q \rightarrow q') \right]_{Z=\infty}, \quad (\text{I-1})$$

where Z_{eff} is an effective Z , to be discussed further below. For hydrogen-like and helium-like ions the results can be expressed very simply in terms of the scaled hydrogenic collision strength $Z^2\Omega_H$ and exchange collision strength $Z^2\Omega_H^e$. The latter is defined like $Z^2\Omega_H$, but with the "direct" contribution to the R-matrix elements set equal to zero. Specifically, the formula applicable for hydrogenic ions is

$$\Omega(n_a \ell_a \rightarrow n'_a \ell'_a) = \frac{2}{Z_{\text{eff}}^2} \left[Z^2\Omega_H(n_a \ell_a \rightarrow n'_a \ell'_a) \right]_{Z=\infty}, \quad (\text{I-2})$$

and those applicable for helium-like ions are

$$\begin{aligned} \Omega(1s n_a \ell_a \begin{smallmatrix} 2S_a+1 \\ L_a \end{smallmatrix} \rightarrow 1s n'_a \ell'_a \begin{smallmatrix} 2S'_a+1 \\ L'_a \end{smallmatrix}) &= \frac{3B^2}{4Z_{\text{eff}}^2} \delta_{\ell_a L_a} \delta_{\ell'_a L'_a} \left[Z^2\Omega_H^e(n'_a \ell'_a \rightarrow n'_a \ell'_a) \right]_{Z=\infty}; S_a \neq S'_a \\ &= \frac{B^2}{Z_{\text{eff}}^2} \delta_{\ell_a L_a} \delta_{\ell'_a L'_a} \left[Z^2\Omega_H(n_a \ell_a \rightarrow n'_a \ell'_a) - \frac{3}{4} Z^2\Omega_H^e(n_a \ell_a \rightarrow n'_a \ell'_a) \right]_{Z=\infty}; S_a = S'_a = 0 \\ &= \frac{3B^2}{Z_{\text{eff}}^2} \delta_{\ell_a L_a} \delta_{\ell'_a L'_a} \left[Z^2\Omega_H(n_a \ell_a \rightarrow n'_a \ell'_a) - \frac{Z^2}{4} \Omega_H^e(n_a \ell_a \rightarrow n'_a \ell'_a) \right]_{Z=\infty}; S_a = S'_a = 1 \end{aligned}$$

(I-3)

where $B^2 = 2$ for transitions from the ground level and is 1 for all other transitions. The factor of 2 on the right-hand side of Eq. (I-2) occurs in order that the well-known relation between Ω and the cross section Q

$$\frac{Q(q \rightarrow q')}{\pi a_0^2} = \frac{I_H}{E} \frac{1}{\omega_q} \Omega(q \rightarrow q') \quad (I-4)$$

be applicable with

$$\omega_q = (2S_a + 1)(2L_a + 1) \quad (I-5)$$

in the case of hydrogenic ions, as well as more complex ions. In most earlier work on hydrogenic ions the spin factor $(2S_a + 1) = 2$ was omitted from ω_q and incorporated into the definition of Ω , causing it to be less by a factor of 2. This has been done in the definition used here for Ω_H to be consistent with earlier work. Hence, one must multiply by a factor of 2, as in Eq. (I-2), in order that Eq. (I-4) with ω_q given by (I-5) be applicable for hydrogenic ions. The Z_{eff}^2 occurring in Eqs. (I-1)-(I-3) is not specified by the theory and one should use the value which is physically most plausible. For the purpose of giving specific numbers to be compared with results obtained by other methods, usually the simple expression

$$Z_{\text{eff}} = Z - N + 1 \quad (I-6)$$

has been arbitrarily used, where N is the number of bound electrons per ion. This gives $Z_{\text{eff}} = Z$ for hydrogenic ions of finite Z ; however, if this is correct, as seems plausible, it then implies complete (or maximum possible) screening by the inactive or spectator electrons in transitions in complex ions (those with $N \geq 2$). One would expect that the appropriate choice for Z_{eff} for complex ions would lie between the value $Z_{\text{eff}} = Z$, corresponding to no screening, and Z_{eff} given by Eq. (I-6), which corresponds to complete screening by the inactive electrons. For He-like ions, where Eq. (I-6) gives $Z_{\text{eff}} = Z - 1$, one would expect the inactive electron to be only partially effective in screening for transitions from the $1s^2 \ ^1S$ ground level. Hence, the results given here for transitions from

the $1s^2\ ^1S$ level correspond to use of $Z_{\text{eff}}^2 = 30$ for C V and $Z_{\text{eff}}^2 = 56$ for O VII, which implies the spectator electron is about 50% effective in screening. The corresponding collision strengths have values $5/6$ and $7/8$ those obtained when Eq. (I-6) is used. On the other hand, for transitions between excited levels one would expect the inactive $1s$ electron to be nearly 100% effective in screening. Thus the results given for transitions of this kind in C V were obtained using Eq. (I-6), or $Z_{\text{eff}}^2 = 25$. Of course, for the hydrogenic ions C VI and O VIII, the values $Z_{\text{eff}}^2 = 36$ and 64 were used. Finally we note that in our previous work the results for $\Delta n = 0$ transitions have been expressed as a function of K_i^2 , where K_i^2 for finite Z was interpreted as $E'/(Z_{\text{eff}}^2 I_H)$ and E' is the final impact electron energy. Thus, in order to express results here as a function of X , the initial impact electron energy in threshold units, we have used the formula

$$X = 1 + \frac{Z_{\text{eff}}^2 I_H K_i^2}{E_{\text{ex}}} . \quad (\text{I-7})$$

Since the $Z = \infty$ results, upon which our results are based, use free electron wave functions in which no account is taken of change in electron energy in transitions involving no change in n value, our results are expected to be somewhat unreliable very near threshold for these transitions. However, since E_{ex} is very small, the important region for determining the collision rates for these transitions is not near threshold, but rather for $X \gtrsim 10$ or 20 .