7. ATOMIC ISSUES

[Edited by Helen Mason, Cambridge]

CDS and SUMER will be used to derive information on the nature of the solar atmosphere by utilising different spectroscopic diagnostics. We plan to obtain temperature and density determinations, emission measure distributions and elemental abundance variations from intensity ratios of spectral lines for sequences of ions; to extract flow patterns and information on non-thermal broadenings from spectral line profiles. Even assuming a perfect calibration for the instruments, we must be aware that the reliability of these techniques depends on our understanding of the atomic physics processes and the accuracy of the atomic data used. Thus, we regard the assessment of atomic data and an investigation of spectroscopic diagnostics as high priorities for CDS and SUMER. For these studies, several atomic physics issues need to be specifically addressed.

7.1 Introduction

CDS is one of the very few instruments that have been designed from the beginning with the primary purpose of determining the physical parameters of the solar atmosphere from measurements of spectral intensities. Together with SUMER and UVCS a very wide spectral range will be covered (151Å to 1600Å) and this will require for its interpretation a correspondingly large amount of reliable atomic data.

An UV spectroscopic diagnostics working group of CDS and SUMER co-investigators and associated scientists (co-ordinator, Helen Mason) is addressing these issues and preparing relevant diagnostic techniques and software. The topics covered include electron density and temperature determination, differential emission measures, elemental abundance variations and basic atomic data - energy levels, radiative data, electron and proton excitation, ionisatio, recombination and charge exchange. Central to the analysis software is the Atomic Data and Analysis Structure (ADAS), which is an interconnected set of computer programs and data collections

for modelling the radiating properties of ions and atoms in plasmas, and for assisting in the analysis and interpretation of spectral measurements. It was developed at JET under the leadership of Hugh Summers (see Summers 1994). A consortium of European and US laboratories, including CDS and SUMER PI laboratories has been formed to port ADAS from the JET IBM mainframe to Unix workstations. See URL http://phys.strath.ac.uk/adas/ on World Wide Web for further detailed information on ADAS.

A review of VUV (100-2000Å) spectroscopic diagnostics for solar and stellar plasmas has recently been published by Mason and Monsignori Fossi (1994). It covers past, present and future observations; plasma diagnostics for optically thin emission lines; atomic processes; recent developments in atomic calculations. Another useful review directly relating to CDS/SUMER diagnostics has been published by Dwivedi (1994).

7.2 Emission line intensities

We are concerned with atomic processes in a hot $(T = 2 \times 10^4 - 10^7$ K$)$ and low density $(N_e < 10^{13} cm^{-3})$ plasma. We assume that the spectral lines are optically thin, which is valid for the outer atmosphere of the Sun. The line emissivity (per unit volume, per unit time) for an optically thin spectral line of wavelength λ_{ij} is given by

$$\varepsilon_{\lambda ij} = N_j A_{ji} \qquad [\text{photons cm}^{-3} \text{ s}^{-1}] \qquad (7.1)$$

where i, j are the lower and upper levels, A_{ji} is the spontaneous transition probability and N_j is the number density of the upper level, j, of the emitting ion.

The emission line intensity, per unit time, per unit solid angle, from a volume V, is then

$$I(\lambda_{ij}) = (1/4\pi) \int_{vol} \varepsilon_{\lambda ij} \, dV \qquad [\text{photons s}^{-1}\text{ster}^{-1}] \qquad (7.2)$$

In low density plasmas the collisional excitation processes are generally faster than ionisation and recombination timescales, therefore the collisional excitation is dominant over ionisation and recombination in populating the excited states. This allows the low lying level populations to be treated separately from the ionisation and recombination processes.

7.3 The Coronal Model Approximation

In the *coronal model* approximation it is assumed that the upper level, j, of the ion X^{+m} is populated via electron collisional excitation from the ground state, g, and that the radiative decay overwhelms any other depopulation process. Thus, assuming equilibrium, we may write

$$N_g(X^{+m}) \, N_e \, C^e_{gj} = N_j(X^{+m}) \, \Sigma_k \, A_{jk} \quad (k<j) \qquad (7.3)$$

Here, the sum of the transition probabilities (the A values) takes account of the possibility that the excited ion may be able to decay radiatively by more than one route. The electron collisional excitation rate coefficient, C^e_{gj}, for a Maxwellian electron velocity distribution with a temperature T_e (K), is given by

$$C^e_{ij} = \frac{8.63\ 10^{-6}}{T_e^{1/2}} \frac{\Upsilon_{ij}(T_e)}{\omega_i} \exp(-\Delta E_{ij} / kT_e) \qquad (7.4)$$

where ΔE_{ij} is the energy difference between levels i and j; ω_i is the statistical weight of level i; k is the Boltzmann constant and Υ_{ij} is the thermally-averaged collision strength,

$$\Upsilon_{ij}(T_e) = \int_0^\infty \Omega_{ij}\ exp\ (-E_j/kT_e)\ d(E_j/kT_e) \qquad (7.5)$$

Here the collision strength Ω is a symmetric, dimensionless quantity, which is related to the electron excitation cross-section; E_j is the energy of the scattered electron relative to the final energy state of the ion.

The population of level g can be expressed as

$$N_g\left(X^{+m}\right) = \frac{N_g(X^{+m})}{N(X^{+m})} \frac{N(X^{+m})}{N(X)} \frac{N(X)}{N(H)} \frac{N(H)}{N_e} N_e \qquad (7.6)$$

Here, $N(X^{+m})/N(X)$ is the ionisation ratio of the ion X^{+m} relative to the total number density of element X. It is usual to assume that the plasma has had time to relax to its steady-state value in which case the ratio is simply a function of temperature, ignoring its slight dependence on density in this approximation. $N(X)/N(H)$ is the elemental abundance Ab(Z); $N(H)/N_e$ is the Hydrogen abundance which is usually assumed to be around 0.8. For allowed transitions (electric dipole), the radiative decay rates are very large ($10^{10}s^{-1}$) compared to the electron excitation rates, so the population of the upper level, N_j is negligible in comparison with the ground level, g, i.e $N_g(X^{+m})/N(X^{+m}) \approx 1$.

From the equations above, we find that the intensity of an optically thin spectral line from a low density plasma integrated over a volume V, is given by

$$I(\lambda_{ij}) = (1/4\pi)\ Ab(Z) \int_{vol} G(T)\ N_e^2\ dV \qquad [\text{photons s}^{-1}\text{ster}^{-1}]\ (7.7)$$

where G(T) contains all of the atomic physics parameters relevant to the transition between levels j and i in the ion X^{+m}. Generally the function G(T), called the *contribution function*, is strongly peaked in temperature. It is given by

$$G(T) = \frac{N(H)}{N_e} \; \frac{N(X^{+m})}{N(X)} \; C^e_{gj} \; \frac{A_{jg}}{S_k \, A_{jk}} \qquad [\text{cm}^3 \, \text{s}^{-1}] \qquad (k < j) \qquad (7.8)$$

We have considered a very simple system in equilibrium. If a radiative transition probability is small, other mechanisms can de-excite the upper level. For example, for forbidden or intersystem transitions, the electron de-excitation rate may become larger than the radiative decay rate as electron density increases. Eventually, at high enough densities, the populations of the upper and lower levels are in statistical equilibrium. A level which has a significant population relative to the ground level is called a *metastable level.* Other levels in the ion can be excited from these metastable levels. In practice the level populations $N_j(X^{+m})/N(X^{+m})$ are determined by solving the statistical equilibrium equations for a number of low lying levels of the ion including all the important collisional and radiative excitation and de-excitation mechanisms,

$$N_j (N_e \, \Sigma_i \, C^e_{ji} + N_p \, \Sigma_i \, C^p_{ji} + \Sigma_{i>j} \, R_{ji} + \Sigma_{i<j} \, A_{ji}) = \Sigma_i \, N_i \, (N_e C^e_{ij} + N_p C^p_{ij}) +$$
$$\Sigma_{i>j} \, N_i \, A_{ij} + \Sigma_{i<j} \, N_i \, R_{ij} \qquad (7.9)$$

with C^e_{ji} and C^p_{ji} the electron and proton collisional excitation rate coefficients (in $\text{cm}^{-3}\text{s}^{-1}$), R_{ji} the stimulated absorption rate coefficient (s^{-1}) and A_{ji} the spontaneous radiation transition probability (s^{-1}).

The atomic contribution function (equation 7.8) can be written as

$$G(T) = \frac{N(H)}{N_e} \; \frac{N(X^{+m})}{N(X)} \; [\sum_g \frac{N_g}{N(X^{+m})} \, C_{gj}] \; \frac{A_{ji}}{\Sigma_k \, A_{jk}} \qquad \text{cm}^3 \, \text{s}^{-1} \qquad (7.10)$$

The factor inside the square brackets represents the collisional excitation processes where account is taken of excitation from metastable levels as well as the ground level.

7.4 Differential Emission Measure Analyses

The emission measure is basically a measure of the amount of plasma as a function of temperature and it is the primary characteristic which any theoretical model should predict. Following Pottasch (1964), techniques have been developed to determine the distribution of plasma as a function of temperature from the UV and X-ray lines.

If one assumes that the spectral line is emitted from a volume V, over a temperature range ΔT around the temperature T_{max} corresponding to the peak value of its contribution function G(T) and that the contribution function is constant over this temperature range at 0.7 $G(T_{max})$ then the intensity can be expressed as:

$$I (\lambda_{gj}) = \frac{1}{4\pi} \; \frac{N(H)}{N_e} \; \frac{N(X)}{N(H)} \; <\text{EM}> \, 0.7 \, G(T_{max}) \; \Delta T \qquad (7.11)$$

where average volume emission measure $\langle EM \rangle$ for that spectral line is defined as:

$$\langle EM \rangle \ = \ \int_V N_e^2 \, dV \qquad\qquad (7.12)$$

This method is used to derive the $\langle EM \rangle$ as a function of temperature using lines emitted for a wide range of values of T_{max}. The average electron density can be crudely deduced assuming that the spectral line is emitted over a homogeneous, isothermal volume estimated from images at that temperature.

More sophisticated methods involve re-writing equation 7.7 in the form

$$I\,(\lambda_{ij}) = \ (1/4\pi)\, Ab(Z) \int_T G(T)\ \varphi(T)\, dT \qquad [\text{photons cm}^{-2}\, \text{s}^{-1}\text{ster}^{-1}] \qquad (7.13)$$

where the intensity is integrated over a volume of unit area along the line of sight, h, and the differential emission measure (DEM) function is defined as

$$\varphi(T) \ = \ N_e^2 \, dh/dT. \qquad\qquad (7.14)$$

The DEM relates to the amount of material in the temperature interval T to T+dT and the temperatue gradient along the line of sight. Often, it is more convenient to express the DEM on a $Log_{10}T_e$ scale. To derive the DEM from the observations one must solve a set of integral equations. The problem, given a set of spectral intensities, I, values of the abundances Ab(Z), and the atomic physics functions G(T), is to invert the integral written above to derive information about the structure of the atmosphere $\varphi(T)$. The inversion problem itself is not simple and requires some assumptions about the nature of the solution.

A series of workshops was sponsored by the SOHO teams to study differential emission measure techniques and in particular the inversion of the intensity integral. These meetings were organised by Richard Harrison and Peter McWhirter. Several groups working on this problem met at Cosener's House, Abingdon in November 1990 (Glasgow, MSSL, Arcetri, RAL, Cambridge, Lindau, Oxford, Wroclaw). The plan was to first compare the available methods by analysis of the same data-set provided from the CHASE experiment observations (Lang et al. 1990). The first meeting comprised discussion of this comparison and of the available methods themselves. A method assessment exercise was performed in the lead up to a second meeting in April 1991. For this exercise some dummy differential emission measures were constructed and line intensities calculated from them. The line intensities were distributed to the participating groups and their ability to reconstruct the known differential emission measures was studied. The results and a full description of the methods are beyond the scope of this report and are discussed in a RAL Report edited by Richard Harrison and Alan Thompson (1992). It is clear that mathematically the problem here is not well defined and that a wide range of solutions are possible. The different codes all eventually gave consistent results, but the DEM derived depends rather critically on the methods used to constrain the solution and the errors in the

observed intensities and atomic data. Attention must be given to the error analysis procedure. For SOHO, some of these DEM routines are being automated and prepared for implementation into the diagnostic software.

The advantage of the differential emission measure method is that it allows one to derive from a set of spectral line intensities an empirical model of the plasma from which the lines are emitted without the need for a detailed model. In order to make this possible it is necessary to adopt a number of underlying assumptions:

(i) The plasma should be optically thin in the lines observed. For lines from neutral atoms and even some ions of charge one this assumption is not tenable and for them it is necessary to solve the equation of radiative transfer. For lines of higher charge, i.e. lines excited in higher temperature regions, the optically thin assumption is better although there is evidence that while all are effectively thin, some show redistribution in a direction determined by the physical shape of the plasma and the direction of viewing. Thus the branching ratio between line pairs from the same upper level are found to depart from the ratio of the transition probabilities. It may be possible to take account of this effect by a slight modification to the emission measure procedure. It may even be possible to take advantage of the effect to deduce additional information about the structure of the plasma.

(ii) The element abundances are assumed to be constant over the full depth of the plasma. There is growing observational evidence that for the solar plasmas of interest here this is not so - and in any case there are well established physical processes that cause separation of the ions depending on their mass and charge, such as thermal diffusion and the long mean-free paths of solar coronal ions.

(iii) It is assumed that the plasma is in steady-state of ionization balance. The time it takes a plasma to reach the steady-state after some disturbance can be estimated as: $\tau = 10^{12}/N_e$. For ions in the solar corona where the electron density is about 10^8cm^{-3}, $\tau \approx 0.5$ hour. Thus it is very likely that for some of the high temperature ions seen in solar plasmas there will not have been time for the steady-state to have been established. Time dependent observations may help to resolve this problem.

We also assume that (i) there is a Maxwellian electron distribution, (ii) that all atomic processes have been included, (iii) that the atomic data are of adequate accuracy, (iv) that the observations include a good intensity calibration, and (v) that we have a reliable means of inverting the intensity integral.

In the usual way in which they are applied, the assumption is made that the plasma emitting the lines whose ratio is used for either temperature or density diagnostics is uniform in both temperature and density. With the differential emission measure method it is not necessary to make this assumption. Thus the intensity ratio between two lines sensitive to temperature may be expressed:

$$I_1/I_2 \ = \ (\textstyle\int G_1(T) \ \varphi(T) \ dT)/(\int G_2(T) \ \varphi(T) \ dT) \qquad\qquad (7.15)$$

This expression is independent of the value of Ab(Z) if the lines are of from the same element, and also independent of the absolute value of $\varphi(T)$. It may be used to derive an averaged value of T but possibly more usefully the value of the slope $d\varphi(T)/dT$ in the region where the G(T) functions have their peaks.

In those cases where the ratio of the population density of the metastable to ground levels is sensitive to electron density (i.e. where there is the possibility of a density diagnostic) the G(T) functions are functions also of N_e. In order to proceed it is necessary to make some assumption about the relation between density and temperature. A natural one is that the plasma pressure is constant over the relatively restricted range of temperature where the lines are emitted so that $N_e = <N_eT>/T$. The line ratio may then be expressed as

$$I_1^{<NeT>} / I_2^{<NeT>} = G_1^{<NeT>}(T) \; \phi(T) \; dT \; / \; G_2^{<NeT>}(T) \; \phi(T) \; dT \qquad (7.16)$$

In this case a measure of the line intensity ratio may be used to derive the value of $<N_eT>$ in the region where the G(T) functions have their peaks.

The discussion above is concerned with spectral line emission. CDS will also view the continuum from free-free and free-bound collisons (Bremsstrahlung and radiative recombination) as well as two-photon decay. In this case the intensity integral becomes

$$I(\lambda_{cont}) = (1/4\pi) \int G_\lambda(T) \; \varphi(T) \; dT \qquad [\text{photons cm}^{-2} \text{ s}^{-1} \text{ster}^{-1} \text{Å}^{-1}] \qquad (7.17)$$

This integral has a similar form to equation (7.13) but the G(T) function has a greater width in temperature space - about 50 times the width of a G(T) value associated with an emission line. Thus, G(T) and I are functions of λ. The greatest uncertainty lies in the G(T) due to the uncertainty of the He abundance. The continuum observations, combined with spectral line intensities can be used to obtain absolute intensities and, therefore the element abundances.

7.5 Elemental Abundance Determinations

There has been a great deal of discussion and controversy recently about variations in the elemental abundances in the solar atmosphere (Meyer, 1993). The details of these studies are beyond the scope of this report. One approach to determining element abundances is to calculate them simultaneously with the Differential Emission Measure (Fludra and Schmelz 1995). One can also use the detailed shape of the <EM> or DEM distribution for ions from the same element and apply an iterative procedure to normalising the curves for different elements. Another procedure is to use the intensity ratios for individual spectral lines which have very similar G(T) functions (Widing and Feldman, 1992). All the methods used depend rather critically on the assumed accuracy for the atomic data (Mason, 1992, 1995).

7.6 Diagnostic Line Ratios

7.6.1 Electron density diagnostics

The electron pressure, N_eT_e, is an important parameter in any theoretical model for the plasma, but why not simply deduce the electron density from the <EM> and an estimate of the emitting volume? This can and has been done in numerous analyses, however, it assumes that the emitting material is homogeneously distributed throughout the assumed volume. Our experience from solar observations is that the plasma is often in unresolved filamentary structures, even down to the best spatial resolution which has yet been obtained. At one extreme is the solar transition region, where only a very small fraction of the observed emitting volume is actually filled. The situation is a little better in the corona, but even here the filamentary nature of the emission is evident. The determination of electron density from spectral line intensity ratios from the same ion, makes no assumption about the size of the emitting volume or the element abundance value. It therefore provides a powerful and important diagnostic for the plasma conditions.

Spectral lines may be grouped into different categories according to the behaviour of the upper level population: allowed lines collisionally excited from the ground level (the coronal model); forbidden or intersystem lines originating from a metastable level; allowed lines excited from a metastable level.

For simplicity we again consider a simple two level model. For forbidden and intersystem transitions, where the radiative decay rate is generally very small (A_{mg} ~ 10^0 - 10^2 s^{-1}), collisional de-excitation then becomes an important depopulating mechanism (A_{mg} ~ $N_eC^e_{mg}$) and may even be the dominant mechanism; moreover the population of the metastable level becomes comparable with the population of the ground level and we have

$$N_m(X^{+m}) = (N_g(X^{+m}) N_e C^e_{gm}) / (C^e_{mg} + A_{mg}) \qquad (7.18)$$

For small electron densities $A_{mg} >> N_eC^e_{mg}$, then the intensity has the same dependence on the density as an allowed line, $I(\lambda_{mg}) \sim N_e^2$.

For very large values of electron density the collisional de-population dominates, $N_eC^e_{mg} >> A_{mg}$; the metastable level is in Boltzman equilibrium with the ground level: the line intensity has the form $I(\lambda_{mg}) \sim N_e$.

For intermediate values of electron density the intensity varies as $I(\lambda_{mg}) \sim N_e^{\alpha}$, where $1 < \alpha < 2$.

If the population of metastable level (m) is comparable with the ground level (g), then other excited levels (k) can be populated from this metastable level as well as from the ground level and the dependence of the intensity on electron density becomes $I(\lambda$
$_{k})$ ~ N_e^{β} where $2 < \beta < 3$

Since the intensities of different spectral lines within the same ion have a different dependence on the electron density, the ratio of the observed intensity ratio allows a determination of the average electron density for the emitting region. The dependence on the ionisation ratio, helium abundance, element abundance and emitting volume cancels. Most of the dependence on temperature also disappears although there sometimes remains a slight temperature sensitivity. A full discussion of these density diagnostic techniques is beyond the scope of this report . More details are given in elsewhere (cf Mason and Monsignori Fossi, 1994).

7.6.2 Electron temperature diagnostics

A determination of electron temperature can be obtained from the intensity ratio of two allowed lines excited from the ground level g but with significantly different excitation energy. The ratio is given by

$$I(\lambda_{gj}) / I(\lambda_{gk}) = (\Upsilon_{gj} / \Upsilon_{gk}) ((\Delta E_{gk} - \Delta E_{gj})/kT_e) \tag{7.19}$$

The ratio is sensitive to the change in electron temperature if $(\Delta E_{gk} - \Delta E_{gj})/kT_e \gg 1$ assuming that the lines are emitted by the same isothermal volume with the same electron density. Such spectral lines are far apart in wavelength and it may be necessary to use lines from different instruments. This gives rise to major uncertainties in the derived temperature due to the relative calibration of the intensities.

7.7 Spectral Line Profiles

Line shifts and broadenings give information about the dynamic nature of the solar atmosphere.

If the optically thin spectral lines can be fitted with Gaussian profiles, the intensity per unit wavelength is defined as

$$I_\lambda = (I/ \sqrt{2\pi} \sigma) \exp [- (\lambda-\lambda_0)2 / (2\sigma2)] \tag{7.20}$$

where I is the integrated intensity and σ is the Guassian width given by

$$\sigma2 = (\lambda2/2c2) (2kT/M) + \xi2 + \sigma_I2 \tag{7.21}$$

for a Maxwellian velocity distribution of temperature T, usually assumed to be the temperature corresponding to peak abundance of the ion. Here M is the ion mass, σ_I is the Gaussian instrumental width and ξ is the most probable non-thermal velocity.

7.8 Atomic Data Requirements

7.8.1 Energy levels, wavelengths and radiative data

It is suprising that the observed energy levels for some of the coronal ions (e.g. the iron ions) are not well known. The tables provided by NIST give a very good basic data-set, but it is sometimes necessary to supplement these with other laboratory measurements or even theoretical values. For refined techniques involving the measurement of Doppler shifts, it is necessary to know the rest wavelength of the spectral lines to a very high precision. This is a problem in particular for some of the transition region lines to be observed by SUMER.

Kelly's spectral line lists are available online, but these are rather too comprehensive and it is necessary to select those spectral lines which are likely candidates for different solar regions. This requires some estimates of the line intensities from synthetic spectra.

Until recently, it was thought that the available theoretical values for radiative decay rates for solar ions were very accurate (10% or better). However, recent laboratory measurements made at the Harvard Smithsonian Center for Astrophysics have thrown doubt on their accuracy, particularly for forbidden or intersystem transitions.

7.8.2 Electron collisional excitation and de-excitation

The line intensities and G(T) functions depend critically on an accurate knowledge of the electron excitation rates. The solution of the electron-ion scattering problem is complex and takes a great deal of computing resources. The accuracy of a particular calculation depends on two main factors. The first is the representation which is used for the target wavefunctions, the second is the type of scattering approximation chosen. The target must take account of configuration interaction and allow for intermediate coupling for the higher stages of ionization. The main approximations used for electron-ion scattering are Distorted Wave (DW), Coulomb Bethe (CBe) and the more elaborate Close-Coupling (CC) approximation. The DW approximation neglects the coupling of the channels (target + scattering electron). Since the scattering electron sees a central field potential, the DW approximation is only valid for systems which are a few times ionized. For high partial wave values of the incoming electron, the CBe approximation is valid, when it is assumed that the scattering electron does not penetrate the target. In the CC approximation, the scattering electron sees individual target electrons, the channels are coupled and a set of integro-differential equations are solved. The CC approximation is the most accurate. It is also the most expensive in terms of computing resources and it has sometimes been necessary to truncate the size of the target, i.e. the number of interacting configurations which are included. In general DW is thought to be accurate to about 25% and CC to better than 10%. Resonance structures, not calculated in the DW approximation, can contribute significantly to the excitation rates, particularly for forbidden and intersystem lines.

A semi-empirical formula commonly used in astrophysics is the effective Gaunt factor or g' approximation. This is based on the CBe approximation and relates the collision strength to the oscillator strength for electric dipole transitions:

$$\Omega_{ij} \; = \; (8\pi/\sqrt{3}) \; \omega_j \; f_{ij} \; (I_H/\Delta E_{ij}) \; g' \qquad (7.22)$$

It is a very crude approximation and should only be used when no calculations are available.

7.8.3 Atomic Data Assessment Study Group

Atoms and ions whose spectra will be observed by CDS or SUMER, or both, are given in Table 7.1. **C**, **S** or **CS** indicate a stage of ionisation of an element with a spectral line or lines lying in the wavelength range of CDS, SUMER or both and included in the electron excitation data assessment exercise (see below), while c, s or cs indicate a stage of ionisation of an element with a spectral line (or lines) lying in the wavelength ranges of CDS, SUMER or both but not included in the data assessment. A + indicates a stage of ionisation included in the data assessment. For CDS the lines lie mainly in isoelectronic sequences for elements up to oxygen while the lines observed only by SUMER are usually from low stages of ionisation of elements from magnesium to argon. Lines from ions heavier than nickel were not considered because of their low solar abundances. Some lines from very high ionisation stages of elements included in the table may be seen during solar flares.

Table 7.1: Atoms and Ions whose Spectra fall in the Wavelength Ranges Detected by CDS and SUMER (see text).

Spec.No.	H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar
I	S	CS	+	+	+	S	S	S	S	cs				s		s	s	s
II		CS	+	+	+	CS	CS	CS	+	CS				S	s	S	s	s
III			+	+	+	CS	CS	CS	+	CS	S		cs	S	s	S	s	s
IV				+	+	CS	CS	CS	+	CS	+	+	s	S	s	CS	s	s
V					+	+	CS	CS	+	CS	+	CS	+		s	s	s	
VI						+	+	CS	CS	CS	+	CS	+	+	s	cs		c
VII							+	+	+	CS	CS	CS	+	C	+		s	cs
VIII								+	+	CS	C	CS	C	CS	+	C		cs
IX									+	S	CS	CS	+	C	+	+	+	
X										+	+	CS	C	CS	+	CS	+	C
XI											+	+	CS	CS	+	CS	+	C
XII												+	+	CS	+	C	+	C
XIII													+	+	C	C	+	CS
XIV														+	+	C	+	C
XV															+	+	+	+
XVI																+	+	+
XVII																	+	+
XVIII																		+

Element: H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar

Spec.No.	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni
I								+		
II								S		s
III								S		
IV		c						+		
V								+		
VI								S		s
VII								+		
VIII		cs						C		
IX	cs	c						C		
X		cs						CS		c
XI	+							CS		
XII	+	+						CS		c
XIII	+	+	+			c		CS		c
XIV	+	C	+	+		c		C		c
XV	+	C	+	+	+			C		c
XVI	+	+	+	+	+	+		C		c
XVII	+	C	+	+	+	+	+	+		c
XVIII	+	+	+	+	+	+	+	+		c
XIX	+	+	+	+	+	+	+	C	+	
XX		+	+	+	+	+	+	+	+	+
XXI			+	+	+	+	+	CS	+	+
XXII				+	+	+	+	C	+	+
XXIII					+	+	+	C	+	+
XXIV						+	+	C	+	+
XXV							+	+	+	+
XXVI								+	+	+
XXVII									+	+
XXVIII										+

Element: K Ca Sc Ti V Cr Mn Fe Co Ni

The electron excitation rates required for SOHO spectra were the subject of an Atomic Data Assessment Workshop held in Abingdon, UK in March 1992. The

proceedings from this workshop, including individual reports and recommendations on all of the iso-electronic sequences of solar interest, are published as a single issue of Atomic Data and Nuclear Data Tables (editor J. Lang, 1994). The data assessment was performed by J. Callaway (H-like), J. Dubau (He-like), R.W.P. McWhirter (Li-like), K. Berrington (Be-Like), D.H. Sampson, L.H. Zhang and C.J. Fontes (B-like), B. Monsignori-Fossi and M. Landini (C-like), T. Kato (N-like), J. Lang and H.P. Summers (O-like) A.K. Bhatia (F-like), P. Dufton and A.E. Kingston (SiII-IV; SII-IV), A.K. Pradhan (FeI-VIII). H.E. Mason (FeIX-XIV), N.R. Badnell and D.L. Moores (FeXV-XVII). The assessors were asked to assess available data, identify work to be done, produce bibliographies etc... and summarize recommended data in similar formats (Υ's). The general conclusions of the workshop were that different approximations for calculating electron excitation rates are converging and the agreement with laboratory measurements is quite good. High accuracy calculations are available for ions with outer electrons in the n=1 or n=2 shells. Ions with outer electrons in the n=3 or n=4 shells are much more difficult to treat well (e.g. FeIX - FeXIV). It is essential to start with a good representation for the target. Time consuming work is in progress on the assessment and storage of electron excitation rates .

7.8.4 New electron scattering calculations

Prompted by the need for better electron excitation rates, several atomic physics groups are carrying out more accurate calculations. The Iron Project (Hummer et al. 1993), an international collaboration of atomic physicists, is calculating new electron excitation rates using the close coupling approximation, with very good targets including relativistic effects. The first stage is to compute collisional excitation rates for the fine structure transitions in the ground configuration of many ions. The second stage is to calculate new electron excitation rates for all the iron ions. A series of papers is being published in Astronomy and Astrophysics.

7.8.5 Proton collisional excitation and de-excitation

The proton collisional excitation and de-excitation rates must also be included. They become comparable with electron collisional processes only for transitions where $\Delta E_{ij} \ll kT_e$. This happens, for instance, for transitions between fine structure levels at high temperatures (Reid, 1988).

7.8.6 Ionisation and recombination processes

A major uncertainty in the calculation of the G(T) functions is variations in the different calculations of the ionisation ratios. This is clearly illustrated in the comparison between the recent calculations of Arnaud and Raymond (1992) with the earlier values of Arnaud and Rothenflug (1985). It can be seen that the temperature of peak ionisation fraction for individual ions is significantly different between the two sets of calculations. This is due to the incorporation of more recent ionisation and recombination rates. So far, results have only been published for the iron ions, so it is

not yet known what effect more accurate atomic data will have on ions from other elements.

The degree of ionisation of an element is obtained by equating the ionisation and recombination rates that relate successive stages of ionisation.

$$N^{+m} (q_{col} + q_{au} + q_{ct}) = N^{+m+1} (\alpha_r + \alpha_d + \alpha_{ct}) \qquad (7.23)$$

The dominant processes in optically thin plasmas are collisional ionization (direct ionization from the inner and outer shells) (q_{col}) and exicitation followed by autoionization (q_{au}); radiative recombination (α_r) and dielectronic recombination (α_d); and charge transfer (α_{ct} and q_{ct}).

Ionisation rates have several components: indirect prossesses via autoionising levels as well as direct outer and inner shell ionisation. A review of indirect processes in electron impact ionisation which covers both the theoretical and laboratory work has recently been written by Moores and Reed (1994). It is found that the structures in the ionisation cross sections are complex but that the agreement between theory and measurements is good.

Dielectronic recombination (DR) is the dominant recombination mechanism at high temperatures, at least a factor of 20 higher than radiative recombination. The DR rates for ions of solar interest have received much attention, in particular with relation to the formation of the satellite lines seen in the X-ray wavelength range. The available atomic data for these should be very accurate. A comparison with the much used Burgess' general formula gives agreement to within 30%. External electric fields can have an important effect on DR rates. Field ionization effects lead to a decrease in the DR rate coefficient, while field mixing effects lead to an increase in the DR rate coefficient.

Recent work of the Opacity Project (Cunto et al. 1993) provided new photo-excitation and photo-ionisation calculations for all of the astrophysically interesting ions. These data are available from a databank. The objective of this project was to calculate the opacity of stellar atmospheres.

7.8.7 Atomic Data Banks.

There is a need for data banks to meet two separate requirements. The first need is to store the results of the very sophisticated calculations in all their detail and is really for use by the atomic physics community (e.g., the Queen's University Belfast Databank). For this data bank where the emphasis is on quality there is a need to have regular meetings of atomic physics experts with a few from the user community to assess the material that it contains or should contain. The second is a users data bank where the aim is not so much to store the best data in detail but to cover the very wide needs of the user community, in providing both primary (e.g. effective collision strengths, ionisation rates) and derived quantities (e.g. ionisation balance, contribution

functions). This is being provided for CDS and SUMER by ADAS. The database requirements are:

(a) It must be up-datable -- a living thing. (b) It should contain routines to estimate data in situations where only an incomplete set is available -- such as iso-electronic interpolation. (c) It should contain a wide range of relevant data of a range of accuracies. (d) It should contain bench-mark data which is well known in the community rather than particularly accurate so that comparisons can be made in a meaningful way when new material becomes available. Another requirement of the bench-mark data is that there should be no ambiguity about its derivation. (e) It will be necessary to be able to manipulate source data to produce composite rate coefficients. These should include routines to do collisional-radiative calculations (f) It should be capable of meeting the needs of those who want to build sophisticated solar models taking account of time-dependence, opacity, diffusion etc. (g) It should provide e.g., reliable G(T) values and ionisation balance for those who don't want to be involved with detailed atomic physics matters.

7.9 CDS Scientific Software

CDS scientific software forms one component of the CDS ground software effort. This effort also includes data acquisition, processing, storage and handling, calibration applications, quick look and planning tools. The CDS Ground Software Leader is David Pike (RAL) and the bulk of the software effort has come from RAL, Oslo and GSFC. The majority of the ground software is written in IDL. Much of the scientific software will be derived from actions taken at meetings of the Atomic Data Assessment Group and the Integral Inversion Group.

The preparation work for CDS and SUMER requires the interfacing of solar analysis programs with the best available atomic data calculations. It is clear from recent work that using accurate ionisation and recombination rates can make a significant difference to ionisation balance calculations. In addition, better electron excitation rates are becoming available for many solar ions and these should be used in preference to estimated values. Assessing and assembling atomic data for the analysis of astrophysical plasma is major task. The core of the CDS scientific software development is the ADAS package, which provides an accurate method of atomic data analysis, storage and processing. It is a very powerful suite of programs, which can solve the collisional radiative model for equilibrium or non-equilibrium conditions. The most recent electron excitation rates are being input, together with high accuracy ionisation and recombination rates. ADAS will provide the G(T) functions, density and temperature diagnostic line ratios and ionisation ratios required for the solar analyses. This work is being co-ordinated by Hugh Summers and Jim Lang.

A synthetic spectrum code for UV wavelengths and for different solar models (quiet Sun, active region, coronal hole etc) is being developed by Ken Dere, Brunella Monsignori Fossi, Helen Mason and co-workers. The electron excitation rates are

fitted using the Burgess and Tully (1992) assessment method. These data will be available to the solar and astrophysics community via anonymous FTP.

A rapid and reliable procedure is being incorporated into the CDS software to invert the intensity integral and produce the DEM in a semi-automated way. Several methods are being considered, including codes by Alan Thompson and Andrzej Fludra.