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Atomic and Molecular Data Exploitation for Spectroscopic Diagnostics of Fusion Plasmas

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Atomic and Molecular data exploitation for spectroscopic diagnostics of fusion plasmas

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Abstract

An overriding requirement of atomic and molecular data for spectroscopy of fusion plasmas is identified as a need to ensure that the most recent and highest quality fundamental data is incorporated in analysis and interpretation of emission from plasmas and that it enters consistently into large scale plasma modelling. It is argued that this can only be achieved by accompanying the product of modern large scale atomic reaction coefficient calculations with an equally sophisticated organisation and utilisation structure for its exploitation. The paper describes a possible form for such a structure which can address both the present and anticipated developments in fusion up to a demonstration reactor. Various illustrations are given of practical implementation of parts of such an atomic data and analysis structure which has supported spectral studies at the Joint European Torus experiment.

A. Introduction

The atomic and molecular data needs for fusion have been discussed and reviewed many times and in general terms these have not changed in marked degree over the last decade. In that sense an article of the present title appears redundant. However, although there has been explosive growth in available experimental and theoretical collision cross-section data to fill the perceived need, there are surprises. For example, in some established beam energy deposition codes and indeed in some very new codes, the cross-section data used dates from the nineteen sixties and is inaccurate to factors $\geq 20\%$. Such errors are quite important in beam

spectroscopy studies. This suggests that there are two separate problems in atomic data for fusion, namely, the generation of high quality collision data on the one hand, and its effective use in fusion plasma studies on the other. The huge amount of data available at the present time makes the latter question quite critical and it is on this that the present article is focussed.

Our article is based on nearly ten years of experience at the JET Joint Undertaking in trying to model the spectral emission from all regions of the tokamak plasma. To achieve this we have created a structured computational approach involving groups of processing codes, fundamental and derived database organisations and linkages to experimental data reduction and to theoretical plasma models. We call this the 'Atomic Data and Analysis Structure', ADAS (Summers & Dickson, 1992); Summers & Wood, 1988; Gordon et al., 1982), and describe the underlying structure here as an illustration of the type of system which can be envisaged and which should accompany large scale atomic data production.

There are some general principles which have influenced us in the establishing this structure. Firstly, atomic data, as well as entering experimental spectroscopic analysis, forms an important part of large scale plasma models, albeit often as a 'package'. It is evident however that spectroscopy is the primary testing ground of high quality items of atomic collision data through precise measurements, while the comparisons of parameters from plasma models are usually more gross. The most detailed atomic data needs are in the spectroscopic realm and it is there that the organisation structure begins. The needs of global models are then derived, being obtained by bundling and condensation procedures. Our structure seeks to make these bundling pathways precise and explicit so that refinement of global atomic data for plasma models is driven by advances at the spectroscopic level. By this means we believe that the separation and inconsistencies between data in spectroscopy and data in global models, so common in the fusion plasma environment, can be avoided. Secondly, it is clear that an atomic data and analysis structure must fit correctly as part of an iterative loop from spectroscopic observation through atomic modelling, plasma modelling, experiment/theory confrontation and back again. We call this the diagnostic loop and its support is basic to our expectations of the atomic data organisation.

In section B, the main analysis needs are identified and divided into four main areas. These are described separately. Then in a smaller section C, some organisational aspects of particular background fundamental calculations which aid and reinforce the application are discussed. Attention to these can greatly ease the interface between fundamental researches and the fusion plasma models and interpretations. The conclusions are in section D. Detailed identifications of individual species, fundamental reactions and methods for positioning them in collisional radiative calculations for present and future fusion plasma devices have been made in an associated work (Summers, 1993) and are not repeated here.

B. Areas of Need

It is in general the case that any observed radiation emission from a plasma, such as a spectrum line due to transition in an excited impurity ion, is the resultant of a number and possibly many fundamental reactions. In the early days of high temperature, low density plasma studies it was believed that a particularly simple situation usually occurred, the *coronal approximation*, whereby excitation (or ionisation) was by electron collisions with the ground

states of ions only and was followed by radiative cascade (or radiative recombination). It is now however seen that in most of the critical zones of the modern fusion plasma this simplification is not valid. Metastable states are important in recombination and ionisation, multistep collisional processes matter in beam attenuation, redistribution occurs in low temperature high density divertor plasma and ion/atom collisions are as important as electron collisions. It is indeed true that population of excited levels of an ion in a plasma results from the combined effect of many processes. Thus in interpretation of emission from plasmas it is the *effective* coefficients for reactions which must be sought rather than the fundamental *direct* reactions. The basic organisation of an atomic modelling structure is therefore apparent. It must incorporate and address the problems of a fundamental reaction database, be able to generate a derived database of meaningful atomic coefficients for the various plasma environments and provide appropriate interfaces for their use in experimental data reduction and plasma modelling. This leads naturally to certain groupings of related aspects and manipulations indicated in table B.

Table B.

Application group
1. Entry and validation of fundamental atomic data
2. Evaluation of excited state populations of ions in a plasma
3. Charge exchange and beam emission spectroscopy
4. Recombination, ionisation, radiated power and plasma models

Group 1 activities address fundamental, that is essentially individual reaction data and as such are to be distinguished from the composite effects of many processes which is the subject of the remaining groups. In group 1, we are not concerned with ab initio calculations of individual reaction cross-sections but rather preparation and assessment of such data from other sources for inclusion in a database. Unit conversions, data display, comparison with expected forms for the data, Maxwell averaging, control of asymptotic behaviour and transfer onto preferred standard temperature ranges are the main objectives. In particular, we shall discuss in this group *approximate forms* which will allow a point of comparison and vetting of new numerical data, which link to compact representations of fundamental data and aid interpolation.

Group 2 activities are concerned with evaluating excited populations of specific ions in a plasma environment and then their radiation emission. It relies on availability of a reaction rate data collection for the ion in a suitable database although an important issue is some provision for generating an approximate collection of such data when this is not so. A reaction data set which is complete and self contained for the execution of an excited state population calculation, we call a *specific ion file*. A combined (and usually simpler) data set for an iso-electronic sequence from which a specific ion file can be generated, we call a *general z file*. A further important issue in population calculations is the distinction of states whose populations relax on time scales comparable with plasma dynamical timescales, *metastables* (which includes ground states), and those which relax more rapidly, *excited states*. This distinction influences the way calculations are performed and determines the types of derived coefficients which are required for plasma spectroscopic application. The calculational approach which can

accommodate these aspects is called *generalised collisional radiative theory* (Bates et al., 1962; Summers & Hooper, 1983; Summers, 1993) and it forms the heart of our analysis structure.

Group 3 activities are concerned with those situations in a plasma when charge transfer from neutral hydrogen (or its isotopes) or neutral helium is a primary mechanism. This is the area which has developed very strongly in association with neutral beam heating of plasmas and has given rise to *charge exchange spectroscopy* and *beam emission spectroscopy*. The population manipulations and fundamental and derived data requirements for these latter spectroscopies are specialised.

Group 4 activities are concerned with the dominant ground and metastable populations of ions in a plasma and particularly their preparation and calculation for dynamical plasma models. It therefore operates with generalised collisional dielectronic recombination and ionisation coefficients, associated power loss coefficients and metastable fractions. It is found most convenient in working with atomic data and preparing derived coefficients to address sets of ions with the same number of electrons but different nuclear charges, that is *isoelectronic sequences*, together if possible. This allows powerful interpolations in charge state. Thus group 4 activities also include mediation of transfer from an isoelectronic sequence storage of data which is the preferred choice for atomic data preparation and manipulation to an *isomuclear sequence* storage preferred for applied studies in dynamical plasma models. Finally, group 4 activities recognise the need to provide a number of simplified or extremal plasma models such as the coronal case or the purely dynamically ionising model on which initial emission and spectroscopy expectations can be based. They do not include the large scale magnetohydrodynamic and kinetic models. These are serviced by the provision of the derived database which is created by the procedures of the earlier groups.

1. Fundamental data entry and verification

It is found that we have to deal with at least seven types of atomic data. These and the manipulations required are indicated in table B.1.

Table B.1

Data type	Processing required
a. Electron-impact excitation cross-sections	graphing and up-silon evaluation
b. Electron-impact excitation rate coefficients	graphing and interpolation
c. Electron-impact ionisation cross-sections	graphing and rate evaluation
d. Electron-impact ionisation rate coefficients	graphing and interpolation
e. Radiative recombination rate coefficients	graphing and interpolation
f. Dielectronic recombination rate coefficients	graphing and interpolation
g. Charge exchange cross-sections	graphing and interpolation

a. Electron collision cross-sections for individual reactions frequently come under direct scrutiny. Such data are presented in the general literature in a variety of forms including collision strengths, excitation and deexcitation cross-sections and effective Gaunt factors. The problem is often that the data is given at very few energy points and Maxwellian averages are required for the electron collision database. Also, since we wish the rates to be valid over extended temperature ranges, the behaviour of the cross-section beyond the tabulated values is of concern. As a first step it is helpful to convert the data to a standard

form, the most favoured by atomic collision workers being the collision strength, Ω , mapped as a function of the threshold parameter $X (=E/\Delta E)$. The collision strength is nearly constant, tending to a finite value at threshold for ions. The asymptotic behaviour varies depending upon whether the transition is of dipole, non-dipole or spin change character. Collision strength data are conveniently examined by forming a ratio of them to a simple, adjustable, one or two parameter approximate form of appropriate character. Such a ratio is often very close to unity and makes evident typographical errors in data. Also flat asymptotic behaviours can be forced on the ratio providing a stable interpolant and extrapolant for the data in preparation of Maxwell averages. We make use of this comparison with approximate forms in all the data entry procedures of this section, documenting the comparative plot. Figure B.1.a shows such a comparative plot. With spline interpolation of the ratio, it is then straightforward to form an accurate Maxwellian average. In practice, it is the rate parameter, sometimes written as Y (upsilon) or γ (gamma) which is usually computed since this is slowly varying, simply related to the excitation and deexcitation rate coefficients and equal to the threshold collision strength at low temperature. Also Y is usually prepared at a standard set of z-scaled (*reduced*) temperatures ($\theta=T_e/z_1^2$).

ANALYSIS OF EXCITATION CROSS SECTIONS

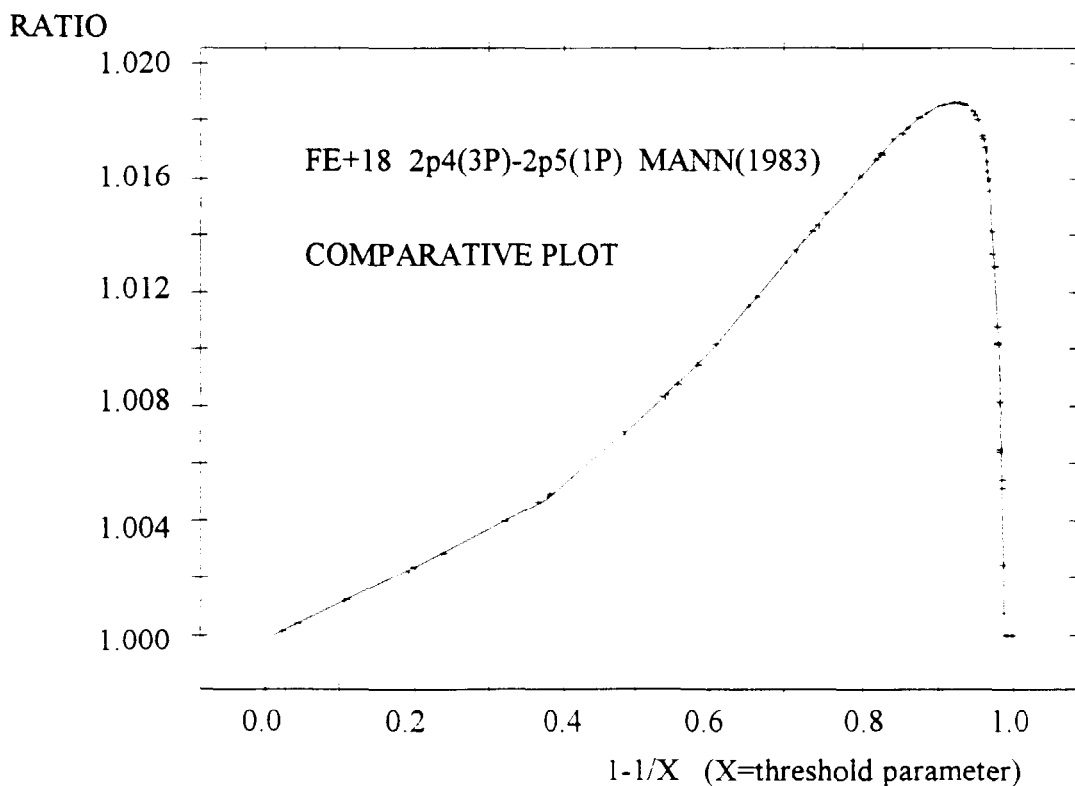


Fig. B.1.a Comparative plot of the ratio of tabular collision strength data for the FeXIX ($2p^4 ({}^3P) - 2p^5 ({}^3P)$) transition to an approximate form of dipole type matched to the first and last data values. The very small excursion of the ratio from unity is noted. Crosses mark interpolated points used in forming the Maxwellian averages.

b. A similar situation occurs for excitation rate coefficients. Data in the literature is presented as excitation rate coefficients, deexcitation rate coefficients, rate parameters and Maxwell averaged Gaunt factors. The rate parameter is preferred for standardised presentation and storage since it has a close relationship to the collision strength and excludes the rapidly varying exponential from the excitation rate coefficient. Ratio comparisons of individual rate parameter data to simple one or two parameter approximate forms of suitable character are again desirable. The approximate forms for the collision strength can usually be analytically integrated over Maxwellians and so consistency is maintained between the cross-section and rate coefficient examination. The ratio again provides a good basis for interpolation and extrapolation by splines matched to flat asymptotic behaviour. In virtually all fusion plasma applications, it is the Maxwell averaged rate coefficients which are required and so the primary electron collision database is maintained in this form.

c. Ionisation cross-section data are frequently required from tabulations in the general literature. The ionisation cross-section itself is usually presented as a function of electron temperature, z-scaled temperature or energy scaled temperature. Also it is the Maxwell averaged ionisation rate coefficient which is sought for applications. A number of questions arise in assessing such data of theoretical origin, which may not be explicitly answered in the source papers. These include whether excitation/autoionisation pathways and all inner shell ionisations have been included. There is also a major problem in that at the present time most data is not at a state selective resolution level appropriate for generalised collisional radiative application. Thus ionisation only from the ground state may be given with the cross-section summed over all final state channels. The data verification and examination procedure must seek to provide some guidance on a tentative breakup of the composite coefficient. The use of a suitable approximate form as a comparator is of considerable value here. In studies at JET, we have used the approximate form of Burgess-Chidichimo (1983) type and follow the philosophy of Summers and Hooper (1983) on the flexible use of threshold energies and numbers of equivalent electrons. Particularly, we allow two ionisation shell groups and two excitation shell groups. Each ionisation shell group can consist of several individual shells with their own threshold energy and number of equivalent electrons, but in adjustment of the approximate form to fit external data, the group is scaled as a whole. The excitation groups are designed for adjustment to match the opening of large excitation/autoionisation steps and consist of a weighted simple excitation cross-section form. The source data to approximate form ratio is used to check the inclusion of all shells and expected features and then by optimising the fit, to provide overall scaling adjustment of the approximate form. The breakdown of a composite cross-section is then achieved by separating the parts of the approximate form appropriately. Also omissions in the source data can be amended by adding in the appropriate approximate form part. Figure B.1.c illustrates a comparative plot for the ionisation cross-section. Ionisation cross-section data is converted to Maxwell averaged ionisation rate coefficients for the electron impact ionisation database.

d. Similar examination of ionisation rate coefficient data is required. The procedure is the same as for the cross-section in the previous subsection since the same approximate form

usage is possible. The Burgess-Chidichimo cross-section expression yields an analytic rate coefficient expression. The comparative plot for the ionisation rate coefficient ratio is however a less sensitive one for assessment of details of the rate coefficient because of the Maxwellian averaging. We do not illustrate this case.

ANALYSIS OF IONISATION CROSS SECTIONS

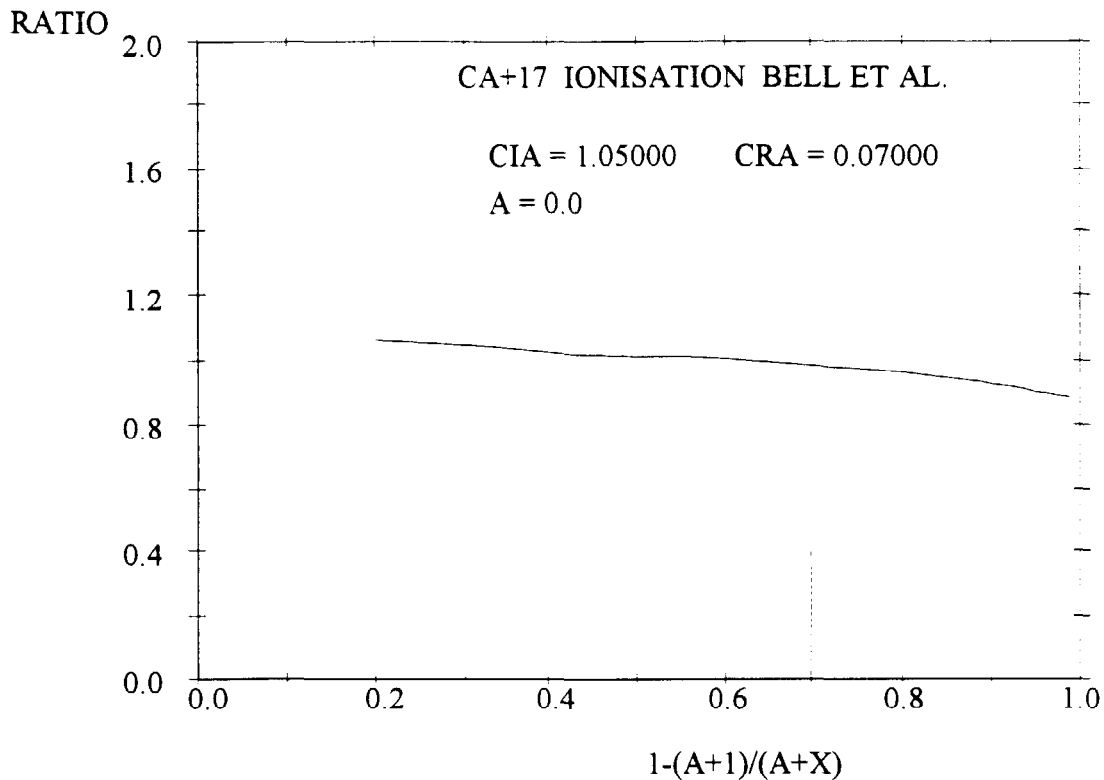


Fig. B.1.c Comparative plot of the ratio of tabular ionisation cross-section data from Lennon et al. (1986) to an adjusted approximate form for Ca^{+17} ionisation. The approximate form includes $2s$ direct ionisation and an effective excit./autoionis. resonance contribution from $1s2s^2$. It is evident that the source does not include the $1s$ shell direct ionisation. This needs to be included for our preferred data. The dotted line is the position of the excitation/autoionisation threshold.

e. Radiative recombination and dielectronic recombination in the next subsections present a somewhat more complicated problem. The fundamental measurement or calculation is of the photoionisation cross-section from a particular state. The radiative recombination rate coefficient for a Maxwellian free electron distribution is obtained from the Milne relation. In the general literature, it is often the radiative recombination coefficient summed over all levels of the recombined ion which is presented. This would be the actual ionisation stage to ionisation stage effective recombination coefficient in a plasma of zero density when ionisation from excited states is negligible. More occasionally, the radiative recombination coefficient to the ground state is given. The total zero density coefficient is composed of a ground level part which is a major contribution and most influenced by the core electron structure and an excited level part which approaches hydrogenic. It is the ground level part which requires most scrutiny. There is a second issue, namely, that collisional radiative

calculations for finite density plasma requires the separate radiative recombination coefficients into individual excited levels. Thus the examination and verification procedure must suggest a tentative subdivision. This is analogous to the final state problem in the ionisation cross-section. In a moderate accuracy approach, we assume that the excited state captures are correctly represented by hydrogenic values and by the hydrogenic subdivisions into n and l shells. Our comparative approximate form is then a simple adjustable two parameter form for the ground state capture added to exact hydrogenic values for the other levels. The ratio adjustment then is then essentially a fit of the ground state capture while resolved coefficients in applications are given by the approximate form. Figure B.1.e illustrates the comparative plot. The product of the data examination and verification is source data interpolated to preferred temperatures together with parameters of the best approximate form fit.

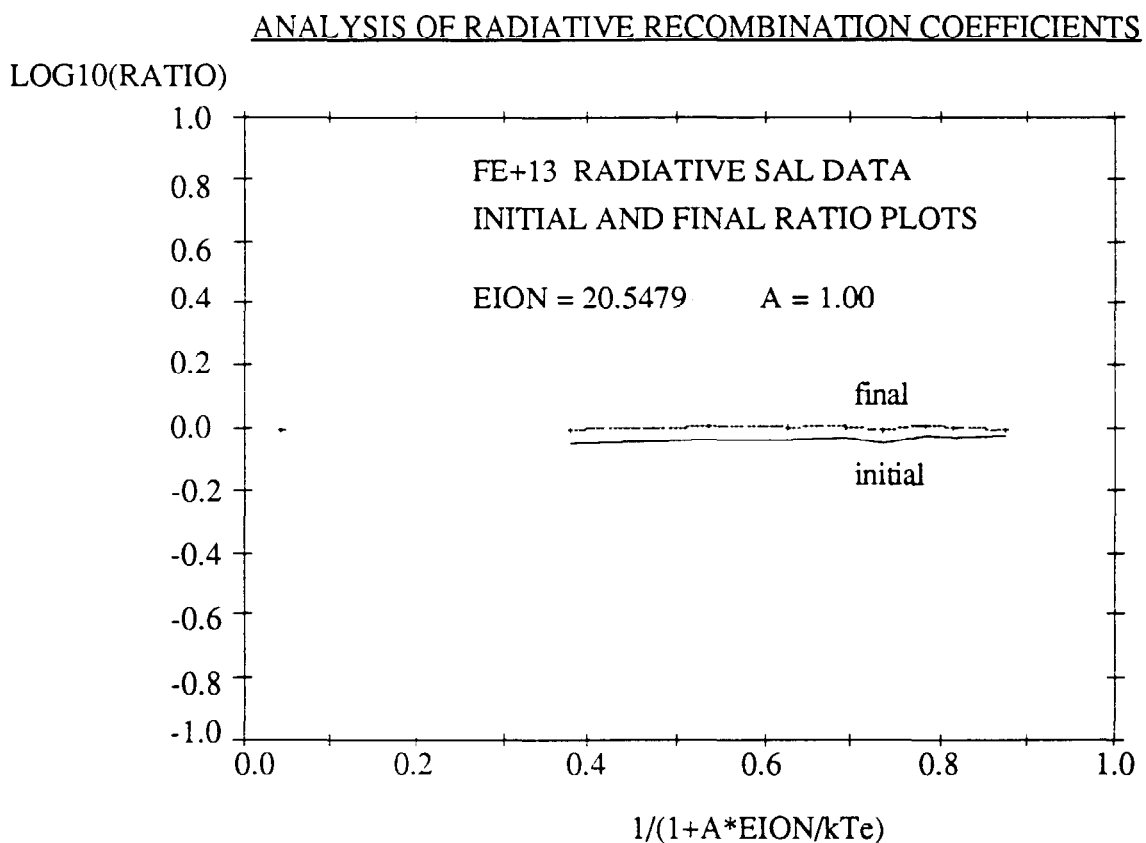


Fig. B.1.e Comparative plot of the ratio of some tabular total zero density radiative recombination data for $Fe^{+13} + e$ commonly used in fusion (Behringer, 1987) matched to the approximate form. The solid line is the initial ratio and the dashed line the ratio after adjustment of the approximate form. The approximate form includes an effective principal quantum number and an effective fractional shell occupancy number for the lowest level. The optimised form includes a temperature dependent shift and a constant scaling.

f. For dielectronic recombination also, it is usual to find the total zero density coefficient presented as a function of electron temperature in the literature. Resolution of the

coefficient into the capture to separate n and l levels is necessary for population calculations, but in this case there is no simple hydrogenic assumption to use. Dielectronic recombination is markedly dependent on the detailed core structure of the recombining ion and this must be taken into account. We prefer to examine data by comparing it with two approximate forms. The first is the Burgess General formula (Burgess, 1965) for the total zero density coefficient. Inaccuracies in the formula arise from the mean resonance energy factor in the exponential which affects the low temperature behaviour and errors in the mean Auger/radiative branching ratio which acts as a constant shift. Our two parameter form allows adjustment in these respects. Our second approximate form is in fact a numerical algorithm for the nl resolved dielectronic coefficients based upon the computer program of Burgess (1964). It was upon the results of this code, summed over all levels, that Burgess prepared his general formula. The program is very rapid and a more fundamental view can be taken to it's adjustment as an approximate form. This approximate form program, adjusted so that the total coefficient agrees with the source data then provides the moderate accuracy level resolution of the dielectronic coefficient. Figure B.1.f shows a typical comparative plot of the source to approximate form ratios.

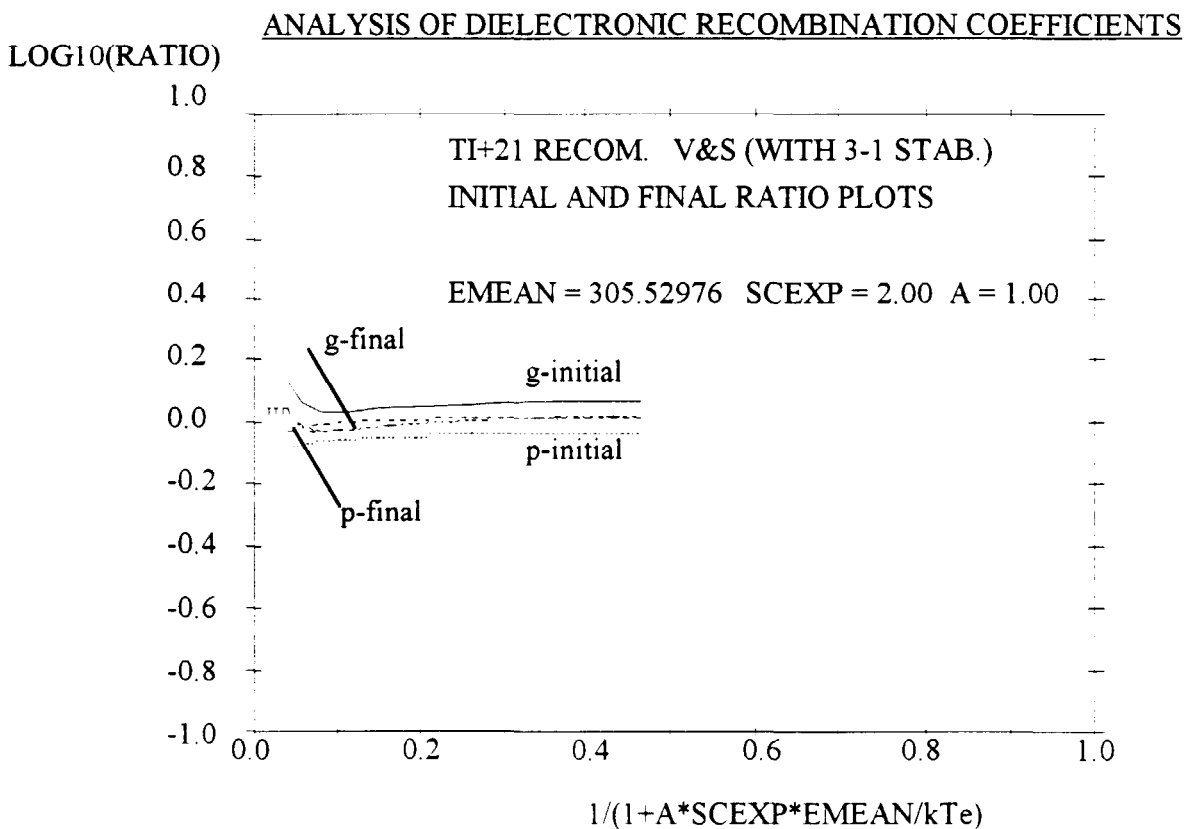


Fig. B.1.f Comparative plot of the ratio of tabular total zero density dielectronic data for $Ti^{+21} + e$ from Vainshtein & Safronova (1978) to approximate forms based on the Burgess General formula (g) and the Burgess general program (p). The data is for the 1s-2p parent transition and includes outer n=3 electron stabilisation. The approximate forms before and after parameter optimisation for the fit are shown. The crosses mark interpolated values and the flat extrapolation is noted.

The product of the data examination and verification is source data interpolated to preferred temperatures together with parameters of the best approximate form fit for storage in the database. It should be noted that there are a number of further details in dielectronic fitting including numbers of parent transitions and their grouping for adjustment, recombination from metastable parents and alternative Auger channel cut-offs.

g. The cross-sections we wish to consider here are those relevant to charge exchange spectroscopy using hydrogen or helium isotope fast beams. Also, it is capture by bare nuclei. The situation is similar to the previous two cases, in that it is not only immediate comparative examination of data which is required but also guidance on resolution of a summed up coefficient. Charge exchange data is required at least at nl-resolution for realistic population calculations and preparation of useful derived data. Some important sources give only total or n-resolution data.

ANALYSIS OF CHARGE EXCHANGE CROSS-SECTIONS

LOG10(RATIO)

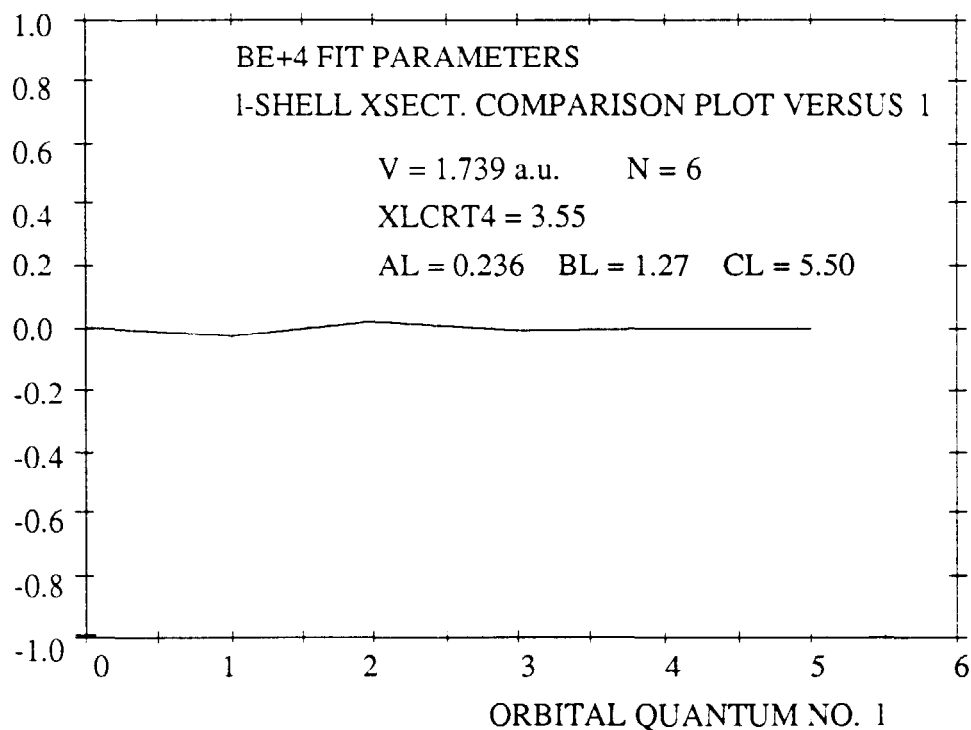


Fig. B.1.g Comparative plot of the ratio of tabular 1-shell charge exchange cross-section capture data into the $n=6$ shell for $Be^{+4} + H$ from Ryufuku (1978) to the approximate form. The approximate form is optimised to the tabular data and is for the collision energy of 75 keV/amu. The fit parameters are $xlcrit4$, al , bl and cl .

Also available data may be rather curtailed in n -shell for an adequate examination of the cascade contributions to observed visible charge exchange spectrum lines. We seek adjustable approximate forms which can represent the total coefficient, the n -shell distribution of the capture, the asymptotic behaviour at high n as a function of collision

energy, and finally, the shape of the l-shell distribution of capture for a given n-shell. In practice, we treat these as three separate stages, using only those required by the source data. Examination of data in this manner has been helpful at JET in building up an appreciation of charge exchange cross-section behaviour and in focussing attention on parts requiring detailed study and calculations. In fact, the product of these detailed calculations in comprehensive fully resolved data has been very impressive in recent years. Comprehensive data in machine readable form obviates much of the need for intensive direct examination of data in the above way, a subject we consider further in section C.

2. Population processing and spectral emission

The resultant of the data verification and conversion steps of the previous section is that prepared fundamental data can be assembled into suitable collections for further use. The variety and purposes to which these can be put in population calculations will be described in the following subsections. A point of principle is that all data collections should be able to be interrogated and sample data extracted, interpolated, fitted, displayed and printed. Thus the processing procedures to be described include such interrogation routines as well as the true collisional radiative population calculations. This section is primarily concerned with population and emissivity calculations where electron collisions are the main reactions although ion collisions are not excluded. There are first of all the interrogation routines on the fundamental data collections. Then there are the collisional radiative population calculations for individual ions and manipulations allowing investigation of an ion's theoretical line emissivities and ratios of emissivities as spectral diagnostics. Finally there are the interrogation routines on the derived database collections obtained from these calculations. Table B.2 summarises the main processing required.

Table B.2

Stored data type	Processing applied
a. Specific ion excitation file	graph and fit coefficient
b. General z recom./ionis.file	extraction from general z file
c. General z excitation file	extraction from general z file
d. Specific z recom.ionis. file	process ACD, SCD and populations
e. Specific z excitation file	process meta./excit. population
f. Specific z excitation file	process line/total power
g. Meta./excit. population file	process line emissivities
h. Ionelec PEC file	graph and fit coefficient
i. Ionelec SXB file	graph and fit coefficient

a. One of the most important data collection types is the *specific ion excitation file*. Such a file applies to a particular ion and identifies for that ion a set of energy levels. The set is complete in the sense that it includes the ground and metastable levels and all excited levels for a low group of principal quantum shells (perhaps only one or two). The data set includes the ionisation potential, energies of the levels, statistical weights and all spontaneous emission coefficients and electron impact rate parameters (for a wide range of temperatures) connecting pairs of levels from the set. The dataset may be in LS or J

resolution. The first routine extracts any individual collisional rate from the file, fits cubic spline and minimax polynomials to it so allowing interpolation, graphing and useful tabulation of it in various forms. Figure B.2.a shows a typical graph. In their simplest form specific ion files include only electron impact excitation collisional data and are targetted at a population calculation which includes spontaneous and electron collision reactions amongst the low level set. However, in it's complete form the *specific ion file* also includes further blocks of proton impact excitation, state selective recombination, ionisation and charge exchange rate coefficients associated with defined parent states. The collection of comprehensive data for such advanced specific ion files is a difficult task and is discussed further in section C.

EXCITATION RATE COEFFICIENT VERSUS TEMPERATURE

File: JETSHP.HELIXE.DATA(BSC80B)

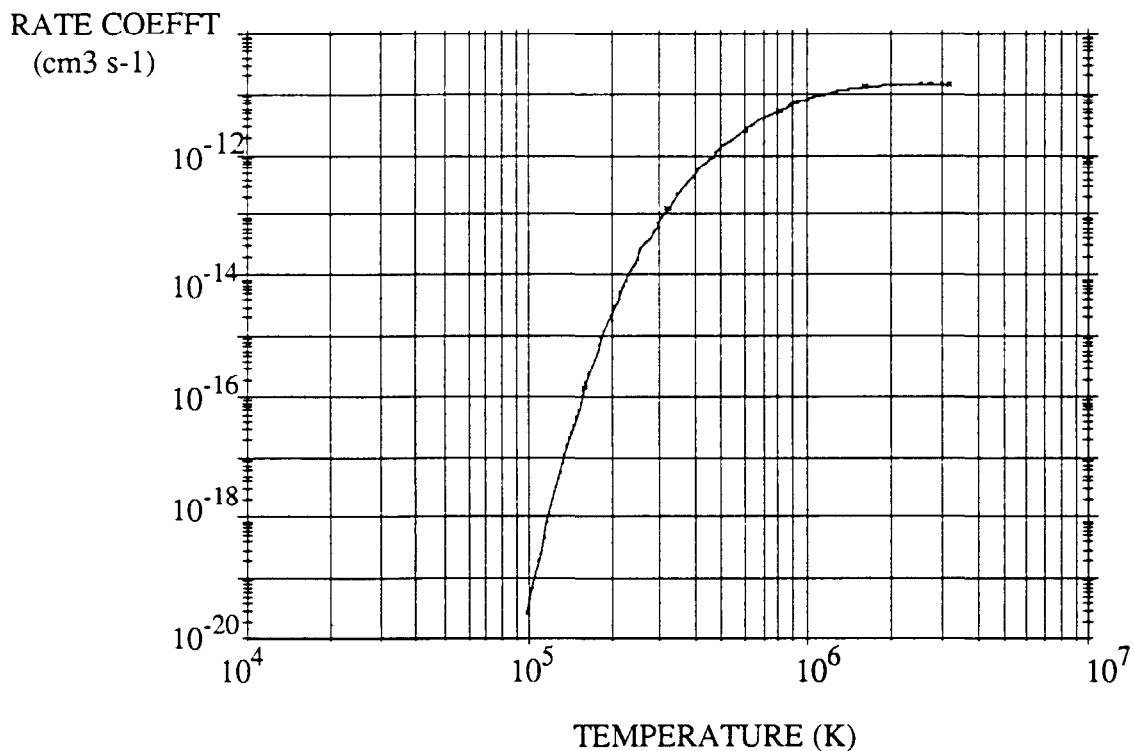


Fig. B.2.a Extracted electron impact excitation rate coefficient data from a specific ion file. The excitation rate coefficient is given for the BIV($1s^2 1S - 1s2s 3S$) transition from original data of Sampson et al. (1983). The solid line is the cubic spline fit, the dashed line a minimax approximation and the crosses are interpolated values at temperatures requested by the interrogation program.

b. Another useful type of fundamental data collection assembles data resulting from the examination and verification of ionisation and recombination data. This is for a number of members of the same isoelectronic sequence. The relevant data are the approximate form fitting parameters for ionisation, radiative recombination and dielectronic recombination separately together with accurate numerical data for the total zero density coefficients at a standard z-scaled set of temperatures. Such a file is called a *general z ionis/recom file*.

The approximate form parameters can be interpolated with z as well as the numerical rate coefficients and so for an intermediate ion provides the tentative decomposition of the coefficients into their state selective components. The routine extracts such data for use by processing codes of type d.

c. Energy level, A-value and electron impact rate parameter data from compatible sources for several members of an isoelectronic sequence can also conveniently be grouped together in a single data set. For this purpose, the rate parameters for a specified transition for the sequence members must be evaluated at the same reduced temperatures.

EXTRACTION FROM A GENERAL Z EXCITATION FILE

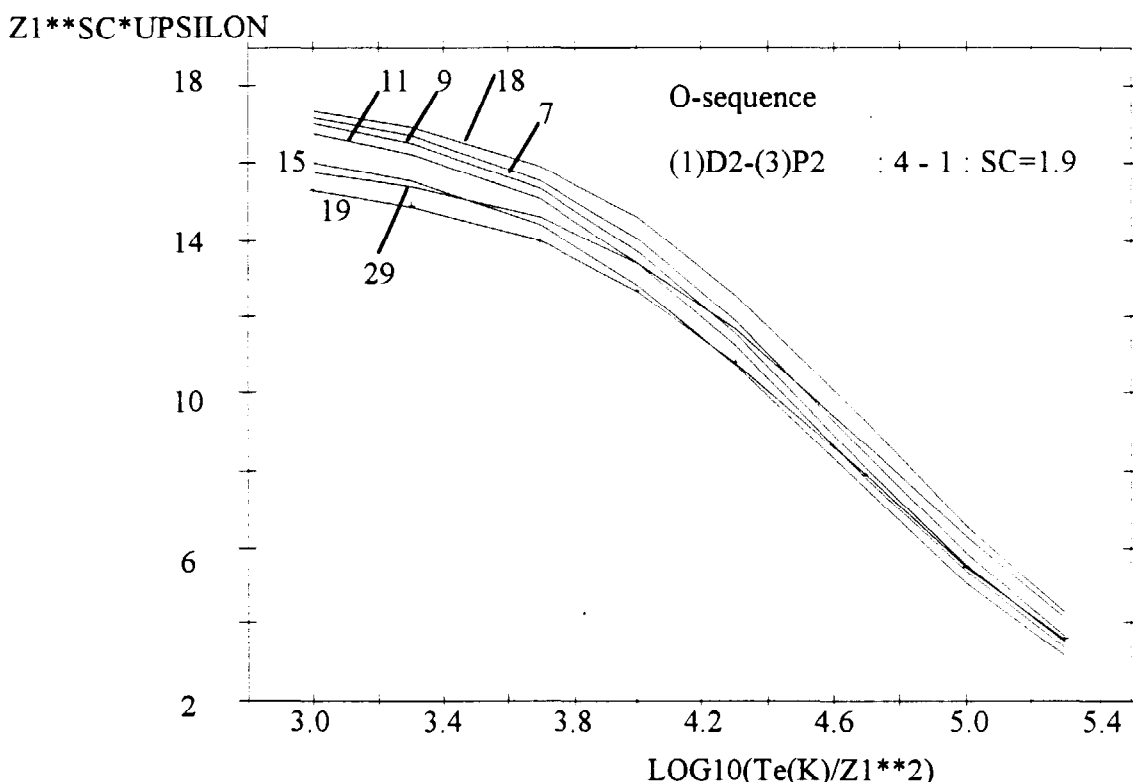


Fig. B.2.c Scaled rate parameters mapped as a function of reduced temperature for a transition in the oxygen isoelectronic sequence. Crosses mark interpolated data for an intermediate ion, in this case a check on one of the tabulated ions. SC is the z scaling parameter which is adjusted to give maximum compression of the set of curves prior to interpolations in z . The curves are labelled by $z1$, the ion charge +1.

Such a collection is called a *general z excitation file*. It is effectively a set of specific ion excitation files reorganised into one datafile representing an isoelectronic sequence. By interpolations in z as well as in temperature, specific ion excitation data can be created easily for an intermediate ion of the sequence for which explicit data is not available. Although there is some reduction in precision in this process, the procedure allows initial studies to be made on new species which can be followed up by detailed fundamental cross-section calculations and tailored specific ion excitation files later, if required. Figure B.2.c illustrates the extraction of rate parameters for a particular transition from general z

excitation file data. By z-scaling of the stored rate parameters and mapping as a function of scaled temperature, it can be seen that quite sound interpolation to an intermediate ion is possible. Practical implementation allows complete *specific ion excitation file* generation from a *general z excitation file*.

Turning now to the populations and emissivities, in practice, a number of variants of population calculations need to be carried out to generate all the derived data at appropriate accuracies and resolution levels for application to the range of situations occurring in spectroscopy and plasma modelling.

d. The first population calculation is required to establish the effective recombination and ionisation coefficients connecting different ionisation stages of an element. These effective coefficients are different from the zero density total coefficients because in a finite density plasma the processes of reionisation of an excited state (following a recombination to it) before cascade to the lowest levels, ionisation from an excited state following excitation from the lowest levels and redistribution of excited populations have important effects. This is especially so for dielectronic recombination even at modest densities. A requirement in addressing this problem is that many excited state populations should be included, perhaps up to the $n=1000$ principal quantum shell, but on the other hand populations of sub-levels of the same principal quantum shell can be grouped. There is a complication in that in a proper generalised collisional radiative viewpoint, the ground and metastable populations of each ionisation stage have to be treated explicitly. We use a *bundle-nS* population model which allows us to distinguish separate parent states of the recombining ion, spin systems and (approximately) lowest metastables of the recombined ion. Such calculations produce generalised collisional radiative recombination coefficients (*acd*), ionisation coefficients (*sca*) and recombination/cascade/bremsstrahlung radiated power coefficients (*prb*) as functions of density and temperature. Usually such calculations are conducted for several members of an isoelectronic sequence at once at a fixed set of reduced temperatures and densities. The basic fundamental data is drawn from an appropriate general z ionis/recom file (see however section C). The structured output data sets are called (*partial*) *isoelectronic master files* and replace the simple stage to stage zero density data often used in the past. We sometimes add the term *partial* when describing fully metastable resolved data as distinct from single ground state data. The bundle-nS model is not at a sufficient resolution to treat low level excited state populations and their emission precisely enough for spectroscopic studies. This is examined in the next subsection. However the coupling to the continuum through high levels is a factor of concern in such low level studies to which the bundle-nS model can contribute. To this end a *condensation* of the bundle-nS model generalised collisional radiative matrix onto a low set of n-shells is simultaneously performed and the resulting condensed matrices form an additional set of coefficients (*cbnm*) which are available to be used in the most sophisticated low level calculations if required. Illustrations of these data are shown in subsection B.4.

e.f. The low level population calculation is the one most pertinent to spectroscopy. It starts with a specific ion file from which the collisional-radiative matrix giving all the connections between the level populations of the specified set can be computed. It is

necessary to take a generalised collisional-radiative viewpoint separating the level set into the *dynamical group* (excited states) and the *quasi-static group* (ground and metastable states). The solution assumes an equilibrium of the excited populations relative to the instantaneous ground and metastable populations. Then any excited population can be expressed in terms of coefficients multiplying the metastable populations (Summers, 1993). The result of the calculation is illustrated in figure B.2.e. Also effective coefficients giving the generalised collisional radiative coefficients between metastables can be obtained. Such metastable cross-coupling coefficient data are stored in isoelectronic master files (*xcd*) and it is convenient in addition to evaluate and store the metastable to ground population ratios (*met*) which occur in a full statistical balance of all the states in the low level set. With the excited populations determined, radiative power from the low level set can be evaluated for the isoelectronic master files (*plt*) also. We perform this as a separate operation (f) using a simplified version of the low level population code. The isoelectronic master files, comprising *acd*, *scd*, *prb*, *plt*, *xcd*, *met*, some extension involving charge transfer driven processes (*ccd*, *prc*) and finally the pure bremsstrahlung radiated power (*pbb*), for each isoelectronic sequence form the derived database for plasma models.

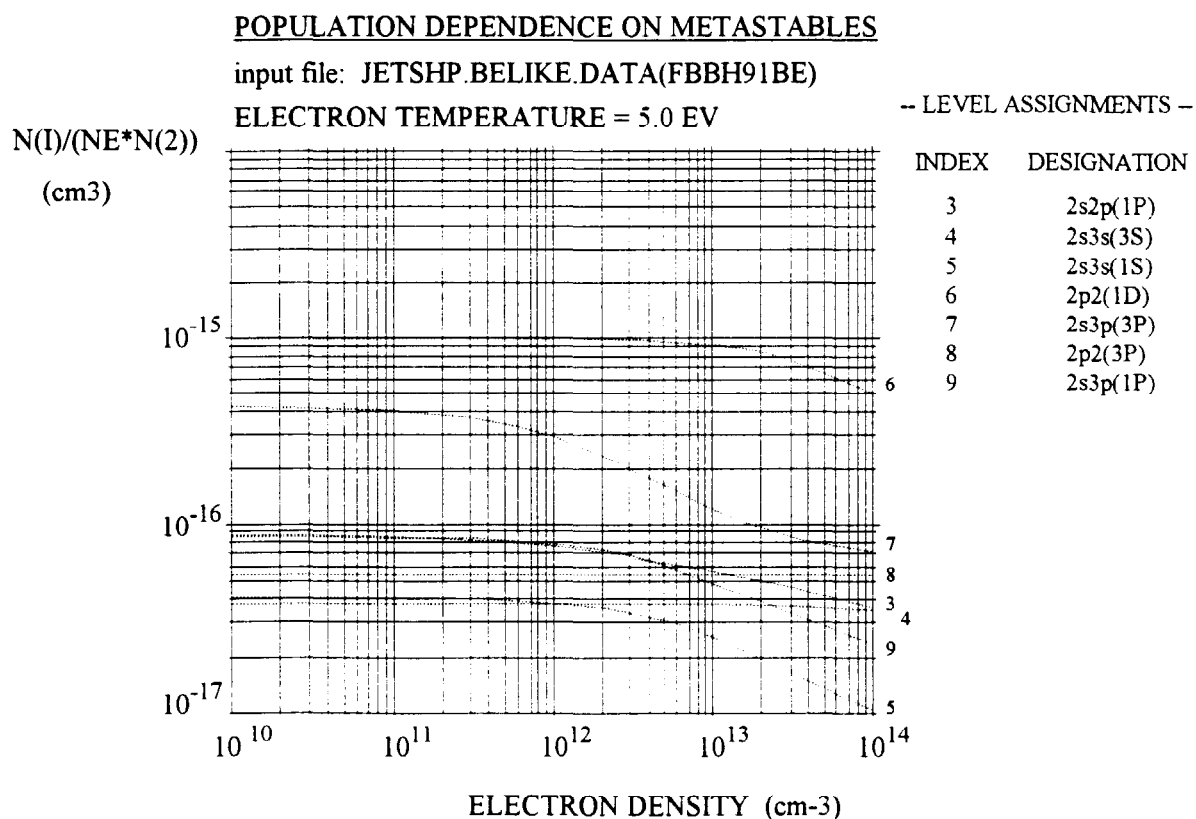


Fig. B.2.e The plot shows the coefficients giving the dependence of the population of some excited states (indexed by I) of neutral beryllium on the 2s2p ³P metastable (indexed 2). There are similar curves giving the part of the dependence on the ground state. The curves are mapped as a function of electron density for a single temperature and show the departure from the flat 'coronal' behaviour at low density.

These datafiles are quite large since they are tabulated both as a function of reduced temperature and density. Turning to spectroscopy, the emissivity of any spectral line originating from a level of the included set in the specific ion file can be evaluated. The emissivity is expressible as a sum of coefficients multiplying each metastable population. When the metastable populations are known from a dynamical plasma model, the individual absolute line emissivities can be computed immediately from these 'photon emissivity coefficients' (*pec*). We find it convenient to store such data as indexed lists for each ion of each element which are easily interrogated by applications. A further derived coefficient relating to a particular spectrum line emission with it's origin in electron impact excitation from a ground or metastable state (directly or indirectly) is the 'photons per ionisation' (*sxb*) (Behringer et al., 1989). The reciprocal of this quantity is the 'photon efficiency'. We also store these in indexed lists. A more advanced technique is appropriate in higher density regions, for low stages of ionisation in cool plasma and for spectrum lines from levels belonging to fairly highly excited n-shells (for example, n=3 or 4) at the top of the specific ion file set. The divertor is such an environment.

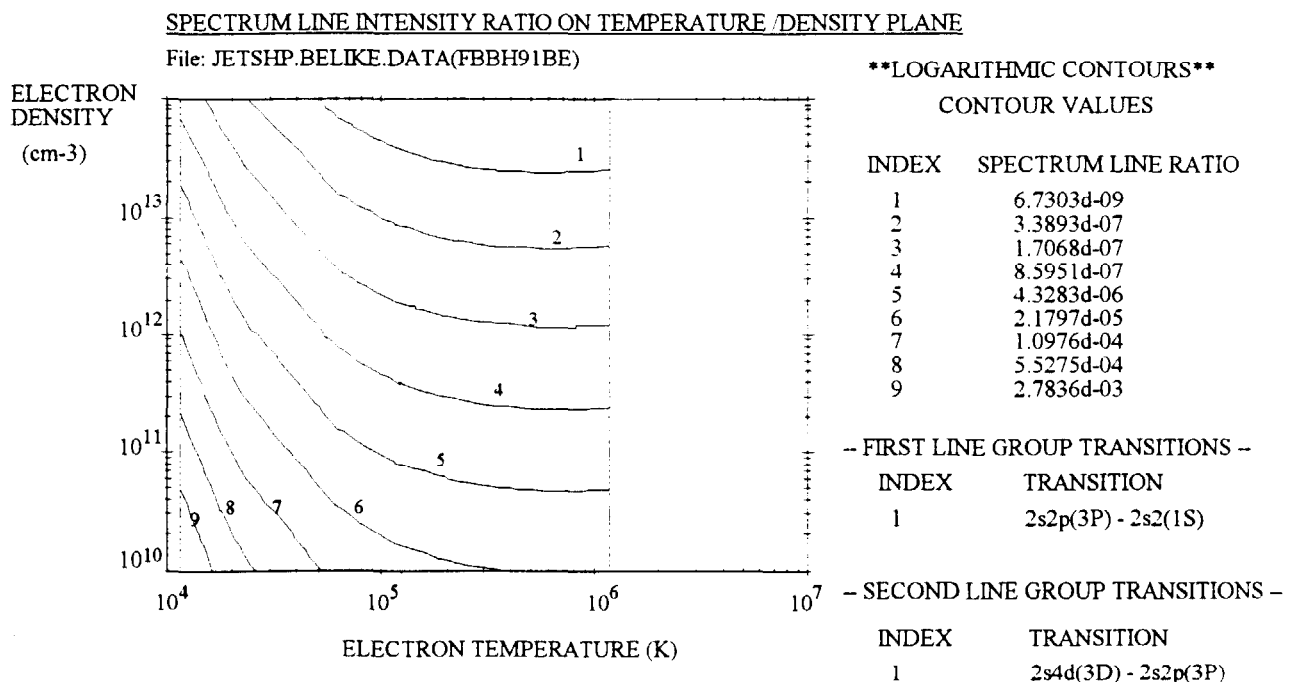


Fig. B.2.g The diagnostic plot of line emissivity ratio on the electron temperature / electron density plane is shown for an arbitrary pair of lines from neutral beryllium. The curvature shows the movement from greater temperature dependence to greater density dependence as the density increases. In this case each line group consists only of a single line. The ground and metastable populations are set at their statistical equilibrium ratio for the plot. The fundamental collision cross-section data originates with Fon et al. (1992)

Then the coupling to higher omitted levels and to the continuum via ionisation or recombination matters. It is here that the condensed matrices (*cbnm*) from the bundle-nS calculations of the previous sub-section can be exploited. The specific ion file collisional radiative matrix can be merged with a projected and expanded *cbnm* matrix to give all the

couplings. The result of such calculations is a regeneration of the isoelectronic master files, but at greater precision together with additional terms in the *pec* data coming from recombination from the various metastables of the parent ion. Such *pec* data are then applicable to emission from ions in any arbitrary state of dynamic ionisation or recombination far from equilibrium. For important species such as beryllium, carbon or oxygen in divertor plasma such elaborations are justified (see section D).

g. Examination of theoretical predictions of spectral line emissivities and emissivity ratios is an important part of diagnostic investigation. In particular, ratios of lines from the same ion which show sensitivity to electron density or temperature are valuable since independent of the ionisation balance. The low level population solution from the previous section provides all the necessary information for such an investigation.

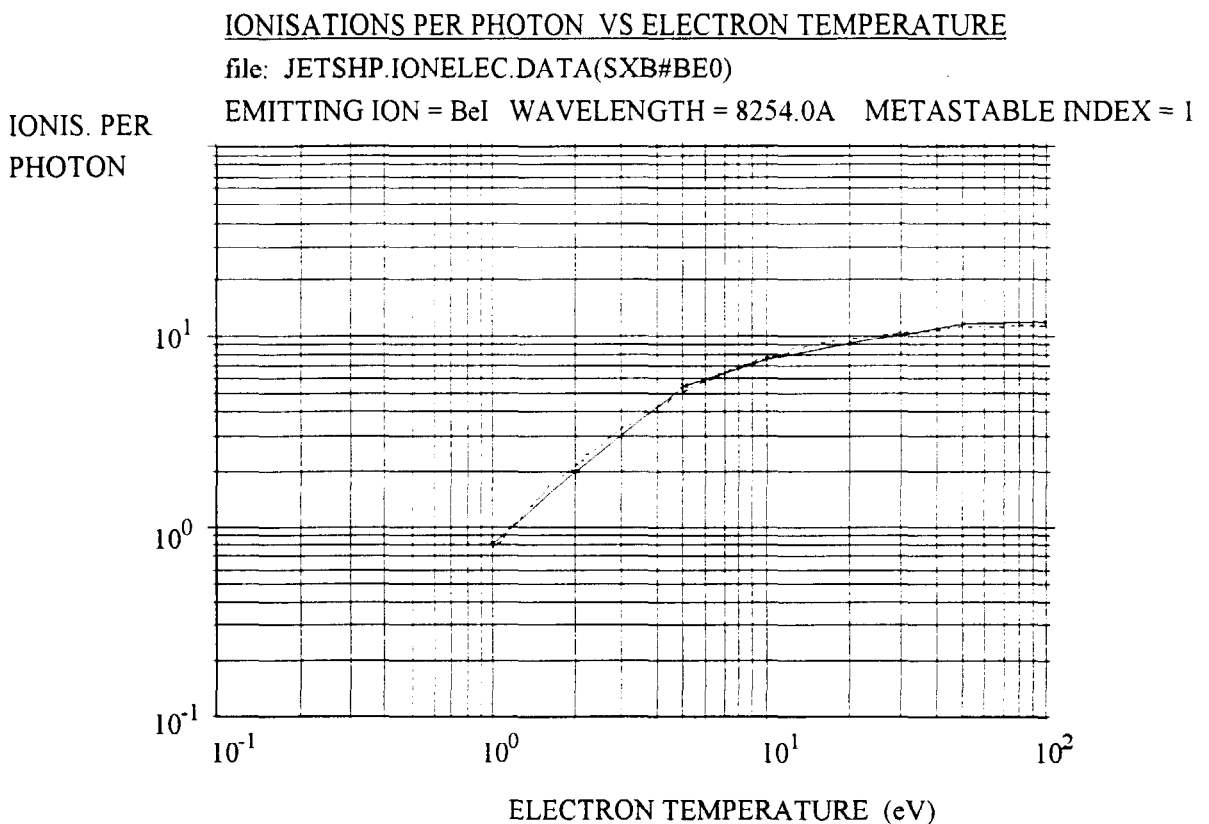


Fig. B.2.i The plot gives the ionisation per photon value for a principal line BeI ($2s3s\ ^1S - 2s2p\ ^1P$) used for influx measurements on neutral beryllium. The solid line is a spline fit used for the main interpolation and the dashed curve is a minimax fit. The data is stored in a derived database and collections accessed by element and charge state. All lines of interest are recorded in an indexed list.

We find it helpful to consider line groups and their ratios rather than pure lines to encompass practical limitations which may occur in spectroscopic observations such as overlapping lines or limiting resolving power. We use a procedure which draws a passing file directly from the low level population calculation, allows line groups to be assembled

arbitrarily for the ion and then maps the line group emissivities or ratios as a function of temperature or density or maps contours in the temperature/density plane. Figure B.2.g shows a typical line ratio contour plot.

h.i. These are the interrogation routines on the *pec* and *sxb* derived data sets respectively. The data are stored in indexed tables as functions of electron density and temperature. The routines satisfy the requirements specified earlier of interpolation, fitting and provision of graphs and tables. Such derived data is used directly in reduction of experimentally observed spectral line photon counts. For each derived data set type, as well as the interactive interrogation routine, a library subroutine is provided for embedding in experimental analysis codes which draws the data by index number from the centrally stored and maintained files. The figure shows the graph resulting from interrogation of an *sxb* file.

3. Charge exchange and beam emission spectroscopy

Analysis of charge exchange spectroscopy and beam emission spectroscopy presents three atomic modelling tasks. These are theoretical calculation of beam attenuation into a plasma, evaluation of the effective emission coefficients for charge exchange spectroscopy lines from the (hydrogenic) recombined receiver ion and evaluation of the emission coefficients of the beam atoms themselves (hydrogen isotopes or helium isotopes). To a first approximation, valid provided the plasma density is sufficiently low, the beam attenuation can be evaluated from the direct losses from the ground state beam atoms only. More complete calculations, necessary at higher densities include the stepwise losses through excited states for which a multilevel population calculation is required.

Table B.3

Data type	Purpose
a. Chexdata file	graph and fit cross-section
b. Ionatom file	graph and fit cross-section
c. Chexdata file	process effective coefficients - l resolved
d. Chexdata file	process effective coefficients - l resolved/scan
e. Chexdata file	process effective coefficients - j resolved
f. Chexdata file	process effective coefficients - j resolved/scan
g. Multiple files	process stopping and beam emission coefficients
h. Ionatom QEF#CX file	graph and fit coefficient
i. Ionatom QEF#STK file	graph and fit coefficient

The charge exchange reaction from fast neutral hydrogen and helium donors can populate highly excited quantum shells of the receiver and it is radiation from such states which give the visible charge exchange lines of convenience for observation. There is substantial redistribution of population by collisions and fields before emission which must be calculated by collisional radiative models (Spence and Summers, 1987). Likewise the calculation of beam emission must be evaluated by collisional radiative models in a Stark basis of states (Boileau et al, 1989). This is because of the large motional Stark electric field present in the frame of the moving beam atoms. The speed of the beam atoms means that ion impact collisions are more

important than electron collisions for stopping and redistribution. Also in charge exchange emission, the near degeneracy of the hydrogen like states ensures that ion impact redistribution is important. The atomic data and analysis structure in this area needs special fundamental database collections and interrogation routines, charge exchange and beam emission collisional radiative population modelling codes and finally derived data collections with their interrogation routines. The requirements are summarised in table B.3 below.

a. The fundamental data collections for charge exchange spectroscopy are of state selective charge exchange cross-sections tabulated as a function of relative collision energy (eV/amu). These are required for both hydrogen and helium donors and for each bare nucleus receiver. Additional collections for excited donor states and for helium-like receivers can also be useful in some investigations.

CHARGE EXCHANGE CROSS SECTION VERSUS ENERGY

file: JETSHP.CHEX#H.DATA(BE4)

PREFERRED DATA - BLOCK 4 PRINC. QUANT. NO. N=5

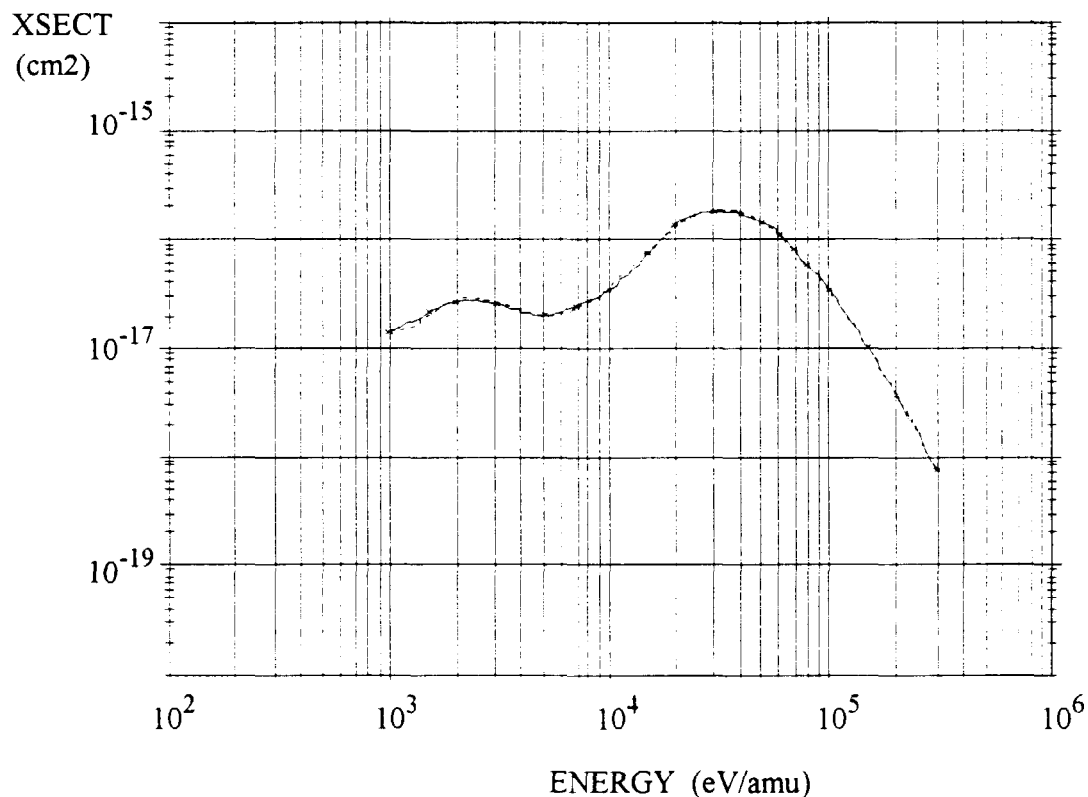


Fig. B.3.a The plot shows data extracted from the fundamental state selective charge exchange database for $\text{Be}^{+4} + \text{H}$. Data collections are held for each fully stripped impurity ion in up to four approximations (usually of different theoretical origin or principal energy range) and an extended energy range preferred set. Similar collections are held for He donor and for excited donor states.

The data must be stored as cross-sections since the simplification of stationary targets and very fast projectiles, which allowed use of Maxwell averages in the electron collision case.

is not valid. Ideally, the tabulations include the total cross-section, n and l resolved partial cross-sections up to some n -shell and some strategy for extrapolation of partial cross-sections beyond the highest tabulated value. Because of ambiguity in the l -shell behaviour (a situation which is now much improved), at JET we have also parametrically fitted l -shell partial cross-section behaviours and stored the parameters in the data collection (c.f. section B.1). Two types of data extraction from these data collections are required, namely, the cross-sections themselves at interpolated collision energies and then the rate coefficients which are displaced Maxwell averages representing a target particle Maxwellian distribution and a monoenergetic beam donor particle. The interrogation routine follows the usual pattern and an illustration is given in figure B.3.a.

b. The second set of fundamental data collections relate to the needs of beam stopping principally. They are held for each beam species, that is hydrogen and helium, and contain cross-sections for the dominant reactions.

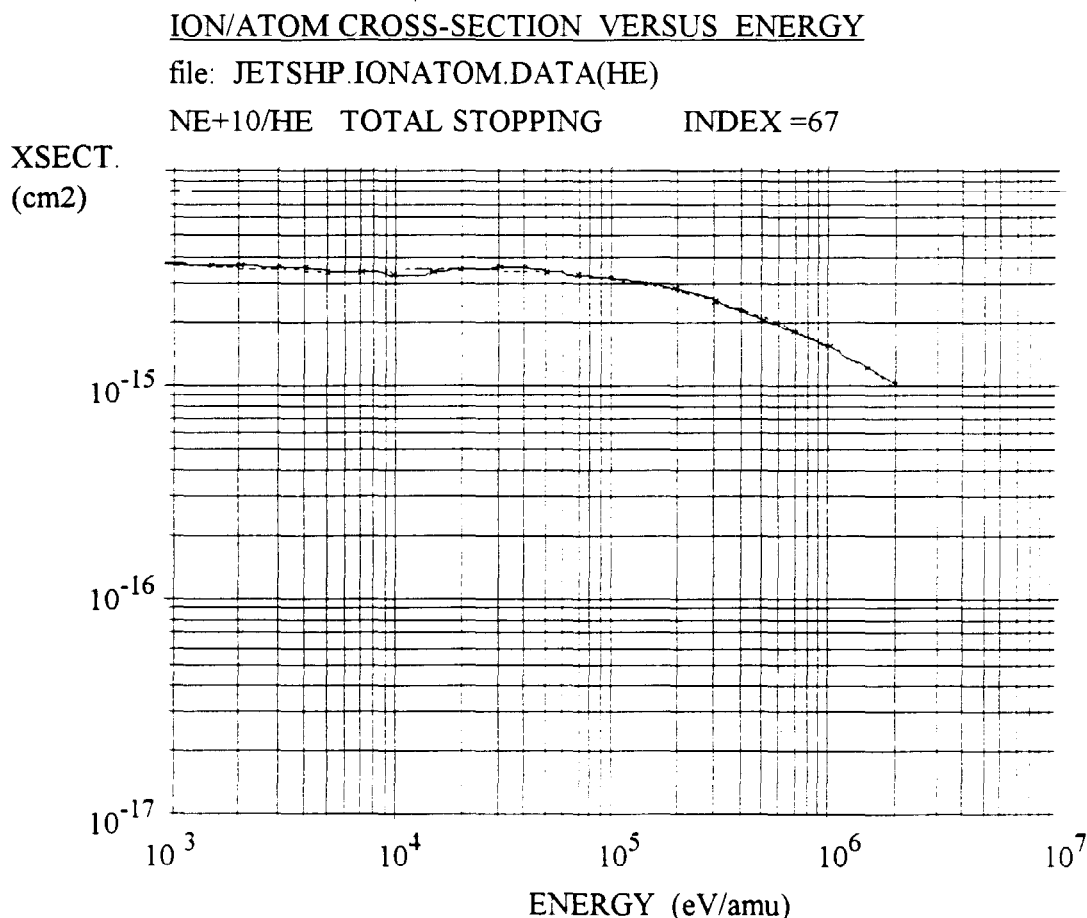


Fig. B.3.b The plot shows data extracted from the fundamental dominant ion / atom data collection in which He is a participant. The data are for the total zero density stopping due to collision of He in it's ground state with Ne^{+10} . The data are selected by index value in a list and are the sum of single ionisation, single charge transfer, double charge transfer and double ionisation including transfer ionisation. These parts are also stored individually under separate indices. The solid line is the spline fit and the dashed line a minimax approximation.

These include ionisation of ground state hydrogen by protons, alpha particles and the bare nuclei of the principal impurities, total charge exchange loss cross-sections to these reactants, excitation cross-sections to the lowest principal quantum shells of hydrogen induced by these reactants etc. Accuracy in these cross-sections is essential for determining beam stopping and so for the consequent charge exchange spectroscopy. We prefer to hold this data in indexed lists which are frequently re-examined and upgraded. Also it is convenient to store some sums over these coefficients in the lists as well since these are useful in particular applications. For example, the total loss cross-section for ground state helium in collision with an alpha particle, composed of single ionisation, single charge transfer, double charge transfer and double ionisation (including transfer ionisation) is provided. We hold a range of comparative data and identify among them preferred data for JET usage.

CHARGE EXCHANGE EMISSION FEATURES

EMITTING ION = CVI DONOR = D(1s)

TI = 3000 EV NI = 2.5×10^{13} CM⁻³ ZE_{EFF} = 2.0

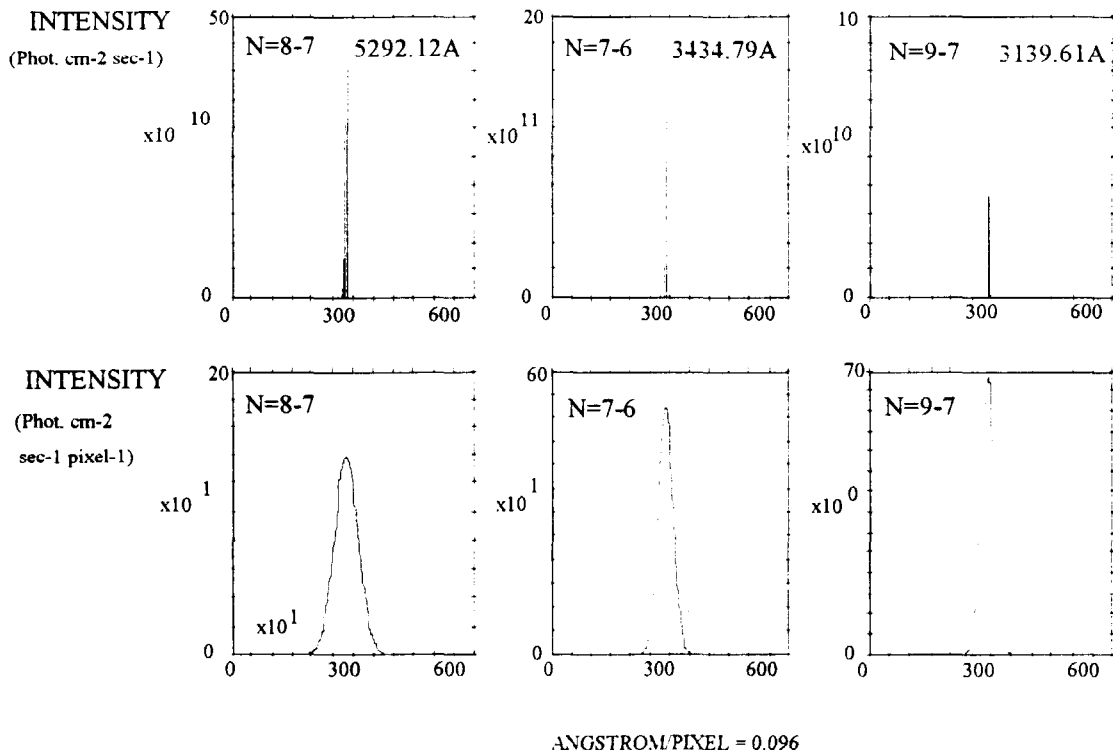


Fig. B.3.c The plots show line of sight emissivities for some charge exchange spectroscopy lines of CVI due to the D beams at JET. Both totals in each line component and the Doppler broadened profiles are shown. The calculation is normalised to an intensity for the whole CVI (n=8-7) line of 10^{12} ph. cm⁻² sec⁻¹.

c,d. In subsections c and d, we are concerned with collisional radiative models in the bundle-nl picture for emission of charge exchange spectroscopy lines principally by hydrogenic ions such as C⁺⁵ although the calculations extend without complication to

lithium-like ions. The capture to the separate nl shells is taken into account and then redistribution by electron and ion collisions within the n-shell. Precise energy levels must be calculated to allow determination the nearly degenerate collision cross-sections correctly. In general there is partial redistribution after capture and before emission. At plasma densities $\leq 10^{14} \text{ cm}^{-3}$, collisional transitions between n-shells is of less importance for the usual charge exchange lines and can be omitted to a good approximation. On the other hand, cascade from high n-shells above the radiating shell is important, since charge transfer cross-sections at fast beam energies fall fairly slowly with principal quantum number ($\sim n^{-3}$). With these assumptions a helpful organisation of the calculation for interpreting charge exchange spectra is possible. Thus if more than one charge exchange line intensity is available originating in different n-shells, then the collisional radiative inversions can be reversed, an emission measure estimated and a comparison of theoretical and experimentally implied n-shell fundamental (before redistribution) capture rate coefficients made. These techniques are used in the interactive routine c. For completion of the calculation, account is taken of the wavelengths of the separate components of the multiplet and transition arrays contributing to the nearly degenerate total line and the Doppler broadening in predicting a final line feature shape. Figure B.3.c illustrates this. However in systematic reduction of the observational data it is the effective emission coefficients for the charge exchange lines which must be prepared as a function of collision energy, ion temperature, ion density, Z effective etc. Multi-parameter arrays for this would be very large and we have preferred to identify a representative set of plasma parameters. Then the one-dimensional variation of the effective emission coefficient with each plasma parameter separately is scanned. This organisation forms the basis of the derived database (*qeff#cx*) and is prepared directly by routine d, a 'scanning' version of the population calculation c. It is to be noted that the effective emission coefficient must be tabulated as a function of the collision energy because the formation of a shifted Maxwellian average over the plasma impurity ion temperature with the beam particle speed must be performed in conjunction with the spectrometer viewing line and beamline geometry to predict final 'cross-section dependent' spectral feature shapes and distortions.

e,f. Sub-sections e and f provide similar routines to c and d but with a more sophisticated collisional radiative model in the bundle-nlj picture.

g. This subsection addresses beam stopping and beam emission in a finite density plasma where secondary collisions with excited states play a role. It is of relevance in the higher density plasmas envisaged in the future. The organisation of the calculations in this part follows closely the steps of section B.2.d and B.2.e. The initial calculation is in the bundle-n approximation but, since it is beam atoms which are of concern, with attention to the more important ion/atom collisions and to drawing the best available data on these from the fundamental database described in B.3.b. The effective stopping coefficients are calculated for each impurity separately and multi-dimensional tables prepared in (*bmstop*) files in the derived database. Condensation of the bundle-n calculations onto a low level set is again performed with the difference that the low level set in this case is in a Stark representation. The augmented low level solution then includes the high level loss pathways and provides a complete picture of the Stark resolved multiplet emission by the beam atoms. This allows

also creation of a derived data collection for the effective emission coefficients (*qef#stk*). A typical Stark emissivity picture for the D α line is shown in figure B.3.g for illustration.

DEUTERIUM BEAM EMISSION STARK FEATURES

TRANSITION = D(N=3-2) CENTRAL WAVELENGTH = 6526.87Å

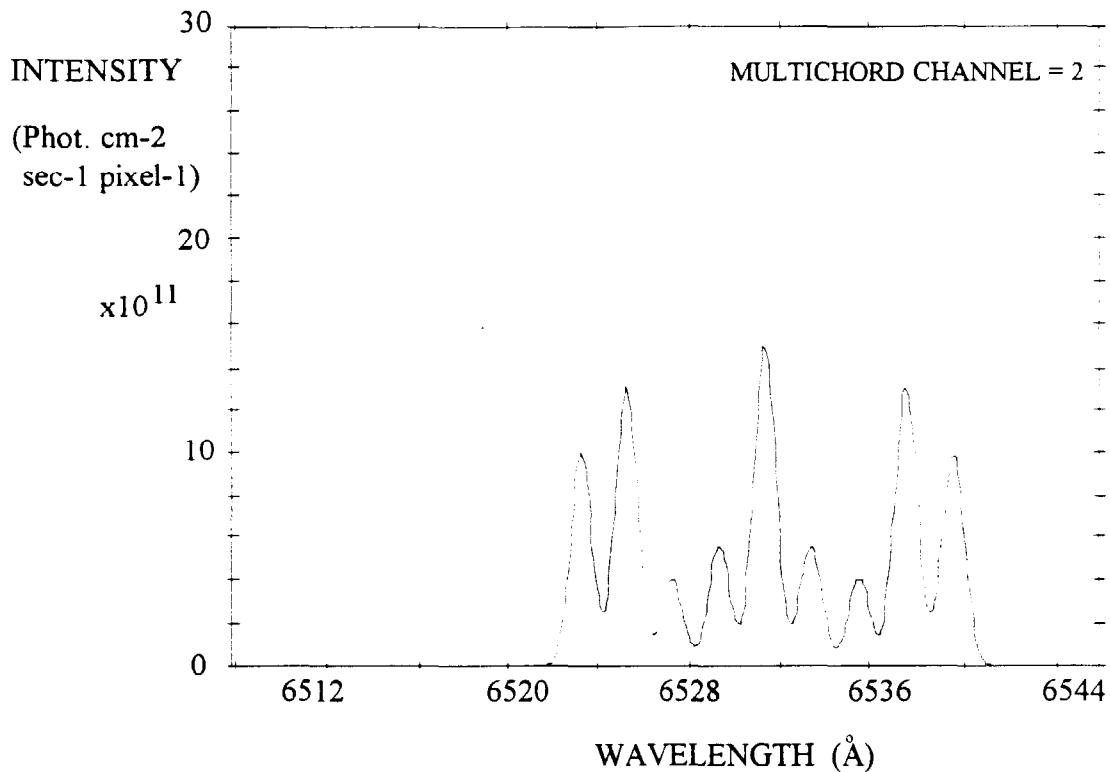


Fig. B.3.g A typical Stark multiplet shape for the D (n=3-2) line emitted by the deuterium beams at JET. The plot corresponds to one of the horizontal array viewing lines and includes corrections for the transmission of π and σ components.

h.i. These are the interrogation routines on the derived data sets for charge exchange emission lines (*qef#cx*) and beam emission lines (*qef#stk*) respectively. The data are stored in indexed tables as functions of plasma parameters. The routines satisfy the requirements specified earlier of interpolation, fitting and provision of graphs and tables. Such derived data is used directly in reduction of experimentally observed spectral line photon counts. For each derived data set type, as well as the interactive interrogation routine, a library subroutine is provided for embedding in experimental analysis codes which draws the data by index number from the centrally stored and maintained files. Figure B.3.h shows the graph resulting from interrogation of a *qef#cx* file.

4. Recombination, ionisation, radiated power and plasma models

The section is concerned with final assembly of all the parts of the derived database for the various particular plasma models under study. In most circumstances the models make use

CX EFFECTIVE EMISSION COEFFICIENTS

file: JETSHP.IONATOM.DATA(QEF#H)

EMITTING ION = CVI TRANSITION N=7-6 DONOR = D(1s)

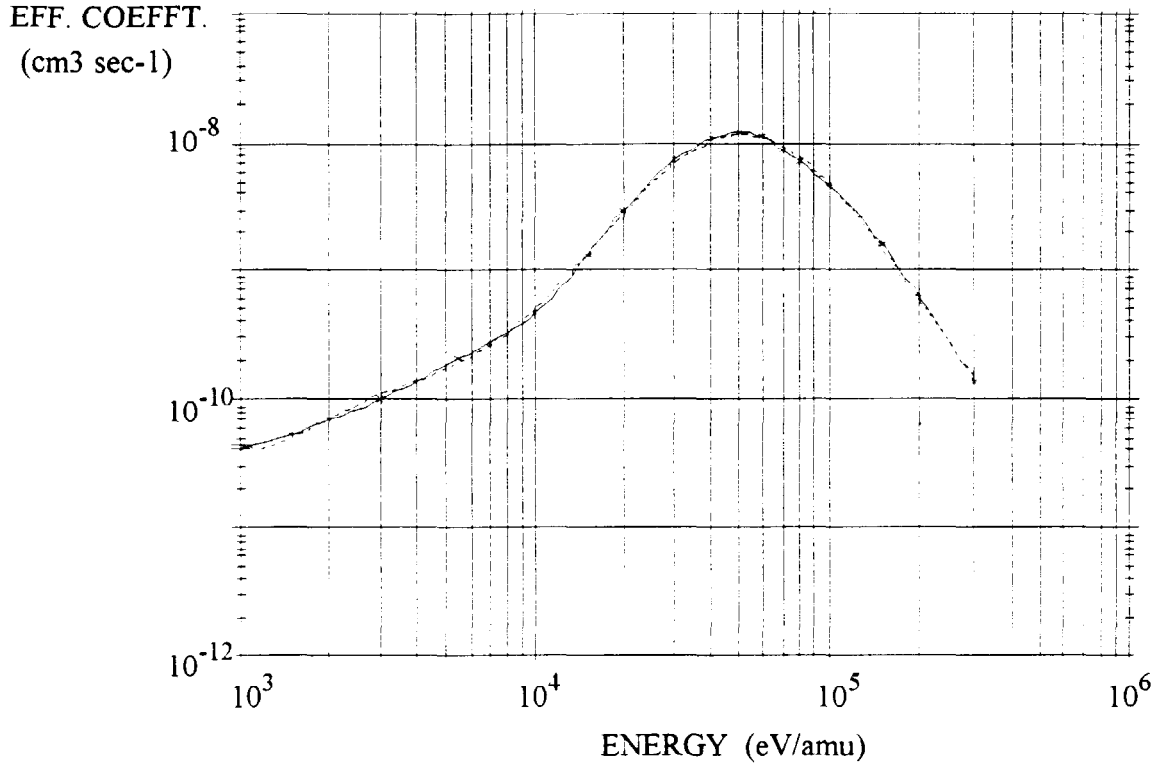


Fig. B.3.h The plot shows the effective mono-energetic emission rate coefficient for the CVI (n=7-6) line extracted by index number from the derived data collection. The data is interpolated from stored one dimensional parameter scans from a standard set of conditions. The solid line is a spline fit to the data at the specified plasma conditions and the dashed curve is a minimax fit.

initially of ionisation and recombination and radiated power functions in a dynamical calculation. Then with primary populations (ground and metastables of each ionisation stage of each elemental species present) determined in the dynamical calculation, the detailed emission in particular spectrum lines and continua are predicted.

Table B.4

Data type	Purpose
a. Iso-electronic sequence	graph and fit coefficient
b. Iso-nuclear sequence	graph and fit coefficient
c. Iso-electronic master file	merge partial iso-electronic files
d. Iso-nuclear master file	extract from iso-elec. master file
e. Iso-nuclear master file	equilibrium ionisation balance
f. Iso-nuclear master file	time-dependent ionisation model

There are three useful operations, namely, reorganisation and interpolation of generalised collisional radiative data from isoelectronic sequence storage to isonuclear storage, merging of *partial* generalised collisional radiative data to the more familiar stage to stage coefficients for the simpler applications and provision of a few basic plasma models. Table B.4 summarises some of these possibilities and we illustrate them in the following subsections.

OXYGEN RECOMBINATION COEFFICIENTS VERSUS TEMPERATURE

file: JETSHP.ACD89#O.DATA

ELECTRON DENSITY = $2.51 \times 10^{13} \text{ CM}^{-3}$

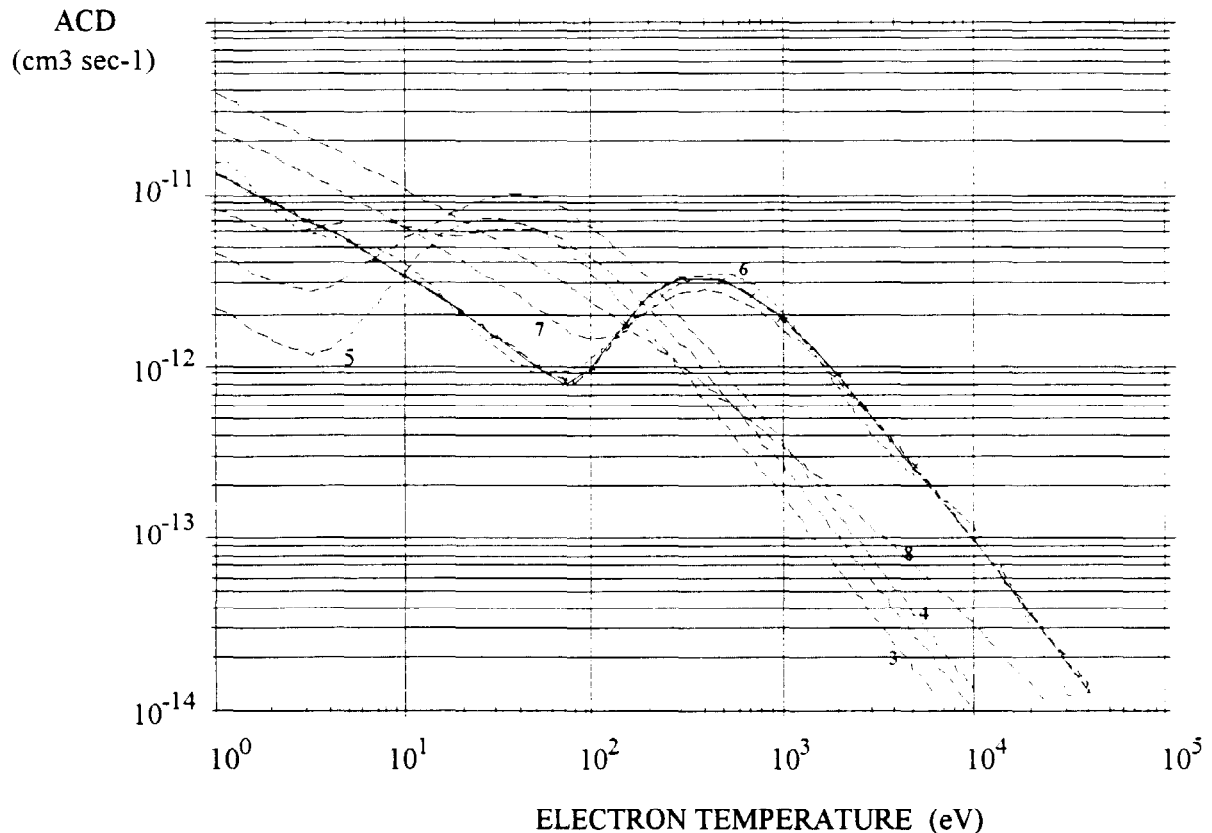


Fig. B.4.b The plot show collisional dielectronic recombination coefficient data extraction from an iso-nuclear master file for oxygen. Data is interpolated to a recombining ion charge $z1 = 6$ and shown as the solid line. The recombination coefficients for other ionisation stages are shown as dashed lines and labelled by the recombining ion charge. The data is extracted for display at a single electron density.

a. As described in earlier sections, extensive generalised collisional radiative data sets, (for example *acd*, *scd* etc.- up to nine types) are combined into isoelectronic sequence collections. Typically these are stored for up to ten ions of the sequence at up to fifteen *z*-scaled (reduced) temperatures and ten *z*-scaled (reduced) densities. We call these *isoelectronic master files* and store them by year number. Significant upgrades are done approximately annually. As well as recent generalised collisional radiative data, older zero density and simpler collisional radiative data are held. The first interrogation routine accesses the isoelectronic master files and returns tabulations and graphs for any ion and

temperature/density pair sets spanned by the data. The graphical display is similar to that of sub-section b below and is not illustrated.

b. Then complete data collections of the same types are assembled for isonuclear sequences, that is for each ion of an element. We call these *isonuclear master files* and have such files for each important element in fusion research. As before they are stored by year number. We have within the collections a baseline data set. This is numerical equivalent to the results of the standard simple empirical formulae often used directly in plasma models. Also it is useful to have available comparative data such as the favoured zero density data used in coronal astrophysics (see for example Arnaud & Rosenflug, 1985). The interrogation routine accesses and displays these data and an example is shown in figure B.4.b.

c. The routine addresses the merging of the generalised collisional radiative *partial isoelectronic master files* by assuming specific values for the ratios of the metastable populations of an ionisation stage to the total population of the stage. The step is necessary to support modelling which uses the stage to stage view. We use the equilibrium metastable fractions for this step stored in *met* files.

d. Conversion from isoelectronic storage in isoelectronic master files to isonuclear storage in isonuclear master files is achieved in this step. Since isoelectronic storage is in terms of reduced temperatures and densities this requires substantial multi-dimensional interpolation.

CARBON IONISATION BALANCE - PROJECTION DATA

file: JETXLE.XCD#C.RDATA

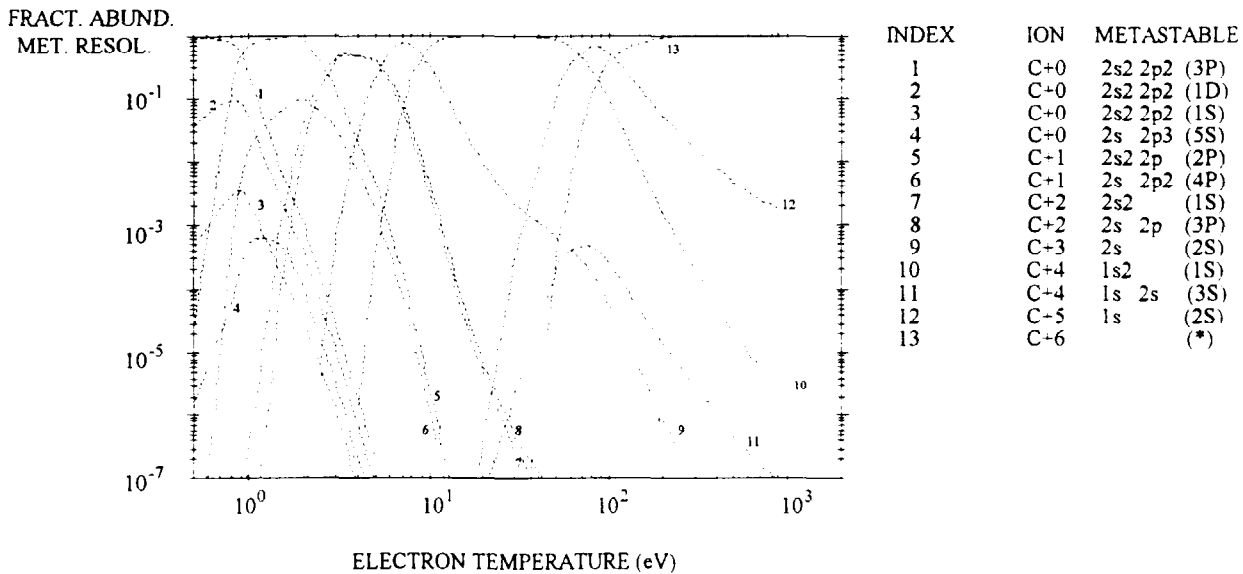


Fig. B.4.f.1 The plot shows ionisation equilibrium fractional abundances for all the metastables states of carbon evaluated using the generalised collisional radiative coefficients. The balance is at the electron density 10^{13} cm^{-3} .

e. Turning to plasma models, the simplest situation is the equilibrium ionisation balance. This is often approached in the high temperature core of plasmas and is nearly always used in initial efforts to analysis emission phenomena. We provide an interactive code for this case. It begins by drawing data for a specified year number from the isonuclear master files of each type at a set of temperature / density pairs of choice. If data of a particular type for the requested year is not available then a default year number is used. The extraction subroutines which perform this task are needed in all the more complex plasma models and are conveniently placed in a centralised subroutine library. For the most thorough studies it is metastable resolved master files which are used. In both metastable resolved and unresolved cases the balance is straightforward and it is again convenient to provide a subroutine version of it in the library. The procedure continues to evaluate radiated power and the contributions to it, mean charge state and ionisation potential energy etc. These are the more global parameters of general relevance. The further operations are then to do with spectroscopic predictions. Emissivity coefficient (*pec*) files are accessed so that the absolute emissivities (per atom of the species in any ionisation stage) can be predicted. The contributions of excitation from the different metastable states, recombination from different parent metastable states, inner shell ionisation contributions and charge exchange contributions can all be included depending on the completeness of the *pec* files.

CARBON EQUILIBRIUM RADIATED POWER - PROJECTION DATA

file: JETXLE.XCD92#C.RDATA

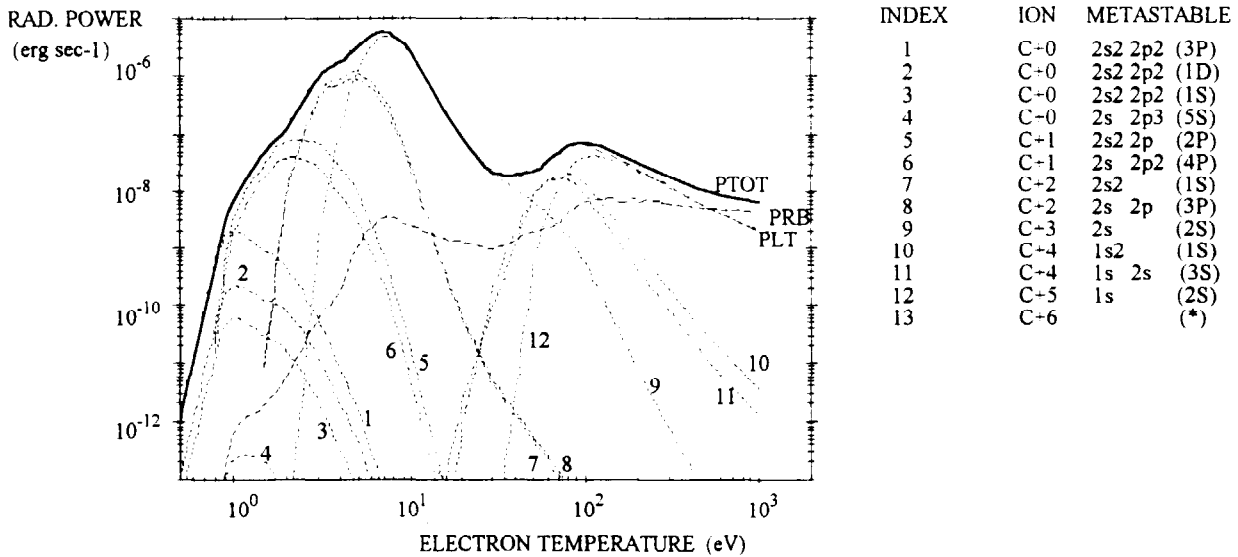


Fig. B.4.f.2 The plot shows the total equilibrium radiated power (PTOT) for carbon, the separation into recombination + bremsstrahlung power (PRB) and total line power (PLT) and the line power contributions from each of the metastables states evaluated using the generalised collisional radiative coefficients. The balance is at the electron density 10^{+13} cm^{-3} .

This in turn depends on the completeness of the *specific ion files* and the inclusions in the calculation B.2.e. The combination of the emissivity coefficient for a particular line with the ionisation balance is sometimes called the $G(\text{Te})$ function for the line. This is a term used in coronal analysis where it is the theoretical input to the integral inversion problem for the differential emission measure. A similarly defined $G(\text{Te})$ function is useful in fusion but

without the assumption of solar elemental abundances. It is the immediate quantity required for experimental data reduction within the assumption of ionisation balance. The procedure displays $G(\text{Te})$ functions as required. For some purposes, it is useful to do automatic and complete $G(\text{Te})$ generation for all the lines of an ion at a wide range of temperatures for fixed pressure for storage in large look-up tables. We provide a separate routine for this purpose.

CARBON G(TE) FUNCTIONS - PROJECTION DATA

file: JETXLE.XCD92#C.RDATA

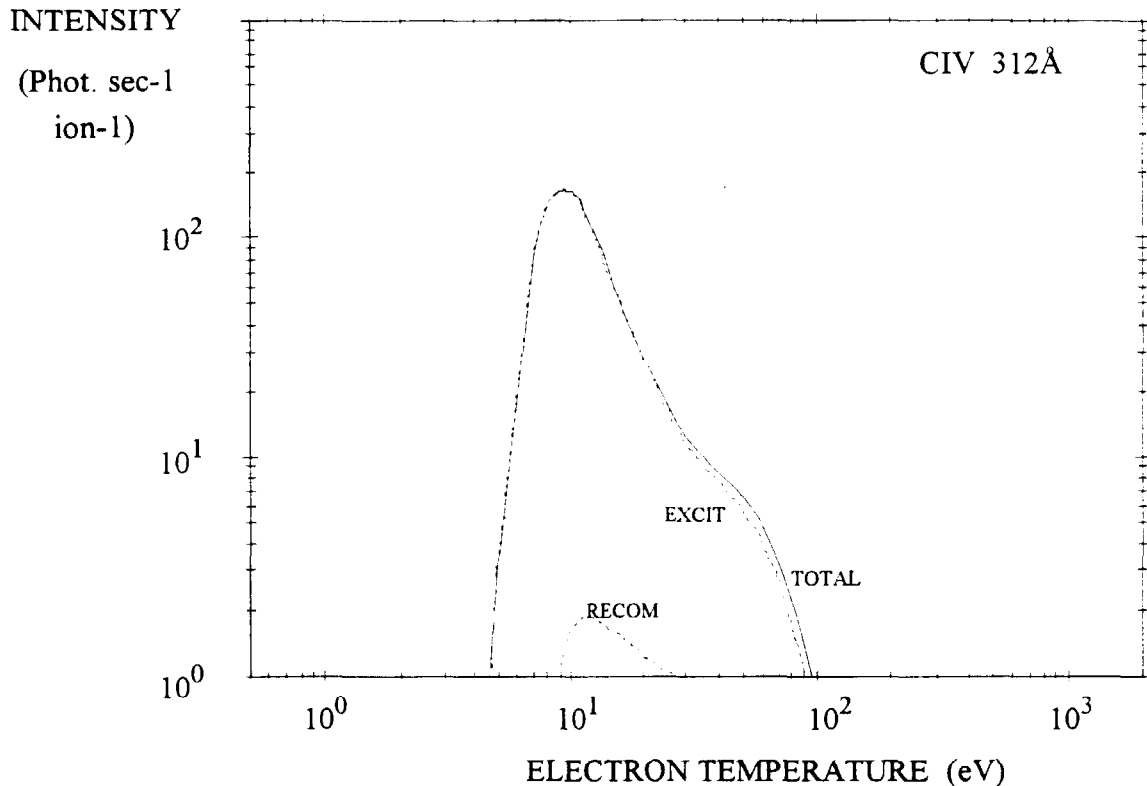


Fig. B.4.f.3 The plot shows the equilibrium $G(\text{Te})$ function for the CIV (2s-2p) resonance line. It is evaluated using the ionisation equilibrium fractional abundances including all the metastables states of carbon and with projected high level and recombination parts included in the excited population. The contributions from recombination and excitation are shown as dashed lines. The $G(\text{Te})$ function omits the $N(\text{C})/N(\text{H})$ and $N(\text{H})/N(\text{e})$ factors usually included in the solar coronal definition. The balance is at the electron density 10^{+13} cm^{-3} .

f. Our final procedure is a time dependent ionisation model, that is of a species with some initial distribution of ionisation stage ground and metastable populations evolving in a plasma of specified electron temperature, electron density and possible neutral hydrogen density. The temperatures and densities can vary with time. This model can equally well provide spatial distributions of populations in an influx picture. From the solution for the time dependent metastable populations, all the equivalent power (transient energy emission

and equilibrium power) and absolute emissivity predictions to those of sub-section e can be made and displayed. Our final illustrations in figures B.4.f.1, B.4.f.2 and B.4.f.3 are for carbon using this procedure, but giving the final equilibrium solution at infinite time in fixed temperature and density. It is therefore the same as provided by e above. Atomic data supply to more advanced diffusion models follows the same pattern as in the procedures e and f. However, we do not provide these models themselves as part of our atomic data and analysis structure.

C. Background support

It is inevitable, that following successful penetration of more comprehensive atomic population and emission modelling for light species such as helium, beryllium carbon and oxygen into spectral interpretation and plasma models, there is a interest in similar sophistication for heavier species. These may include medium weight metals such as iron and nickel and then heavier species such as molybdenum. Also the interest in these species will be more in their role close to the plasma edge and in divertors than in their more familiar role in the hot core. In complex ions with more than one open shell, or when the detailed emission from excited principal quantum shells is of interest, there is a very rapid increase in the total number of levels which must be included in population equations and in the size of the generalised collisional radiative matrices. Also the more accurate atomic collision data are themselves produced by very large interlinked codes including many complex target states (see for example Badnell et al, 1993). In the effort to bring this data into use, we have found it helpful to give quite detailed attention to the interface between the important collision codes and the fundamental database, specific ion files and so on of the atomic data and analysis structure. We have addressed this issue for dielectronic data, excitation cross-section data and charge exchange data and have found it helpful to begin at the atomic data and analysis structure end and the needs of the generalised collisional radiative models. We prepare detailed prescriptions of the required parameters, data formatting and layout, units, variable identifications and descriptions for the target fundamental datasets. A data format prescriptions is called an *adf*. After some iterations with the workers operating the primary collision code, the *adf* is finalised and postprocessing routines tailored to write output directly to the *adf* specification. These files can be transferred electronically and enter into immediate use. An additional issue in some of the usages of very large data files is a progressive approach to condensation and bundling of data, a subject touched upon in earlier parts of this work.

Finally, it is usually necessary to have immediate, 'on site', access to robust, but perhaps more modest accuracy cross-section codes which can provide 'data fill-in'.

D. Conclusions

There is a continuing use and need of fundamental atomic collision data for the activities and developments on current large fusion machines. However the atomic data need for spectroscopy is only partly for new fundamental data. It is equally important that data production and presentation is appropriate for the present usages. Most spectral studies require

collisional radiative calculations and therefore quite large, complete collections of fundamental atomic rate coefficient data. This has to be in direct computer usable form.

We have described a organisation for atomic data and analysis consisting of a fundamental database, generalised collisional radiative calculations and a derived database which can meet some of these needs. A description has been given of how parts of this organisation are implemented and illustrations given of results. At JET, such a system has been effective in closing the gap between experimental spectroscopic measurements and theoretical atomic calculations. This has allowed an enhanced level of interpretation to take place.

For the future, it will be important to ensure that the large scale fundamental cross-section calculations generate output to precise formats suited to the atomic data and analysis structures. It is only in this way that the fundamental efforts and volume of data will be able to be exploited effectively in fusion.

There has been no discussion of molecular data in this work inspite of it's appearance in the title. Collisional-radiative studies of molecular populations and emission are at present in their infancy. Nonetheless, the increasing availability of sophisticated collision cross-section calculations for diatomics makes progress in this area likely in the near future.

Acknowledgements

In the study and development of atomic modelling for spectroscopy at JET Joint Undertaking, we have been grateful for many profitable discussions and much code development to Mr. W. Dickson, Dr. J. Spence, Dr. P. Briden, Dr. L. Horton, Dr. R. W. P. McWhirter and Dr. J. Lang.

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