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Report



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EMISSION FROM PLASMAS
II. The Organisation and Use of Basic Atomic Data

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CULHAM LABORATORY
Abingdon, Oxfordshire
1985

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THE CALCULATION OF SPECTRAL LINE EMISSION FROM PLASMA

II. The Organisation and Use of Basic Atomic Data

by

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ABSTRACT

A set of computer codes has been developed for verification, display and conversion of atomic cross-section and rate data drawn from the literature. Data for isoelectronic sequence members are prepared as rates in standard forms over standard reduced parameter ranges. Regularities in this 'general z' representative data are exploited to infer rates for arbitrary ions and to generate input for spectral prediction codes. The H, He, Li, Be and Na-like isoelectronic sequences have been incorporated in the database. The operation of the procedures is illustrated.

Work supported by an EMR grant from the UKAEA Culham Laboratory

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July 1985

ISBN:0-85311-136-7

1. INTRODUCTION

This paper is the second in a series of papers describing computational procedures for the analysis of atomic spectra from laboratory fusion plasmas. In the first paper of the series (Gordon, Summers and Tully, 1982), known as paper I, techniques were described for calculating spectral emission, ion populations and ionization stage abundances for impurities in thermal plasmas. These were developed into a collection of computer codes known as COPASE which could be applied to a wide range of physical conditions in both equilibrium and non-equilibrium plasmas.

A necessary preliminary to the application of these codes to the details of the emission of a particular impurity is the preparation of a suitable set of basic collision excitation coefficients, spontaneous emission coefficients and energy levels for that ion. The completeness and precision of the predictions depends absolutely on the quality of this fundamental data.

A number of problems arise in the creation of such a data collection. Firstly we have special interest in application to thermonuclear plasmas, such as the investigation of impurity spectral emission from large tokamak devices such as DITE and JET. The range of impurity elements and their respective ions which can occur is large. Besides including common low Z-elements such as carbon and oxygen, many metals from the first and second long periods are also important. By comparison the number of ions for which atomic data (both experimental and theoretical) of sufficient accuracy is available, is much smaller and is sparsely distributed throughout the literature. Secondly, the full data of reaction matrices etc resulting from each detailed cross-section calculation which is required for the full description of the cross section and its resonance structure is over complex for our present purposes. For thermal plasmas it is usually the Maxwellian integrated rate coefficient which matters. Finally, for population calculation, a complete or fairly complete set of transition rates amongst the various levels is usually required. This raises questions of consistency of data from mixed sources and of having available simple approximations to fill in gaps in higher accuracy data.

In the light of these comments, we have adopted two approaches, namely

- (a) the collection of data of the best available quality for specific ions of special importance;
- (b) the assembly of interpolable data for whole isoelectronic sequences from which values for a specific member can be derived rapidly but with some reduction in precision compared with the data derived from (a).

It is the contention of this paper that such 'general z' data, as described in (b), can be prepared and that with care in the organisation and interpolation any resulting loss of accuracy of the data can be minimised. In the present paper data has been compiled for the H-I, He-I, Li-I, Be-I and Na-I isoelectronic sequences, however the overall structure of the suite of programs is such that it can be employed for any isoelectronic sequence where suitable data is available. The assembly of data, its upgrading and revision will be continuing tasks as new data becomes available.

The computer codes which are used to assemble and organise the data feature graphical display and interactive computer dialogue which allow both verification of raw data and optimising interpolation, extrapolation and quadratures over the data. They have proved useful in their own right for atomic data manipulation and have been combined into a comprehensive data handling computer package.

In section 2, the broad behaviour of the various atomic coefficients required for the data base are described. In section 3, the numerical techniques used to represent the data and extend it in parameter space are summarised. The detailed description is given in appendix A. The computer programs are described in section 4. In section 5 the sources of data currently employed and the present state of the data collection are described. Finally, in section 6, some case studies are presented which are of particular interest to interpreting impurity spectral emission from tokamak devices.

2. THE BEHAVIOUR OF ATOMIC RATES

Data tabulated in the literature is given in a large variety of approximations and forms and therefore inevitably for a given ion under study, it is often the case that it is the one for which the atomic data is incomplete, or presented for a range of energies out with the range of current interest, or requires conversion. It is therefore helpful to develop techniques to allow interpolation and in some cases extrapolation of atomic data along a given isoelectronic sequence where the data for some of the members is available. To achieve this while keeping any loss of accuracy to a minimum, it is necessary to be aware of the broad theoretical form of the relevant coefficients and especially of their asymptotic behaviour.

To this end, we now review the dominant behaviour of transition energies, A-values and collision cross-sections.

2.1 Transition Energies

Transition energies are required for the COPASE suite of programs for the evaluation of transition rates in the rate equations for the populations of ionic levels. In this case spectroscopic accuracy is not required, as would be essential in the case of line identification studies.

The present study spans from low charge states for which the energies are dominated by the correlation terms of the Hamiltonian to highly charged states for which relativistic effects are prominent.

For an ion of charge z , the ionization potential I_i with the ion in level of principal quantum number n_i can be expanded as

$$\frac{I_i}{I_H} = \frac{z_1^2}{n_i^2} + a_0 z_1 + b_0 z_1^4 + \dots \quad (1)$$

Likewise, for an ion of charge z , the transition energy ΔE_{ij} between levels of principal quantum number n_i and n_j can be expanded as

$$\frac{\Delta E_{ij}}{I_H} = z_1^2 \left(\frac{1}{n_j^2} + \frac{1}{n_j^2} \right) + a_0 z_1 + b_0 z_1^4 + \dots \quad (2)$$

We use the following notation conventions: z is the ion charge, z_0 the nuclear charge and $z_1 = z+1$. a_0 and b_0 are the coefficients of the leading terms of the correlation and relativistic corrections respectively.

2.2 A-Values

An important aspect of the study of the atomic physics of plasmas is the exploitation of the sensitivity of metastable level populations to plasma conditions. Therefore, as well as being concerned with the emission of resonance lines with electric dipole A-values, we cannot ignore the importance of the weak radiative decay of metastables associated variously with A-values for non-dipole, LS breakdown, two photon decay, etc. The A-values vary smoothly with ion charge, or effective ion charge and behave asymptotically as some power of the charge characteristic of the particular type of radiative transition. A-values are also sensitive to the transition energy.

For electric dipole transitions the alternative forms of absorption oscillator strengths, $f_{i \rightarrow j}$, and line strengths, S_{ij} , are also used and may exhibit simpler behaviour with z than the A-values. In the present work only A-values are employed in the final data collection. We have the following relations

$$A_{j \rightarrow i} = \frac{\alpha^4 c}{2a_0} \left(\frac{\Delta E_{ij}}{I_H} \right)^2 \frac{\omega_i}{\omega_j} f_{i \rightarrow j} = \frac{\alpha^4 c}{6a_0} \left(\frac{\Delta E_{ij}}{I_H} \right)^3 \frac{1}{\omega_j} S_{ij} \quad (3)$$

The ω_i and ω_j are statistical weights. Other notation is conventional.

Generally we can write

$$A = a_0 z_1^{b_0} + \dots \quad (4)$$

where a_0 and b_0 are only weakly dependent on z_1 along an isoelectronic sequence and are characteristic of the particular type of transition. Note however that the effective power b_0 can change significantly on moving from correlation to relativistic dominated atomic structure regions.

2.3 Electron Collisional Cross-Sections and Rates

As described in Paper I, the COPASE suite of programs calculate directly proton induced collision rates for quadrupole transitions between nearly degenerate fine structure levels. These are only ones for which proton collisions are important (ignoring highly excited states involved in recombination and cascade events). For all other transitions the electron collision rates are much more important than the proton rates. It is the assembly of the electron collision rates which we are concerned with here.

For our general z data compilation, we have chosen to express all collisional data in terms of the collisional rate parameter, γ , specified at a standard set of reduced electron temperatures. We define the reduced temperature θ_e in terms of the electron temperature as

$$\theta_e = \frac{T_e}{z_1^2} \quad (5)$$

It is evident in practice that a fixed set of reduced temperatures can be chosen which spans all relevant actual electron temperatures for ions along an isoelectronic sequence. For a specified transition, γ varies smoothly with z_1 along an isoelectronic sequence at fixed reduced temperature θ_e , and at fixed z_1 it varies smoothly with θ_e .

Collision cross-section data is provided in published works in various equivalent forms, namely excitation cross-sections, $Q_{i \rightarrow j}$ (with $I_i > I_j$ where the I 's are ionisation potentials), de-excitation cross-sections, $Q_{j \rightarrow i}$, collision strengths, Ω_{ij} , z -scaled collision strengths, $z^2 \Omega_{ij}$ and effective Gaunt factors,

\bar{g}_{ij} , as tabulated functions of colliding electron energy in various forms, namely, energy with ion in initial state, E_i , initial wave number, k_i , energy with ion in final state, E_j , final wave number, k_j , parameter, X , and threshold parameter, ϵ . If the transition energy is ΔE_{ij} , I_H the ionisation energy of hydrogen in its ground state and a_0 the Bohr radius, then we have the following relations

$$\Delta E_{ij} = I_i - I_j = E_i - E_j$$

$$\frac{E_i}{I_H} = \frac{\Delta E_{ij} + E_j}{I_H} = k_i^2 a_0^2 = k_j^2 a_0^2 + \frac{\Delta E_{ij}}{I_H} \quad (6)$$

$$\frac{E_i}{\Delta E_{ij}} = X = 1 + \epsilon$$

$$\frac{E_i \omega_i Q_{i \rightarrow j}}{I_H \pi a_0^2} = \frac{E_j \omega_j Q_{j \rightarrow i}}{I_H \pi a_0^2} = \Omega_{ij} = \frac{1}{z_{\text{eff}}^2} (z^2 \Omega_{ij}) \quad (7)$$

$$= \frac{8\pi}{\sqrt{3}} \frac{I_H}{\Delta E_{ij}} \omega_i f_{i \rightarrow j} \bar{g}_{ij}$$

Ω , X and ϵ are dimensionless quantities and Ω is symmetrical between initial and final states. z_{eff} is an effective ion charge chosen to give good correspondence with best results. We have chosen Ω and X as the most convenient for tabulation of collision cross-section data. Ω is a smooth, slowly varying function of X except in the vicinity of resonances where it changes rapidly. The detailed variation due to resonances is not of importance here, since we are only concerned with averages over free electron distributions close to Maxwellian. Usually collision strengths averaged over energy intervals much greater than the resonance widths are available from the source papers. We shall use Ω for this average without distinction.

Collisional rate data is also provided in several equivalent forms, namely excitation rates $q_{i \rightarrow j}$, de-excitation rates $q_{j \rightarrow i}$, the rate parameter, γ_{ij} , the Maxwell averaged scaled collision strength, $\langle z^2 \Omega_{ij} \rangle$ and the 'P-factor', P_{ij} introduced by Van Regemorter (1962). All these forms denote integrals over Maxwellian free electron distributions and are tabulated as functions of T_e , θ_e , $\Delta E_{ij}/kT_e$ or some composite of them. The following relations hold

$$\begin{aligned}
 q_{j \rightarrow i} &= \frac{\omega_i}{\omega_j} \exp(\Delta E_{ij}/kT_e) \quad q_{i \rightarrow j} = 2\sqrt{\pi} \propto c a_0^2 \frac{1}{\omega_j} \left(\frac{I_H}{kT_e} \right)^{1/2} \gamma_{ij} \\
 &= 8\pi/3 \left(\frac{2\sqrt{\pi} a c a_0^2}{3} \right) \left(\frac{I_H}{kT_e} \right)^{1/2} \left(\frac{I_H}{\Delta E_{ij}} f_{i \rightarrow j} \right) \frac{\omega_i}{\omega_j} P_{ij} \\
 \gamma_{ij} &= \frac{1}{2 \cdot z_{\text{eff}}} \langle z^2 \Omega_{ij} \rangle
 \end{aligned} \tag{8}$$

γ and $(z^2 \Omega)$ are dimensionless and symmetrical between initial and final states. We have chosen γ and θ_e as most convenient for tabulation of general z rate data.

2.3.1 Asymptotics and Approximate Forms

Three types of collisional transition are distinguished here, namely dipole allowed, non-dipole and spin change. These are not mutually exclusive types and transitions with intermediate character do occur. The extreme behaviours are as follows:

$$\begin{aligned}
 \text{(i) dipole} \quad & \lim_{X \rightarrow 1} \Omega \rightarrow c_1 & \Omega & \sim 4/3 S \log X & X \rightarrow \infty \\
 \text{(ii) non-dipole} \quad & \lim_{X \rightarrow 1} \Omega \rightarrow c_1 & \Omega & \sim c_2 & X \rightarrow \infty \\
 \text{(iii) spin change} \quad & \lim_{X \rightarrow 1} \Omega \rightarrow c_1 & X^2 \Omega & \sim c_2 & X \rightarrow \infty
 \end{aligned} \tag{9}$$

c_1 and c_2 are constants, and S is the line strength.

It is found that fairly good representation of the collision strengths over their whole energy can be obtained by simple modification of the asymptotic forms, namely:

$$\begin{aligned}
\text{(i)} \quad \Omega &\approx F_3 S \log(X + F_2) \\
\text{(ii)} \quad \Omega &\approx F_3 \\
\text{(iii)} \quad \Omega &\approx \frac{F_3}{(X + F_2)^2}
\end{aligned} \tag{10}$$

where F_2 and F_3 are constants to be determined by fitting to source data. These approximate forms have been identified by a number of other authors.

Integrating these approximate forms over a Maxwellian electron distribution, the equivalent expressions for the corresponding rate parameters, γ , are obtained, namely:

$$\begin{aligned}
\text{(i)} \quad \gamma &\approx F_3 S [\log(1 + F_2) + EEI((1 + F_2)\Delta E/kT_e)] \\
\text{(ii)} \quad \gamma &\approx F_3 \\
\text{(iii)} \quad \gamma &\approx \frac{F_3(\Delta E/kT_e)}{1 + F_2} EE2((1 + F_2)\Delta E/kT_e)
\end{aligned} \tag{11}$$

where $EEI(x) = \exp(x)E_1(x)$ and $EE2(x) = \exp(x)E_2(x)$ with E_1 and E_2 the first and second exponential integrals.

Note that further terms in the asymptotic series could be given and more elaborate approximate forms deduced from them. We have chosen here the simplest useful forms. They are used in the next section as an aid to interpolation and extrapolation of cross-section and rate data.

3. INTERPOLATION AND INTEGRATING PROCEDURES

Numerical procedures are used for interpolation and extrapolation of ionisation potentials and transition energies with respect to z_1 ; A 's with respect to z_1 ; Ω 's with respect to X ; γ 's with respect to θ and z_1 . Also numerical quadrature procedures perform conversion of Ω 's to γ 's. Our work is based on the use of cubic splines for interpolation. The advantages are the

generally stable and convincing trajectory of the spline in interpolation and the latitude for choice in end conditions which allows smooth extrapolation into specified asymptotic behaviour.

Our general strategy has been to convert the input data value pairs to 'reduced' values such that the reduced dependent variable is as nearly constant as possible over the whole independent variable range and is asymptotically constant. Also the reduced independent variable is chosen, if possible, to convert the infinite theoretical source ranges to convenient finite ranges. For interpolation in z , the above requirements are met by z -scaling of the dependent values, with the reduced independent variable usually taken as $1/z_1$. z_1 itself is sometimes convenient in spite of its infinite range. For interpolation of cross-section data with energy, the source data is first used to generate an approximate form based on equations (10), if possible. The difference or ratio of the source and approximate values provides suitable reduced values.

With regularly spaced nodal values and pure transition types, spline interpolation is very reliable, but frequently the data is very sparse, of mixed character or badly distributed. Then it is much less clear what accuracy expectations can be placed on interpolated and extrapolated values. It is often necessary to 'experiment' with the fitting. We have found it useful to have a 4th type of transition (used when the primary transition type is unclear) (cf. equation (10)) which simply converts to logarithmic reduced values. For collision strength interpolation in energy, an approximate form based on two input values sometimes cannot be obtained. We have also available forms based on one input value. For the dipole case, this one point form forces the exact asymptotic behaviour (equation (9i)). Where data is badly distributed the spline may be too flexible and it is safest to revert to simple linear interpolation. Alternatively, some improvement can be effected by rescaling of the independent spline variable. Finally, collision data for transitions of mixed type can often be interpolated successfully in two stages by first subtracting the approximate form obtained by treating the transition as one type and interpolating the remainder as a

transition of the other type. We have found our use of graphic display and interactive computing helpful in the above manipulations. The details of the interpolations are in appendix A.

4. THE COMPUTER PROGRAMS

There are six Fortran program units as follows:

- (1) QQPROG interpolates and extrapolates tabular excitation cross-section data to different energies;
- (2) QRPROG integrates over tabular cross-section data to provide Maxwell averaged rates;
- (3) RRPROG interpolates and extrapolates tabular excitation rate data to different temperatures;
- (4) EAPROG interpolates and extrapolates tabular energy and A value data to different z's;
- (5) IPPROG generates impact parameter approximation excitation rates at selected temperatures;
- (6) GZPROG generates a COPASE compatible specific ion atomic rate data set from a 'general z' data file.

All these programs are written in Fortran and are designed for interactive execution from a graphic terminal. Graphic plotting is done through calls to the GINOF or GHOST subroutine libraries. The organisation of programs (1) to (5) are similar and require prompted console input as follows:

(a) Transition title information, ion charges z_0 , z and z_{eff} , principal quantum numbers, energies and statistical weights of initial and final states.

(b) Source tabular data values. The various equivalent forms of the input data, described in section 2.3 are allowed and immediate conversion is made to our standard forms.

(c) Selection of independent variable values at which output results are required. Various output forms are allowed.

During execution, graphical display of both source and output data values is selectable under program prompt. This allows visual verification of data and of successful interpolation. Also, under program prompt, choices are offered for altering interpolation and display formats and for selecting different output values. Finally, result listing and graph hard copy can also be obtained. These five routines operate independently and require no additional input data files from disc or tape. They make use of a library of subroutines for spline interpolation, approximate form fitting and graphic output.

These programs have been used to produce 'general z data files'. Each such file is for a particular isoelectronic sequence over a range of ion charge and usually based on specific theoretical approximations. It contains atomic data for each transition for a representative set of z's (or ions) stored in a form suitable for easy interpolation to any ion in the range. For the representative ions, energy levels, transition energies and A values are stored directly. Collision data is stored for each representative ion as γ 's at a standard set of reduced temperatures. Each stored transition has an associated parameter line. These parameters are preset to allow best interpolation in general. There is at least one such general z datafile for each isoelectronic sequence and there may be several corresponding to different approximations and ranges of z spanned by the representative data. We have used partitioned data set organisation to store the separate members under an isoelectronic sequence group name such as HELIKE.DATA. Thus the general z data file for He-like ions containing primarily the data of Pradhan, et al.(1981) is HELIKE.DATA(PNH1981). Each sequence partitioned data set may also contain members with specific ion data. This is necessary for few times ionised ions where interpolation based on z-scaling is poor.

Program (6), in addition to console input, requires a general z data file entered on Fortran stream 7. As for programs (1) to (5), program (6) initially prompts for the nuclear charge, ion charge and effective ion charge of the ion for which data is required. Also a set of output temperatures (or reduced

temperatures) are sought. Thereafter the program works successively through each transition stored in the general z file, computing for the given ion, the transition energy, A value and γ values at the output temperatures. As mentioned in the previous paragraph, each transition has an associated parameter line. These parameters are chosen for best interpolation in general (see section 3), but improvement is possible in certain cases. For this reason, the option can be selected to use the preset parameters or to search for the best parameters and hence interpolation under interactive dialogue using the display facilities. Operation in this latter circumstance is similar to that of programs (3) and (4). Program (6) can produce an output data file of the assembled energy. A value and rate parameter results for the requested ion and temperatures in the form required for re-entry to the COPASE package described in paper I.

5. SOURCES OF ATOMIC DATA

The programs described in the previous section have been used to prepare atomic data for population calculations for a number of specific ions. However the particular concern has been to prepare general z data files for a number of the principal sequences of interest to fusion. At present data in the H-I, He-I, Li-I, Be-I and Na-I sequences have been assembled. It must be stressed that this is not an exhaustive compilation of all results on these sequences. Rather, the principal theoretical calculations expected to have reasonable accuracy have been sought. For most of the sequences, it has been possible to assemble general z data files in more than one approximation. This has proved most useful for making realistic accuracy assessments and for investigating the consequences of basic data variation for predicted populations and emissivities. In the following subsections, sources used for the various sequences are described. Note that although transition energies, A-values and γ 's are treated as separately compiled quantities in the data files, in the actual generation of γ 's from cross-section data, A-values and energies consistent with the original collision calculations involved were used.

5.1 Hydrogen-like Data

Only transitions between terms of different principal quantum shells are considered. The exact non-relativistic theoretical z -scaling with the nuclear charge has been used to obtain transition energies and electric dipole A -values for low and medium z ions from the hydrogen values. Term energies with relativistic corrections have been calculated for higher z ions (Fe^{+25} and Mo^{+41}) using the SUPERSTRUCTURE code. (Eissner et al. 1974). Transition probabilities for hydrogen were taken from Corney (1979). Only electric dipole transition probabilities were included except for the $1s$ - $2s$ two-photon decay and magnetic dipole decay. The A value for the former scales as z_1^6 and the latter as z_1^{10} . The composite A value of Parpia and Johnson (1982) has been adopted here.

The partitioned data set of general data files for the H-I sequence is called HLIKE.DATA with the following members

- (a) SGC1983;
 - (b) HS1977;
 - (c) HS1978;
- and a specific ion member for hydrogen
- (d) CMCD83H.

(a) SGC1983 contains collision data in the infinite z Coulomb Born approximation of Sampson et al. (1983). This latter work is an extension of the tables of z -scaled collision strengths ($z^2\Omega$) of Golden and Sampson (1978) to higher X values and to some further higher angular momentum transitions. The variation between the two calculations is small ($<2\%$). Results are available for $1s-n\ell$ ($2 \leq n \leq 5$, $\ell \leq 4$) $2s-n\ell$ ($3 \leq n \leq 5$, $\ell \leq 4$) and $2p-n\ell$ ($3 \leq n \leq 5$, $\ell \leq 2$). The appropriate z_{eff} is z_1 , the nuclear charge (cf equation (7) and Golden and Sampson (1977)). The γ 's scale exactly with z_1^{-2} , in this case (by definition) apart from very small variations at high z due to relativistic transition energy variation. We have simply put this data into our general z structure by storing the data for a set of ions of the sequence, viz, C^{+5} , O^{+7} , Si^{+11} , Ar^{+17} , Fe^{+25} and Mo^{+41} .

(b) HS1977 This is a small data file containing only the $1s$ - $2s$ and $1s$ - $2p$ transitions for He^+ , Li^{+2} , C^{+5} and Ne^{+9} from the close

coupling calculations of Hayes and Seaton (1977). Collision strengths were provided in this latter paper for $1 \leq x \leq 4$ and we have converted them to γ 's at the standard reduced temperature set. These results do not include resonances. Hayes and Seaton (1978) indicate that the resonances converging on the $n=3$ level increase the collision strength of the $1s-2s$ transition by 20% and the $1s-2p$ transition by 10% between the $n=2$ and 3 thresholds. A rough assessment of this is contained in the following data file.

(c) HS1978 is as HS1977, but with the $1s-2s$ collision strength increased by 20% between excitation and ionization threshold and the $1s-2p$ collision strength by 10% similarly.

(d) CMCD83 is a specific data set for neutral hydrogen. It was produced directly from the recommended collision strengths of Callaway and McDowell (1983) and includes the $1s-2s$, $1s-2p$, $1s-3s$, $1s-3p$, $1s-3d$ transitions.

5.2 Helium-like Data

Transitions between resolved fine structure levels are of interest here and especially the detailed decays of the $1s2\ell$ levels at high z . Energy level data for the helium sequence is available from a number of sources. Of note are theoretical data from Sampson and Clark (1980) associated with their infinite z Coulomb-Born calculations, from Padhan (1983) based on the SUPERSTRUCTURE code, from Ermolaev and Jones (1974) and from the high precision multiconfiguration Dirac-Fock calculations of Hata and Grant (1983). We carried out calculation some time ago for a number of helium-like ions conveniently spaced in charge for interpolation purposes. It has been informative to compare these older results with the newer calculations. Agreement is very good in general with typically 0.1% variation between the various sources, with the exception of the well recognised weakness of some of the calculations in obtaining the correct ordering of the 2^3P_0 , 2^3P_1 and 2^1S_0 levels along the isoelectronic sequence. This difficulty arises in the vicinity of $z=14$. This is of little importance for the calculation of level populations and our SUPERSTRUCTURE calculations were adopted in the present study.

For He-like ions the $1s2s^1S_0$ and $1s2s^3S_1$ levels are metastable. Additionally at higher z , the decay of the $1s2p^3P_{1,2}$ levels to the ground level $1s^2^1S_0$ matter. The $1s2s^1S_0 - 1s^2^1S_0$ decay is predominantly two photon with the A value varying as z_1^6 . The $1s2s^3S_1 - 1s^2^1S_0$ decay is through a relativistic magnetic dipole transition, $A \sim z_1^{10}$. The $1s2p^3P_0 - 1s^2^1S_0$ decay is strictly forbidden. The $1s2p^3P_1 - 1s^2^1S_0$ occurs through breakdown of LS coupling which allows a weak (but strongly z dependent) electric dipole decay, $A \sim z_1^8$. The $1s2p^3P_2 - 1s^2^1S_0$ decay is magnetic quadrupole with $A \sim z_1^8$. The results of Lin et al.(1977) have been used for all these with interpolation and extrapolation where necessary using program EAPROG (see section 4). All other important transitions are electric dipole type, however for decay within the $1s2^1$ complexes it should be noted that the behaviour of the A value with z can be substantially different from z^4 . For example, the $1s2p^3P_{0,1} - 1s2s^3S$, A values are nearly linear in z_1 . We have used a combination of results of Lin et al.(1977) and our own calculations for the electric dipole decays.

The partitioned data set of general z files for the He-I sequence is called HELIKE.DATA with the following members

- (a) KT1983
- (b) PNH1981
- (c) PRAD1983
- (d) SPC1978
- (e) SC1980

(a) KT1983 This is a small data file containing the collision data of Tayal and Kingston (1984) and Kingston and Tayal (1983). There are close coupling calculations with inclusion of resonance contributions, for the transitions $1s^2^1S - 1s2s^3S$ and $1s^2^1S - 1s2p^3P$. Fine structure is not resolved. The calculations are available for $z_1 = 5, 7, 11$.

(b) PNH1981 These are the extensive distorted wave calculations of Pradhan et al.(1981). They extend up to high z ($z_1 \leq 25$) and include all transitions between terms in the $1s^2$

and $ls2\ell$ complexes. The calculations are in LS coupling. Resonance contributions are included although it is to be noted that the radiative branching of the resonant states at high z is not included. The resonant enhancements in this work at high z are very large.

(c) PRAD1983 These are the intermediate coupling distorted wave calculations of Pradhan (1983a) for some high z ions. (Fe^{+24} , Se^{+32} , and Mo^{+40}) for an extensive set of transitions from $n=1-2$, 3 and from $n=2-2$, 3 fine structure levels. These calculations do not incorporate resonances. Our datafile contains the $n=1-2$ transitions only. Pradhan (1983b) assesses the enhancement of these results by resonances and, in turn, the reduction of the resonant enhancement through radiative branching (c.f. dielectronic recombination). Insufficient results are given for preparation of a full datafile, however it is evident that the radiative branching does reduce the resonant enhancement at high z substantially. The enhancements in Pradhan et al. (1981) are much too large.

(d) SC1980 This comprises the calculations of Sampson and Clark (1980) for transitions within the $ls2\ell$ complexes. These are based on the authors' infinite z Coulomb-Born techniques but are in intermediate coupling. Fine structure resolved data is given for all the possible transitions for a wide range of z 's. Our datafile has been assembled with representative ions between $z_1=5$ and $z_1=41$. The collision strength data in this case is tabulated as a function of K_2^2 , which leads to bad data distribution in the region near threshold at high z . We have used the bad data option in our codes in these cases. This region of uncertainty is not of great physical importance under normal excitation conditions.

(e) SPC1978 This comprises the calculations of Sampson et al. (1978) for transitions with $\Delta n \neq 0$ based again upon their infinite z Coulomb-Born techniques. The results are in intermediate coupling, giving fine structure resolved transition data. The data includes $z_1=13, 25, 41$. The values at the lowest z_1 where intermediate coupling is small are close to the

'no mixing' values. The no mixing values can be extended to lower z , using the standard prescriptions for the method. We have produced a general z datafile on that basis, spanning the range $z_1=5$ to $z_1=41$ as for SC1980. The two files SPC1978 and SC1980 provide an extensive compilation of Coulomb-Born data.

5.3 Lithium-Like Ions

Transitions between terms are of most importance here. The lithium-like system is well known and available data is of good quality. There are no metastable levels and only electric dipole transitions matter. We have taken transition energies from Baskin and Stoner (1975) supplemented with our own SUPERSTRUCTURE calculations for Fe^{+23} and Mo^{+39} . A-values are taken from the critical compilations of Martin and Weise (1976) which spans from Li^{+0} to Ni^{+25} . Omitted transitions for Fe^{+23} and Mo^{+39} are obtained from our own calculations. It should be noted that fine structure separation of the levels is occurring for $z_1 \gtrsim 23$ with associated changes in the simple low z component f -value ratios.

The partitioned data set of general z files for the Li-I sequence is called LILIKE.DATA with the following members:

- (a) CMCW1983
- (b) GCS1981

(a) CMCW1983 This is based on the study of Li-like ion collision cross-sections by Cochrane and McWhirter (1983). This is a fairly complete study which has assessed best available data and especially close coupling calculations. Cochrane & McWhirter have a similar approach to our own in seeking the trends of collision rate data with z . However, their results are provided as ad hoc empirical fits for the fP factor (equation 81) (so-called $\bar{g}f$ by the authors). We have converted this data to our standard forms of γ 's at our standard reduced temperatures. The general z file spans from $z_1=12$ to $z_1=40$.

(b) GCS1981 These are the infinite z Coulomb-Born calculation of Golden et al. (1981). The required z_{eff} for the Li-like sequence transitions is given by Golden and Sampson (1977). It

has been informative to contrast some of the transitions in GCS1981 with the data of CMCW1983. The Coulomb-Born data often gives a very good representation of the latter values but with different z_{eff} . For example, for Fe^{+23} the 2s-3d transition required $z_{\text{eff}}=25.5$ whereas the 2s-3p transition gave agreement to within a few per cent with $z_{\text{eff}}=26$ the nuclear charge. The general z file spans from $z_1=4$ to $z_1=40$.

5.4 Beryllium-Like Ions

The beryllium-like sequence has been extensively studied, especially for the lower z members of the sequence. There are substantial calculations of energy levels, transition probabilities and collision data. Fine structure resolution of the terms is of interest here. The $2s2p^3P$ level is metastable and the $2s3p^3P$ level relatively long-lived. We have concentrated on two separate regions, namely $11 \leq z_1 \leq 39$ and $3 \leq z_1 \leq 9$: and on transitions within the $n=2$ complexes. For the former we have chosen representative ions Si^{+10} , Ar^{+14} , Fe^{+22} and Mo^{+38} . Energy levels for Si^{+10} , Ar^{+14} and Fe^{+22} were taken from Edlen (1979) and for Mo^{+38} from Nussbaumer and Storey (1979a). For the second range, we have chosen representative ions C^{+2} , O^{+4} , Ne^{+6} and Si^{+10} . Transition energies are taken from Baskin and Stoner (1975) and transition probabilities from Nussbaumer and Storey (1978, 1979a, b) and from Muhlethaler and Nussbaumer (1976).

The partitioned dataset of general z files for the Be-I sequence is called BELIKE.DATA with the following members:

- (a) CSP1980
- (b) BBDK1984
and an ion specific member for O^{+4}
- (c) D19780

(a) CSP1980 This is the data of Clark et al.(1980) and Sampson et al.(1980) and is fine structure resolved intermediate coupling data based on the authors' infinite z Coulomb-Born techniques. The general z file spans $11 \leq z_1 \leq 39$ and for all transitions with $\Delta n=0$ and $n=2$.

(b) BBDK1984 Consists of the close coupling calculations of Berrington et al.(1984). The collision rates are based on the extension of their older collision strength data to higher energies with an expected improvement in the rates.

Data is available for C^{+2} , O^{+4} , Ne^{+6} and Si^{+10} and has simply been converted to γ 's at our reduced temperature set. These calculations are in intermediate coupling and take account of resonances.

(c) D19780 Is an ion specific file for O^{+4} . The collision data is based on the close coupling calculations of the Queen's University, Belfast Group, but is drawn from a range of their papers. Also the $n=3$ levels are included. Data is drawn from Dufton et al.(1978), Berrington et al.(1979), Widing et al.(1982) and Tayal et al.(1983). Supplementary A value data is taken from Hibbert (1980). A fine structure resolved picture is used. Separation of term collision strengths into fine structure components has been achieved using the data of Malinowsky (1975) for reference.

5.5 Sodium-Like Ions

Fine structure resolved transitions between the 3s and 3p terms are of interest and possibly also resolution of the 3d term. For transitions involving higher levels, term averages are sufficient. Only electric dipole transition probabilities matter, there are no metastables. There have been a number of calculations of transition energies for this sequence. The range from Si^{+3} to Mo^{+31} is relevant. We have taken level energies from Baskin and Stoner (1975) for Si^{+3} to Ca^{+9} , from Corliss and Sugar (1982) for Fe^{+15} and from Blaha and Davis (1978) beyond Fe^{+15} up to Mo^{+31} . For transition probabilities, and representative ions, we have chosen two ranges: namely from $z_1=4$ to $z_1=16$ and from $z_1=10$ to $z_1=32$. For the former fine structure resolved transition probabilities between the 3s, 3p and 3d levels are used. Comparative data is available, including Flower and Nussbaumer (1975), Froese-Fischer (1976) and McEachan and Cohen (1983). Agreement is good with the largest divergence $\sim 12\%$ for Si^{+3} and much smaller divergences for higher z 's. For

the second range, data of Blaha and Davis (1978) is also available and the spread in A-values at Fe^{+15} is at most $\sim 8\%$. We have used the data of Flower et al. (1975) for the first range and of Blaha and Davis (1978) for the second.

The partitioned data set of general z files for the Na-I sequence is called NALIKE.DATA, with the following members:

- (a) FN1975
- (b) BD1978
- and an ion specific member for M_g^+
- (c) B1972MG

(a) FN1975 Consists of the distorted wave (with exchange) calculations of Flower and Nussbaumer (1975). These are fine structure resolved calculations for the 3s, 3p and 3d levels. We have converted this data to γ 's at the reduced temperature set for the representative ions Si^{+3} , S^{+5} , Ca^{+9} and Fe^{+15} . It should be noted that the source collision strength data is available at three impact energies only ranging from near threshold to about twice threshold.

(b) BD1978 Consists of the distorted wave (no exchange) calculations of Blaha and Davis (1978). The multiplet component transitions are resolved only for the $3s_{1/2}-3p_{1/2}$ and $3s_{1/2}-3p_{3/2}$ transitions for $z_1 \geq 20$ (Zn^{+19}) below which the splitting is effectively statistical. This data includes all multiplets between the 3s, 3p, 3d, 4s, 4p, 4d and 4f terms. Collision strength data is tabulated for $1 \leq X \leq 4$. We have converted this data to γ 's for the representative ions Ca^{+9} , Fe^{+15} , Zn^{+19} and Mo^{+31} .

(c) B1972MG Is an ion specific file for M_g^+ based on the unitarised Coulomb-Born (no-exchange) collision strengths derived by Blaha (1972), including the 3s, 3p, 3d, 4s and 4p levels. Comparative collision data is available for 3s-3p, 3p-3d, 3s-4s, 3p-4s and 4s-3d transitions from the close coupling calculation of Mendoza (1981). There is broad agreement (within $\sim 25\%$) between these calculations. Transition

probabilities have been taken from Hibbert et al.(1983). It should be noted that there is some controversy over the 3s-4p transition probability. There is a factor of ~ 2 variation between calculations. The Hibbert et al.(1983) value is at the low end of the range.

6. CASE ILLUSTRATIONS

6.1 Examples of Output from the Programs

The product of this work is the computer data collection and set of programs for its generation and manipulation. It is intended for direct use from a computer terminal. In this section we wish to illustrate simply the form of output, graphical and tabular, which may be obtained from the programs.

Table 1 shows the printed output from the program QQPROG for the $1s^2 1S-1s2p^1P_1$ transition of C^{+4} . This is a dipole transition (type 1) and requires an A-value (f or S) as input. The alternative forms are returned as output. The parameter IDIFF=0 indicates that ratio fitting was used (see Appendix A) and IBPTS=0 indicates that the 'bad point' option was not required. The parameters of the approximate form are FXC2 and FXC3 ($\approx F_2$ and F_3 in equation (10i)). IFPTS = 2 indicates that two point approximate form fitting was used. The difference column shows the difference between the approximate form and the input data. The program interpolates or extrapolates the input cross-section data to the requested set of energies, yielding the required output collision strengths. Figure 1 shows the 'reduced plot'. We use the term 'reduced plot' to indicate that the x and y axis correspond to the actual interpolation variables used (cf. Appendix A). In this case $x = 1/x$ and $y = \Omega/\Omega_{\text{approx}}$. Source values are connected by straight lines and interpolated values marked by crosses. The quality of the interpolation is immediately evident from the graph.

Table 2 shows the printed output from the program QRPROG for the 3s-4s transition of M_g^+ . This is a non-dipole (type 2) transition. The program returns the rate parameter, γ , together

with other equivalent forms at a set of requested temperatures. fP is the absorption oscillator strength times the P-factor. The product is meaningful even for non-dipole transitions. Figure 2 shows the associated reduced plot. The crosses here indicate the values used by the quadrature routines and again provide a clear indication of the accuracy of the interpolation. The graphical display also helps the verification of input data values.

Table 3 shows the output from RRPROG for the $2s^21S-2s2p^3P$ transition in O^{+4} . This is a spin change transition (type 3). The data input in this case consists of rates or an equivalent form at a set of temperatures and the program returns rate parameters and equivalent forms at a requested set of temperatures. For rate interpolation, there is no choice of difference option. If an approximate form can be obtained, ratio interpolation is carried out, otherwise the difference is formed and interpolated. Figure 3 shows the reduced plot. The crosses mark the interpolated values. Note also from the table the characteristic decrease of γ with increasing T_e for spin change transitions.

Table 4 shows the output from EAPROG. This program interpolates transition energies and A-values. The parameter FAC2 is the z-scaling parameter (b_0 in equation (4)). The parameters IECl and IACl indicate the choice of independent variable for the energy and A interpolation respectively (z_1 selected by 1, $1/z_1$ selected by 2). Graphical output is also available.

Table 5 shows the printed output from the impact parameter program IPPROG for a typical case. Note that this program requires binding energies rather than excitation energies for the levels of the transition. It can only provide dipole transitions and requires an A-value as input.

Figure 4 shows the graph of the scaled γ 's versus $\log(\theta_e)$ for a transition using the program GZPROG. The general z data file is NALIKE.DATA (FN1975) and the transition displayed is $3s-3p$. The continuous curves are the scaled γ 's of the representative ion transitions and the crosses mark the values for the ion for which

data is sought - in this case Cl^{+6} . The program allows a search for the best scaling factor, FGC2 (see appendix A) that is, which makes the curves superimpose as nearly as possible. In this case $\text{FGC2} = -1.1$ is most suitable. The program also provides the transition energy and A-value and returns an output file to disk for direct input to the COPASE programs described in paper I. The structure of such a file has been described in paper I.

6.2 A Study of O^{+4}

Spectral emission from this ion is prominent in the edge region of the JET plasma and is in a strongly ionising environment. Electron temperature and density in the region of its emission may be uncertain. It is of interest to investigate the theoretical ratio of the emissivities of two spectral lines emitted by this ion to see if the ratio is markedly dependent on density, temperature or both. A COPASE type datafile BELIKE.DATA (D19780) for O^{+4} was used. This datafile contains the atomic data necessary to calculate the local populations of low excited levels of O^{+4} in statistical equilibrium at arbitrary temperatures and densities, and hence the local emissivities of spectrum lines of O^{+4} . This is achieved by re-entering the datafile into the COPASE programs. The various possibilities have been described in paper I. In dynamic conditions (such as the edge region of JET, where impurity ions are diffusing rapidly), metastable populations may differ from their statistical equilibrium values. It is useful to be able to isolate the dependence of the population of the upper emitting level of a line on the ground and metastable level abundances (see equation (6) of paper I). The populations of the excited levels may be determined in these circumstances by a new subroutine in the COPASE package called METPOP. Table 6 shows typical results for O^{+4} . Table 6a shows the level assignments and the plasma parameters. The first four levels are designated as metastable, indexed by IMET and the remainder as ordinary, indexed by IORD. The columns in Tables 6b and 6c correspond to the different densities. Only one temperature is shown. The final population of a level is obtained by multiplying the dependence on each metastable by the metastable population and summing. Equilibrium metastable populations are shown at the top

of Table 6b. From this point it is straightforward to determine line emissivities and ratios of emissivities in conditions of either equilibrium or arbitrary metastable filling. Figure 5 shows the emissivity ratio

$$\frac{\epsilon(2s2p^3P-2s3s^3S)}{\epsilon(2s2p^1P_1-2s3d^1D_2)}$$

plotted as contours in the electron temperature/electron density plane. Equilibrium metastable populations have been adopted in this case. (The metastable multipliers are set to unity.) The line composition and the contour values are also shown on the right hand side of the graph. LGS=1 indicates that the contours are logarithms of the emissivity ratio. The graph is generated by the subroutine METCON after the call to METPOP.

ACKNOWLEDGEMENTS

This work was supported by EMR grant from Culham Laboratory, UKAEA.

We wish to thank Dr N J Peacock for numerous helpful discussions.

APPENDIX A

The choices of independent variable, x , and dependent variable, y , for interpolation are as follows:

A.1 Energies and A-values

(i) Binding energy interpolation with respect to z_1 .

$$y = (I_i/I_H)/z_1 - z_1/n_i^2$$
$$x = z_1$$
$$\left. \frac{d^2 y}{dx^2} \right|_{x_0} = \left. \frac{d^2 y}{dx^2} \right|_{x_{\max}} = 0$$

(ii) Transition energy interpolation with respect to z_1 .

$$y = \frac{(\Delta E_{ij}/I_H)}{z_1} - z_1 \left(\frac{1}{n_i^2} - \frac{1}{n_j^2} \right)$$
$$x = z_1 \quad \text{or} \quad 1/z_1$$
$$\left. \frac{d^2 y}{dx^2} \right|_{x_0} = \left. \frac{d^2 y}{dx^2} \right|_{x_{\max}} = 0$$

(iii) A-value interpolation with respect to z_1 .

$$y = A_{j \rightarrow i}/z_1^{\text{FAC2}}$$
$$x = z_1 \quad \text{or} \quad 1/z_1$$
$$\left. \frac{d^2 y}{dx^2} \right|_{x_0} = \left. \frac{d^2 y}{dx^2} \right|_{x_{\max}} = 0$$

FAC2 is selected interactively to make the $y(x)$ curve approximately constant in the interpolation region.

A.2 Collision strength Ω with respect to X

(i) Dipole

$$y = \Omega - \Omega_{\text{approx}} \quad \text{or} \quad \Omega/\Omega_{\text{approx}} \quad (F_2 \neq 0)$$

$$x = 1/X$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\text{max}}} = 0$$

where Ω_{approx} is given by (1Ci) with the choices

$$(a) F_2 = 0$$

$$F_3 = 4/3$$

$$(b) F_2 = \exp(\Omega_0/(F_3 S)) - X_0$$

$$F_3 = 4/3$$

$$(c) F_2 = -X_0 + (X_{\text{max}} + F_2)^{\Omega_0/\Omega_{\text{max}}} \quad F_3 = \Omega_0/(S \log(X_0 + F_2))$$

(X_0, Ω_0) and $(X_{\text{max}}, \Omega_{\text{max}})$ are the first and last members of the tabular source data pairs with $X_0 < X_{\text{max}}$. Options (b) and (c) for F_2 and F_3 are called the 1pt and 2pt approximate forms. The 2pt form for F_2 is obtained iteratively with solution possible only if Ω is an increasing function of X . (b) is used if only a single data pair is available.

ii) Non-Dipole

$$y = \Omega$$

$$x = 1/X$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\text{max}}} = 0$$

(iii) Spin Change

$$y = \Omega/\Omega_{\text{approx}}$$

$$x = 1/X$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\text{max}}} = 0$$

where Ω_{approx} is given by (10iii) with the choices

$$(a) \quad F_2 = 100 \quad F_3 = \Omega_0(X_0 + F_2)^2$$

$$(b) \quad F_2 = \frac{(X_{\text{max}} \sqrt{(\Omega_{\text{max}}/\Omega_0)} - X_0)}{(1 - \sqrt{(\Omega_{\text{max}}/\Omega_0)})} \quad F_3 = \Omega_0(X_0 + F_2)^2$$

Options (a) and (b) are called the 1pt and 2pt approximate forms. The 2pt form is obtainable only if Ω is a decreasing function of X . (a) is used with a single source data pair.

(iv) Other

$$y = \log \Omega$$

$$x = 1/X$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\text{max}}} = 0$$

Note that the line strength, S , is required in (i).

As has been mentioned earlier, the collision types are not exclusive. LS coupling breakdown at high Z leads to a dipole component in some intersystem transitions. When this mixed character is clearly expressed, the approximate form (ia) may be used for F_2 and F_3 and the difference between this and the actual Ω 's interpolated using type (iii).

A.3 Rate parameter γ with respect to T_e at fixed z_1

(i) Dipole

$$y = \gamma - \gamma_{\text{approx}} \quad \text{or} \quad \gamma/\gamma_{\text{approx}} \quad (F_2 \neq 0)$$

$$x = (\Delta E/kT_e) / ((\Delta E/kT_e) + 1)$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\text{max}}} = 0$$

where γ_{approx} is given by (10i), with the choices

$$(a) \quad F_2 = 0$$

$$F_3 = 4/3$$

$$(b) \quad F_2 \text{ soln. of } \gamma^{(0)} = \gamma_{\text{approx}}^{(0)}$$

$$F_3 = 4/3$$

$$(c) \quad F_2 \text{ soln. of } \frac{\gamma^{(0)}}{\gamma^{(\max)}} = \frac{\gamma_{\text{approx}}^{(0)}}{\gamma_{\text{approx}}^{(\max)}}$$

$$F_3 \text{ soln. of}$$

$$\gamma^{(0)} = \gamma_{\text{approx}}^{(0)}$$

$\gamma^{(0)}$ and $\gamma^{(\max)}$ are the tabular values corresponding to the lowest and highest reduced temperatures in the source data. In cases (b) and (c), F_2 and F_3 are obtained iteratively.

(ii) non-dipole and other

$$y = \gamma$$

$$x = (\Delta E/kT_e) / ((\Delta E/kT_e) + 1)$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\max}} = 0$$

(iii) Spin change

$$y = \gamma/\gamma_{\text{approx}}$$

$$x = (\Delta E/kT_e) / ((\Delta E/kT_e) + 1)$$

$$\left. \frac{dy}{dx} \right|_{x_0} = \left. \frac{dy}{dx} \right|_{x_{\max}} = 0$$

where γ_{approx} is given by (10iii), with the choices

$$(a) \quad F_2 = 100$$

$$F_3 \text{ soln. of}$$

$$\gamma^{(0)} = \gamma_{\text{approx}}^{(0)}$$

$$(b) \quad F_2 \text{ soln. of}$$

$$F_3 \text{ soln. of}$$

$$\frac{\gamma^{(0)}}{\gamma^{(\max)}} = \frac{\gamma_{\text{approx}}^{(0)}}{\gamma_{\text{approx}}^{(\max)}}$$

$$\gamma^{(0)} = \gamma_{\text{approx}}^{(0)}$$

In many cases Ω_{approx} and γ_{approx} are very good approximations to the tabulated Ω and γ over their whole range. However, often F_3 in the dipole case is different from 4/3 contrary to the theoretical expectation. This is probably attributable to deficiencies in the higher partial wave treatment in the source data (provided a consistent S is used). We have chosen to continue to use 2pt approximate fitting where possible, since this usually provides the optimum representation of the source data. We have made no effort to 'correct' or 'adjust' source data.

A.4 Rate parameter γ with respect to z_1

This is at the standard set of reduced temperatures θ_e .

$$\begin{aligned} y &= \frac{\gamma}{z_1^{\text{FGC2}}} \\ x &= z_1 \quad \text{or} \quad 1/z_1 \\ \left. \frac{dy^2}{dx^2} \right|_{x_0} &= \left. \frac{dy^2}{dx^2} \right|_{x_{\text{max}}} = 0 \end{aligned}$$

FGC2 is chosen interactively to make the $y(\theta_e)$ curves approximately coincident in the interpolation region.

A.5 Quadrature of Ω over a Maxwellian

$$\gamma = \gamma_{\text{approx}} + \sum w_i (\Omega(X_i) - \Omega_{\text{approx}}(X_i))$$

$$\text{where } X_i = \frac{x_i}{(\Delta E/kT_e)} + 1$$

with the x_i and w_i the nodes and weights of N-pt. Gauss-Laguerre quadratures with N selectable from 4, 6 and 8.

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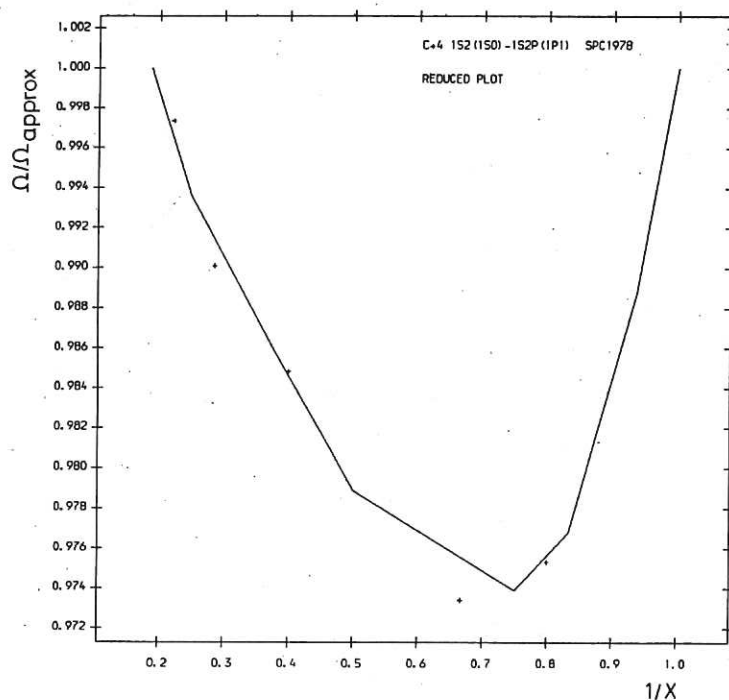


Fig. 1 Reduced plot for $C^{+4} 1s^2 1S - 1s2p^1$ from QQPROG. (+'s denote interpolated values) Note the small variation of the ration Ω/Ω_{approx} over the whole range of $1/\chi$. $\chi = \Delta E_i$ is the incident electron energy and ΔE_{ij} the translation energy. Ω_{approx} is the approximation to Ω in equation(10(i)).

CLM-R250

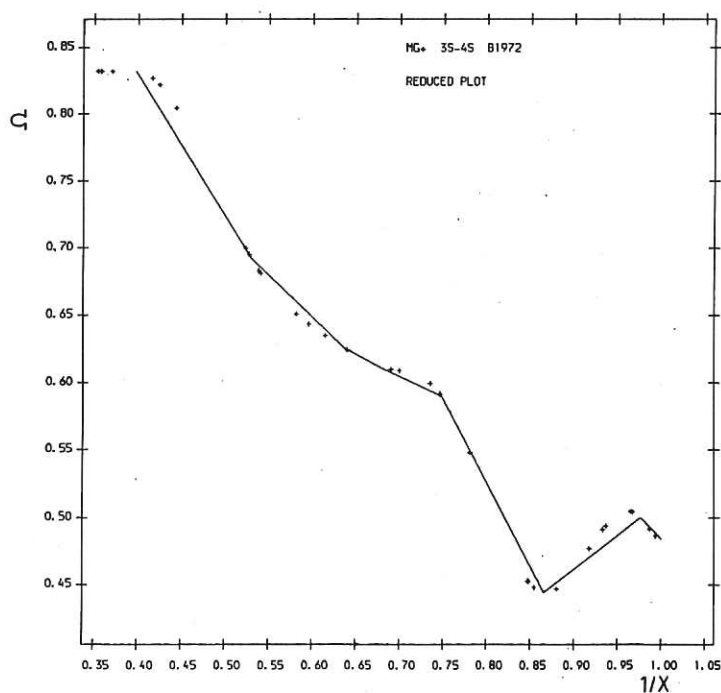


Fig.2 Reduced plot for $Mg^+ 3s - 4s$ from QRPROG.

CLM-R250

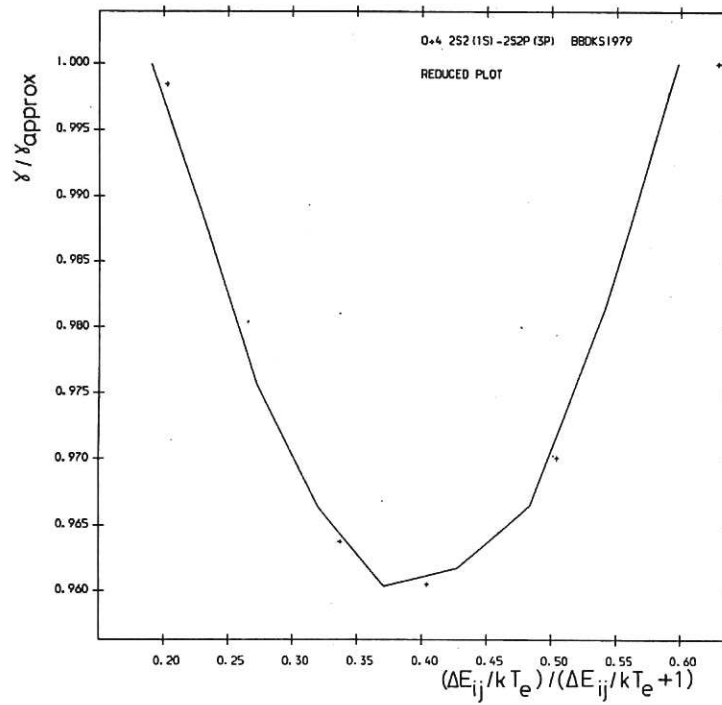


Fig.3 Reduced plot for $O^{+4} 2s^2 1S-2s2p 3P$ from RRPROG. Note the small variation of the ratio γ/γ_{approx} over the whole range of the independent variable. γ_{approx} is the approximation to γ in equation (11(iii)).

CLM-R250

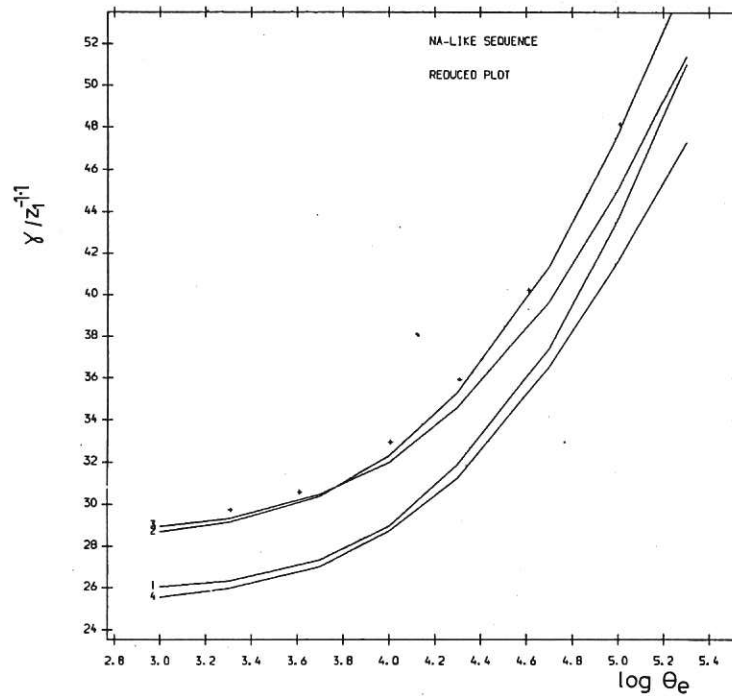


Fig.4 Scaled γ versus $\log(\theta_e)$ plot for sodium-like $3s-3p$ from GZPROG. (+'s denote interpolated values for Cl^{+6}) θ_e is the reduced electron temperature (equation (5)). -1.1 is the scaling factor. FGC2 in appendix A4. The continuous curves are for 1: Si^{+3} , 2: S^{+5} , 3: Ca^{+9} , 4: Fe^{+15} .

CLM-R250

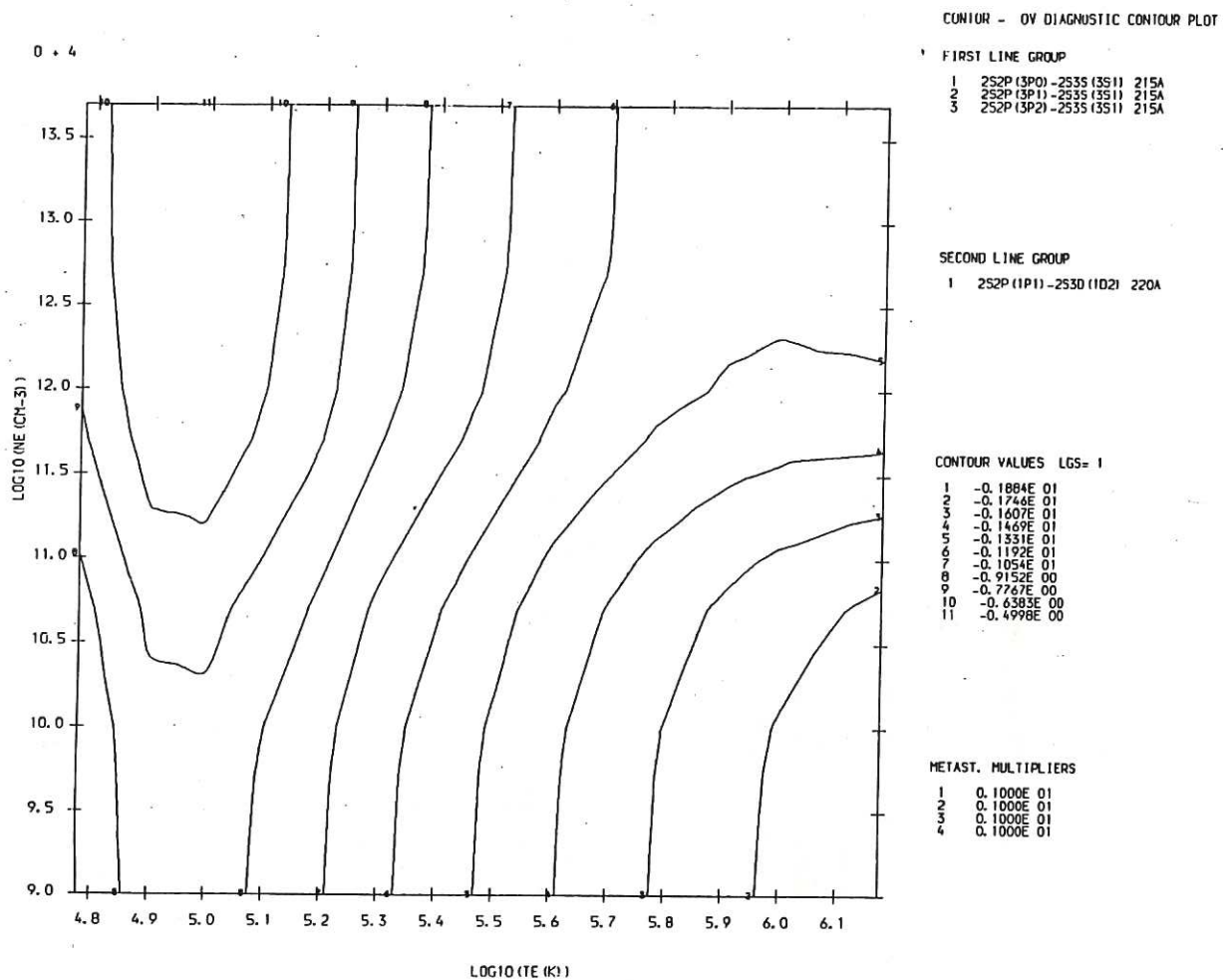


Fig.5 Diagnostic contour plot O^{+4} from METCON.

CLM-R250

Table 1. Output for C⁺⁴ 1s² 1S-1s2p 1p from QQPROG.

C+4 1S2(1S0)-1S2P(1P1) SPC1978

NUCLEAR CHARGE = 6.00 ION CHARGE = 4.00 EFFECTIVE ION CHARGE = 5.50

LOWER INDEX = 1 UPPER INDEX = 2

LOWER ENERGY = 0.00000000 UPPER ENERGY = 22.629013

LOWER WEIGHT = 1.0 UPPER WEIGHT = 3.0

ACOEFF = 8.87000+11 S = 8.57090-02 FABS = 6.46950-01 ENERGY DIFFERENCE = 22.629013

XSECT TYPE= 1 XSECT OPTIMISATION FACTORS ,FXC2 = 4.23310-01 FXC3 = 1.79180+00 IBPTS = 0 IFPTS = 2 IDIFF = 0

X	OMEGA	APPROX. OMEGA	DIFFERENCE
1.00000+00	5.42480-02	5.42480-02	6.93890-18
1.05700+00	6.06280-02	6.13170-02	-6.89130-04
1.20000+00	7.27270-02	7.44550-02	-1.72730-03
1.33300+00	8.42980-02	8.65570-02	-2.25930-03
2.00000+00	1.33160-01	1.36030-01	-2.87350-03
2.66700+00	1.70980-01	1.73400-01	-2.42150-03
4.00000+00	2.20040-01	2.28510-01	-1.46890-03
5.33300+00	2.68990-01	2.68990-01	-6.85420-08

X	OMEGA	APPROX. OMEGA
1.25000+00	7.71650-02	7.91170-02
1.50000+00	9.78440-02	1.00520-01
2.50000+00	1.62360-01	1.64860-01
3.50000+00	2.07990-01	2.10080-01
4.50000+00	2.44320-01	2.44970-01

Table 2. Output for Mg⁺ 3s-4s from QRPROG.

NUCLEAR CHARGE = 12.00		ION CHARGE = 1.00		EFFECTIVE ION CHARGE = 2.00	
LOWER INDEX = 1		UPPER INDEX = 4			
LOWER ENERGY = 0.000000		UPPER ENERGY = 0.636112			
LOWER WEIGHT = 2.0		UPPER WEIGHT = 2.0			
ACOEFF = 0.0000D+00		S = 0.0000D+00		FABS = 0.0000D+00	
XSECT TYPE= 2		XSECT OPTIMISATION FACTORS , FXC2 = 0.0000D+00		FXC3 = 0.0000D+00	
				IBPTS = 0	
				IFPTS = 0	
				IDIFF = 1	
				ENERGY DIFFERENCE = 0.636112	
X		OMEGA		DIFFERENCE	
1.0000D+00		4.8400D-01		4.8400D-01	
1.0242D+00		5.0000D-01		5.0000D-01	
1.1553D+00		4.4400D-01		4.4400D-01	
1.3367D+00		5.9000D-01		5.9000D-01	
1.4815D+00		6.1200D-01		6.1200D-01	
1.5721D+00		6.2600D-01		6.2600D-01	
1.8865D+00		6.9200D-01		6.9200D-01	
2.5153D+00		8.3200D-01		8.3200D-01	
TE(K)		GAMMA		EX. R. ATE	
4.0000D+03		4.9114D-01		4.1736D-19	
8.0000D+03		4.8797D-01		8.3084D-14	
2.0000D+04		5.0801D-01		1.0219D-10	
4.0000D+04		5.8558D-01		1.0259D-09	
8.0000D+04		6.1386D-01		2.6687D-09	
2.0000D+05		7.4309D-01		4.3395D-09	
4.0000D+05		7.6233D-01		4.0464D-09	
8.0000D+05		8.2827D-01		3.5246D-09	
		APPROX. GAM		DEXC. RATE	
		0.0000D+00		3.3511D-08	
		0.0000D+00		2.3542D-08	
		0.0000D+00		1.5501D-08	
		0.0000D+00		1.2635D-08	
		0.0000D+00		9.3656D-09	
		0.0000D+00		7.1702D-09	
		0.0000D+00		5.2014D-09	
		0.0000D+00		3.9961D-09	
				GBARF	
				1.0765D-02	
				1.0696D-02	
				1.1135D-02	
				1.2835D-02	
				1.3455D-02	
				1.6288D-02	
				1.6710D-02	
				1.8155D-02	

Table 3. Output for O⁺¹⁴ 2s² 1S - 2s2p ³p from RRPROG.

O+4 2S2(1S)-2S2P(3P) BBDKS1979									
NUCLEAR CHARGE = 8.00		ION CHARGE = 4.00		EFFECTIVE ION CHARGE = 5.00					
LOWER INDEX = 1	UPPER INDEX = 2								
LOWER ENERGY = 0.000000		UPPER ENERGY = 0.747925							
LOWER WEIGHT = 1.0		UPPER WEIGHT = 9.0							
ACOEFF = 0.00000+00		S = 0.00000+00		FABS = 0.00000+00		ENERGY DIFFERENCE = 0.747925			
GAMMA TYPE = 3		GAMMA OPTIMISATION FACTORS,				FXC2 = 5.38670+00		FXC3 = 2.55570+01 IBPTS = 0 IFPTS = 2	
TE(K)		GAMMA		APPROX. GAMMA		DIFFERENCE			
7.94000+04	5.24530-01		5.24530-01		9.71450-17				
1.00000+05	4.95390-01		5.04770-01		-9.38260-03				
1.26000+05	4.66270-01		4.82420-01		-1.61490-02				
1.50000+05	4.40620-01		4.58130-01		-1.75060-02				
2.00000+05	4.13430-01		4.30580-01		-1.70740-02				
2.51000+05	3.88490-01		4.01970-01		-1.34810-02				
3.16000+05	3.62560-01		3.71560-01		-8.99980-03				
3.98000+05	3.36410-01		3.40130-01		-3.71620-03				
5.01000+05	3.08380-01		3.08390-01		-9.62760-06				
TE(K)		GAMMA		APPROX. GAM		EX. RATE		GBARF	
6.96320+04	5.34640-01		5.34640-01		3.20690-09		1.94260-09		2.75580-02
1.16050+05	4.76010-01		4.90570-01		4.35840-09		1.33970-09		2.45350-02
1.74080+05	4.29380-01		4.47040-01		4.50630-09		9.86700-10		2.21320-02
2.32110+05	3.97070-01		4.11990-01		4.27580-09		7.90190-10		2.04660-02
4.64220+05	3.18440-01		3.18910-01		3.12670-09		4.48050-10		1.64110-02
6.96320+05	2.63520-01		2.63530-01		2.29990-09		3.02700-10		1.35830-02
1.16050+06	1.98560-01		1.98560-01		1.43660-09		1.76720-10		1.02340-02
1.74080+06	1.53680-01		1.53680-01		9.38660-10		1.11620-10		7.91700-03
2.32110+06	1.26010-01		1.26020-01		6.78320-10		7.93030-11		6.49530-03
4.64220+06	7.46270-02		7.46290-02		2.91370-10		3.32090-11		3.84660-03

Table 4. Output for sodium-like 4p-3d from EAPROG.

TRANSITION SPECIFICATION
NA-SEQUENCE 4P-3D MC&BD

ENERGY LEVEL DATA

ION CHARGE	TRANS.ENER.(RYD)	TRANS.ENER.(CM-1)
1.00	8.3370240D-02	9148.8
2.00	2.5269964D-01	27730.5
6.00	1.9907403D+00	219445.5
9.00	4.4034601D+00	483222.5
15.00	1.1090060D+01	1304779.5
19.00	1.8075990D+01	2071394.5
25.00	3.2201000D+01	3542420.1
31.00	4.9209010D+01	5400049.1

OUTPUT PARAMETERS IEC1 = 1 IEC2 = 1

ION CHARGE	TRANS.ENER.(RYD)	TRANS.ENER.(CM-1)
5.00	1.3907440D+00	153494.0
6.00	1.9907403D+00	219445.5
9.00	4.4034601D+00	483222.5
13.00	8.9964614D+00	987244.7
15.00	1.1090060D+01	1304779.5
17.00	1.5184896D+01	1666344.9
31.00	4.9209010D+01	5400049.1

A VALUE DATA

ION CHARGE	A VALUE(SEC-1)	F(ABS)	S(AT. UNITS)
1.00	1.65000D+07	1.7733D-01	6.3809D+01
2.00	1.45000D+06	1.6962D-01	2.0137D+01
6.00	4.6000D+09	8.7046D-02	1.3059D+00
9.00	1.6600D+10	6.3948D-02	4.3567D-01
15.00	7.8500D+10	4.1477D-02	1.0465D-01
19.00	1.6700D+11	3.5011D-02	5.5644D-02
25.00	4.1200D+11	2.9533D-02	2.7447D-02
31.00	8.6000D+11	2.6529D-02	1.6173D-02

OUTPUT PARAMETERS IAC1 = 1 IAC2 = 1 FAC2 = 4.00

ION CHARGE	A VALUE(SEC-1)	F(ABS)	S(AT. UNITS)
5.00	2.7305D+09	1.0425D-01	2.2360D+00
6.00	4.6000D+09	8.7046D-02	1.3059D+00
9.00	1.6600D+10	6.3948D-02	4.3567D-01
13.00	5.1396D+10	4.7435D-02	1.5818D-01
15.00	7.8500D+10	4.1477D-02	1.0465D-01
17.00	1.1604D+11	3.7591D-02	7.4267D-02
31.00	8.6000D+11	2.6529D-02	1.6173D-02

Table 5. Output for He⁺ 1s-2p from IPPROG.

```

HE+ 1S-2P

NUCLEAR CHARGE = 2.00  ION CHARGE = 1.00  EFFECTIVE ION CHARGE = 2.00
LOWER INDEX = 1          UPPER INDEX = 2
LOWER ENERGY = 4.000000  UPPER ENERGY = 1.000000
LOWER WEIGHT = 2.0       UPPER WEIGHT = 6.0

ACOEFF = 1.0029D+10  S = 8.3239D-01  FABS = 4.1619D-01  ENERGY DIFFERENCE = 3.000000

TE(K)
2.00000D+04
5.00000D+04
1.00000D+05
2.00000D+05
5.00000D+05
1.00000D+06

GAMMA
6.3235D-01
6.3551D-01
6.5600D-01
7.0761D-01
8.3880D-01
1.0213D+00

EX. RATE
9.9964D-19
9.4277D-13
7.8487D-11
6.3934D-10
1.9852D-09
2.7443D-09

DEXC. RATE
6.4318D-09
4.0882D-09
2.9840D-09
2.2760D-09
1.7065D-09
1.4690D-09

GBARF
6.5369D-02
6.5695D-02
6.7814D-02
7.3149D-02
8.6718D-02
1.0557D-01

```

Table 6. Output for O^{+4} from METPOP. Table (6a) shows the energy levels and designations for the ion, the selected metastable levels and the electron and proton temperatures and densities. Table (6b) shows the populations. Successive columns correspond to the different densities. The first four rows give the metastable populations in equilibrium. The following four groups of rows show the excited level populations resolved as multipliers of the metastable populations. Only one temperature is shown.

ION		Z0	Z1	ION.POT.(W.NO.)		ENER.(RYD)	
0 + 4		8	5	918657.			
ENERGY LEVELS		CONFIG.	(2S+1)L(J)	W.NO.	B.V.NO.		
1			(1)0(0.0)	0.	918657.	0.0000000	
1	2S2		(3)1(0.0)	81939.	836718.	0.7466847	
2	2S1 2P1		(3)1(1.0)	82075.	836582.	0.7479240	
3	2S1 2P1		(3)1(2.0)	82382.	836275.	0.7507216	
4	2S1 2P1		(1)1(1.0)	158798.	759859.	1.4470769	
5	2S1 2P1		(3)1(0.0)	213459.	705198.	1.9451857	
6	2P2		(3)1(1.0)	213615.	705042.	1.9466073	
7	2P2		(3)1(2.0)	213884.	704773.	1.9490586	
8	2P2		(1)2(2.0)	231721.	686936.	2.1116016	
9	2P2		(1)0(0.0)	287910.	630747.	2.6236346	
10	2P2		(3)0(1.0)	546969.	371688.	4.9843589	
11	3S1		(1)1(1.0)	561276.	357381.	5.1147342	
12	2S1 3S1		(3)1(0.0)	580825.	337832.	5.2928782	
13	2S1 3P1		(3)1(1.0)	582803.	335854.	5.3109031	
14	2S1 3P1		(3)1(2.0)	582840.	335817.	5.3112402	
15	2S1 3P1		(3)2(1.0)	582917.	335740.	5.3119419	
16	2S1 3D1		(3)2(1.0)	600746.	317911.	5.4744084	
17	2S1 3D1		(3)2(2.0)	600756.	317901.	5.4744995	
18	2S1 3D1		(3)2(3.0)	600776.	317881.	5.4746845	
19	2S1 3D1		(1)2(2.0)	612616.	306041.	5.5825797	
20	2S1 3D1						

Table 6a

METASTABLE LEVEL DESIGNATION, NUMBER = 4

1 2 3 4

ELECTRON TEMPERATURES

6.00D+04 8.00D+04 1.00D+05 1.50D+05 2.00D+05 4.00D+05 6.00D+05 8.00D+05

PROTON TEMPERATURES

6.00D+04 8.00D+04 1.00D+05 1.50D+05 2.00D+05 4.00D+05 6.00D+05 8.00D+05

ELECTRON DENSITIES

1.00D+09 5.00D+09 1.00D+10 5.00D+10 1.00D+11 5.00D+11 1.00D+12 5.00D+12

PROTON DENSITIES

0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00

Table 6b

EQUILIBRIUM METASTABLE POPULATION DEPENDENCE ON DENSITY AT $T_e = 6.000 \pm 0.04$

IMEF	1	2	3	4
1	1.00000+00	1.00000+00	1.00000+00	1.00000+00
2	1.40190-02	1.45310-02	1.51460-02	1.57220-02
3	4.26220-04	2.12270-03	4.21860-03	2.83520-01
4	7.98670-02	8.24320-02	8.54010-02	4.78160-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

1.00000+00
1.00000+00
3.03660-01
5.06480-01

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 1

10RD	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	8.95590-10	4.47800-09	8.95590-09	4.47800-08	8.95590-08	4.47790-07	8.95580-07	4.47760-06	8.95460-06	4.47460-05	8.95360-05	4.47360-04	8.95260-04	4.47160-03	8.95060-03	4.46960-02	8.94860-02	4.46760-01	8.94660-01	4.46560-01
2	5.57980-14	2.78990-13	5.57980-13	2.79000-12	5.58010-12	2.79080-11	5.58360-11	2.79960-10	5.61350-10	2.88730-09	5.68360-09	2.94470-08	5.73330-08	2.99470-07	5.88480-07	2.99420-06	5.88420-05	2.99320-04	5.88220-03	2.98120-02
3	1.62880-13	8.14400-12	1.62880-12	8.14430-11	1.62890-11	8.14670-11	1.62990-10	8.17170-10	1.63990-09	8.42310-09	1.63990-09	8.42310-08	1.63990-07	8.42310-06	1.63990-05	8.42310-04	1.63990-03	8.42310-02	1.63990-01	8.42310-01
4	2.77180-13	1.38590-12	2.77180-12	1.38590-11	2.77200-11	1.38630-10	2.77360-10	1.39040-09	2.78990-09	1.43140-08	2.78990-09	1.43140-08	2.78990-07	1.43140-06	2.78990-05	1.43140-04	2.78990-03	1.43140-02	2.78990-01	1.43140-01
5	2.48790-11	1.20400-10	2.48800-10	1.20400-09	2.48810-09	1.20440-08	2.48840-08	1.20480-07	2.42880-07	1.25590-06	2.42880-07	1.25590-06	2.42880-05	1.25590-04	2.42880-03	1.25590-02	2.42880-01	1.25590-01	1.25590-01	1.25590-01
6	2.23810-13	1.11910-12	2.23820-12	1.11910-11	2.23840-11	1.11980-10	2.24100-10	1.12620-09	2.26670-09	1.19050-08	2.26670-09	1.19050-08	2.26670-07	1.19050-06	2.26670-05	1.19050-04	2.26670-03	1.19050-02	2.26670-01	1.19050-01
7	2.83470-17	1.41740-16	2.83470-16	1.41740-15	2.83470-15	1.41740-14	2.83470-14	1.41740-13	2.83470-13	1.41740-12	2.83470-13	1.41740-12	2.83470-11	1.41740-10	2.83470-09	1.41740-08	2.83470-07	1.41740-06	2.83470-05	1.41740-04
8	5.16400-10	2.57750-09	5.16400-09	2.57780-08	4.94960-08	2.51930-07	3.59350-07	8.10180-07	9.60870-07	1.12880-06	9.60870-07	1.12880-06	9.60870-05	1.12880-04	9.60870-03	1.12880-02	9.60870-01	1.12880-01	1.12880-01	1.12880-01
9	4.69660-17	2.34830-16	4.69660-16	2.34830-15	4.69660-15	2.34830-14	4.69660-14	2.34830-13	4.69660-13	2.34830-12	4.69660-13	2.34830-12	4.69660-11	2.34830-10	4.69660-09	2.34830-08	4.69660-07	2.34830-06	4.69660-05	2.34830-04
10	1.47800-12	7.38080-12	1.47730-11	7.37230-11	1.47890-10	7.21480-10	1.47890-09	5.94470-09	9.94420-09	2.15350-08	9.94420-09	2.15350-08	9.94420-07	2.15350-06	9.94420-05	2.15350-04	9.94420-03	2.15350-02	9.94420-01	2.15350-01
11	1.30190-14	6.50960-14	1.30190-13	6.50950-13	1.30190-12	6.50910-12	1.30170-11	6.50480-11	1.30000-10	6.46200-09	1.30000-10	6.46200-09	1.30000-08	6.46200-07	1.30000-06	6.46200-05	1.30000-04	6.46200-03	1.30000-02	6.46200-01
12	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07	1.43520-07
13	2.48680-18	1.24340-17	2.48680-17	1.24340-16	2.48680-16	1.24340-15	2.48680-15	1.24340-14	2.48680-14	1.24340-13	2.48680-14	1.24340-13	2.48680-12	1.24340-11	2.48680-10	1.24340-09	2.48680-08	1.24340-07	2.48680-06	1.24340-05
14	4.17830-18	2.08910-17	4.17830-17	2.08910-16	4.17830-16	2.08910-15	4.17830-15	2.08910-14	4.17830-14	2.08910-13	4.17830-14	2.08910-13	4.17830-12	2.08910-11	4.17830-10	2.08910-09	4.17830-08	2.08910-07	4.17830-06	2.08910-05
15	5.75630-18	2.87810-17	5.75630-17	2.87810-16	5.75630-16	2.87810-15	5.75630-15	2.87810-14	5.75630-14	2.87810-13	5.75630-14	2.87810-13	5.75630-12	2.87810-11	5.75630-10	2.87810-09	5.75630-08	2.87810-07	5.75630-06	2.87810-05
16	2.33880-17	1.16900-16	2.33880-16	1.16900-15	2.33880-15	1.16900-14	2.33880-14	1.16900-13	2.33880-13	1.16900-12	2.33880-13	1.16900-12	2.33880-11	1.16900-10	2.33880-09	1.16900-08	2.33880-07	1.16900-06	2.33880-05	1.16900-04

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 2

10RD	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	8.35260-11	4.17630-10	8.35260-10	4.17630-09	8.35260-09	4.17630-08	8.35260-08	4.17620-07	8.35240-07	4.17570-06	8.35240-07	4.17570-06	8.35240-05	4.17570-04	8.35240-03	4.17570-02	8.35240-01	4.17570-01	4.17570-01	4.17570-01
2	9.43230-12	4.71620-11	9.43230-11	4.71620-10	9.43230-10	4.71620-09	9.43230-09	4.71620-08	9.43230-08	4.71620-07	9.43230-08	4.71620-07	9.43230-06	4.71620-05	9.43230-04	4.71620-03	9.43230-02	4.71620-01	9.43230-01	9.43230-01
3	1.10450-09	5.52240-08	1.10450-08	5.52240-07	1.10450-07	5.52230-06	1.10450-06	5.52160-05	1.10410-05	5.51360-04	1.10410-05	5.51360-04	1.10410-04	5.51360-03	1.10410-02	5.51360-01	1.10410-01	5.51360-01	5.51360-01	5.51360-01
4	1.27340-11	6.36690-10	1.27340-10	6.36700-09	1.27340-09	6.36770-08	1.27370-08	6.37430-08	1.27630-07	6.44070-07	1.27630-07	6.44070-07	1.27630-06	6.44070-05	1.27630-04	6.44070-03	1.27630-02	6.44070-01	6.44070-01	6.44070-01
5	9.94770-11	4.97390-10	9.94770-10	4.97390-09	9.94770-09	4.97380-08	9.94760-08	4.97350-07	9.94640-07	4.97850-06	9.94640-07	4.97850-06	9.94640-05	4.97850-04	9.94640-03	4.97850-02	9.94640-01	4.97850-01	4.97850-01	4.97850-01
6	2.46510-13	1.23260-12	2.46510-12	1.23260-11	2.46520-11	1.23270-10	2.46570-10	1.23390-09	2.47070-09	1.24630-08	2.47070-09	1.24630-08	2.47070-07	1.24630-06	2.47070-05	1.24630-04	2.47070-03	1.24630-02	2.47070-01	1.24630-01
7	3.07620-16	1.53810-15	3.07620-14	1.53810-14	3.07620-14	1.53810-13	3.07620-13	1.53810-12	3.07620-12	1.53810-11	3.07620-12	1.53810-11	3.07620-10	1.53810-09	3.07620-08	1.53810-07	3.07620-06	1.53810-05	3.07620-04	1.53810-03
8	8.99460-11	4.48940-10	8.99460-10	4.48940-09	8.99460-09	4.48940-08	8.99460-08	4.48940-07	8.99460-07	4.48940-06	8.99460-07	4.48940-06	8.99460-05	4.48940-04	8.99460-03	4.48940-02	8.99460-01	4.48940-01	4.48940-01	4.48940-01
9	6.98300-17	3.34920-16	6.98300-16	3.34920-15	6.98300-15	3.34920-14	6.98300-14	3.34920-13	6.98300-13	3.34920-12	6.98300-13	3.34920-12	6.98300-11	3.34920-10	6.98300-09	3.34920-08	6.98300-07	3.34920-06	6.98300-05	3.34920-04
10	2.08920-10	1.04440-09	2.08920-09	1.04440-08	2.08920-08	1.04440-07	2.08920-07	1.04440-06	2.08920-06	1.04440-05	2.08920-06	1.04440-05	2.08920-04	1.04440-03	2.08920-02	1.04440-01	2.08920-01	2.08920-01	2.08920-01	2.08920-01
11	8.38810-14	4.19410-13	8.38810-13	4.19410-12	8.38810-12	4.19410-11	8.38810-11	4.19410-10	8.38810-10	4.19410-09	8.38810-11	4.19410-09	8.38810-08	4.19410-07	8.38810-06	4.19410-05	8.38810-04	4.19410-03	8.38810-02	4.19410-01
12	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07	9.42860-07
13	2.98730-16	1.49370-15	2.98730-15	1.49370-14	2.98730-14	1.49370-13	2.98730-13	1.49370-12	2.98730-12	1.49370-11	2.98730-12	1.49370-11	2.98730-10	1.49370-09	2.98730-08	1.49370-07	2.98730-06	1.49370-05	2.98730-04	1.49370-03
14	2.26510-17	1.13260-16	2.26510-16	1.13260-15	2.26510-15	1.13260-14	2.26510-14	1.13260-13	2.26510-13	1.13260-12	2.26510-13	1.13260-12	2.26510-11	1.13260-10	2.26510-09	1.13260-08	2.26510-07	1.13260-06	2.26510-05	1.13260-04
15	2.36090-17	1.18040-16	2.36090-16	1.18040-15	2.36090-15	1.18040-14	2.36090-14	1.18040-13	2.36090-13	1.18040-12	2.36090-13	1.18040-12	2.36090-11	1.18040-10	2.36090-09	1.18040-08	2.36090-07	1.18040-06	2.36090-05	1.18040-04
16	5.93990-17	2.96990-16	5.93990-16	2.96990-15	5.93990-15	2.96990-14	5.93990-14	2.96990-13	5.93990-13	2.96990-12	5.93990-13	2.96990-12	5.93990-11	2.96990-10	5.93990-09	2.96990-08	5.93990-07	2.96990-06	5.93990-05	2.96990-04

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 3

POP	1	5	8.09860-11	4.04530-10	8.09860-09	4.04530-08	8.09860-07	4.04530-06	8.09860-05	4.04530-04	8.09860-03	4.04530-02	8.09860-01	4.04530-00
1	1	5	8.09860-11	4.04530-10	8.09860-09	4.04530-08	8.09860-07	4.04530-06	8.09860-05	4.04530-04	8.09860-03	4.04530-02	8.09860-01	4.04530-00
2	2	6	3.02110-10	1.91060-09	3.82110-08	1.91060-07	3.82110-06	1.91060-05	3.82110-04	1.91060-03	3.82110-02	1.91060-01	3.82110-00	1.91060-00
3	3	7	2.79280-10	1.39640-09	2.79280-08	1.39640-07	2.79280-06	1.39640-05	2.79280-04	1.39640-03	2.79280-02	1.39640-01	2.79280-00	1.39640-00
4	4	8	4.96370-10	2.48480-09	4.96370-08	2.48480-07	4.96370-06	2.48480-05	4.96370-04	2.48480-03	4.96370-02	2.48480-01	4.96370-00	2.48480-00
5	5	9	9.13470-11	4.56740-10	9.13470-09	4.56740-08	9.13470-07	4.56740-06	9.13470-05	4.56740-04	9.13470-03	4.56740-02	9.13470-01	4.56740-00
6	6	10	2.36590-13	1.18350-12	2.36590-11	1.18350-10	2.36590-09	1.18350-08	2.36590-07	1.18350-06	2.36590-05	1.18350-04	2.36590-03	1.18350-02
7	7	11	3.13460-16	1.56730-15	3.13460-14	1.56730-13	3.13460-12	1.56730-11	3.13460-10	1.56730-09	3.13460-08	1.56730-07	3.13460-06	1.56730-05
8	8	12	4.9910-11	4.24210-10	8.46580-09	4.24210-08	8.46580-07	4.24210-06	8.46580-05	4.24210-04	8.46580-03	4.24210-02	8.46580-01	4.24210-00
9	9	13	6.98870-17	3.49030-16	6.98870-15	3.49030-14	6.98870-13	3.49030-12	6.98870-11	3.49030-10	6.98870-09	3.49030-08	6.98870-07	3.49030-06
10	10	14	9.37990-12	4.68900-11	9.37990-10	4.68900-09	9.37990-08	4.68900-07	9.37990-06	4.68900-05	9.37990-04	4.68900-03	9.37990-02	4.68900-01
11	11	15	6.99600-13	3.49800-12	6.99600-11	3.49800-10	6.99600-09	3.49800-08	6.99600-07	3.49800-06	6.99600-05	3.49800-04	6.99600-03	3.49800-02
12	12	16	9.81260-07	9.81260-06	9.81260-05	9.81260-04	9.81260-03	9.81260-02	9.81260-01	9.81260-00	9.81260-00	9.81260-00	9.81260-00	9.81260-00
13	13	17	8.44920-17	4.22460-16	8.44920-15	4.22460-14	8.44920-13	4.22460-12	8.44920-11	4.22460-10	8.44920-09	4.22460-08	8.44920-07	4.22460-06
14	14	18	2.23570-16	1.11790-15	2.23570-14	1.11790-13	2.23570-12	1.11790-11	2.23570-10	1.11790-09	2.23570-08	1.11790-07	2.23570-06	1.11790-05
15	15	19	2.57200-17	1.28600-16	2.57200-15	1.28600-14	2.57200-13	1.28600-12	2.57200-11	1.28600-10	2.57200-09	1.28600-08	2.57200-07	1.28600-06
16	16	20	5.62510-17	2.81260-16	5.62510-15	2.81260-14	5.62510-13	2.81260-12	5.62510-11	2.81260-10	5.62510-09	2.81260-08	5.62510-07	2.81260-06

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 4

POP	1	5	8.18170-11	4.09080-10	8.18170-09	4.09080-08	8.18170-07	4.09080-06	8.18170-05	4.09080-04	8.18170-03	4.09080-02	8.18170-01	4.09080-00
1	1	5	8.18170-11	4.09080-10	8.18170-09	4.09080-08	8.18170-07	4.09080-06	8.18170-05	4.09080-04	8.18170-03	4.09080-02	8.18170-01	4.09080-00
2	2	6	2.69680-12	1.34840-11	2.69680-10	1.34840-09	2.69680-08	1.34840-07	2.69680-06	1.34840-05	2.69680-04	1.34840-03	2.69680-02	1.34840-01
3	3	7	2.98280-10	1.49140-09	2.98280-08	1.49140-07	2.98280-06	1.49140-05	2.98280-04	1.49140-03	2.98280-02	1.49140-01	2.98280-00	1.49140-00
4	4	8	8.86340-10	4.43170-09	8.86340-08	4.43170-07	8.86340-06	4.43170-05	8.86340-04	4.43170-03	8.86340-02	4.43170-01	8.86340-00	4.43170-00
5	5	9	1.02310-10	5.14560-09	1.02310-08	5.14560-07	1.02310-06	5.14560-05	1.02310-04	5.14560-03	1.02310-02	5.14560-01	1.02310-00	5.14560-00
6	6	10	2.49120-13	1.24560-12	2.49120-11	1.24560-10	2.49120-09	1.24560-08	2.49120-07	1.24560-06	2.49120-05	1.24560-04	2.49120-03	1.24560-02
7	7	11	3.20560-16	1.60280-15	3.20560-14	1.60280-13	3.20560-12	1.60280-11	3.20560-10	1.60280-09	3.20560-08	1.60280-07	3.20560-06	1.60280-05
8	8	12	8.64720-11	4.31600-10	8.64720-09	4.31600-08	8.64720-07	4.31600-06	8.64720-05	4.31600-04	8.64720-03	4.31600-02	8.64720-01	4.31600-00
9	9	13	7.40420-17	3.70210-16	7.40420-15	3.70210-14	7.40420-13	3.70210-12	7.40420-11	3.70210-10	7.40420-09	3.70210-08	7.40420-07	3.70210-06
10	10	14	9.72230-12	4.86020-11	9.72230-10	4.86020-09	9.72230-08	4.86020-07	9.72230-06	4.86020-05	9.72230-04	4.86020-03	9.72230-02	4.86020-01
11	11	15	8.43070-14	4.21530-13	8.43070-12	4.21530-11	8.43070-10	4.21530-09	8.43070-08	4.21530-07	8.43070-06	4.21530-05	8.43070-04	4.21530-03
12	12	16	5.13610-06	5.13610-05	5.13610-04	5.13610-03	5.13610-02	5.13610-01	5.13610-00	5.13610-00	5.13610-00	5.13610-00	5.13610-00	5.13610-00
13	13	17	1.32840-17	6.64180-16	1.32840-15	6.64180-14	1.32840-13	6.64180-12	1.32840-11	6.64180-10	1.32840-09	6.64180-08	1.32840-07	6.64180-06
14	14	18	6.19940-17	3.09970-16	6.19940-15	3.09970-14	6.19940-13	3.09970-12	6.19940-11	3.09970-10	6.19940-09	3.09970-08	6.19940-07	3.09970-06
15	15	19	2.60740-16	1.30370-15	2.60740-14	1.30370-13	2.60740-12	1.30370-11	2.60740-10	1.30370-09	2.60740-08	1.30370-07	2.60740-06	1.30370-05
16	16	20	6.00170-17	3.00090-16	6.00170-15	3.00090-14	6.00170-13	3.00090-12	6.00170-11	3.00090-10	6.00170-09	3.00090-08	6.00170-07	3.00090-06

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PRINTED IN ENGLAND
