# Electron Collisions With Atomic Ions

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## 1 Introduction

Electron impact excitation of ions is one of the primary processes for spectral formation in laboratory and astrophysical plasmas. The cross sections and rates for a large number of ions are therefore required for the diagnostics and modeling of plasma sources as diverse as the interstellar medium, with temperatures as low as a few degrees Kelvin, and X-ray objects such as supernova remnants or nuclear fusion plasmas at a few million degrees. Owing to the wide range of temperatures a large variety of atomic ions in various ionization stages need to be studied.

Nearly all atomic data for practical applications is obtained theoretically. Experimental measurements are difficult and have been done for a relatively small number of ions and transitions essentially to ascertain the accuracy of theoretical calculations. Theoretical methods have been developed or improved in recent years to meet many of the needs with high precision, although much work remains to be done. Most of the excitation data available is still from earlier works. It is therefore necessary to determine the accuracy of the excitation data in literature. A very large number of theoretical calculations have been carried, but mostly in relatively simple approximations that exclude one or the other of the important atomic effects determining the accuracy of the cross sections. On the ohter hand practical applications increasingly require a large number of atomic transitions to be taken into account, such as in non-local thermodynamic equilibrium (NLTE) atomic models for astrophysical spectroscopy. A huge amount of data is required and the users therefore need to be aware of the uncertainties in the available data.

Related to the requirement of theoretical calculations, appropriate methods need to be employed depending on the electronic structure and nuclear charge of the ion and associated atomic effects. Theoretical methods must, in principle, be able to accurately account for both the extensive electron correlation effects and the effect of relativity generally important in multiply charged ions when fine structure must be considered. A brief introduction to the methods and atomic effects, important in the assessment of a given calculation, is given.

In this review we present results from some recent calculations, as well an assessment of recent theoretical data sources compiled in the bibliographies by Itikawa 1996,1998). A comprehensive compilation and evaluation of data up to 1990 was carried out by Pradhan and Gallagher (92P1), including a discussion of the primary methods and atomic effects. The present review is therefore concerned with progress made since 1990 in the theoretical methods and atomic effects (section 2), comparison with new experiments (section 3), scaling laws, analysis of data, and databases (section 4), and data tables and accuracy ratings (section 5). Only those data are presented herein that are of reliable accuracy. For some important ions the data given may be of uncertain accuracy but are the only ones available. A special effort is made to present the data, as compleletly as possible, for all Iron ions; these are of special importance in both laboratory and astrophysical sources and comprehensive datasets for the complex low-ionization stages of iron have recently been calculated.

## 2 Theory

A number of approximations are usually employed to satisfy the two criteria of correlation and relativistic effects, respectively stated as: (i) coupling between the excited states as manifested, for example, in autoionizing resonances in the energy regions between states, and (ii) angular momenta and spin coupling schemes for the fine structure and relativistic operators in the hamiltonian for the (e + ion) system. Some of the major approximations for (i) are (a) the close coupling (CC) approximation that allows for strong coupling between the states of the target ion, and (b) weak-coupling approximation such as the distorted wave (DW) which accounts only for coupling between the initial and the final target states. Some of the approximations for fine structure transitions are: (a) non-relativisitic re-coupling of the total $L$ and $S$ of the (e+ion) system to yield the total $J$ symmetry, i.e. $\mathbf{L} + \mathbf{S} \longrightarrow \mathbf{J}$, (b) a term-coupling scheme allowing for relativistic atomic structure effects in the target ion alone, (c) intermediate coupling scheme via the Breit-Pauli hamiltonian for the (e + ion), (d) a fully relativistic Dirac hamiltonian.

In electron scattering calculations over the past three decades or so the CC approximation has been widely employed to account for the coupling between the electron scattering channels. The most powerful CC method has proven to be the R-matrix method (93B1) that is particularly suited for calculations for cross sections at a large number of energies needed to resolve resonance structures. The R-matrix method has been extended for cases (a),(b), (c), and (d) to include fine structure and relativistic effects. For exmaple a number of calculations have been carried out in recent years using the Breit-Pauli R-matrix (BPRM) method under the Iron Project (93H1).

For sufficiently highly charged ions the coupling between channels is weak, since the scattering is dominated by the coulomb potential, and the DW approximation yields accurate results. Several formulations of the DW approximation have been developed, for example a package developed by Eissner & Seaton (72E1). Relativistic effects have also been incorporated into the DW formulation and relativistic distorted wave (RDW) codes have been developed (e.g. Zhang *et al.* , 89Z1).

Although most of the calculations for electron scattering cross sections have been carried out using the CC or the DW methods, a number of calculations using other approximations are also found in literature.

## 2.1 Definitions and formulae

The total electron + ion wave function may be represented as

$$\Psi = A\sum_{i=1}^{NF} \psi_i\theta_i + \sum_{j=1} C_j\Phi_J, \tag{1}$$

where $\psi_i$ is a target ion wave function in a specific state $S_i$ $L_i$ and $\theta_i$ is the wave function for the free electron in a channel labeled as $S_iL_ik_i^2\ell_i(SL\pi)$, $k_i^2$ being its incident kinetic energy relative to $E(S_iL_i)$ and $\ell_i$ its orbital angular momentum. The total number of free channels is $NF$ ("open" or "closed" according to whether $k_i^2$ < or > $E(S_iL_i)$. $A$ is the antisymmetrization operator for all $N+1$ electron bound states, with $C_j$ as variational coefficients. The second sum in Eq. (1) represents short-range correlation effects and orthogonality constraints between the continuum electron and the one-electron orbitals in the target. The radial asymptotic form of $\theta_i$ is expressed as follows:

$$F_i(r) \underset{r\to\infty}{\sim} sin(\xi r) + cos(\xi r)\,\tilde{K}, \tag{2}$$

where $\xi$ is the Coulomb phase and $\tilde{K}$ is a real matrix called the *reactance* matrix. The *scattering matrix*, which is complex, is given by

$$\tilde{S} = (1+i\tilde{K})(1-i\tilde{K})^{-1}, \tag{3}$$

and the *collision strength* for the transition from the initial state of the target ion $S_iL_i$ to the final state $S_jL_j$ is

$$\Omega(S_iL_i - S_jL_j) = \frac{1}{2}\sum_{SL\pi}\sum_{\ell_i\ell_j}(2S+1)(2L+1)|S^{SL\pi}(S_iL_i\ell_i - S_jL_j\ell_j)|^2, \tag{4}$$

where $SL\pi$ is the total (e + ion) symmetry, i.e. the total spin and orbital angular momenta and parity, and $\ell_i\ell_j$ are contributing partial waves of the incident, scattering electron. The *cross section* $Q$ is expressed in terms of the collision strength as

$$Q(i,j) = \frac{\Omega(i,j)}{\omega_i k_i^2}(\pi a_o^2), \tag{5}$$

in units of Bohr area, ($\omega_i = (2S_i+1)(2L_i+1)$ and $\pi a_0^2 = 8.797 \times 10^{-17}\mathrm{cm}^2$); $k_i^2$ is the energy of the incident electron in Rydbergs (1 Ryd = 13.61 eV). For practical applications the quantity of interest is the *Maxwellian averaged collision strength*, sometimes referred to as the rate parameter or the *effective collision strength*, given by

$$\Upsilon(T) \text{ or } \gamma(T) = \int_0^\infty \Omega_{ij}(\epsilon_j)e^{-\epsilon_j/kT}d(\epsilon_j/kT). \tag{6}$$

Finally, the excitation *rate coefficient* is given by

$$q_{ij}(T) = \frac{8.63(-6)}{\omega_i T^{1/2}}e^{-E_{ij}/kT}\gamma(T)\ cm^3s^{-1}, \tag{7}$$

with $T$ in K and $E_{ij} = E_j - E_i, E_i < E_j$ in Rydbergs $[(1/kT) = (157885/T)]$; j is the excited upper state.

It follows from detailed balance that the *de-excitation* rate coefficient $(E_i < E_j)$ is given by

$$q_{ji} = q_{ij}\frac{\omega_i}{\omega_j}e^{E_{ij}/kT}. \tag{8}$$

In general $\Omega$ is an energy dependent function which consists of a slowly varying part, the background or nonresonant $\Omega$, and a rapidly varying part due to autoionizing resonances that can significantly affect the scattering rate.

## 2.2 Principal Methods

This section describes briefly the principal methods, the R-matrix and the DW methods, employed in most of the computations.

### 2.2.1 The Close Coupling approximation and the R-matrix method

The Schrödinger equation for the electron-ion collision problem may be expressed in terms of the scattering electron moving in the potential of the target ion. The radial part of the wave function of the scattering electron is written as

$$[\frac{d^2}{dr_i^2} - \frac{\ell_i(\ell_i+1)}{r_i^2} + k_i^2]F(i,r) = 2\sum_{i'}\{V_{ii'} \pm W_{ii'}\}F(i',r), \tag{9}$$

where $F$ is the radial function in a given channel (represented by $i$ or $i'$). The summation on the RHS of Eq. (9) is over all discrete and continuum states. $V_{ii'}$ and $W_{ii'}$ are direct and exchange potential operators respectively. The $W_{ii'}$ are integral operators and therefore Eq. (9) represents an infinite set of coupled integro-differential equations. The following sections discuss the various approximations found in literature for solving Eq. (9).

Truncating the sum on the RHS of Eq. (9) to a finite number of excited states of the target ion and solving the remaining coupled equations exactly yields the $n$CC approximation, where $n$ is the number of states included. The method of solution based on the R-matrix method has been computerized in the RMATRX package of codes developed at the Queen's University of Belfast by P. G. Burke and associates (93B1). It is important to ensure that the basis set of eigenfunctions that represent the $n$ states of the target ion be obtained with high precision. These atomic structure calculations may be carried out using the computer program CIV3 (75H1), based on the Hartree-Fock method (with configuration interaction) for computing one- electron orbitals, or the program SUPERSTRUCTURE based on a Thomas-Fermi-Dirac-Amaldi type potential (94E1).

The Breit-Pauli R-matrix method (82S1) considers the scattering problem in intermediate coupling to take account of relativistic effects. The $(N+1)$-electron Breit-Pauli hamiltonian includes the one-body, non-fine structure mass-velocity and Darwin terms, and the spin-orbit interaction leading to fine structure. The one-body non-fine- structure operators and may be included in R-matrix calculations in an otherwise LS-coupling non-relativistic calculation. In the full BPRM calculations the total angular momenta states are LSJ and parity.

### 2.2.2 The distorted wave and the relativistic distorted wave approximations

Usually for ions more than two or three times ionized, the distorted wave (DW) method can be used, since coupling is not very strong. In the DW method the relavant matrix elements need include only the initial and final states. However, the method allows for the distortion of the channel wave functions, from their asymptotic Coulomb form, in the target potential. The collision strength in terms of the transition matrix $\tilde{T}$ is

$$\Omega(i-j) = \frac{1}{2}\sum_{s_i,s_j}\omega|T(s_i;s_j)|^2, \tag{10}$$

where $i$ and $j$ are the initial and final target states in appropriate representation, $s_i$ and $s_j$ represent the overall quantum numbers of the $(N+1)$-electron ion, obtained by coupling the continuum functions to the target states, and $\omega$ is the corresponding statistical weight, such as $(2S+1)(2L+1)$ in Eq. (4) for $LS$ coupling. The $\tilde{T}$-matrix elements are obtained from the $\tilde{S}$ matrix as

$$\tilde{T} = 1 - \tilde{S} = -2\mathrm{i}\tilde{K}(1-i\tilde{K})^{-1} \simeq -2\mathrm{i}\tilde{K}, \tag{11}$$

where the last expression indicates that the unitarity constraint is neglected, valid for highly-charged ions in which $\tilde{K}$-matrix elements are usually much smaller than unity. It is generally accepted that, for ion charge $Z > 30$, a fully relativistic treatment is preferred.

The DW results for electron-ion scattering are usually accurate for highly charged ions or for high energies and should be a good complement to the CC results. Most DW results in literature usually do not include resonance contributions. However, there are a number of ways to include the resonance contributions. In the UCL formulation, bound channel wave functions can be introduced in the total eigenfunction expansion for the e + ion system. These give rise to poles in the scattering matrix in the continuum energy region and thus account for a limited number of resonances in the cross sections. Another way to implement the resonances is that described by Cowan (80C1) as a two step process of electron capture followed by autoionization with radiative decay of the continuum included.

For ions with very high $Z$, i.e., $Z > 50$, the lowest order of QED corrections, in particular the generalized Breit interaction, to the Coulomb interaction in the scattering matrix, could be important, especially for excitation of the $1s$ orbital. The effect of the generalized Breit interaction on electon-ion scattering was first studied by Walker (75W1) for H-like ions. Fontes *et al.* (93F1) studied this effect for more complex ions and inluded it as an option in the general RDW codes of Sampson *et al.* and Zhang *et al.* (89S1 and 89Z1).

In addition to the total cross section for excitation by electron impact, the differential cross section and the partial cross section for transitions between the magnetic sublevels can also be calculated, e.g., Zhang *et al.* (90Z1) and Inal & Dubau (93I1). The results for the transitions between the magnetic sublevels are useful for comparison with and interpretation of experimental results in the electron-beam ion-trap (EBIT) experiments. These can also be used to study the polarization of emmision lines. It should be mentioned that results for the hyperfine structrure transitions may also be of astrophysical interest and can be obtained readily (97S1).

### 2.2.3 High partial waves and the Coulomb-Bethe approximation

The basis of the Coulomb-Bethe (CBe) approximation is that the collisional transition may be treated as an induced radiative process. It is employed for optically allowed transitions where, due to the long-range dipole potential involved, it is usually necessary to sum over a large number of orbital angular momenta ($\ell$) of the incident electron. The method is valid for $\ell$-waves higher than a given $\ell_o$, which depends on the ionic charge, and is often used in conjunction with DW or CC approximations for low $\ell$-waves. If one takes $\bar{r}$ to be the mean radius of the target ion of charge z, the condition for the validity of the CBe approximation is

$$\ell > (k^2\bar{r}^2 + 2z\bar{r} + \frac{1}{4})^{1/2} - \frac{1}{2} \equiv \ell_0. \quad (12)$$

Thus, for allowed transitions the scattering calculations may be divided according to the sets of partial waves $\ell \leq \ell_o$ and $\ell_o < \ell < \infty$; the former are treated in the DW or CC approximations that take account of the detailed close-range interaction and the latter in the CBe approximation. The partial wave summation for forbidden transitions usually converges for $\ell \geq \ell_0$. A discussion of the general forms of the Born and the Bethe approximations is given by Burgess and Tully (92B1). The CBe approximation overestimates the cross sections due to the fact that the approximation is invalid for close encounters, i.e. low $\ell$-waves and the neglect of coupling among target states. The contribution due to high partial waves is further discussed by Burke and Seaton (86B1) who describe a "top-up" scheme, in LS coupling, implemented as an option in the R-matrix codes.

### 2.2.4 The Iron Project

Employing the R-matrix method large-scale close coupling calculations for radiative transitions, oscillator strengths and photoionization cross sections, were carried out under the Opacity Project for astrophysically abundannt elements with $Z$ = 1-14,16,18,20,26 in all ionization stages (95O1, 94S1). Collisional calculations using the BPRM method are now being carried out in a systematic manner under the Iron Project (93H1). The primary emphasis is on fine structure transitions in all ions of iron and iron-peak elements, although a number of calculations for other atomic systems are also being done. The close coupling calculations may be complemented, for high energies and partial waves, by the other methods discussed above such as the DW, RDW, or CBe. This is often necessary since the close coupling method is intended for low energies and partial waves (typically $\ell \sim 10$) requiring a detailed consideration of short range electron interactions. However for many transitions, such as electric dipole and quadrupole, the partial wave expansion needs to be more extensive for the convergence of the collision strengths, i.e. up to $\ell \sim 10 - 100$.

The Iron Project data is being made available electronically, together with data from the the Opacity Project, in a database called TOPbase/TIPbase (93C1). Links to the Iron Project work, papers, and data are available from the Web site www.astronomy.ohio-state.edu/∼pradhan.

## 2.3 Atomic effects

The primary atomic effects that determine the accuarcy of theoeretical calculation for electron impact excitation, and are usually incoportated in the theoretical methods employed are: (a) electron exchange, (b) coupling between the scattering channels, (c) accuracy of the eigenfunction expansion, i.e. the configuration interaction included to represent the basis of target states, (d) relativistic effects and fine structure when necessary. The uncertainty in a given calculation depends not only on the principal method employed but also on these contributing atomic effects included. The relative importance and magnitude of these effects varies widely from ion to ion. Even within an iso-electronic sequence large variations with $Z$ may be found; for example, pure LS coupling calculations become invalid for some transitions in high $Z$ ions. Another example is where, for the same ion, a close- coupling calculation may be less accurate than a distorted-wave calculation if the target wave functions in the latter take into account configuration interaction but the former do not. Also, at high energies a close-coupling calculation may not be accurate if the target states corresponding to the incident electron energies are not explicitly included in the target eigenfunction expansion, although otherwise it may represent short range electron correlation accurately and the low-lying transition cross sections may be reliable at low energies.

Following is brief description of the atomic effects.

### 2.3.1 Electron exchange

Almost all present day calculations fully include electron exchange. However, there are still many older sources of data in literature that are from calculations neglecting exchange (92P1). The total e + ion wave function should be an antisymmetrized product of the N+1 electron wave function in the system with N electrons in a bound state of the target ion and one free electron. It has been shown that apart from spin-flip transitions, which proceed only through electron exchange, it may be necessary to include exchange even for optically allowed transitions when the low $\ell$-wave contribution is significant, e.g., $1^1S - 2^1P$ in He-like ions where neglect of exchange leads to an error of about 50% (see Fig. 1 in 92P1).

### 2.3.2 Channel-coupling

For low-stages of ionization, with energetically closely spaced energy levels, electron scattering couples the probabilities of excitation of more than one level. When the coupling between the initial and the final levels is comparable to or weaker than the coupling with other levels included in the target expansion, then the scattered electron flux is diverted to those other states and coupling effects may significantly affect the cross sections. Thus the weak-coupling approximations such as the Born or the CB tend to overestimate the cross sections. As the ion charge increases, the nuclear Coulomb potential dominates the electron-electron interaction and correlation effects (such as exchange and coupling) decrease in importance. Whereas for neutrals and once or twice charged ions coupling between several states is usually strong and only a close-coupling calculation may yield accurate results, for multiply charged ions a distorted-wave treatment often suffices. Optically allowed transitions are generally not affected much, however, although there are exceptions such as in Li-like ions where the $2p - 3s$ transition is strongly influenced by the stronger coupling between the $2p$ and the $3d$. In such cases, resonance contributions to the cross sections are also large (81H1).

### 2.3.3 Target representation

An accurate representation for the wave functions of the target ion is essential to obtain accurate cross sections since the error is of the first order with respect to the error in the target ion wave functions. For complex atomic systems (e.g. low ionization stages of iron; see Refs. in Bautista and Pradhan 1998, 98B1) it is necessary to include a large configuraton interaction (CI) basis in order to obtain the proper wave functions for states of various target (angular + spin) symmetries $SL\pi$. The accuracy may be judged by comparing the calculated eigenenergies and the oscillator strengths (in the length and the velocity formulation) with experimental or other theoretical data for the states of interest in the collision. The advent of increasingly powerful serial and massively parallel supercomputers has enabled some very large atomic systems to be dealt with, e.g. Fe II (95Z1). To circumvent the problem of computer memory restrictions, the target state expansion may include pseudo-states, with adjustable parameters in the total eigenfunction expansion over the target states for additional CI. Transitions involving the pseudo-states themselves are ignored. Single configuration (SC) calculations are generally less accurate than the ones including CI. In the asymptotic region the coupling potentials are proportional to $\sqrt{\mathrm{f}}$ where f is the corresponding oscillator strength. It is therefore particularly important that the wavefunctions used should give accurate results for these oscillator strengths.

### 2.3.4 Relativistic effects

As mentioned earlier, the relativistic effects may be taken into account in several ways. However, the necessity to include these, and the method to be employed, depends on the ion under consideration. As the ion charge increases, relativistic effects may become prominent and have to be considered explicitly. For low-Z or z (nuclear charge or ionization state) ions the cross sections for fine structure transitions may be obtained by a pure algebraic transformation from the LS to LSJ or an intermediate-coupling scheme e.g., through programs JAJOM or STGFJ as part of the R-matrix package of codes (93H1). In general, the ratio of the fine structure collision strengths to multiplet collision strengths depends on the recoupling coefficients, but for the case of $S_i = 0$ or $L_i = 0$ we have

$$\frac{\Omega(S_iL_iJ_i, S_jL_jJ_j)}{\Omega(S_iL_i, S_jL_j)} = \frac{(2J_j+1)}{(2S_j+1))(2L_j+1}). \tag{13}$$

For example, consider the transitions in $p^3$ open-shell ions where the terms dominated by the ground configuration are: ${}^4S_{3/2}, {}^2D_{3/2,5/2}, {}^2P_{1/2,3/2}$. The ratio $\Omega({}^4S_{3/2} - {}^2D_{3/2})/\Omega({}^4S - {}^2D) = 4/10$ and $\Omega({}^4S_{3/2} - {}^2D_{5/2})/\Omega({}^4S - {}^2D) = 6/10$.

As the relativistic effects become larger one may employ three different approaches. The first one, for high-Z and z, is based on the Dirac equation. The Dirac R-matrix package of codes (DARC) has been developed by Norrington and Grant (87N1). The second method is to generate term coupling coefficients $< S_iL_iJ_i|\Delta_iJ_i >$ which diagonalize the target Hamiltonian including relativistic terms (Breit-Pauli Hamiltonian); $\Delta_iJ_i$ is the target state representation in intermediate coupling. These coefficients are then used together with the transformation procedure mentioned above to account for relativistic effects. The second method is incorporated in the program JAJOM or STGFJ (93H1). The third approach, the BPRM method is by Scott and Taylor (82S1) who extended the close-coupling nonrelativistic RMATRX package to treat the entire electron-ion scattering process in the Breti-Pauli scheme. The BPRM method appears particularly well suited for elements up to the Iron group (Z $<$ 30) to account for both the electron correlation and the relativistic effects accurately. However, for very heavy and highly charge systems the DARC approach may be needed and further studies are required to determine the precise validity of each of the methods.

A comparison of the various relativisitic approximations, the Dirac R-matrix, BPRM, and term-coupling, for electron scattering with Boron-like Fe XXII shows that the term-coupling approximation is not particularly accurate but that there is good agreement between the DARC and the BPRM calculations including the fine structure resonances that are important for several transitions (95Z2,96A1).

### 2.3.5 Radiation damping of autoionizing resonances

In the close coupling approximation the channels corresponding to each target state and angular momemtum of the incident electron, are coupled together. Resonances occur at energies below a target threshold due to coupling between the 'open' channels, corresponding to the excitation of energetically accessible target states, and the 'closed' channels corresponding to higher, energetically inaccessible target states that may be excited during electron collision but leaving the free electron temporarily bound in an autoionising resonant state. The R-matrix calculations include the resonance effects in an ab initio manner and the resonance profiles are obtained in detail by calculating the cross section directly at a large number of energies. The autoionizing resonances may enhance the excitation rates by up to several factors, with some reduction due to radiation damping in the continuum for highly charged ions (discussed below).

Electron scattering flux may undergo recombination with the target ion with emission of a photon. Such recombination may take place both through direct recombination, i.e. radiative recombination (RR), or indirectly through autoionizing resonances, i.e. dielectronic recombination (DR). The DR process thus diminishes the influence of resonances in electron impact excitation (EIE) cross section via radiation damping (e.g. Pradhan, 81P1). In a combined study of fine structure, autoionization, and radiative decays of *high-n* resonances up to the Rydberg series limits at target thresholds, Pradhan (83P1,2) found maximum reductions in the EIE rate coefficients for the metastable $1\ ^1S_0 - 2\ ^3S_1$ transition of 9% for He-like Fe XXV and 19% for Mo XLI. Fig. 1 shows the cross sections for EIE of He-like Ti XXI including relativistic and radiative damping effects (95Z3); Fig. 2 compares the theoretical results with the experimentally measured values from the Electron-Beam-Ion-Trap (EBIT) at Livermore.

Thus DR and EIE are complementary processes and related through the unitarity of the generalized scattering matrix including both the electron and the photon channels. This follows from the conservation of (photon + electron) flux during the scattering process. A general theory of DR was developed by Bell and Seaton (85B1) that provided a rigorous theoretical framework for radiation damping, and precise expressions for practical calculations, combined with multi-channel quantum defect theory, appropriate for Rydberg series of atomic states, and coupled-channel wavefunctions that allow for resonances in an *ab initio* manner.

As is physically evident, the RR and the DR processes are unified in nature. Extending the CC approximation and the R-matrix method to electron-ion recombination, Nahar and Pradhan (92N1) have developed a computationally unified approach to obtain total e+ion recombination cross sections and rate coefficients. Further, employing BPRM method the calculations have been extended to highly charged ions including relativistic effects and associated couplings (Zhang and Pradhan 97Z1,97P2). Fig. 3 illustrates the unification process, and relation to EIE, for electron scattering and recombination with He-like carbon: e + C V $\rightarrow$ C IV. The photo-recombination cross sections labeled 'PR' are unified elctron-ion recombination cross sections, including both RR and DR, obtained via the detailed balance relation from photoionization cross sections. At sufficiently high-$n$ the resonant contribution (DR) is very large compared to the background, non-resonant part and the total recombination cross section may be approximated accurately by simply the DR cross section. This is verified in Fig. 3 where the PR (including RR and DR) matches the DR cross section precisely at about $n = 10$. Finally, the DR cross section merges with the EIE cross section at the threshold for excitation of the dipole transition $1^1S_0 - 2^1P_1^o$ It may be noted that the resonances are completely damped out radiatively as $n \longrightarrow \infty$, even as the DR cross section rises to equal the EIE cross section at the threshold (98Z1).

# 3 Comparison with experiments

Although experimental measurements of electron-ion scattering cross sections are difficult, a number of advances have been made in recent years. The advent of merged-beam techniques, synchrotron ion storage rings, and electron-beam-ion-traps (EBIT) have made it possible to measure the cross sections to unprecedented accuracy.

Most of the recent experimental work employs the merged beam technique and cross sections for a number of ions have been measured. In nearly all cases the experimental results agree with the most sophisticated coupled channel calculations to within the typical experimental uncertainties of 10-15% – the range of uncertainty often quoted for such theoretical calculations. However, it needs to be emphasized that the details of resonance structures in the experimental data are subject to beam resolution; the theoretical data are convolved over the FWHM beam width in comparing with experiments. A few of the merged-beam cross sections and corresponding theoretical works are presented below.

The cross sections for C II in Fig. 4a,b,c are for the three lowest transitions from the ground state: the intercombination transition $1s^22s^22p\ ^2P^o \longrightarrow 1s2s2p^2\ ^4P^o$ (Fig. 4a), and the next two dipole allowed transitions to $1s^22s2p^2\ (^2D,\ ^2S)$ (Figs. 4b,c). The latter two final states lie relatively close together in energy and are coupled, as indicated by the fact that the proportion of the collision strengths is quite different from that of the oscillator strengths (90L1). It follows that simple formulae such as the Van Regemorter formula, or the "g-bar" approximation, for the collision strengths gives incorrect collision strengths (90L1). All three cross sections in Fig. 4 show considerable resonance structures; therefore approximations neglecting channel couplings, such as the distorted wave, are also likely to yield inaccurate collision strengths.

The measured cross sections in Figs. 4b and 4c for C II are for relatively strong dipole allowed transitions and therefore not as sensitive to channel coupling effects and resonances as the weaker intercombination or $LS$ forbidden transitions. However, recent experimental work has also been carried out for the $LS$-forbidden transitions in O II (95Z4) and S II (97L1). Both ions have the same $LS$-term structure. The measured cross sections are from the ground state $^4S^o \longrightarrow (^2D^o,\ ^2P^o)$, and for the dipole allowed transitions up to the higher $^4P$ terms. Figs. 5a and 5b show the experimental and theoretical results for the forbidden transition $(2s^22p^3\ ^4S^o \rightarrow ^2 D^o)$, and the dipole allowed transition $(2s^22p^3\ ^4S^o \rightarrow 2s2p^4\ ^4P)$ in O II. Theoretical data from two different sets of R-matrix calculations (95Z4) agree with experiment well within experimental error bars.

Fig. 6 presents the measured and theoretical collision strengths for the dipole allowed transtion 3s – 3p in Mg II (95S1). All experimental points except the last one agree with theoretical results within experimental uncertainties. It might be noted that the agreement holds true even at energies that span a number of excited n = 4 and n = 5 thresholds.

Fig. 7a,b,c show the results for three transitions in S II (97L1): $3s^23p^3\ ^4S^o \longrightarrow 3s^23p^3\ ^2D^o$ and $^2P^o$, and $3s^23p^3\ ^4S^o \longrightarrow 3s3p^4\ ^4P$. The theoretical data curves are based on two 19-state close coupling calculations (solid line and dash-dot line) and a 12-state close coupling calculation (dashed curve). While the all theoretical results agree with experiment for the first transition $^4S^o\ \ --\ ^2D^o$ (Fig. 7a), there is considerable disagreement for the transition $^4S^o\ \ --\ ^2P^o$ (Fig. 7b) between the 12-state calculation and experiment owing to the presence of a near-threshold resonance structure that is delineated by the 19-state, but not by the 12-state, close coupling calculation. This illustrates the importance of the configuration interaction expansion used in close coupling calculations; although the transition in question is only to the second excited state, the 12-state target expansion is not sufficiently accurate to reproduce the large resonance structure. Similarly, the 12-state results are also considerbly lower than experiment for the even higher transition up to $3s3p^4\ ^4P$ (Fig. 7c).

Electron impact excitation cross sections for multicharged ions have also been measured using the Merged Electron-ion Beams Energy Loss (MEIBEL) technique (94B1). Measured cross sections include:
$C^{3+}\ 2s\ ^2S - 2p^2P,\ O^{5+}\ 2s^2S - 2p^2P, Si^{2+}\ 3s^2\ ^1S - 3s3p\ ^1P, Si^{2+}\ 3s^2\ ^1S - 3s3p\ ^3P, Si^{3+}\ 3s\ ^2S - 3p\ ^2P, Ar^{6+}\ 3s^2\ ^1S - 3s3p\ ^1P, Ar^{6+}\ 3s^2\ ^1S - 3s3p\ ^3P, Ar^{7+} 3s\ ^2S - 3p\ ^2P$, and $Kr^{6+} 4s^2\ ^1S - 4s4p\ ^3P$. References to the experimental works and comparisons with theory may be obtained from at: www-cfadc.phy.ornl.gov/meibel/meibel.html. There is good agreement, usually within experimental uncertainties, between experimental values and theoretical close coupling calculations using the R-matrix method. It might be noted that the measured transitions are the lowest dipole allowed or intercombination transitions.

Some discrpancies between theory and experiment are evident in the figures given, although the overall structures agree.

In summary, the most elaborate theoretical calculations for up to the third row elements generally agree with experiments for the low-lying transitions that have been experimentally studied. However, detailed comparisons show that several prior theoretical results were in error.

# 4 Scaling laws, analysis of data, and databases

Transitions may be classified according to the range of the potential interaction $(V_{ii'} \pm W_{ii'})$ in Eq. (9). Spin change transitions depend entirely on the exchange term $W_{ii'}$ which is very short range since the colliding electron must penetrate the ion for exchange to occur. Therefore, only the first few partial waves are likely to contribute to the cross section, but these involve quite an elaborate treatment (e.g. close- coupling). For allowed transitions, on the other hand, a fairly large number of partial waves contribute and simpler approximations (e.g. Coulomb-Born) often yield acceptable results. The asymptotic behavior of the collision strengths for allowed and forbidden transitions is as follows (x is in threshold units of energy):

(A) $\Omega(i,j) \underset{x\to\infty}{\sim}$ constant, for forbidden (electric quadrupole) transitions, $\Delta L \neq 1, \Delta S = 0$

(B) $\Omega(i,j) \underset{x\to\infty}{\sim} x^{-2}$, for spin-change transitions, $\Delta S \neq 0$

(C) $\Omega(i,j) \underset{x\to\infty}{\sim} a\ell n(4x)$, allowed transitions, $\Delta\ell = 0, \pm 1, \Delta S = 0$.

The slope $a$ in the last equation is proportional to the dipole oscillator strength. The above forms are valid for transitions in LS coupling. For highly charged ions where one must allow for relativistic effects, through say an intermediate coupling scheme, sharp deviations may occur from these asymptotic forms particularly for transitions labeled as intercombination type (e.g., the transition $1^1S - 2^3P$ in He-like ions). For low $Z$ ions ($Z < 15$) when LS coupling is usually valid, $\Omega(1^1S - 2^3P)$ behaves as (B). With increasing $Z$, the fine structure splitting between $2^3P(J = 0, 1, 2)$ becomes significant and the collision strength $\Omega(1^1S_0 - 2^3P_1)$ gradually assumes form (C).

A useful fact for isosequence interpolation or extrapolation is that $Z^2\Omega(i,j)$ tends to a finite limit, as $Z \to \infty$, as a function of $k^2/Z^2$; i.e., at the $Z^2$ reduced incident electron energy, $\Omega(i,j)$ is constant or a slowly varying function for large $Z$. For highly ionized atoms (e.g. H-like, He-like) the $Z^2$ behavior is valid even for $Z < 10$, but for many-electron ions (e.g. Ne-like) one needs to go to much higher values of $Z$.

Faced with the huge volume of atomic data, calculated with different methods, it is important to be able to analyze, evaluate, compile, and disseminate it in efficient ways. One such approach is to adopt scaling procedures and examine systematic trends in the collision strengths. Burgess and Tully have implemented this approach to fit and extrapolate or interpolate effective (maxwellian averaged) collision strengths in a computer program called OMEUPS (92B1). Although useful in many cases, the limiting values( i.e as $E$ or $T \longrightarrow \infty$) adopted in this approach may not always be accurate, particularly for non-dipole transitions where coupling effects, such as $n$-complexes of resonances, may attenuate the collision strengths even to very high energies and the Coulomb-Born or Coulomb-Bethe limits may not be applicable. Nonetheless the scaled collision strength data can be visualized in a systematic manner, for example along iso-electronic sequences. Deviations from the fits may be investigated to explore possible errors, presence of resonances, convergence of partial wave expansion, etc.

A number of databases are listed in a review article on atomic data by Pradhan and Peng (95P1). As mentioned above a new database, TIPbase, has been developed to include the high precision data from the Iron Project (93H1).

# 5 Data Tables and Accuracy Ratings

Three sets of data tables are presented: 1. an evaluated compilation of theoretical data sources since 1990 (similar to the one by Pradhan and Gallager (92P1) for sources before 1990), 2. recommended data for a number of ions containing the maxwellian averaged or effective collision strengths $\Upsilon(T)$ at a range of electron temperatures, the wavelengths and transition probabilities of associated transitions, and 3. effective collision strengths for all iron ions, for a large number of transitions, taken from the recent Iron Project work or relativistic distorted wave calculations. Most of the data chosen are of high accuracy, rated A or B (10-20 % estimated uncertainty). Data rated lower, with higher uncertainties, are not included in the data tables 2 and 3 (with some exceptions), as many of these are being recalculated at the present time.

## 5.1 Table 1. Theoretical Data Sources

As mentioned earlier, a comprehesive survey and evaluation of theoretical calculations up to 1990 was carried out by Pradhan and Gallagher (92P1). Further compilations of data have been done by Itikawa for theoretical data sources appearing between 1990-1994 (96I1), and from 1995- (97I2). The papers listed in the annotated bibliographies in the latter two publications have been evaluated according to the basic criteria of (i) theoretical method employed and (ii) atomic effects included (these are explained in greater detail in 92P1).

An approximate accuracy rating is assigned according to estimated uncertainties within 10% (A), 20% (B), 30% (C), 50% (D), $>$ 50% (E), and Uncertain (U). Table I presents the data sources along with these ratings. It is noted that unlike most of the calculations prior to 1990, nearly all of the recent calculations for electron impact excitation have been carried out in the close coupling approximation using the R-matrix method, or the distorted wave (relativistic and non-relativistic) approximation. Also, unlike previous calculations the often dominant effect of autoionzing resonances is now well established and most calculations for low-ionization species include or estimate these effects.

It should be emphasized that the accuracy rating assigned is only an overall estimate of the theoretical calculations reported in the corresponding publication. It does not attempt to represent the accuracy of each individual transition or range of energies for which the uncertainties may well vary even for the same method with the same effects included for the same ion. As such, the ratings are meant only as a rough criterion to provide some assessment of the overall reliability of the data, and whether the data needs to be recalculated with improved accuracy.

Sections of Table 1 are divided according to isoelectronic sequences, with the number of electrons in the ion, N = 1 etc., and in order of the atomic number the elements listed. The first author's name is listed. Soemtimes it is not possible to list all the transitions in detail and users should consult the data source(s) before deciding to use a given set of data. The symbols used to represent the available "Data" are as follows:

$\Omega$ - collision strength, $\Upsilon$ - maxwellian averaged collision strength, Q - cross section, q - rate coefficient, f - oscillator strength, DCS - differential cross section, Pol. - polarization data.

The theoretical methods listed in Table 1 are:

RM – R-matrix, BPRM – Breit-Pauli R-matrix, CC – close coupling (R-matrix or others), CCC – convergent close coupling, DW – distorted wave, RDW – relativistic DW, CB – Coulomb Born, CBe – Coulomb Bethe, CDW – Coulomb DW, CBR - Coulomb Born relativistic, QDT – quantum defect theory.

## 5.2 Table 2. Effective Collision Strengths, Wavelengths, and A-values

At electron temperatures around 10000 K the elements in a plasma source are in low ionization stages and low levels of excitation. In astronomy such sources are often "nebular" plasmas such as found in supernova remnants, diffuse and planetary nebulae, stellar atmospheres, active galactic nuclei, and the interstellar medium. In Table 2 we present the maxwellian averaged collision strengths $\Upsilon(T)$, and the observed wavelengths and Einstein A-coefficients, for low-lying transitions in a number of ions. These recommended data are taken from the best available sources and have been interpolated where necessary to obtain the $\Upsilon(T)$ at 5000 K, 10000K, 15000 K, and 20000 K (data sources are listed in the review article by Pradhan and Peng, 95P1).

The decimal and exponent notation for the effective collision strength $\Upsilon(T)$ is 'a.bc-x', where 'x' is the exponent in $10^x$. The "$\Downarrow$" after the *first* fine structure transition within a multiplet indicates that the available value is for the whole LS multiplet, which may be divided according to the fine structure statistical weights among the other transitions as described above for cases *when one of the levels has only one associated J-value* (see $\oint$ 2.3.4), i.e. for levels with L = 0 or S = 0. For transitions such as $^1D\ -\ ^3P$, such division is not possible in a straightforward manner and only the total multiplet value may be used (although Table 2 lists the fine structure levels). The "–" indicate that the data is not available for those transitions.

The order of transitions in Table 2 with respect to the upper and lower levels is mixed, and the initial levels under the column 'Transition' is not usually the lower one. Therefore care must be exercised in using Eq. (7) or (8) to determine the lower and the upper levels $E_i$ or $E_j$. Wavelengths may be converted into excitation energy as $E_{ij}$ (Ryd) = 911.26708 / $\lambda(\mathring{A})$ or $E_{ij}$ (eV) = 12399 / $\lambda(\mathring{A})$ (assuming the Rydberg constant for infinite mass $R_\infty$ = 911.26708).

## 5.3 Table 3. Excitation Data For Iron Ions

Electron-impact excitation data for iron ions are very important for astrophysical and other plasam modeling applications. The Iron Project (IP, 93H1) is mostly devoted to calculating reliable collisional data for all iron ions using the most accurate method, the Breit-Pauli R-matrix close-coupling method, with relativistic fine structure effects. The effective, or maxwellian-averaged, collision strengths tabulated in this section are mostly taken from the collective efforts by the IP. Because this is an on-going endeavor, data for some iron ions by the IP are currently not available. For some of these ions data calculated by the RDW method are also tabulated. It is noted that these RDW data contain only the background, or non-resonant, contribution. It should be accurate if the resonance contributions, by using the method described in §2.2.2, is added.

In Table 5.3 the data tables for the iron ions are summarized. It also lists the methods and the data sources. The theoretical methods listed in Table 5.3 are: DARC – relativistic Dirac R-matix (87N1), BPRM – Breit-Pauli R-matrix, FARM – FARM package of the R-matirx method (95B2), ARRM – R-matrix with algebraic recoupling to obtain fine-structure results, TCC – same as ARRM but with inclusion of term coupling coefficients, and RDW – relativistic distorted wave.

The symbols used in the data tables are: $J$ – the total angular momentum for the fine-structure level, $T$ – temperature, and $\Upsilon$ – the effective or mexwellian-averaged collision strength. The decimal and exponent notation for $\Upsilon$ is '$a.bc[x]$', where '$x$' is the exponent in $10^x$. For most ions there are two tables, a and b, where Table 5.3.2a, for instance, lists the fine-structure energy levels and the observed and theoretical energies, and Table 5.3.2b gives the effective collision strengths $\Upsilon$ as a function of temperatures $T$(K).

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**Table 5.3.** List of the data tables for the iron ions included.

| Tables | | Ion | Method | Ref. |
|---|---|---|---|---|
| 5.3.1a | 5.3.1b | Fe I | FARM | 97P1 |
| 5.3.2a | 5.3.2b | Fe II | ARRM | 95Z1 |
| 5.3.3a | 5.3.3b | Fe III | ARRM | 96Z1 |
| 5.3.4a | 5.3.4b | Fe IV | ARRM | 97Z2 |
| 5.3.5 | | Fe V | BPRM | 95B1 |
| 5.3.6 | | Fe X | ARRM | 95P1 |
| 5.3.7a | 5.3.7b | Fe XII | TCC | 98B2, 98B3 |
| 5.3.8 | | Fe XIV | TCC | 96S1 |
| 5.3.9a | 5.3.9b | Fe XVI | RDW | 90S1 |
| 5.3.10a | 5.3.10b | Fe XVII | RDW | 89Z1 |
| 5.3.11 | | Fe XVIII | ARRM | 98B1 |
| 5.3.12a | 5.3.12b | Fe XXI | RDW | 96Z2 |
| 5.3.13a | 5.3.13b | Fe XXII | BPRM | 97Z1 |
| 5.3.14a | 5.3.14b | Fe XXIII | RDW | 92Z1 |
| 5.3.15a | 5.3.15b | Fe XXIV | BPRM | 97B1 |
| 5.3.16a | 5.3.16b | Fe XXVI | DARC | 96K1 |

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FIGURE CAPTIONS

Fig. 1. Electron impact excitation cross sections for the transitions $1^S_0 - 2^1P_1(w), 1^1S_0 - 2^3P_2(x), 1^1S_0 - 2^3P_1(y)$, and $1^1S_0 - 2^3S_1(z)$ in Ti XXI; left panels: without radiation damping, right panels: with radiation damping (Zhang and Pradhan 1995, 95Z3).

Fig. 2. Comparison of the convolved theoretical electron impact excitation cross sections, solid lines (Zhang and Pradhan 1995, 95Z3) with the EBIT experimental data ,circles with error bars (Chantrenne *et al.* 1992, 92C1) for the transitions in Ti XXI in Fig. 1.

Fig. 3. Correspondence between photo-recombination (PR), dielectronic recombination (DR), and electron impact excitation. The PR cross sections are derived from photoionization cross section via detailed balance and include both resonant and non-resonant (background) recombination; the DR cross sections are computed using the coupled-channel theory of DR (85B1); and the filled circle represents the near-threshold value of electron impact excitation cross section for the dipole transition $1^1S_0 - 2^1P_1$ in C V (Zhang *et al.* 1998, 98Z1).

Fig. 4. Experimental (filled circles) and theoretical R-matrix cross sections for C II convoluted with a 250 MeV FWHM resolution (Smith *et al.* 1996, 96S1); solid line (96S1), dotted line (Luo and Pradhan, 90L1) for the excitation of the (a) ${}^2P^o -{}^4 P$ (intercombination) transition, (b) ${}^2P^o -{}^2 D$ (allowed) transition, and (c) ${}^2P^o -{}^2 S$ (allowed) transition.

Fig. 5. Experimental (filled circles) and theoretical R-matrix cross sections (solid line, Zuo *et al.* 1996, 95Z4) for O II for excitation of the (a) $2s^22p^3\ {}^4S^o -{}^2 D^o$ (forbidden) transition and (b) ${}^4S^o - 2s2p^4\ {}^4P$ (resonance) transition.

Fig. 6. Comparison of the 3s – 3p collision strength with experiment (Smith *et al.* 1993, 93S1); the full curve is the ten-state close coupling (R-matrix) calculation averaged over a Gaussian electron beam of 0.3 eV FWHM (Sigut and Pradhan, 95S1).

Fig. 7. Experimental (filled circles) and theoretical cross sections for excitation of S II. Theoretical results are convoluted with a 250 meV (FWHM) electron energy width: solid line, 19 state R-matrix calculation; dash-dot line, Ramsbottom *et al.* . (1996) 19 state R-matrix calculation; dashed line, Cai and Pradhan (1993) 12 state R-matrix calculation; dotted line, Tayal *et al.* (1987) 6-state R-matrix calculation (as reported in Liao *et al.* 1997, 97L1) – (a) ${}^4S^o \rightarrow{}^2 D^o$ transition, (b) ${}^4S^o \rightarrow{}^2 P^o$ transition and (c) ${}^4S^o \rightarrow{}^4 P$ transition.