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PUBL6: ADAS molecular population modelling for fusion plasmas

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Abstract: *An infra-structure for molecular collisional-radiative modelling of the radiating properties of molecules in the fusion plasma is created. Necessary data classes are defined and prepared to support this modelling. It parallels the organisation of ADAS for atoms and ions by introducing a new ADAS series 9: Molecular Collisional-Radiative Modelling. ADAS precedent is followed by the intrdouction of molecular data formats called mdf numbers. Coding is primarily in FORTRAN and IDL. There is an IDL-driven graphical user interface with a pedagogical capacity, for the interactive user as well as a background subroutine and procedure libraries for the off-line worker. The current release is restricted to* H_2.

Contents

Preface

This article is the one of a series of technical notes which are being prepared as useful extracts during the longer term construction of the next edition of the ADAS user manual. As such it reflects a change in style, planned for the new manual. It will be more book-like, examining and explaining in detail the physics basis behind the commitment to certain approaches in ADAS and how these work out in practice. The new manual will remain technically detailed with extended appendices. However, it is hoped this will be ameliorated by much more emphasis on worked examples. That is to say the actual manoeuvres, adopted by experienced ADAS users in getting the atomic modelling into application scenarios will be mapped, rather as an expert system. It has become clear that, for some, ADAS operates in a somewhat rarefied atmosphere in which too much is assumed. It is this which I wish to improve upon.

Inclusion of molecular data is a large new venture for the ADAS Project. ADAS over its more than thirty years of existence has remained focussed on atoms and ions. It has been primarily an atomic modelling system for the radiating properties of plasmas, which has prepared, assembled and if necessary calculated atomic data as necessary. These ADAS data collections have become very large and a primary source in the world. Although, up until now, not concerned with molecular data, molecular considerations have not been entirely absent from ADAS. Low energy charge transfer takes place through intermediate quasi-molecular states of the collision system, so it is molecular quantum theory experts who have assisted ADAS in these matters.

The molecular extension of ADAS is not simply a collection of molecular data for fusion in one place for the fusion user. ADAS is an modelling system and, true to itself, this extension is designed to be a molecular modelling system with its required data brought with it. It is though just the first step in this direction and should be viewed as such.

H P Summers
13 December 2012

Chapter 1

Introduction

1.1 Molecules in Plasmas

Molecular emission is an edge-localised phenomenon in the fusion plasma. The molecular species originate as the released species from plasma contacted surfaces, or possibly by active gaseous introduction. Historically, in older fusion devices, with limiters or relatively high temperature divertors, molecular species survived only very short distances into the plasma from their point of origin. Since these molecules rapidly catabolised to atoms and since the catabolic pathways to these atoms were often obscure, from a practical point of view, observational studies of influx of species into plasmas could begin with the atomic emission. There has been some change in this situation. Modern tokamaks, to handle the dual problems of high heat fluxes into divertors and the movement of released (possibly heavy) species back into the confined plasmas, have developed strategies of very low temperature divertor plasma regimes in which the survival of molecules is higher. Also, the plasma-surface interaction chemistry has become a central area of study and concern. The effectiveness of the heavily heated-loaded plasma contacted surface in restricting erosion, limiting tritium retention and so on are critical issues. Molecular species, observed in the plasma phase near these surfaces are contributors to the spectroscopic diagnostic tools for divertors. Because of the diagnostic interest in the

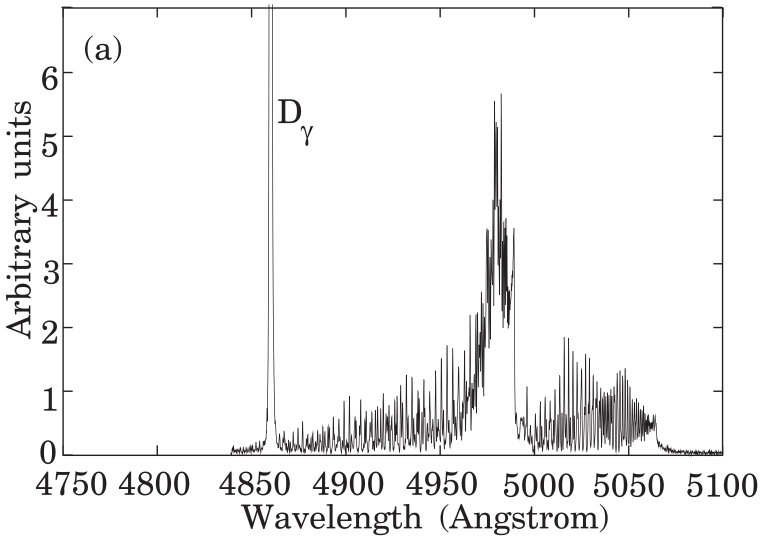


Figure 1.1: Observed spectrum of the 4850-5100Å region (JET Pulse #35687 at 14.5s) showing *BeD* ($A\ ^2\Pi - X\ ^2\Sigma$). The overlapping atomic line, D_β, is indicated [1].

localisation of molecular emission, spectral observation of molecules in fusion devices is usually conducted in the visible range. The available observables are low. Generally only diatomics are observed. For example, in the JET tokamak with variously carbon and beryllium surfaces, the species CD, CD^+, C_2, BeD and of course D_2 are regularly observed. One must also exepect the protium and tritium isotopic forms in active experiments and some other devices and also the mixed forms such as DT. Gaseous introduction of nitrogen may be evident as N_2. Other species, such as more complex hydrocarbons, are only rarely observed in tokamaks and are normally studied in special experiments such as divertor simulators.

A spectrum of the green bands of BeD observed at JET is shown in figure 1.1. Such a detailed band spectrum is on first sight encouraging. The hot 1-1 and 2-2 bands are readily observed. The beating between their slightly differently spaced P branch lines with those of the 0-0 band, and the well defined head in the P branch give a clear identification both of the carrier of the bands, and of the rotational temperature. Rotational and vibrational temperatures appear very similar ($T_r \sim T_v \sim 3500K$). More detailed studies on the localisation of this emission suggested that the emission was coming almost entirely from the strike zone, so that the molecule was emitting and probably breaking up almost on the surface, with no plasma phase chemistry. Also, inspite of the very clear and accurately predicted band-head structure, the differences between BeD and BeT probably precludes discrimination except at nearly 50% proportions. By contrast the Fulcher Band emission of D_2 is shown in figure 1.1. As deuterium is the primary plasma species in JET and most current tokamaks, while deuterium and tritium will be the fuel for the active phase of ITER, the D_2 *molecular system* comprising D, D^+, D_2, D_2^+ and D_3^+ is a central one for current modelling and diagnosis. As is evident in figure 1.1, there is a weak, very dispersed band spectrum arising from the strong coupling between the rotational and vibrational motion. Since the homonuclear molecule has no permanent dipole, there is no dipole matrix element between vibrational substates. These characteristics mean that population modelling cannot rely on the clear atomic time constant separations which simplify the atomic/ionic case in ADAS. Also, ion as well as electron collisions can be influential in the excitation and redistribution of molecules, while the addition of dissociative and attachment pathways removes the linearity of ionisation state modelling of trace atomic impurities. For these reasons, molecular modelling for ADAS must be substantially different in detail from that of its atomic/ionic modelling.

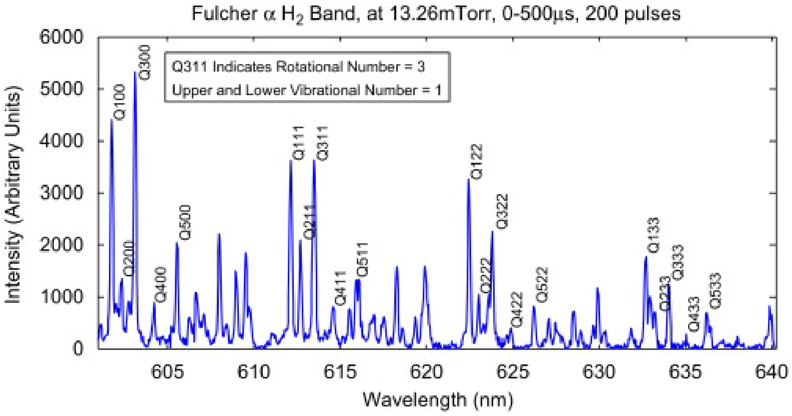


Figure 1.2: Composite spectrum of the D_2 Fulcher-α band emission at viewing chord 7, Pulse No's: 81271, 81272, 81274 bands (EFDA-JET report EFDA-JET-CP(12)02/12).

For spectral analysis of fusion plasma, it is the usual pattern to extract observed line-of-sight emissivities of single lines with simply fitted, usually Gaussian thermal, profiles. These line-of-sight emissivities, together with independently measured electron temperature and density radial profiles allow the confrontation with theory and the extraction of parameters such as diffusion coefficients, non-equilibrium state, impurity densities and impurity influxes. The molecular spectrum requires a different approach. The presence of rovibronic sub-structure means that it is more convenient to work with spectral regions and to use theory to construct composite spectral features for the confrontation with experiment. Such an approach is also necessary for the difficult, sometimes quasi-continuous, spectra which arise from complex heavy element ions such as W^{+20}. Fortunately ADAS, also as part of the ADAS-EU Project, has built-up a powerful new capability in this area (see ADAS-EU report PUBL_2 of this series). The added complexity in the molecular catabolism case, such as the various kinetic energy fragments of dissociated and excited Dα emission also fits well into this framework.

1.2 The H_2 system

The present development of H_2 molecular system modelling is directed at magnetic confinement fusion plasmas. Interest in this system of course extends much further than fusion - to low temperature technical plasmas, high density laser-produced plasmas and to a wide range of photo-ionised and collisionally-ionised astrophysical plasmas. The application practices and hence molecular modelling usages in consequence also vary widely. For fusion, hydrogen atomic emission in the Lyman, but especially Balmer series, is a principal observable. The molecular dimension lies in the pathway to excited H^0 atomic states directly from molecular precursor catabolism. This means that there are cohorts of $H^0(n = 3)$ excited atoms of different kinetic energy distributions emitting Hα. Visible spectral observations willl try to resolve the intensities and widths of these cohorts, while plasam/surface interaction codes, such as DEGAS, attempt to model the whole system. It is a requirement of molecular ADAS that it fulfill the needs of both the theoretical and experimental spectroscopic activities. A fruitful path in atomic/ionic ADAS has been the production of derived, so called *collisional-radiative*, quantities which relate to application more directly than individual fundamental reaction cross-sections. In the molecular context, it is sometimes useful to view collisional-radiative effects as 'dressing' of populations and reactions. Thus the direct excitation of $H^0(n = 3)$ from the ground state $H^0(n = 1)$ in a plasma may be dressed by population of $H^0(n = 3)$ indirectly via excitation to higher levels $H^0(n > 3)$ followed by cascade. In a finite density plasma, the direct excitation of $H^0(n = 3)$ may be 'undressed' by ionising from the $n = 3$ level so reducing the efficiency of the excitation for Hα emission. Also the $H^0(n = 1)$ can be viewed as dressed by the $H(n > 1)$ which it carries with it. In this subsection, the various fusion applications are described and then discussed with a view to identifying the useful collisional-radiative quantities or dressed-reaction rates for these applications.

In recent years, modelling of the scrape-off-layer, the edge plasma and the plasma-surface interaction zone has been dominated by 2- and 3-dimensional Monte Carlo codes, including DEGAS2 [2], EIRENE [3], DIVIMP/NIMBUS [4] and ERO [5]. DEGAS2 adopts the usual effective collisional-radiative coefficients for electron impact recombination of H^+ and ionisation of H. That is to say, it assumes the quasi-static modelling of the H excited population structure and its projection on the H^+ and H(1s) populations (the ADAS *ACD* and *SCD* coefficients). Then only the dressed populations H^+ and H(1s) need to be carried in the Monte Carlo modelling. This assumption in DEGAS2 implicitly sets a timescale for quasi-static behaviour for the complete H_2 molecular system. Thus the electronic excited states of H_2 apart from the $^3\Sigma$ metastable should also be assumed quasi-static so that H_2 $^1\Sigma$ and H_2 $^3\Sigma$ have dressed populations. Of concern for DEGAS2 is the charge transfer reaction $H + H^+ \rightarrow H^+ + H$ which along with other elastic collisions moves neutral hydrogen between different kinetic distributions. Nearly resonant charge transfer occurs between ground states of H as well as between excited states. The latter have much larger cross-sections but much smaller populations which from the previous assumptions should be viewed as dressing populations of the ground state. Thus for DEGAS2 the $H + H^+ \rightarrow H^+ + H$ reaction refers to the ground states but the rate coefficient should be a collisional-radiative one coming from the quasi-static excited population model of H (in ADAS this recombination coeffficient is CCD). Returning to H_2, one would expect to seek equivalent effective coefficients or dressed cross-sections for dissociation etc. However the H_2 electronic states have vibrational (and rotational sub-structure). For the ground $^1\Sigma$ electronic state, the excited vibronic states cannot decay radiatively, so they have lifetimes which place them into the metastable category of generalised-collisional-radiative *GCR* modelling. The singlet excited H_2 electronic states also have vibrational substructure between which radiative decay is not allowed, but the maximum lifetime - that of the electrronic radiative decay, places them in the ordinary quasi-static population structure. H_2 has fourteen vibrational substates and D_2 with twenty in the $^1\Sigma$ ground electronic state (up to the dissociation limit). The explicit handling of this large group of metastables has been explored for EIRENE. It is beyond the normal scope of the above-mentioned codes, but cannot be completely neglected since dissociative collisions are strongly affected by vibrational state of the target. From the point-of-view of molecular ADAS, the full molecular GCR picture of the vibronic system is addressed, but it will be necessary to extract from this a reduced set effective coefficient source terms which condense the vibrational sub-structure for the 2- and 3-dimensional Monte Carlo codes. This means, at minimum, forcing a distribution on the vibrational substate populations of the ground electronic states of H_2 and H_2^+, such as that expected for H_2 released from a tokamak surface. So ADAS in its databases for derived molecular quantities loses the purely local assumption which has been possible for atom/ion ADAS. These issues, although addressed by reference to DEGAS2, apply to all the above Monte Carlo modelling codes.

It must be noted that the independent spectral observables for the H_2 system are limited, especially for flexible localised measurements in the visible. The H_2^+ molecular ion has no primary band emission (the shallow highly excited state potentials give only microwave emission). So H_2 is the only emitter, but with the primary singlet emission in the VUV, the tripet emission (the Fulcher bands) is the main observable. This, along with the familiar H atomic Balmer and Paschen series emission are the targets of the ADAS spectral modelling. For the various molecular and atomic emitters of the H_2 system, the production of emissivities can follow the usual ADAS pattern. Complexity is added by the number of different kinetic cohorts and the band structure of the molecular emission. It is noted that the molecular ADAS population modelling at this stage extends only to vibronic structure, whereas observationally it is superposition of rotational sequence bands which are present. This suggests that it is feature emssivity coefficients which are more relevant for molecules rather than single emissivity coefficients. The H_2 case is particularly problematic since the low nuclear masses and the rotational/vibrational coupling disperses the emission widely in wavelength. Additional derived quantities, such as ionisation per photon quantities (ADAS calls these SXBs), are also useful. In addition to ionisation per photon quantities, however, there will also be dissociations per photon and these may be helpfully resolved into different varieties depending on the kinetic energy imparted to fragments and depending on the resolution of spectrometry. Since the population modelling is vibronic, the rotational splitting for the band structure is determined by a Boltzmann assumption at an arbitrary rotational temperature T_r. The construction of spectral emission will be expanded in chapter **??**.

Since hydrogen is the dominant species, in a low Z_{eff} plasma, charge balance means that the population equations are inherently non-linear. However, electron temperature and density are measured locally, so within the H_2 system the electrons may be prescribed independently of charge balance, assumed Maxwellian, isotropic and fast compared with molecules, atoms and ions in the edge plasma. Thus non-linearity issues apply only to the heavy particle reactions and populations. In general, the ion impact collision cross-sections are small compared with electron impact cross-sections, so the non-linearity can be handled as a small perturbation. Since these non-linear paths in the population equations usually apply to exit paths for species change, the manipulation of the collisional-radiative equations and the condensation onto dominant populations may be performed by the usual matrix techniques. This will be explored further in a later chapter.

1.3 Isotopic scaling

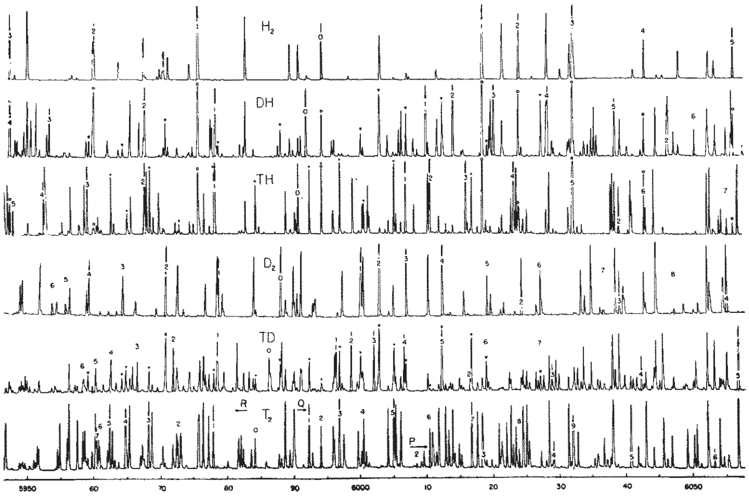


Figure 1.3: Comparison of spectra of H_2 isotopic combinations from Dieke[6].The lines of the 0 → 0 band of $3p\ ^3\Sigma \rightarrow 2s\ ^3\Sigma$ are numbered.

The first release of molecular ADAS is restricted primarily to the H_2 system. Current magentic confinement fusion devices predominantly operate with deuterium as the plasma species, although JET has operated briefly with a mixture of tritium and deuterium. So the requirement is really for the D_2 system and in the medium term also T_2 and the mixed DT, HD and HT systems. From a spectroscopic point-of-view, the Fulcher bands of H_2 are the primary visible spectral molecular features of the whole H_2 system. These features appear complex and very different for the different isotopes, as shown in figure 1.3, because of the open rotational band structure of this light diatomic. But as also shown in the figure, the band compression for the heavier isotopic combinations resolves matters - the spacing in T_2 is one-third that of H_2. These bands are an important discriminating spectrosopic diagnostic.

By far, the substantive molecular collisional data is for the H_2 system which has guided this first step. Although the fundamental data for the other isotopic systems is growing, there is an immediate need. Atomic/ionic ADAS has made extensive use of z-scaling, with much of its data explicitly organised for z-scaling and interpolation in z. It is sought now to extend this type of handling to isotopic scaling in the diatomic molecular picture. There are some simplifications. To a first approximation the electronic structure and collisional cross-sections between electronic states are independent of participant masses. To this extent, the H_2 electronic state database may be applied to all the isotopic combinations. This does not apply to the vibronic system. The vibrational energy eigenvalues depend on the nuclear masses. There have been a number of studies, of particular note being the work of Celiberto and his collaborators [7]. Celiberto relates the v vibrational quantum number of an isotopic system with the non-integer pseudo-vibrational level v' of H_2 through the relation

$$v' = \sqrt{\mu'/\mu}\, v \tag{1.1}$$

where μ' is the H_2 mass and μ is the other isotopic system mass. Celiberto treats v' as interpolable within the set of H_2 vibrational eigenvalues. In this work, the molecular constants of the H_2 system isotopic variants are assembled so that approximate scaling shifts of the H_2 data to the other isotopic combinations can be made. Further details are in the later chapters.

Chapter 2

H_2 data

The availability of collisional data is always a major issue when building collisional-radiative models. Insufficient quality of data and/or its lack of completness can mislead as to the importance of one class of process over another and ultimately yield an unrealistic physical picture. For these reasons, very substantial efforts have been made here on data compilation and completeness. The present intensive study has assembled all available data for the H_2 system and has also created some new data, using relatively simple approaches, when necessary. ADAS-EU has drawn on special expertise in its attempts to ensure the quality of the data and calculations used. In particular, Prof. R. K. Janev has worked with the ADAS-EU team as an advisor. This chapter reviews in detail the assembly of atomic data so that the collisional matrix for the H_2 molecular system (the H_2 molecule and collisional products) is complete and sound.

2.1 Type of data and quality

As discussed earlier, the whole molecular system must in principle be recognised for the collisional-radiative model, since ionisation, dissociation and associative products link the various hydrogen molecules, molecular ions, atoms and ions (see figure 3.8). The important components of the molecular system for the fusion plasma are those species (neutrals and ions) that have significant presence inside the plasma and their dissociation products. In H_2 that includes the molecules H_2, ${H_2}^+$ and the atomic species H, H^+ and H^-. We do not consider at this stage the H_3^+ pseudomolecule which is of low concentration in typical fusion plasmas. Nor do we include explicitly the ${H_2}^-$ anion. For the latter, the vibrational excitation processes that involve the participation of the resonant states of ${H_2}^-$ and the dissociation through electron attachment are considered as just one process. The participation of the ${H_2}^-$ ion is only as an internal step of this composite process.

Molecular collisional data have been hard to obtain in the past and generally were not procured by systematic, self-consistent approaches. Of special note for the present work are the remarkable recent efforts of Celiberto and collaborators. Key papers, used in the compilations here include [8, 7] and especially [9] - where empirical fitting formulas were included. Also of special initial note is the data base for plasma applications [10], used with the code HYDKIN - the online solver for EIRENE (see section 1.2). Recently new efforts have been done on a complete compilation of the H_2 system molecular data, including the calculations from Celiberto group and many others. This critical evaluation, by R. Janev, D. Reiter & U. Samm [11], of the cross sections and rates, give recommended sets and fitting formulas, which ease the extrapolation to higher energies . The data used in the collisional-radiative model here are largely based on this work and references herein. Complementary data have been obtained from other sourses as necessary, such as Celiberto et al. [7] for vibrational excitation by electron attachment and Atems & Wadehra [12] for dissociative attachment. For ion impact, complementary data come from Krystic & Schultz [13, 14] for proton impact vibrational excitation. These data can be found online in the AMBDAS data base [15]. Charge exchange complementary data have come also from Errea et al. [16]. Predissociation data have been obtained from Glass-maujean [17] and autoionization rates from Dehmer & Chupka [18]. Other fundamental H_2 system data, including vibrational energies and Franck-Condon factors, have been obtained from Fantz & Wunderlich [19] whose data can be access freely in an IAEA INDC report [20], by contacting the IAEA at `http://www-nds.iaea.org/` or directly from the authors.

As a point of note, the minimum of the ground potential of the neutral molecule is used as the “zero point” for energy. This is set up according to Wolnniewicz [21] where a corrected potential with respect to the Kolos value [22] is presented. The minimum energy is then set to:

$$E_{\mathrm{min}} = -1.1744756\mathrm{Ha} = 257767.61\mathrm{cm}^{-1} \tag{2.1}$$

and the energy of the other states of all molecular species are calculated with respect to this minimum.

Potential curves for H_2 system are shown in figure 2.1 taken from Sharp [23]. These curves show how some of the potential curves yield vibrational levels which lie vertically over those of the ground state of the ionized molecule. This implies that autoionization may be present via transition of one electron to the continuum. In figure 2.1 is also evident that all the excited states of $H_2{}^+$ are dissociative. Such dissociation will result in H atoms in excited electronic states which, in turn, contribute to the hydrogen spectral line emission in the plasma. In the H_2 system we have included those electronic states for which there are either collisional cross-section or dipole moment data available. Dipole moment data alone does still allow some simpler calculations of cross-sections by which gaps may be filled in the collisional-radiative matrix The list of basic states included in the H_2 models is presented in the ADAS *mdf02* molecular data format files and a summary of these are also given in the associated *mdf33* and *mdf04* data format headers as a guidance for the user. These will be described later. The list of molecular electronic states considered is given in table 2.1. In table 2.1, the zero level of energy is taken as the minimum of the potential energy curve of the ground state of the neutral specie H_2. The energy of the dissociative states has been obtained from the vertical energy difference with this minimum. Energy differences are needed only when new data need to be calculated. As mentioned earlier, vibrational energies from Fantz & Wunderlich [20] are archived. Note that we have omitted here the triplet state $\mathrm{p}\,^3\Sigma_g^+$ as no information about the dipolar transitions or vibrational energies has been found for it in the literature. This state is therefore an uncoupled “dead” channel with no effect on collisional-radiative balance equations.

2.1.1 Present status of fundamental data

As a preliminary remark, we note that in spite of the many sources of molecular collisional transition data in the literature, there are still gaps in the collisional-radiative matrix of the molecular H_2 system. We summarize below he present status of available collisional data as follows:

Excitation data

Electron impact excitation processes considered here are:

$\mathrm{e} + \mathrm{H}_2^{(+q)}(\mathrm{N},v) \rightarrow \mathrm{e} + \mathrm{H}_2^{(+q)}(\mathrm{N'},v')$	vibrationally resolved excitation.
$\mathrm{e} + \mathrm{H}_2(\mathrm{N}) \rightarrow \mathrm{e} + \mathrm{H}_2(\mathrm{N})$	vibrationally unresolved excitation.
$\mathrm{e} + \mathrm{H}_2(\mathrm{N},v) \rightarrow \mathrm{e} + \mathrm{H}_2(\mathrm{N'},v^{**}) \rightarrow \mathrm{e} + \mathrm{H(1s)} + \mathrm{H}(nl)$	dissociative excitation
$\mathrm{e} + \mathrm{H}_2(\mathrm{X},v) \rightarrow \mathrm{H}_2^-(\mathrm{X}\,^2\Sigma_u^+,\mathrm{B}\,^2\Sigma_u^+) \rightarrow \mathrm{e} + \mathrm{H}_2(\mathrm{X},v')$	vibrational excitation via eelectron attachment

Excitation data are available from the ground state of $H_2(X\,^1\Sigma_g^+, v = 0)$ to every upper state up to $N = 4$. Some spin-change data have also been calculated. The primary excitation data source is the compilation of Janev [11]. There is no data available for excitation from excited electronic states except for the transition between triplet states $\mathrm{c}\,^3\Pi_u \rightarrow \mathrm{a}\,^3\Sigma_g$. Cross-section fitting formulas are also given for these data by Janev [11] (see section 2.2). Excitation processes that go to dissociation as dissociative excitation or excitation to a dissociative state (such as $\mathrm{b}\,^3\Sigma_u$) will hereafter be considered as dissociation processes and therefore are simply added to the direct dissociation. The excitation data are normally provided in the form of total cross sections to some electronic state, with all the vibrational states summed up. Then Franck-Condon factors are used to split them up into the separate vibrational transition if required.

Proton impact excitation data can be obtained from the AMDAS web page [15] from calculations performed by Krystic [14] using the IOSA approximation. Fitting formulas are also provided by Janev [11].

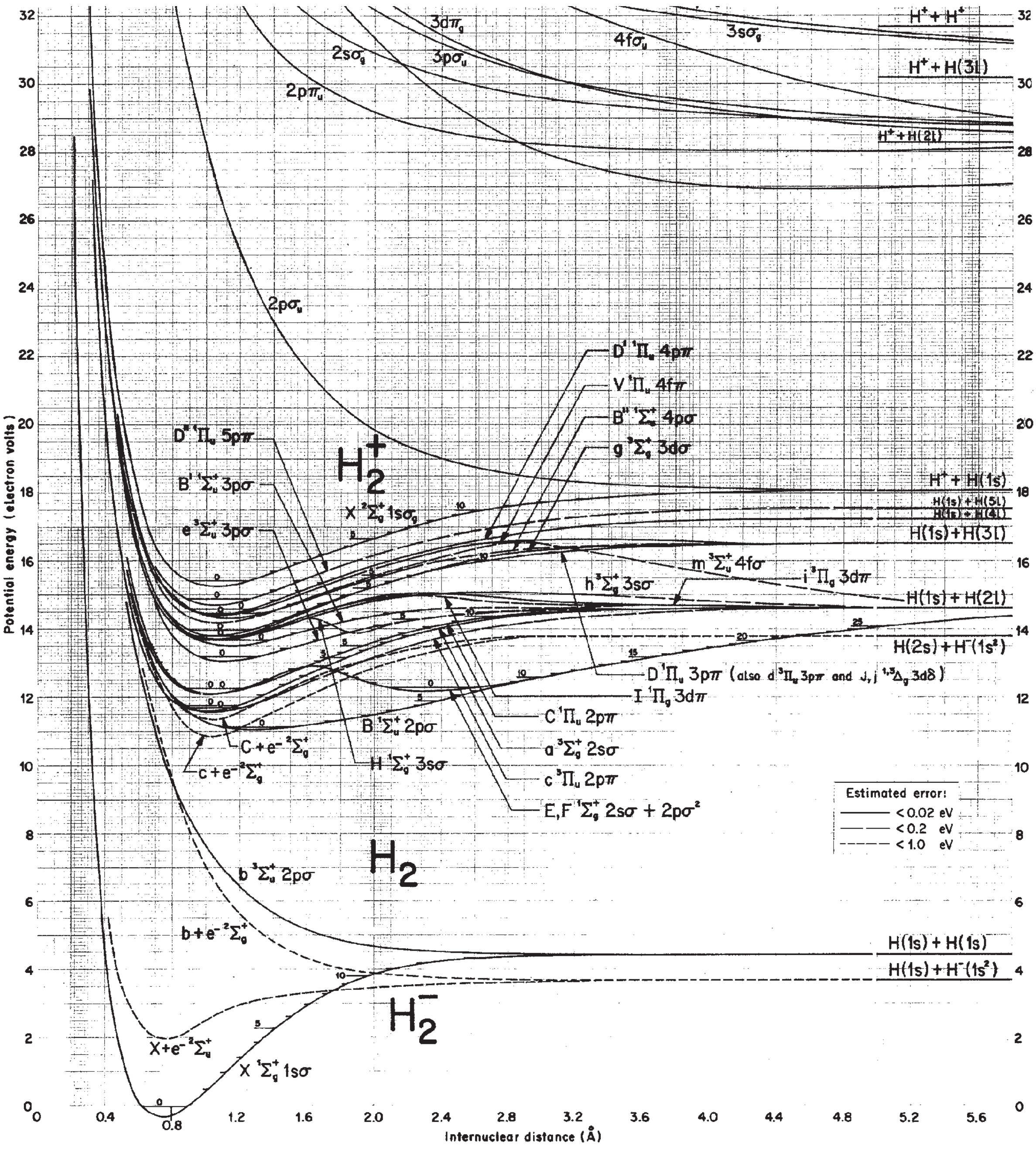


Figure 2.1: Potential energy curves for all the molecular species of H_2 system. In general the $1s\sigma$ has been omitted from state designation for compactness. The figure is taken from Sharp [23].

For H_2							
State	Separated atom config.	Asymptotic levels	coupled config.	$(wt-1)/2$	$E_{\mathrm{min}}\mathrm{cm}^{-1}$	$E_{\mathrm{diss}}\mathrm{cm}^{-1}$	Comments
X	$1s\sigma_g 1s\sigma_g$	H(1s) + H(1s)	$^1\Sigma_g^+$	0.0	0.0	38292.98	ground state
B	$1s\sigma_g 2p\sigma_u$	H(1s) + H(2p)	$^1\Sigma_u^+$	0.0	91691.69	120595.97	
C	$1s\sigma_g 2p\pi_u$	H(1s) + H(2p)	$^1\Pi_u$	0.5	100101.80	120595.97	
EF	$1s\sigma_g 2s\sigma_g$	H(1s) + H(2s)	$^1\Sigma_g^+$	0.0	100146.88	120595.97	
B′	$1s\sigma_g 3p\sigma_u$	H(1s) + H(2s)	$^1\Sigma_u^+$	0.0	111640.12	120595.97	
GK	$1s\sigma_g 3d\sigma_g$	H(1s) + H(2p)	$^1\Sigma_g^+$	0.0	112223.18	120595.97	
I	$1s\sigma_g 3d\pi_g$	H(1s) + H(2p)	$^1\Pi_g$	0.5	113017.64	122442.16	potential barrier
J	$1s\sigma_g 3d\delta_g$	H(1s) + H(3d)	$^1\Delta_g$	0.5	113443.18	135837.26	
D	$1s\sigma_g 3p\pi_u$	H(1s) + H(3d)	$^1\Pi_u$	0.5	113934.45	135837.26	
H$\bar{\mathrm{H}}$	$1s\sigma_g 3s\sigma_g$	H(1s) + H(3d)	$^1\Sigma_g^+$	0.0	114020.67	135837.26	
B″$\bar{\mathrm{B}}$	$1s\sigma_g 4p\sigma_u$	H(1s) + H(3s)	$^1\Sigma_u^+$	0.0	117958.11	135837.26	
P	$1s\sigma_g 4d\sigma_g$	H(1s) + H(3d)	$^1\Sigma_g^+$	0.0	118422.44	135837.26	
R	$1s\sigma_g 4d\pi_g$	H(1s) + H(3p)	$^1\Pi_g$	0.5	118514.31	135837.26	
S	$1s\sigma_g 4d\delta_g$	H(1s) + H(4f)	$^1\Delta_g$	0.5	118703.93	141171.72	
D′	$1s\sigma_g 4p\pi_u$	H(1s) + H(4p)	$^1\Pi_u$	0.5	118910.00	141171.72	
O	$1s\sigma_g 4s\sigma_g$	H(1s) + H(3p)	$^1\Sigma_g^+$	0.0	118954.12	135837.26	
b	$1s\sigma_g 2p\sigma_u$	H(1s) + H(1s)	$^3\Sigma_u^+$	1.0	66178.12	66178.12	dissociative state
c	$1s\sigma_g 2p\pi_u$	H(1s) + H(2p)	$^3\Pi_u$	2.5	95888.20	120595.97	triplet metastable
a	$1s\sigma_g 2s\sigma_g$	H(1s) + H(2s)	$^3\Sigma_g^+$	1.0	95977.76	120595.97	
e	$1s\sigma_g 3p\sigma_u$	H(1s) + H(2s)	$^3\Sigma_u^+$	1.0	107766.65	120595.97	
d	$1s\sigma_g 3p\pi_u$	H(1s) + H(3p)	$^3\Pi_u$	2.5	112750.43	135837.26	
h	$1s\sigma_g 3s\sigma_g$	H(1s) + H(2p)	$^3\Sigma_g^+$	1.0	112787.69	123870.60	potential barrier
g	$1s\sigma_g 3d\sigma_g$	H(1s) + H(3s)	$^3\Sigma_g^+$	1.0	112937.71	135837.26	
i	$1s\sigma_g 3d\pi_g$	H(1s) + H(2p)	$^3\Pi_g$	2.5	113006.18	123897.40	potential barrier
f	$1s\sigma_g 4p\sigma_u$	H(1s) + H(2p)	$^3\Sigma_u^+$	1.0	116631.81	131018.27	potential barrier
k	$1s\sigma_g 4p\pi_u$	H(1s) + H(3d)	$^3\Pi_u$	2.5	118418.65	135837.26	
r	$1s\sigma_g 4d\pi_g$	H(1s) + H(3d)	$^3\Pi_g$	2.5	118509.87	135837.26	
For ${H_2}^+$							
X	$1s\sigma_g$	H(1s) + H^+	$^2\Sigma_g^+$	0.5	124418.00	148030.30	ground state
2pσ_u	$2p\sigma_u$	H(1s) + H^+	$^2\Sigma_u^+$	0.5	274666.12	274666.12	dissiociative state
2pπ_u	$2p\pi_u$	H(2s) + H^+	$^2\Pi_u$	0.5	318289.02	318289.02	dissiociative state

Table 2.1: Parameters of the states of H_2 taken in account. wt is the statistical weight, E_{min} is the energy of the potential minimum, E_{diss} is the asymptotic dissociative energy for this potential.

Ionization data

Electron impact ionization processes considered here are:

$e + H_2(N,v) \rightarrow e + e + H_2^+(N',v')$	vibrationally resolved ionization.
$e + H_2(N) \rightarrow e + e + H_2^+(N')$	vibrationally unresolved ionization.
$e + H_2(N,v) \rightarrow e + e + H_2^+(N',v'^{**}) \rightarrow e + H + H^+$	dissociative ionization.
$H_2(N^{**},v^{**}) \rightarrow H_2^+(N',v') + e + hv$	autoionizacion.

In the case of dissociative ionization, the neutral molecule is ionized to an excited state of $H_2{}^+$. Excited states of $H_2{}^+$ are all dissociative producing a proton and a hydrogen atom. In the latter case the vibrational levels of the excited electronic states of H_2 with principal quantum number $N = 4$ become autoionizing for $v \geq 4$ as their energy is over the vibrational levels of the ground state of $H_2{}^+$ (see figure 2.1). These autoionization rates are stored in *mdf38* format files.

Ionization data are only available for the processes from the ground state of neutral H_2. This handicap would affect the mechanisms for ionization plus subsequent dissociation of $H_2{}^+$ and then the population of ionized and dissociated states. An approach, internal to the present work, is therefore necessary for calculating ionization from excited states to combine with the excitation and dissociation. Especially important is ionization from the triplet ortho-hydrogen metastable $c\,^3\Pi_u$ as it is one of the main routes to depopulatation of this state. The calculation method is explained in section 2.5.2.

Dissociation data

Dissociation (excluding dissociative excitation or ionization) processes considered here are:

$e + H_2(^+)(N,v) \rightarrow e + H_2(^+)(d) \rightarrow e + H(1s) + H(nl)$	vibrationally resolved dissociation.
$e + H_2(^+)(N) \rightarrow e + H_2(^+)(d) \rightarrow e + H(1s) + H(nl)$	vibrationally unresolved dissociation.
$e + H_2(N,v) \rightarrow H_2^-(X\,^2\Sigma_u^+ \rightarrow H^- + H(1s)$	diss. electron attachment through $H_2{}^-(X)$ and H^- production
$e + H_2(N,v) \rightarrow H_2^-(B\,^2\Sigma_g^+ \rightarrow H^- + H(1s)$	diss. electron attachment through $H_2{}^-(B)$ and H^- production
$e + H_2(X,v) \rightarrow H_2^-(X/B^2\Sigma_{(u/g)}^+ \rightarrow e + H(1s) + H(1s)$	diss. electron attachment

d means that the dissociative states $H_2^-(X)$ and $H_2{}^-(B)$ are resonant states. Dissociative attachment data come from the calculations of Atems & Wadehra [12] and Celiberto [7]. They have been compiled by Janev [11]. There are no calculations for dissociative attachment from excited states of the H_2 molecule although relatively high values of $\sim 6 \times 10^{-}5\mathrm{cm}^3/\mathrm{s}$ have been suggested in order to explain some experimental results [11]. Excitation to dissociative states exist from the ground state of the H_2 and $H_2{}^+$ species. However, also needed are rates for excited state (singlets) excitation, de-excitation or decay to $b\,^3\Sigma_u^+$ as even being a forbiden transition could determine the importance of dissociative paths in the collisional-radiative models.

Ion impact dissociative data is given in the form of fitting formulae [11] which come from IOSA theoretical calculations.

Recombination data

Recombination processes are listed as follow for H_2:

$H + H_2^+(N,v) \rightarrow H^+ + H_2(N',v')$	vibrationally resolved inverse CX
$H + H_2^+(N) \rightarrow H^+ + H_2(N)$	vibrationally unresolved inverse CX
$e + H_2^+ \rightarrow H_2{}^{**} \rightarrow H(n) + H(n)$	dissociative recombination

Recombination by electron impact takes place in low temperature plasmas (up to ∼ 11 eV for relevant cross sections) and it is a dissociative process of direct capture into a double excited state of H_2 or by vibrational excitation of $H_2{}^+$ and simultaneous capture of the electron into a dissociative auto-ionizing Rydberg state [11]. Non-dissociative processes need to be then by charge-transfer with a neutral atom in what is called here "inverse charge transfer" to separate it from from the "direct" charge transfer process of $H^+ + H_2$. Dissociative recombination fitting formulas are given by Janev [11] up to 11eV for individual initial vibrational states. No information is given for the n level of atomic products save for a statistical average from a calculation at threshold energy and a recommendation to use the n^{-3} law. Better data comming from direct calculation are desirable. Inverse charge exchange cross sections have been calculated by Krystic [14] using IOSA approximation calculation and are given by Janev [11]. Data can also be retrieved from the ALADDIN-AMBDAS data base [15]. A major drawback from these calculation is the lack of data for energies higher than 7 eV. In figure 2.2 are plotted the inverse CX values for $H_2{}^+(\nu = 0 - 5)$ from [15].

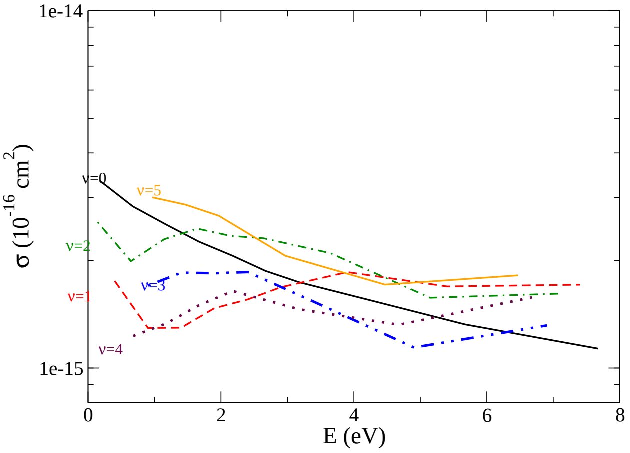


Figure 2.2: $H_2{}^+9\nu + H \rightarrow H^+ + H_2$ process for the first vibrational values $\nu = 0 - 5$ in center of mass energy.

Charge Exchange data

Charge exchange (CX) processes comprise the following:

$H^+ + H_2(N,\nu) \rightarrow H(1s) + H_2^+(N',\nu')$	vibrationally resolved direct CX.
$H^+ + H_2(N) \rightarrow H(1s) + H_2^+(N')$	vibrationally unresolved direct CX.
$H^+ + H_2(N,\nu) \rightarrow H(1s) + H + H^+$	dissociative CX.
$H^+ + H_2(\nu) \rightarrow H(1s) + H^+ + H^+ + e$	transfer ionization.

Charge exchange processes are a way to create neutral atoms and contribute to dissociation by two possible processes - dissociative charge exchange and electron transfer ionization. CX cross sections are and fitting formulas are given in [11] from a compilation of different sources. Vibrationally resolved charge transfer is quasi resonant on the dissociation energies of the initial and final vibrational level. However, the formulas provided in [11] do not comprehend final state vibronic resolution and only give fits for total cross sections. It has been decided then to take the cross section from AMBDAS database [15]. These data come from IOSA approximation calculations by Krstic *et al.* at low and intermediate center of mass energies [14, **?**]. Charge exchange of $H_2{}^+$ molecular ions with hydrogen atoms known in this document as "inverse charge exchange" has been obtained from the same source. Properties as microreversibility of the processes have been checked to be correct. Classical overbarrier model can be employed for excited states charge tranfer. Dissociative charge transfer and transfer ionization have been obtained from the crossed beam experimental results of [24] in a range of 10 to 100keV/amu. This energies are too large for having molecules on the plasma but they can be realistic in a beam molecule collision.

2.1.2 Autoionization and Predissociation data

The treatment of autoionization can be important in a collisional-radiative model. Sawada and Fujimoto [25] combine the excitation to autoionizing vibrational levels with direct ionization so only count the non-autoionizing levels for excitation. It is assumed that autoionization is fast and the autosionising states have no time to de-excite or suffer a secondary collision. However, in the case of autoionizing levels, the rates from experiments suggest that lifetimes of the autoionizing levels at $N = 3$ and $v \geq 7$ are of the order of μs [26, 18] and that only for levels $N \geq 5$ do lifetimes start to be of $\sim 10^{-9}$s which is comparable to excitation lifetimes. In our approach we prefer to use the impact parameter (IP) calculations of section 2.5.2 to calculate excitation and ionization cross sections. The strategy here is not to neglect excitation to autoionizing states and to count autoionizing rates as one more process that affects the balance of populations in those vibrational levels. The result is to make ionization more density dependent as the collisional picture has a bigger part to play in it. Predissociation processes correspond to transition to the dissociative continuum of a lower state after absorption of light. These processes can have appreciable rates and constitute an extra channel for dissociation. Predissociation of B′ $^1\Sigma_u^+$ and D $^1\Pi_u$ to the ground state continuum is obtained from [17].

2.1.3 Electronic and fully vibrational resolutions

2.2 Fitting formulae

The fitting formulae of Janev et al. in [11] have been created so that they force the correct asymptotic behaviour at high energies. ADAS codes exploit such formulae for better analytical treatment of the data. The formulae stored in ADAS are listed in appendix E. It is always preferred to have cross section data (rather than rates) for fundamental data, so that flexibility is maintained for averaging over distribution functions. Thus formulae for cross section are preferred over formulas for rate coefficients. Only in cases where there is no possibility of having cross section, are rate coefficient formula adopted. Apart from the obvious fact that interpolation and extrapolation are easier using fitting formulae, fitting formulae assist in discrimination between the results obtained from various different forms for a process and provides a recommended value for it. Fitting formulas from Janev et al. [11] give us an expert view of the fundamental data allowing us to concentrate on the collisional-radiative modelling.

As an illustration of formulaic behaviour in the different situations, figure 2.3 shows the different data sets for vibrational excitation via electron attachment contrasted with fitting formula number 1. The formula is influenced by the more modern experimental results of Brunger[27] rather than the T-matrix expansion calculations of Klonover [28]. The latter underestimate cross sections by a factor of ~ 2 for energies below 10eV. The formula also provides a correct high energy range behaviour.

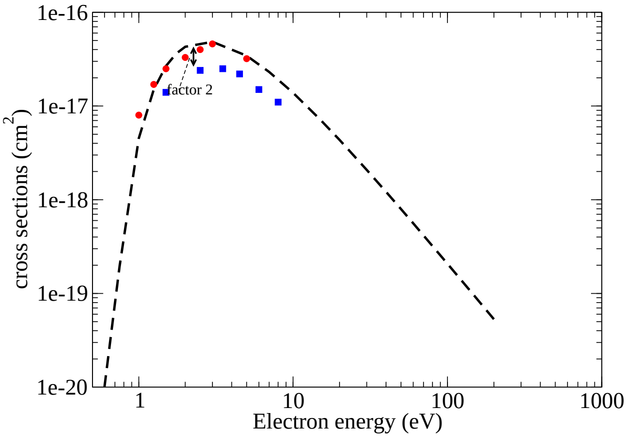


Figure 2.3: Vibrational excitation of ground state X $^1\Sigma_g^+$ $v = 0 \rightarrow v = 1$ of H_2 via electron attachment to resonant states of H_2^-. ■ T-matrix expansion [28]. ● experimental measurements [27]. (- - -), fitting formula 1 from [11].

In figure 2.4 excitation cross-sections from different authors and fitting formula 3 are plotted for vibrationally unresolved excitation from the ground state to state B′. An alternative fitting formula from Celiberto [8] is also plotted for comparison. Whereas the latter chose to rely on the first Born approximation calculations of Arrighini [29], the fitting formula of Janev [11] chooses a compromise between the distorted wave approach of Mutao [30] at low energies and the first Born approximation at higher energies. As this formula seems to give good results with other dipole allowed transitions, we have preferred to use it.

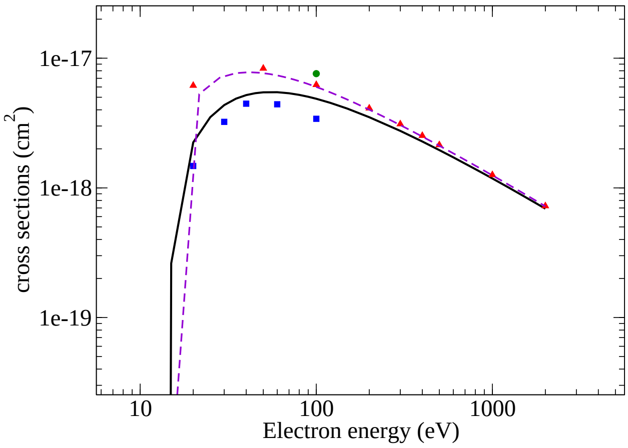


Figure 2.4: Vibrationally unresolved excitation cross section for the process $H_2(X\,^1\Sigma_g^+, v = 0) + e \rightarrow H_2(B'\,^1\Sigma_u^+) + e$. - - - fitting formula from [8]; ▲ first Born approximation [29]; ■ distorted wave approximation [30];● experimental measurements [31];— , fitting formula 3 from [11].

Finally, as a last example, in figure 2.5 a fitting formula from Janev [11] (no. 2 in appendix E) chooses to follow the first Born approximation only above 100eV but falls to threshold in a smoother way which Born calculationsdo not reproduce.

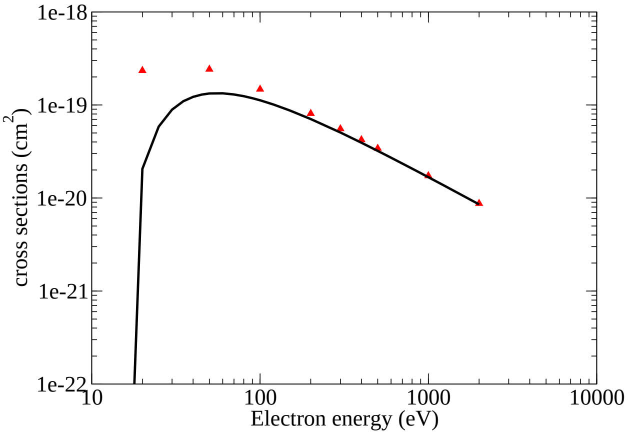


Figure 2.5: Vibrationally unresolved excitation cross section for the process $H_2(X\,^1\Sigma_g^+, v = 0) + e \rightarrow H_2(H\bar{H}\,^1\Sigma_g^+) + e$.▲ first Born approximation [29];— , fitting formula 2 from [11].

Fitting formulas are chosen in ADAS series 9 by default in preference to the numerical data as they have been obtained from the most up-to-the-date assessment of calculations and experimental results. Fitting formulas are properly frequently reappraised in the light of new results. A formula may be updated if appropriate or discarded in favour of the numerical data if its validity comes in question and/or more detailed trends in numerical data, concealed by the fitting formulae, are recognized as real. The latter route was followed for electron impact cross-section data for atoms and ions in ADAS many years ago.

2.3 Extrapolation and interpolation of data

As discussed in section 2.2, fitting formulae for cross-sections (normally in fact collision strengths), with properly specified low and high energy behaviour, eliminate the problems of interpolating and extrapolating of numerical data to any desired energy range. It must be recognised though that exact asymptotic behaviour is frequently not known for molecular cross-sections and so application of a particular formula may be constrained to a specific energy range. Large scale collisional-radiative modelling can be testing, in the sense of requiring cross-section evaluation in energy extremes, without the user necessarily being aware. It is helpful to ensure that even formula applicable to finite energy ranges include a strategy for 'safe' extrapolation.

For interpolation and extrapolation of true numerical tabulations of collision strength data, the general practice used here is cubic spline interpolation. ADAS spline procedures exploit spline end conditions to fit smoothly to correct asymptotic behaviour when available or failing that to 'safe' behaviour. Such asymptotic behaviour or behaviour constraints are generally part of the parametrisation of collision strengths. As is well known from the atomic case, high precision collision strength data may include resonant structure. The fundamental data starting point for collisional-radiative modelling then must be smoothed, perhaps 'interval-averaged' data which balances preservation of grosser structure against distribution function energy scale lengths and spline interpolation. At this stage, the molecular collision strength data in ADAS is not at this level of precision, although the database design does anticipate this for the future. It is for this reason that the pattern of molecular collision strength database storage, molecular data format *mdf02* includes both fitting formula parameters and numerical preferred data (see appendix A section A.2 for the full specification). In the following sub-sections some considerations are given to establishing physically based simple, safe, analytic asymptotic behaviours for key cross-section types.

2.3.1 Charge exchange overbarrier model

The classical overbarrier model [32] has been applied to slow collision $E \sim 10$ eV with highly charged projectiles. As we are in a slow energy range, the overbarrier model can be used as a rough approximation for the extrapolation of charge exchange cross sections. However it is necessary consider its extension to the molecular case to be secure about its correct application. In the collision $H_2 + A^{Z+}$ the barrier will be defined by the potential that the electron experinces. That can be written (in a.u.) as:

$$V(\vec{r}) = -\frac{q}{\vec{r}} - \frac{Z}{(\vec{R}_{CM} - \vec{r})} \tag{2.2}$$

where the first term correspond to the Coulomb attraction of the molecule using some screening effective charge q and the second is the Coulomb potential of the projectile A^{Z+}. A schematic of the system is shown in figure 2.6. If

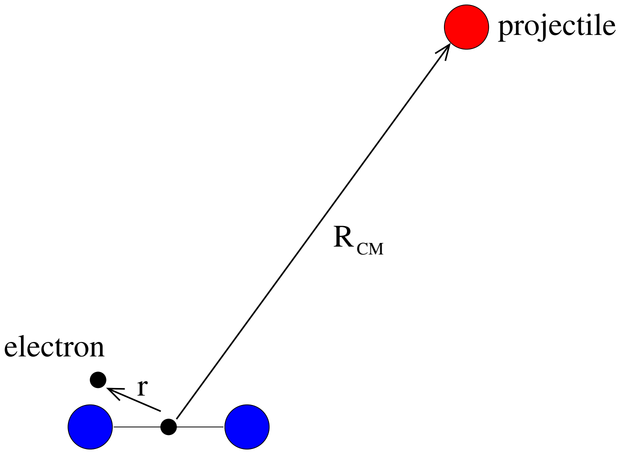


Figure 2.6: Coordinates for the $H_2 + A^{Z+}$ system.

we consider that the distance from the projectile to the bound electron is much greater than from the electron to the molecule, $R_{CM} \gg r$, then we can approximate $(\vec{R}_{CM} - \vec{r})$ by $(R_{CM} - r_z)_z$ where the z component is taken in the direction of $\vec{R}_{CM}$. Then the maximum of the potential is

$$V_{max} = -\frac{\left(\sqrt{Z} + \sqrt{q}\right)^2}{R_{CM}} \tag{2.3}$$

so that the condition for the electron be be released is

$$E_{H_2} - \frac{Z}{R_{CM}} = -\frac{\left(\sqrt{Z} + \sqrt{q}\right)^2}{R_{CM}} \tag{2.4}$$

wher E_{H_2} is the binding energy of the electron in the molecule. Then the electron release distance R_r is:

$$R_r = \frac{Z - \left(\sqrt{q} + \sqrt{Z}\right)^2}{E_{H_2}} \tag{2.5}$$

Following [33] we can establish a minimum condition for capture, balancing the potential energy of the electron in the projectile reference frame and its kinetic energy.

$$\frac{1}{2}V^2 = \frac{Z}{R_c} \tag{2.6}$$

to obtain $R_c = 2Z/V^2$ as the maximun capture distance. When $R_r \leq R_c$ the capture ocurrs automatically after the release and the cross section is

$$\sigma = \pi R_r^2 = \pi \frac{\left(Z - \left(\sqrt{q} + \sqrt{Z}\right)^2\right)^2}{E_{H_2}^2} \tag{2.7}$$

This happens at low energies. As we are considering extrapolation to higher energies we can consider that the release is done before the capture takes place, i.e. $R_c \leq R_r$. Then the capture probability is the ratio between the probability per unit time of release v/a (where v is the velocity of the electron in the molecule orbit and a its radius) and the probability of capture per unit time R_c/V [33]. Then the overbarrier extrapolation cross section is

$$\sigma^{\mathrm{OB}} = \pi * R_c^2 \left(\frac{vR_c}{a * V}\right) = C * \frac{1}{E_P^{7/2}} \tag{2.8}$$

where $E_P = \frac{1}{2}M_p V^2$ is the energy of the projectile. This result coincides with the classical overbarrier results for atomic collisions. Furthermore we can estimate from equation 2.6 the energy needed for the condition $R_c \leq R_r$ using the ionization energy of the $\nu = 0$ level of the ground state of H_2 obtaining an energy of around ~50 eV which is compatible with the energy ranges of molecules in plasmas. To avoid discontinuity from the extrapolation (overbarrier) values being different from the tabulated values, the extrapolation overbarrier results are normalized to the last tabular value. In the asymptotic region, the overbarrier extrapolation follows an $E^{-7/2}$ trend.

2.3.2 Bethe approximation

The Bethe approximation [34] is relevant to the high energy behaviour of ionization and excitation cross-sections by electron (and ion) impact. Extension to molecules can be done if the molecule is treated as as frozen, indivisible heavy particle.

Ionization

We adopt the general Bethe ionization formula [35] depending on constants A and C. The A coefficient is related to the bound-free Gaunt factor for the transition, which is non-vanishing for ionisation. Although the Gaunt factor is determinate, in usual practice, it is preferable to treat it as an effecive Gaunt factor adjusted to fit more exact data. In the present case, the coefficients may be traeted as adjustable parameters allowing differential continuity with tabular data into the high energy extrapolation zone.

$$\sigma^{\text{ion}} = \frac{A}{2E\Delta E}\left(\ln\left\{\frac{4E}{\Delta E}\right\} - C\right) \tag{2.9}$$

Specifying as σ_1 and σ_2 the last two values from the cross-section tabulation, the constants are obtained as

$$\begin{aligned} \frac{A}{2E_1\Delta E}\left(\ln\left\{\frac{4E_1}{\Delta E}\right\} - C\right) &= \sigma_1 \\ \frac{A}{2E_2\Delta E}\left(\ln\left\{\frac{4E_2}{\Delta E}\right\} - C\right) &= \sigma_2 \end{aligned} \tag{2.10}$$

Excitation

For high energy asymptotic behaviour in the Bethe limit, molecular electron (and ion) collision cross-sections follow the same behaviour as for collisions with atoms and ions. This has been described extensively in ADAS documentation, a small portion of which is repeated here for completness. It is convenient to switch to collision strengths, rather than cross-sections. The relationships are:

$$\Omega_{ij} = \omega_i(\epsilon_i/I_H)(\sigma_{i\to j}(\epsilon_i)/\pi a_0^2) = \omega_j(\epsilon_j/I_H)(\sigma_{j\to i}(\epsilon_j)/\pi a_0^2) \tag{2.11}$$

where ϵ_i is the incident electron energy, ϵ_j the final electron energy, E_i is the initial molecular state and E_j the final molecular state so that the transtion energy $\Delta E_{ij} = E_j - E_i = \epsilon_i - \epsilon_j$. Ω_{ij} is the collision strength, $\sigma_{i\to j}$ is the excitation cross-section and $\sigma_{j\to i}$ is the de-excitation cross-section. ω_i and $omega_j$ are statistical weights and other notation is conventional. Three types of collisional transition are distinguished, namely,(1) dipole; (2) non-dipole; (3) spin change which have characteristics high energy asymptotic behaviours as follow:

$$\begin{aligned} \Omega_{ij} &\sim F_3\log(X + F_2) && \text{dipole} \\ \Omega_{ij} &\sim F_3 + F_2/X && \text{non-dipole} \\ \Omega_{ij} &\sim F_3/(X + F_2)^2 && \text{spin change} \end{aligned} \tag{2.12}$$

It is convenient to use the scaled energy parameter $X = \epsilon_i/\Delta E_{ij}$. The parameter F_3 in the dipole case is known independently of the collision calculation to be $4S_{ij}/3$. S_{ij}, the line strength, bears the usual relationships to the oscillator strength $f_{i\to j}$ and the Einstein A-coefficient $A_{j\to i}$, namely,

$$A_{j\to i} = \frac{\alpha^4 c}{2a_0}\left[\frac{\Delta E_{ij}}{i_h}\right]^2 \frac{\omega_i}{\omega_j} f_{i\to j} = \frac{\alpha^4 c}{6a_0}\left[\frac{\Delta E_{ij}}{i_h}\right]^3 \frac{1}{\omega_j} S_{ij} \tag{2.13}$$

The forms 2.12 are fitted to the last or last two tabular collisions strength values for extrapolation of numerical data. It is prefarable to use the dipole limit point if possible. Also the non-dipole limit point F_3 may be available from Born calculations. For molecules, as for atoms and ions, it is advisable to verify numerical collision strength data by the Burgess C-plot method [**?**]. See for example figure 2.9 in section 2.3.4. In the atomic case, in the early days of R-matrix calculations, the higher energy collision strengths sometimes did not correctly approach the limit point - due to unconverged partial wave sums. High quality molecular cross-section data and its availability is still at this ealier phase. Some assessment of electron impact cross-section data for molecules can be done with the interactive ADAS108 code (see also Summers & Kato [**?**]).

2.3.3 Low energy behaviour

Collision strengths for electron impact excitation of neutral molecular targets are zero at threshold. The usual practice of spline interpolation of numerical data in the logarithmic plane, suited to high energy extrapolation cannot be continued to threshold in this case. Specific behaviour, power law or other, should be parametrically specified. For ion impact collisions, exothermicity or endothermicity determines the behaviour. Practically, the behaviour is usually unknown so linear behaviour from theshold to the first tabular value is used.

2.3.4 Comparisons

Comparisons of the different cross-section behaviours and illustrations of the extrapolation strategies describe above are shown in the examples and figures below.

Figure 2.7 shows a comparison of Charge eXchange extrapolation for the process $H_2(X\,^1\Sigma_g^+, v = 0) + H^+ \rightarrow {H_2}^+(^2X_g^+)$. The numerical data (obtained from the formula 106 from appendix E) values stored in *mdf02* are extended with different extrapolation mechanisms. The recommended fitting formula coming from [11] has a positive slope after a minimum. The extrapolation by splines follow this last slope that in this case is correct. However, splines cannot account for an slope change and can give incorrect results. The classical overbarrier model is in any case changing the slope and falling down in the value of the cross section. This illustrates that extrapolation models are simple model that deal in case that there is no other data. Obviously overbarrier model account for the negative slope that in the end the CX data should have maybe at higher energies where the projectile are too fast for influence the target molecule.

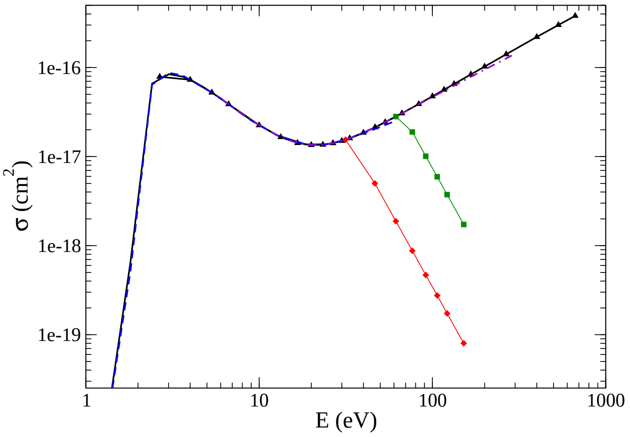


Figure 2.7: Cross section for charge exchange $H_2(X\,^1\Sigma_g^+, v = 0) + H^+ \rightarrow {H_2}^+(^2X_g^+)$. Data: (▲) Numerical data (from formula); (—) Fitting formula 106 from appendix E; (◆—) overbarrier extrapolation from 60 eV; (■—) overbarrier extrapolation from 60 eV;(- - -) spline interpolated (extrapolation from 30eV); (- · -) spline interpolated (extrapolation from 60eV).

In figure 2.8 where electron impact ionization from $H_2(X\,^1\Sigma_g^+, v = 0)$ to the grond state of ${H_2}^+$ is given we can see a different case where spline is not giving a good result. In this case bethe model extrapolation from 200eV follows well the formula and the data while the spline is steeply falling down.. Splines must be taken in linear scale to well reproduce the low energy side near the threshold and avoid big oscillation that happen in the case of logarithmic scale interpolation. That is the reason why small variation on the curvature of the data can make that the spline departs of the reight trend as can be seen on figure 2.8

Cross section for for excitation $H_2(X\,^1\Sigma_g^+, v = 0) + e \rightarrow H_2(^1B_u^+)$ are plotted on figure 2.9 where Bethe extraploation is evaluated. As in the CX case the Bethe cross sections tendency is to fall to lower values for higher energies and the spline follows well the data curve.

It is necessary then to take care on the extrapolation of data and follow a compromise between the numerical data and the best model and point for extrapolate these data. It is here taken priority on the recommended formulas which are use to extrapolate assuming that they have a correct asymptotic behaviour, if there is no formula available then the extrapolation models are preferred over the splines to avoid dangerous artifact which could give to an errounoeus anhancement of the importance of a process.

2.4 Maxwellian rates

The fundamental data are stored as cross sections or collison strength in *mdf02*. Rate coefficients are only stored when cross section data are not available. These cross sections or collision strengths must be integrated over distributions

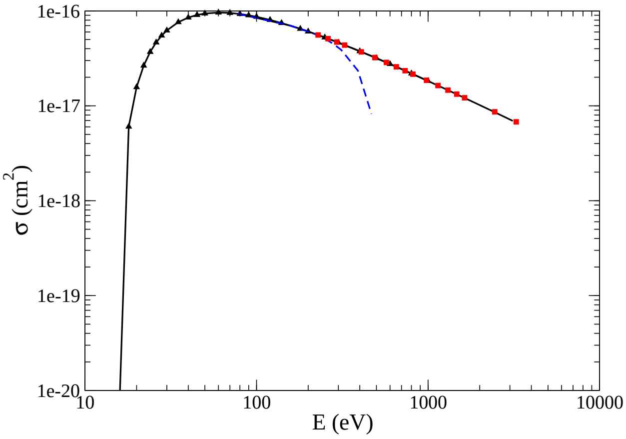


Figure 2.8: Cross section for electron impact ionization $H_2(X\,^1\Sigma_g^+, \nu = 0) + e \rightarrow H_2{}^+(^2X_g^+)$. Data: (▲) Numerical data (from formula); (—) Fitting formula 8 from appendix E; (■—) Bethe formula (2.9) extrapolation from 200 eV; (- - -) spline interpolated (extrapolation from 200eV).

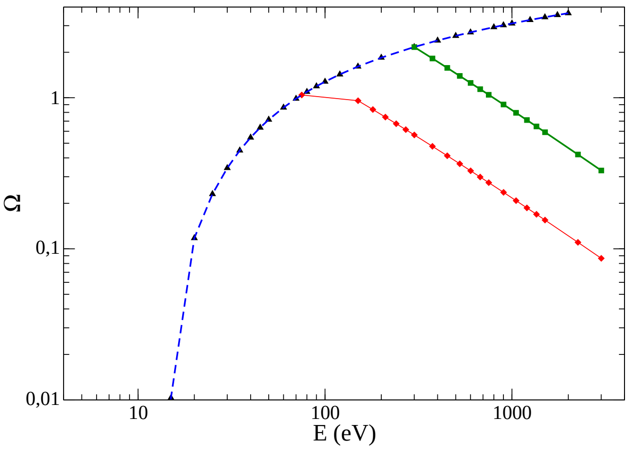


Figure 2.9: Cross section for electron impact excitation $H_2(X\,^1\Sigma_g^+, \nu = 0) + e \rightarrow H_2(^1B_u^+)$. Data: (▲) Numerical data (from formula 3 on appendix E); (♦—) Bethe extrapolation from equation (**??**) (from 80 eV); (■—) Bethe extrapolation from equation (**??**) (from 300 eV).

of participant velocities in order to obtain the collisional rate coefficients required for collisional-radiative application. Under most circumstances a Maxwellian assumption is made for the distribution functions of the colliding particles. For electron collisions, the target heavy molecule may be assumed stationary and so only the electron Maxwellian distribution function matters. A single quadrature over the electron Maxwellian distribution alone is required. For the heavy particle collisions, however, each species may have its own distribution function in principle. So it necessary to perform a double Maxwellian integration in these cases.

2.4.1 Single Maxwellian integrations for electron-impact collisions

In the case of single Maxwell integration we can obtain the Maxwellian rate from:

$$q_{i\to j} = \left\langle \sigma_{i\to j}\vec{v} \right\rangle = \int \mathrm{d}\vec{v}\, \sigma_{i\to j}(\vec{v})\, \vec{v} f(\vec{v}) = \left(\frac{\beta}{\pi}\right)^{3/2} \int \mathrm{d}\vec{v}\, \sigma_{i\to j}(\vec{v})\ \vec{v} \exp(-\beta\, v^2) \tag{2.14}$$

where $f(\vec{v})$ is the Maxwellian distribution function and $\beta = m_e/2kT_e$ with k the Boltzmann constant, m_e the electron mass and T_e the electron temperature. It is useful to express the integral in terms of the impact energy ϵ and assume isotropy. Then, the equation (2.14) transforms to:

$$q_{i\to j} = \sqrt{\frac{8}{\pi m_e \left(kT_e\right)^3}} \int_0^\infty \mathrm{d}\epsilon \sigma(\epsilon)\ \epsilon\ \exp(\epsilon/kT_e) \tag{2.15}$$

Dimensionally, collisional rate coefficients are usually given in cm^3/s units and are the basic data for collisional-radiative calculations. It is useful to obtain a dimensionless quantity from the collisions strength, the Maxwell-averaged collision strength, called “Upsilon” (Υ) as:

$$\Upsilon_{ij} = \int_0^\infty \Omega_{ij}(\epsilon)\, \exp(-\epsilon/\mathrm{kT_e})\, \mathrm{d}(\epsilon/\mathrm{kT_e}) \tag{2.16}$$

Υ_{ij}, like the collision strength ω_{ij}, is symmetric between initial and final states. The relationships between Υ_{ij}, the excitation rate coefficient $q_{i\to j}$ and de-excitation rate coefficient $q_{j\to i}$ are

$$q_{j\to i} = \frac{\omega_i}{\omega_j} exp(\Delta E_{ij}/kT_e)\; q_{i\to j} = 2\sqrt{\pi}\alpha c a_0^2 \frac{1}{\omega_j}[I_H/kT_e]^{1/2}\Upsilon_{ij} \tag{2.17}$$

Excitation processes are usually stored in Υ form since it is a slowly varying functional form with temperature. However, dissociative/ionization processes for which the inverse processes are not easily obtainable are stored as rate coefficients.

2.4.2 Double Maxwellian integrations for ion-impact collisions

The distribution functions of molecular species in the plasma edge are in principle complex, influenced by mechanisms of release, chemical catabolism and reactions. Also ions, which thermalise efficiently among themselves, may tie neutral atoms with them by recombination reactions. For binary reactions between heavy molecular, atomic or ionic species, a minimal assumption is that the individual reactants are thermalised with Maxwellian distributions which differ between reactants. Suppose the ions (molecular aor atomic) of the plasma are thermalized with temperature T_i and neutrals (molecules or atoms) are thermalised with temperature T_m. It is then necessary to make a double Maxwell quadrature over the reaction cross-section to form the rate coefficient. Define the constants $\beta_i = m_i/2K_BT_i$ and $\beta_m = m_m/2K_BT_m$. Then the Maxwellian integration may be written as (see for example [39]):

$$q_{i\to j} = \left\langle \sigma_{i\to j}\vec{v} \right\rangle = \left(\frac{\beta_i}{\pi}\right)^{3/2} \left(\frac{\beta_m}{\pi}\right)^{3/2} \int_{-\infty}^{\infty} \mathrm{d}\vec{v}_i \int_{-\infty}^{\infty} \mathrm{d}\vec{v}_m \sigma_{i\to j}(\vec{v})\, \vec{v} \exp(-\beta_i v_i^2 - \beta_m v_m^2) \tag{2.18}$$

Define the relative velocity $\vec{v}_{\rm rel} = \vec{v}_1 - \vec{v}_2 = \vec{v}$ and operate to reduce to only a single integral:

$$q_{i\to j} = \left(\frac{\beta_{\rm rel}}{\pi}\right)^{3/2} \int_{-\infty}^{\infty} {\rm d}\vec{v}_{\rm rel}\sigma_{i\to j}\left(\vec{v_{\rm rel}}\right) \vec{v_{\rm rel}} {\rm exp}(-\beta_{\rm rel}v_{\rm rel}^2) \tag{2.19}$$

where

$$\beta_{\rm rel} = \frac{\beta_i\beta_m}{\beta_i + \beta_m} \tag{2.20}$$

Express in energy terms and assume isotropy. In the centre of reference mass frame:

$$\vec{v}_i^{\rm CM} = \vec{v}_i - \vec{V}_{CM} = \frac{m_m}{M_{\rm T}}\left(\vec{v}_i - \vec{v}_m\right) \tag{2.21a}$$

$$\vec{v}_m^{\rm CM} = \vec{v}_m - \vec{V}_{CM} = -\frac{m_i}{M_{\rm T}}\left(\vec{v}_i - \vec{v}_m\right) \tag{2.21b}$$

where $M_{\rm T} = m_i + m_m$ the total mass. In this frame the kinetic energy is:

$$\epsilon^{\rm CM} = \frac{1}{2}m_i(\vec{v}_i^{\rm CM})^2 + \frac{1}{2}m_m(\vec{v}_m^{\rm CM})^2 = \frac{1}{2}\mu\vec{v}_{\rm rel}^2 = \epsilon_{\rm rel} \tag{2.22}$$

where in this case the relative velocity is $\vec{v}_{\rm rel} = \vec{v}_i - \vec{v}_m$ and $\epsilon_{\rm rel}$ is the relative kinetic energy. It is straightforward to see that if we situate the laboratory reference frame in the target (molecule), then for H_2 $\epsilon_{\rm CM} = 2/3\ \epsilon_{\rm lab}$. Finally the $\beta_{\rm rel}$ parameter can be written as:

$$\beta_{\rm rel} = \frac{1}{2k}\frac{m_i m_m}{T_i m_m + T_m m_i} = \frac{\mu}{2k\tau} \tag{2.23}$$

with $\mu = m_i m_m/(m_i + m_m)$ and

$$\tau = \frac{T_i m_m + T_m m_i}{m_m + m_i} \tag{2.24}$$

The double maxwellian excitation rate coefficient becomes:

$$q_{i\to j} = \sqrt{\frac{8}{\pi\mu\left(k\tau\right)^3}} \int_0^{\infty} {\rm d}\epsilon_{\rm rel}\sigma(\epsilon_{\rm rel})\ \epsilon\ {\rm exp}(\epsilon_{\rm rel}k\tau) \tag{2.25}$$

τ is a reduced temperature which allows reduction of the integration to a single Maxwell integration in terms of energy. It is clear that if $T_m = 0$, then $\beta_{\rm rel} = \beta_i$ and equation (2.25) reduces to (2.15) for a single maxwellian.

As before we can obtain the Υ from the rate coefficient since

$$q_{i\to j} = \frac{2^{3/2}\pi^{1/2}}{\mu^{1/2}\left(k\tau\right)^{1/2}}\frac{I_H a_0^2}{w_i}\Upsilon_{ij} \tag{2.26}$$

where μ is the reduced mass of the system. The reverse reacton rate coefficient is

$$q_{j\to i} = \omega_i q_{i\to j}{\rm exp}(\Delta{\rm E_{ij}}/{\rm k}\tau)/\omega_{\rm j} \tag{2.27}$$

2.5 Calculation of new data

In section 2.1.1 has been shown that the data present in the literature are not yet sufficient to complete the collisional matrix for fully reliable population modeling. It is desirable to have some methods, albeit perhaps over-simple and approximate, to make estimates of these lacking data. The easiest is the use of scaling laws, such as the well-known n^{-3} law [40]. This is widely exploited in atomic population modelling and, in the molecular case, has been used by K. Sawada and Fujimoto (1995) [25] to calculate excitation cross sections from ground state of H_2 assuming the same dependence on energy as that of atomic hydrogen. Two simplified theories, which have proved very helpful in the atomic collisional-radiative case, are the IP (impact-parameter) method and the related ECIP (exchange-classical-impact-parameter) method The current IP method as implemented in ADAS was an extension by Burgess & Summers [43] of earlier work by Seaton [41]. It is a Bethe-type separation approximation for dipole allowed transitions in which the 'free-free Gaunt factor' part is evaluated by describing the colliding projectile particle, which may be an electron or ion, as on a classical rectilinear (for neutral targets) or hyperbolic (for charged targets) orbit of specified impact parameter. The method has some control of unitarity by restricting the probability of transition as a function of impact parameter in strong coupling situations. ECIP combines a classical-exchange-binary-encounter model (see Burgess [**?**] and Burgess & Percival[**?**]), with the IP approach for distant collisions as described in Burgess & Summers[43]. It has often been used for ionisation with the IP part adjusted to match experiment. These methods have some flexibility for application to collisions with molecules. Since transition probabilities are required for the IP method, these are first considered in the rovibronic case for molecules.

2.5.1 Oscillator strengths from dipolar integrals

Oscillator strengths can be written interms of dipolar integrals and so related to Einstein coefficients to be easily calculable.

We can write the line strength for a rotational line ($J \rightarrow J'$) as[42]:

$$S_{JJ'} = \sum_{M} \sum_{M}^{\prime} |\langle \Psi_M |\mu| \Psi_{M'} \rangle|^2 = \tag{2.28}$$

where Ψ_M are the wavefunction for the magnetic substates and μ is the dipole operator. In the Born-Oppenheimer approximation of fixed nucleai we can simplify by:

$$S_{JJ'} = F_{ij} \mathcal{D}_{vv'}(\bar{r}) \mathcal{S}_{JJ'} \tag{2.29}$$

In equation (2.29) $\mathcal{S}$ is the dimensionless Hönl-London factor and has the property that:

$$\sum_i \mathcal{S}_{JJ'} = (2 - \delta_{0,\Lambda+\Lambda'})\,(2S+1)(2J+1) \tag{2.30}$$

being Λ the angular momentum of the molecular state and S the total spin momentum; the sumation is carried over all the rovibrational states and substates of Λ that is represented here as an i. In equation (2.29), $\mathcal{D}(\bar{r}_{vv'}) = \mathcal{D}_{vv'}$ is the dipolar momentum in a fixed internuclear distance $\bar{r}$ defined as the r-centroid ($\bar{r}_{vv'} = \langle v|r|v' \rangle / F_{vv'}^{1/2}$). Finally $F_{vv'}$ is the overlaping integral known as Franck-Condon factor:

$$F_{vv'} = \left| \langle v|v' \rangle \right|^2 \tag{2.31}$$

The oscillator strength $\mathcal{F}_{vv'}$ dependence on the dipole momentum is[42]:

$$\mathcal{F}_{vv'} = \frac{4\pi^4 mc^2 \alpha^2}{3 I_H} \frac{\Delta E}{I_H} \frac{g_{\Lambda'}}{g_{\Lambda}} g F_{vv'} \, |\mathcal{D}_{vv'}|^2 \tag{2.32}$$

where $g_\Lambda = (2 - \delta_{0,\Lambda})(2S + 1)$ is the statistical weigth of state v, $\mathcal{D}$ is in a.u. (ea_0 units), m is the electron mass, a_0 is the Bohr radius, α is the fine structure constant, c is the speed of light, I_H is the Rydberg energy and ΔE is the energy difference. Here, g is an statistical factor that writes:

$$g = \frac{(2 - \delta_{0,\Lambda+\Lambda'})}{(2 - \delta_{0,\Lambda'})} \tag{2.33}$$

and comes from the Hönl-London factor.. g value is either 1 or 2 and makes the difference with the atomic case.

The Einstein coefficients can be calculated in the dipole aproximation as:

$$A_{v' \leftarrow v} = \frac{\alpha^4 c}{6 a_0} \left(\frac{\Delta E}{I_H} \right)^3 g F_{vv'} \mathcal{D}_{vv'} = g \mathrm{AVAL}_{v' \leftarrow v} \tag{2.34}$$

where AVAL are the “A-values” which are the quantities stored in the *mdf00* formats (see section 4.3) as they have been obtained doing the dipolar integration on the vibrational wavefunctions.

It is now straightforward to relate the oscillator strength with the Einstein coefficients:

$$\mathcal{F}_{vv'} = mc\alpha^2 a_0 \frac{I_H}{\Delta E^2} \frac{g_{\Lambda'}}{g_\Lambda} g A_{v' \leftarrow v} \tag{2.35}$$

2.5.2 IP model

For an incident electron of energy ϵ_i and final energy ϵ_j, the excitation cross-cross-section is written as

$$\sigma_{i \to j}(\epsilon_i) = \int_0^\infty P_{i \to j}(R) 2\pi R dR \tag{2.36}$$

with the probability of transition expressible as

$$P_{i \to j}(R) = 4 \left(\frac{I_H}{\Delta E_{ij}} f_{i \to j} \right) \frac{\sqrt{\epsilon_i / I_H} \sqrt{\epsilon_j / I_H}}{(\sqrt{\epsilon_i / I_H} \sqrt{\epsilon_j / I_H} \, R^c + z/a_0)^2)} X(\xi, \delta) \tag{2.37}$$

where $\xi = z \left| \sqrt{I_H/\epsilon_i} - \sqrt{I_H/\epsilon_j} \right|$ and $\delta = R^c \left| \sqrt{\epsilon_i/I_H} - \sqrt{\epsilon_j/I_H} \right|$. The impact parameter R and distance of closest approach R^c are distinguished so that, with inclusion of symmetrising,

$$R^2 = \frac{I_h}{\epsilon_i} \left[\sqrt{\epsilon_i / I_H} \sqrt{\epsilon_j / I_H} (R^c)^2 + 2 z a_0 R^c \right] \tag{2.38}$$

z, the target charge, is zero for neutrals. Practical application of formula 2.36 then considers that the lower limit of the integral should not be zero, but at a radius characteristic of the molecule, R_0^c. This is provided $P_{i \to j}(R)$ remains less that unity (called *weak coupling*) otherwise there would be a breakdown of unitarity at some impact parameter (called *strong coupling*). There is no difference in application of the IP approximation to atoms and ions or molecules, since the oscillator strength is specified, except in the controlling of unitarity breakdown. For a two level atom, breakdown might be likely to occur at around $P_{i \to j}(R) = 1/2$. For excitation to closely spaced vibrational sub-states a more stringent condition of $P_{i \to j}(R) < 1/2$ might be appropriate, such as $1/N$, where N is the number of closely coupled vibrational states. This gives the IP expressions in weak and strong coupling for application to molecules as

$$\sigma^w_{i \to j}(\epsilon_i) = \frac{I_h}{\epsilon_i} \left[8 \left(\frac{I_H}{\Delta E_{ij}} f_{i \to j} \right) Y(\xi, \delta_0) \right] \pi a_0^2 \tag{2.39}$$

$$\sigma^s_{i \to j}(\epsilon_i) = \frac{I_h}{\epsilon_i} \left[8 \left(\frac{I_H}{\Delta E_{ij}} f_{i \to j} \right) Y(\xi, \delta_1) + \frac{1}{N} \left(\frac{2z}{a_0} R_1^c + \sqrt{\epsilon_i / I_H} \sqrt{\epsilon_j / I_H} \left(\frac{R_1^c}{a_0} \right)^2 \right) \right] \pi a_0^2 \tag{2.40}$$

δ_0 in the weak coupling expression corresponds to evaluation at R_0^c. δ_1 and R_1^c in the strong coupling expression corrsponds to evaluation at the impact parmater R_1 such that $P(R_1) = 1/N$. The functions X and Y are part of the ADAS Fortran libraries (*xip.for* and *yip.for* respectively).

Franck-Condon factor distribution of partial cross sections

Impact parameter aproach made with EIQIP is used to obtain vibrational cross sections for excitation electron impact processes. However some care must be taken in order to maintain the coherence for having a correct Franck-Condon distribution when these cross section are summed up to obtain the total electronic excitation cross section. This is automatically done when using the EIQIP approaches.

In sections 2.5.2 has been shown how Impact Parameter model can be used to calculate vibrational transitions. In the previous paragraphs it has been shown that oscillator strength can be written in function of the dipolar momentum. Usin imnpact parameter approach for th calculation of vibrational transition cross sections in the two state approachWe can prove now that the sum of the partial cross sections calculated in the IP approach fullfils the unitarity of the Franck-Condon factors and total cross sections can be splitted in partial cross sections multiplying by the corresponding Franck-Condon factors.

Writing the cross section for the generic vibrational states v to v' transition in the weak coupling approximation of EIQIP [43] we have:

$$Q_{v\to v'} = \frac{I_H}{E}\left[8\left(\frac{I_H}{\Delta E}\mathcal{F}_{vv'}\right)Y(\xi,\delta_0)\right]\pi a_0^2 \tag{2.41}$$

where E is the initial energy of the incident electron, $\xi = (z/a_0)\left|\frac{1}{k_v} - \frac{1}{k_{v'}}\right|$, $\delta = R^c\,|k_v - k_{v'}|$ and $Y(\xi,\delta_0)$ is a tabulated function (see section 2.5.2). If we assume a weak dependence of $Y(\xi,\delta_0)$ on the cut-off radius R^c (see [43] for details) we can substitute equation (2.32) in equation (2.41) to obtain a linear dependence on Franck-Condon factors:

$$Q_{v\to v'} = \left[\frac{32\pi^4 mc^2\alpha^2}{3E}Y(\xi,\delta_0)\frac{g_{\Lambda'}}{g_\Lambda}gF_{vv'}\,|\mathcal{D}_{vv'}|^2\right]\pi a_0^2 = A\times\frac{g_{\Lambda'}}{g_\Lambda}gF_{vv'}\,|\mathcal{D}_{vv'}|^2 \tag{2.42}$$

where all the factors have been group in the A constant. Total cross section will be obtain by the sum of partials as:

$$Q_v^{\mathrm{TOT}} = \sum_{v'+\mathrm{continuum}} A\times\frac{g_{\Lambda'}}{g_\Lambda}gF_{vv'}\,|\mathcal{D}_{vv'}|^2 \simeq A\times\frac{g_{\Lambda'}}{g_\Lambda}g\left|\bar{\mathcal{D}}\right|^2 \tag{2.43}$$

where in the last equalty we have applied:

$$\sum_{v'+\mathrm{continuum}}\frac{g_{\Lambda'}}{g_\Lambda}gF_{vv'}\,|\mathcal{D}_{vv'}|^2 \simeq \frac{g_{\Lambda'}}{g_\Lambda}g\left|\bar{\mathcal{D}}\right|^2\sum_v F_{vv'} \tag{2.44}$$

and the unitarity rule $\sum_v F_{vv'} = \sum_{v'} F_{vv'} = 1$ including the continuum in the summation has been applied as well. The statistical factors can exit the summation as the angular momemntum Λ_v of the upper and lower vibrational states remain the same. We can asume the dipole moments to be approximately constant in the vibrational states after having done the approximation of equation (2.29), so the vibrational dependence in all contained in the Franck-Condon factors.

That proves that the partial cross section for vibrational transitions are correctly distributed with the Franck-Condon probabitlities due to the linear dependence on the oscillator strength.

A similar proof can be carried out in the strong coupling case (see [43]) obtaining the same result.

2.5.3 ECIP model

Following the interest in classical approaches to electron and ion impact in the 1960s, Burgess developed an approximation for electron impact which combined a classical binary encounter model for low energy collisions combined with an IP treatment of high energy collisions. The classical part, including electron exchange is

$$\sigma^c_{i\to\epsilon} = 4\pi a_0^2 \frac{I_H}{\epsilon_i + \epsilon_b + \chi}\left[\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\right) + \frac{2}{3}\frac{\epsilon_b}{I_H}\left(\frac{I_H^2}{\chi^2} - \frac{I_H^2}{\epsilon_i^2}\right) - \frac{I_H \ln(\epsilon_{\rm i}/\chi)}{\epsilon_i + \chi}\right] \tag{2.45}$$

where ϵ_i and ϵ_b are the kinetic energies of the incident and bound electrons respectively and χ is the ionisation potential. The bound kinetic energy and ionisation potential refer to a specific molecular orbital. The cross-section is summed over orbitals, weighted by the orbital occupancies. In application to population modelling, Burgess and Summers simply the above expression by setting ϵ_b to zero yielding

$$\sigma^c_{i\to\epsilon} = 4\pi a_0^2 \frac{I_H}{\epsilon_i + \chi}\left[\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\right) - \frac{I_H \ln(\epsilon_{\rm i}/\chi)}{\epsilon_i + \chi}\right] \tag{2.46}$$

To this is added the IP part. It is obtained from the weak coupling expression (equation 2.39), but with the oscillator strength analytically continued into the continuum (bound state j becomes a free electron state of energy ϵ), so that it becomes a differential cross-section in the ejected electron energy. The cut-off closest approach R_0^c is replaced by $R_0^c + 2I_H\sqrt{(\epsilon_i + \chi - \epsilon)/\epsilon}/(\epsilon_i + \chi)$. ϵ is the ejected electron energy. A quadrature over this energy from zero to one-half of the incident electron energy (to avoid double counting with exchange) gives the IP contribution to the ionisation cross-section. ECIP has been used almost exclusivl;ey for ionisation of atoms and ions. For ionisation of molecules, a number of other approximations, very similar in concept to ECIP, have been more widely applied and tested against experiment. These include the BEB (binary-encounter-Bethe) approximation developed by Kim [**?**] and the DM formalism of Deutsch and Maerk [**?**]. These authors reintroduce the bound electron kinetic energy ϵ_b and some other adjustments. The molecule is again treated as built from molecular shells with orbitals and occupancies. The occupancies, ionisation potentials of orbitals and average kinetic energies of orbitals are essentially treated as free parameters. Values for these parameters are given in the literature for many systems - atomic, molecular and cluster. It is convenient to have these approximations available here also for comparisons. The BEB approximation [**?**] is

$$\sigma^c_{i\to\epsilon} = 4\pi a_0^2 \zeta_i \frac{I_H}{\epsilon_i + \epsilon_b + \chi}\left[\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\right) + \frac{\ln(\epsilon_{\rm i}/\chi)}{2}\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\frac{\chi}{\epsilon_i}\right) - \frac{I_H \ln(\epsilon_{\rm i}/\chi)}{\epsilon_i + \chi}\right] \tag{2.47}$$

where the orbital occupancy ζ_i is now included explicitly. A modification is made to the expression for ionisation of singly charged molecular ions, namely

$$\sigma^c_{i\to\epsilon} = 4\pi a_0^2 \zeta_i \frac{I_H}{\epsilon_i + (\epsilon_b + \chi)/2}\left[\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\right) + \frac{\ln(\epsilon_{\rm i}/\chi)}{2}\left(\frac{I_H}{\chi} - \frac{I_H}{\epsilon_i}\frac{\chi}{\epsilon_i}\right) - \frac{I_H \ln(\epsilon_{\rm i}/\chi)}{\epsilon_i + \chi}\right] \tag{2.48}$$

The DM approximation [**?**] for ionisation from a single orbital writes the cross-sections as

$$\sigma^c_{i\to\epsilon} = g_i \pi r_i^2 \zeta_i f(u) \tag{2.49}$$

where r_i is the radius of highest probability density of the atomic (molecular) orbital, g_i is an empirical weighting factor and $u = \epsilon_i/\chi$. In turn the function $f_i(u)$ is written as

$$f_i(u) = d\frac{1}{u}\left(\frac{u-1}{u+1}\right)^a \left[b + c\left(1 - \frac{1}{2u}\right)\ln\left(2.7 + ({\rm u}-1)^{1/2}\right)\right] \tag{2.50}$$

a, b, c and d are empirical parameters determined by matching to experimental data. Deutsch et al. [**?**] also introduce a modified form designed to have better behaviour in the higher energy regime through to the Born-Bethe limit. This non-classical form is

$$\sigma^{nc}_{i\to\epsilon} = g_i \pi r_i^2 \zeta_i b_i(u)\,[\ln({\rm c_i u})/{\rm u}] \tag{2.51}$$

where

$$b_i(u) = \frac{A_1 - A_2}{1 + (u/A_3)^p} + A_2 \tag{2.52}$$

leaving four empirical parameters, A_1, A_2, A_3, p and c_i to be specified for each orbital. These formulae, with elaborated empirical forms and larger numbers of empirical parameters lose some of the simple classical scattering basis of ECIP and BEB. They are perhaps best considered as more precise fitting formulae, but with less *ab initio* predictive capability. Here, we prefer to use ECIP, and its progenitor classical differential cross-sections (see Burgess & Perival

[?], suitably restricted in energy space and phase space, as tentative predictors of unknown cross-sections. The full differential cross-section for transfer of energy in the range ϵ to $\epsilon + d\epsilon$ is

$$\frac{d\sigma_i^c}{d\epsilon} = \frac{4\pi a_0^2}{I_H}\frac{I_H}{\epsilon_i+\epsilon_b+\chi}\left[\left(\frac{I_H^2}{\epsilon^2}+\frac{4}{3}\frac{I_H^2\epsilon_b}{\epsilon_i^3}\right)+\left(\frac{I_H^2}{(\epsilon_i+\chi-\epsilon)^2}+\frac{4}{3}\frac{I_H^2\epsilon_b}{(\epsilon_i+\chi-\epsilon)^3}\right)-\frac{I_H}{(\epsilon_i+\chi)}\left(\frac{I_H}{\epsilon}+\frac{I_H}{(\epsilon_i+\chi-\epsilon)}\right)\right] \tag{2.53}$$

The corresponding differential cross-section expression for an incident postive ion of charge z_i and mass m_i and target ion (bound in the molecule) of charge z_b and mass m_b is

$$\frac{d\sigma_i^c}{d\epsilon} = \frac{4\pi a_0^2}{I_H}\frac{I_H}{\epsilon_i}\frac{z_i^2 z_b^2 m_i}{m_b}\left[\left(\frac{I_H^2}{\epsilon^2}+\frac{4}{3}\frac{I_H^2\epsilon_b}{\epsilon_i^3}\right)\right] \tag{2.54}$$

Finally, the double differential cross-section for energy transfer $d\epsilon$ and momentum transfer dq is also helpful in considerations of rotational excitation. For prior momenta $p_i(= m_i v_i)$ and $p_b(= m_b v_b)$, this is

$$\frac{d^2\sigma_i^c}{d\epsilon dq} = \frac{8\pi a_0^2}{I_H}\frac{I_H}{\epsilon_i}\frac{z_i^2 z_b^2 m_i m_b I_H^2}{p_b q^4} \tag{2.55}$$

2.5.4 IP and ECIP Results

In order to have a qualitative idea of the goodness of the approaches made here, comparison of data with the previous recommended theoretical data from [11] have been performed.

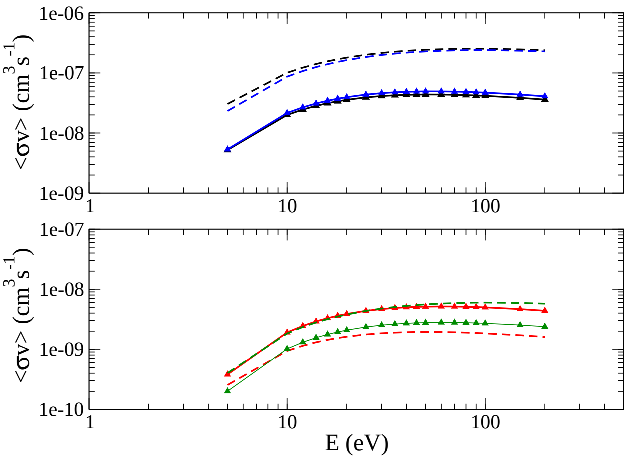


Figure 2.10: Maxwell rates for excitation process H(X $^1\Sigma_g^+$; $v = 0$) + e → H_2(A) + e. (▲—): original data from [11]; (- - -): EIQIP calculations. Black: A=B $^1\Sigma_u^+$ (top graph); Blue: A=C $^1\Pi_u$ (top graph); Green: A=B″B $^1\Sigma_u^+$(bottom graph); Red: A=D′ $^1\Pi_u$ (bottom graph).

In figure 2.10 this comparison is shown for excitation from ground state at the $v = 0$ level of H_2 to B,C (top) and B″B and D′ (bottom) states. It is possible to see that this approximation overestimate in a factor ~5-6 the calculations of cross section to B and C states from R. Celiberto and T. M. Rescigno [44] made with a more elaborated impact parameter calculations. As EIQIP models could have problems in the molecular cut-off radious (the molecular nucleus is taken as a diffuse ball and with no structure), it could be expected that the situation improve when dealing with transition between excited states. Unfortunately htere are no calculation nor experiments given in the literature for transition between excited states of H_2 molecule. It has been only possible for us to compare excitation cross sections to higher states. Indeed, as it can be seen on figure 2.10 (bottom), the comparisons improve when compared excitation to B″B($N = 3$) and D′($N = 4$) being now the ratio of a factor ~2-3 with the original data from [8].

EICIP can be tested as well for the ionization and dissociation processes in H_2. That has been don in figures 2.11 for ionization and 2.12 for dissociative excitation.

Ionization ECIP calculations are not appropriate for the range of ionizing and dissociative process resulting in two orders of magnitude difference with the original data from SOURCE OF ORIGINAL DATA.

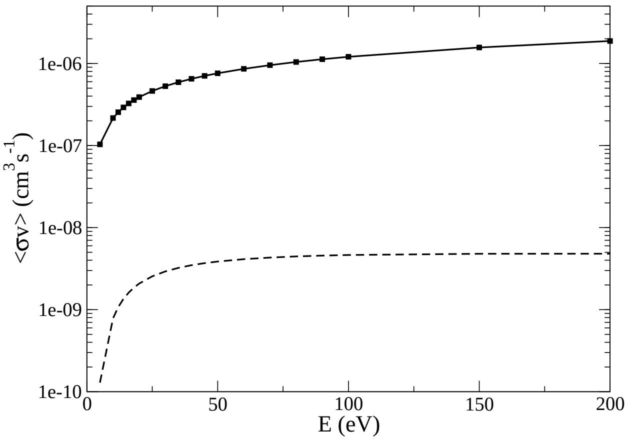


Figure 2.11: Maxwell rates for direct ionization process H(X $^1\Sigma_g^+$; v = 0) + e → H_2^+ + e. (■—): original data from [11]; (- - -): ECIP calculations.

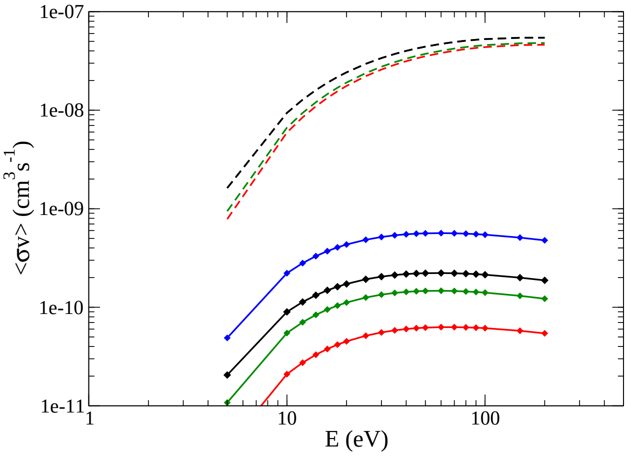


Figure 2.12: Maxwell rates for dissociative excitation process H(X $^1\Sigma_g^+$; v = 0) + e → H_2(A) + e → H + H + e. (♦—): original data from [11]; (- - -): ECIP calculations. Black: A=B $^1\Sigma_u^+$; Blue: A=C $^1\Pi_u$; Green: A=B″B $^1\Sigma_u^+$; Red: A=D′ $^1\Pi_u$.

Chapter 3

Collisional-Radiative model for molecules

Collisional-radiative models have been applied to hydrogen molecule in the past [25, 45]. However that has been an individual effort in order to obtain an specific quantity or to know the neutral contribution to molecules. We have used the big experience of ADAS [46] in generalized collisional radiative models in order to create one for molecules which gives effective coefficients and spectroscopic derived quantities appropriate for the plasma edge as well as molecular and dissociacion product populations. In this chapter the theory will be explained.

3.1 Molecular Generalized Collisional-Radiative Model

In this section the balance equations for the model will be obtained. Firstly, an analysis of time scales is made, then the collsional radiative coefficients deduced. Finally, the role of the vibrational and electronic resolutions will be explained.

3.1.1 Time Scales

As it has been already seen in chapter 2 the different processes in the H_2 system have different temperature ranges in which they either can strongly influence the evolution of the system or have a negligible influence in the MCR model.

In order to make a correct approach to the population modelling it is nessary to pay atention to the relaxation lifetimes of the different molecular and atomic states that are part of our collisional system. In the atomic case it happens in most plasmas [47] that:

$$\tau_{plasma} \sim \tau_m \gg \tau_o \gg \tau_{ee} \tag{3.1}$$

where $\tau_{plasma} \sim 1 - 10$s is the charachteristic plasma time (relaxation time, diffusion time), τ_m is the metastable radiative decay time, $\tau_0 \sim 10^{-8} - 10^{-10}$s is the ordinary states radiative decay time and τ_{ee} is the thermalization time given by[48]:

$$\tau_{ee} = \frac{m^{1/2}(3kT)^{3/2}}{8 \times 0.714\pi n_e^4 Z^4 \ln\Lambda} \tag{3.2}$$

where m is the electron mass, k is the Boltzman constant, n is the density in cm^{-3} and T is given in K. For a plasma of 1KeV and $n_e = 10^{13}$cm^{-3}, $\tau_{ee} \sim 10^{-10}$. That allows us to have a situation of “quasi-equilibrium” where the excited population can be assumed to be relaxed with respect to the metastables.

In the molecular case is expectad that time scales will have a similarity with atomics. Iin the case of H_2, the triplet state $c\,^3\Pi_u$ metastable radiative decay relaxation time is around 1ms [49] which is much less than τ_{plasma} and could be compared to some ion impact relaxation times depending on the temperature (see section 3.1.1. Thus, it has been decided to obtain the time scales for the maxwellian processes in the H_2 molecule and the it will be possible to discriminate between the processes that could be important in a CR model and the ones that are in a much longer time scale and do not compite with the formers. In order to achieve that, processes in the routine *adas901.for* (see 4.2.1) has been created. That routine interrogates the collisional rates format files *mdf33*, *mdf34*, *mdf04* and *mdf14* and obtain the relaxation times from them as is shown in the section 3.1.1.

Molecular relaxation times

In a first approach to the problem, each of the collisional radiative coupled equations can be approximated by:

$$\frac{\mathrm{d}}{\mathrm{d}t}N_i = \Sigma_j C_{ij} + r_i - \frac{N_i}{\tau_0} \tag{3.3}$$

where N_i represents the initial state we are looking at, C_{ij} the coupling coefficients with other states (here C_{ii} represent the looses), r_i is a source term that represents the processes that input from other species and the original influx of molecules and the last term refers to the looses by other means different from collisional or decay processes depending on a time constant τ_0. Let's N_i be the initial state on which the molecules are born. We need to know which processes are dominant here and in which temperature and density conditions, which ones can be neglected in these conditions and how to compare them. This will give us an idea of the completeness needed for our model. The most obvious way to do that without actually doing a collisional radiative model is comparing the time constants of the different processes:

$$\tau^P = \frac{1}{C_{ii}^P} = \frac{1}{\Sigma_j N^S q_{i\to j}} \tag{3.4}$$

where N^S is the density of the species S involved in the collisional processes of class P and $q_{i\to j}$ are the maxwellian coefficients of each process from initial state i. Thus, it is the first task to obtain the maxwellian time constant for the different processes such as ionization from electron and ion impact, excitation from collisions with electrons, protons, neutrals (H) or other molecules, charge exchange processes,etc.

Importance of the collisional matrix completion

Looking at the time constants it is possible to have an idea of how important could be the collisional processes that lack. In figure 3.1 the time constant for total dissociation from all vibrational levels of the gorund state are compared. Dashed line rpresents the fundamental data from *mdf33* format files and the continuous line data from *mdf04* where ECIP approach have been used to complete the lacking data from excited vibrational levels. Here, in total dissociation are included all process which drive to dissociation of the H_2 molecule.

In the figure the new data correspond of a time constant of two orders of magnitude lower and that can be compared with excitation processes as can be seen in table 3.1. Dissociation has an special importance here as this process cannot be reversed in plasmas and drives directly to the formation of neutrals and protons. This a dramatic example of how the processes in excited vibrational levels and states can influence the collisional-radiative picture.

Excitation, ionization and dissociation processes

In figures 3.2, where excitation and total dissociation from all vibrational levels of ground state are represented.

In these figures it is well seen to see that here dissociation and excitation processes have similar order of magnitude in time constants. As before, we have considered total dissociation as the sum of all process that finish in dissociation. Dissociation and excitation processes are decaying as temperature and density increases as the collisionality of the system is higher. Even when contour diagrams are good enough to give a general picture, a careful look in some

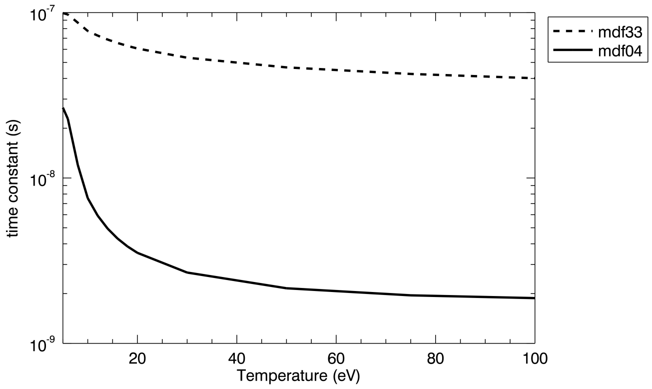


Figure 3.1: Time constants for H_2 + e → H + H(H^+) processes for 3×10^{13}cm^{-3}. Dashed line: fundamental data from *mdf33* file; continuous line: fundamental and calculated data from ECIP approach in *mdf04* file.

chosen temperatures and densities can stablish what are the driver processes. In the figure 3.3, where dissociation and excitation times from all vibronic levels of ground state are plotted in function of the electron density and temperature, can be apreciated that excitation and total dissociation are on the same order of magnitude and both porcesses will compite. As dissociative processes are irreversible we can conclude that all the molecules in the plasma will disappear sooner or later, it will be needed then a source term to have a balance equilibrium. The source terms, assumed constant will be discussed in section 3.2. Ionization processes are of the order of excitation processes as can be seen in figure 3.6.

Looking at dissociation. The main dissociative mechanism is different in low and intermediate temperatures. Dissociative excitation dominates at the whole range of temperatures and at low temperatures ($T_e \lesssim$ 10eV) excitation to dissociative state b $^3\Sigma_u^+$ contributes to dissociation at low energies as shown in figure 3.4. Both mechanism should be taken in account in the plasma edge plasmas where the molecules are expected to play a role. Dissociative excitation will have a bigger importance after the collisional-radiative model as the contributions must be summed after.

It is necessary to be cautious, however, with the densities relevant for the different processes. Heavy ion impact can play a significant role when the proton density is in the same order of magnitude that the electron density (as $n_{H^+} \sim n_e$). in the case of neutral atoms impact, models on passive charge exchange spectroscopy suggest that neutral density can be between 100 to 1000 times lower in the divertor[50] and in some cases of high CX recombination between 100 and 10 times lower[51]. So the H_2 + H collision processes would be irrelevant unless the rates are two or three order of magnitude bigger than electron impact excitation ones. The unknown density of molecules in the plasma could be crucial to dischard the molecule-molecule collisions that could lead to non-linearities of the CR model.

Proton impact dissociation rates are compared with electron impact in the figures 3.5. Here is possible to see that electron impact time constants are two orders of magnitude lower than the proton impact ones. Also, in figure 3.6 $H_2{}^+$ production is compared. Ion-impact processes are driven by charge exchange and electron impact processes by ionization[1]. H_2+ is a molecular ion in which all its bound level behave as metastables. Therefore, given that there are very few path to recombination (only inverse charge exchange), it can be considered as a intermediate stage to dissociation.

That leaves electron impact processes as the dominant processes in those plasma conditions. However, proton impact CX can be a significant contribution for the $H_2 \leftrightarrow H_2{}^+$ balance and neutral impact contribution must be studied in the future.

---

[1] ion impact ionization is negligible at these temperatures as it can be seen on the figure 3.6.

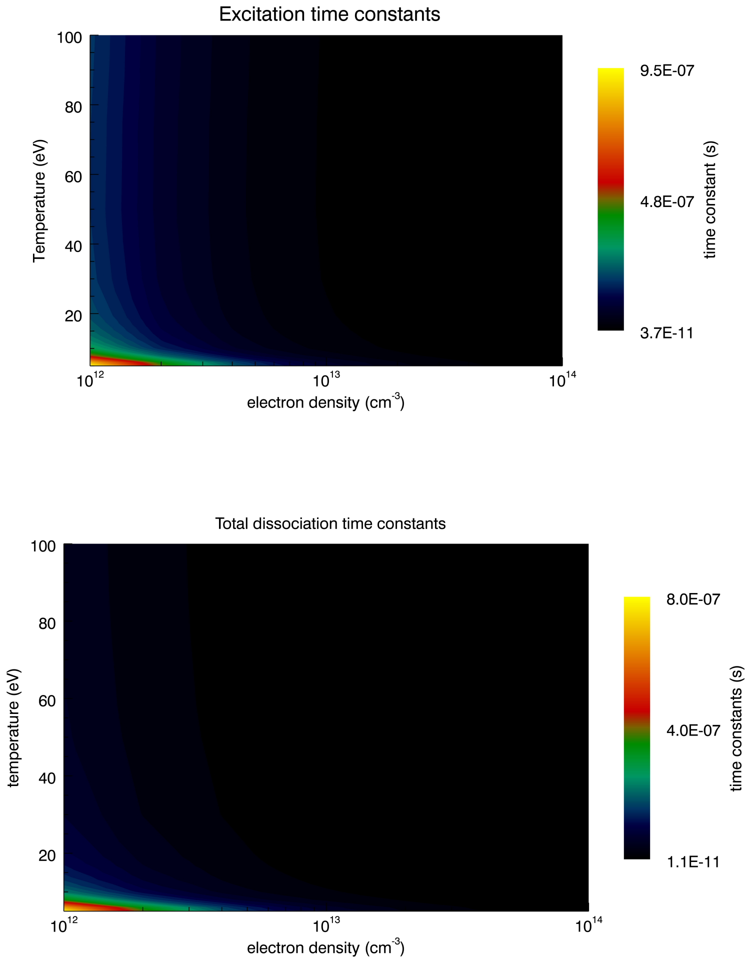


Figure 3.2: Contour diagrams of total dissociation (as in figure 3.1 and excitation time constant in electronic temperature and density. From the scales it can be seen that both processes are competing.Top: excitation; bottom: total dissociation.

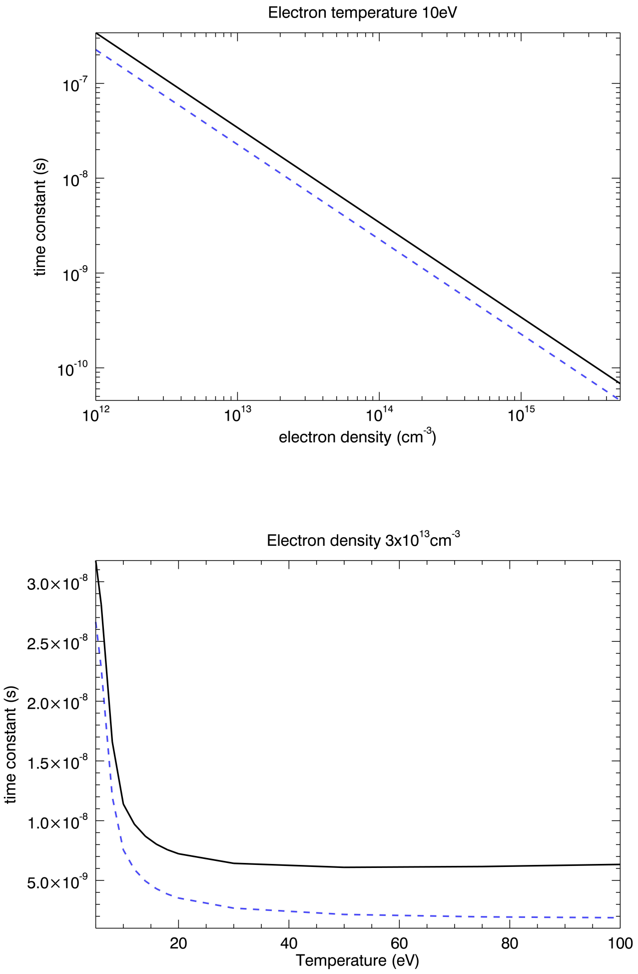


Figure 3.3: Comparative graphs where dissociation and excitation can be seen for a selected temperature or density. Top: excitation (—) and total dissociation (- -) time constant for $T_e = 10$eV; bottom: time constant versus temperature for $n_e = 3 \times 10^{13}\text{cm}^{-3}$.

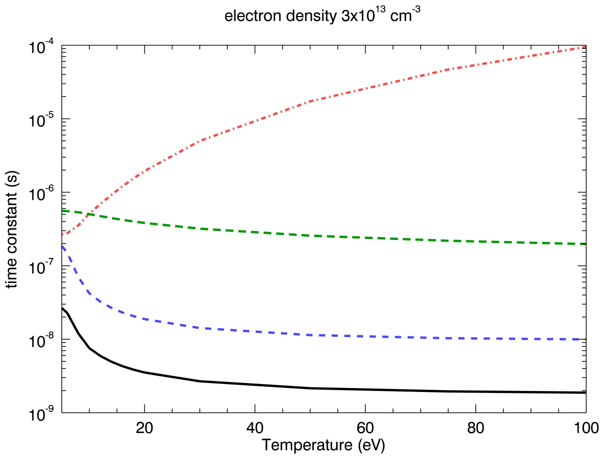


Figure 3.4: Contributions to time constants from dissociative processes to total dissociation from $H_2(X,\nu = 0-14)$.— Total dissociation; - - dissociative excitation; -·- excitation to dissociative $b\,^3\Sigma_u^+$ state; — — Dissociative electron attachment.

Vibrational lifetimes

The H_2 molecule null permanent dipole moment implies that in the initial electronic stae there are in fact fourteen vibrational states that do not decay anywhere and behave as metastables. However, the higher metastables can be excited to the dissociation continuum more easily. That could suposse different levels of "metastability". In the figure 3.7 the time constant for a reprensentative temperature and density and electronic collisional processes are plotted. The time constants have a sharp drop at $\nu = 2$ and stays very similar until $\nu = 14$. It is surprising that only the two lower levels $\nu = 0$ and $\nu = 1$ time constants are one order of magnitude higher and that is much easier to excite form $\nu = 2$. It is not excluded that could be a artifact coming from the different calculations that the data from $\nu \geq 2$ and $\nu \leq 1$ have been obtained in [11]. That enhances the necessity of having reliable and good quality data avalaible. Finally, it is needed to pass through the collisional-radiative model to study the real influence of these differences on the final populations.

Molecular Time Scales

Comparing the diferent relaxation times from in equation (3.1) it is possible to get a picture of the time scales of the H_2 molecules problem. In the table 3.1 are given the different times calculated before for the different representative processes. The times are similar for the different processes and only charge exchange is one order of magnitude over the rest. However, CX is the only mechanism that creates neutrals and molecular ions and should be counted. In the molecular ADAS model (see Chapter 4), CX can be switch on and off interactively.

Temp.	$\tau^{(e)}_{exc}$	$\tau^{(e)}_{ion}$	$\tau^{(e)}_{diss}$	$\tau^{(I)}_{CX}$
5 eV	$\sim 10^{-8}$s	$\sim 10^{-8}$s	$\sim 10^{-8}$s	$\sim 10^{-7}$s
10 eV	$\sim 10^{-8}$s	$\sim 10^{-9}$s	$\sim 10^{-9}$s	$\sim 10^{-7}$s

Table 3.1: Maxwellian relaxation times for representative collisional processes of H_2 for an electronic and ionic density $n = 3\times10^{13}\text{cm}^{-3}$. $\tau^{(e)}_{exc}$: electron-impact excitation relaxation time, $\tau^{(e)}_{ion}$ electron-impact ionization relaxation time, $\tau^{(e)}_{diss}$ electron-impact dissociation relaxation time, $\tau^{(I)}_{CX}$ proton-impact charge exchange relaxation time.

The table 3.1 and the inequalty (3.1) are giving a picture where ordinary states excite and radiate in a local thermodynamic equilibrium and the metastables ionize and dissociate with the same velocity. However, the fact that molecules exist in plasma as experimental measures confirms means that it must exist some external input flux of

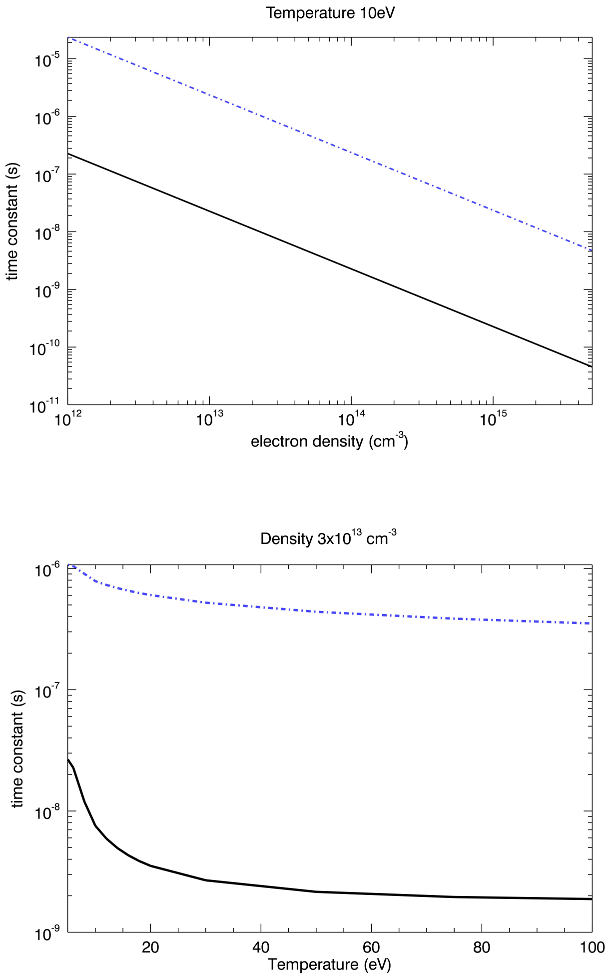


Figure 3.5: Comparative graphs where ion and electron impact dissociation are plot for a selected temperature or density. Density refers to ion and electron density ($n_e = n_i$) Top: electron impact (—) and ion impact (-··-) dissociation time constants for $T_e = 10$eV; bottom: excitation and total dissociation time constant for $n_e = 3 \times 10^{13}\text{cm}^{-3}$.

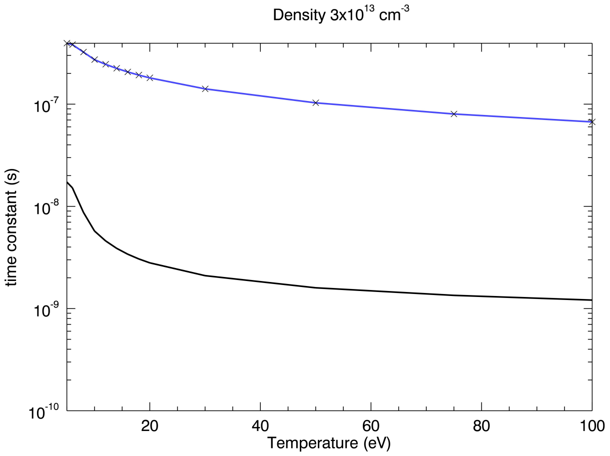


Figure 3.6: $H_2(X,v = 0 - 14) + P \rightarrow H_2^+(X)$ processes being P either electron or protons in each case. (—) electron impact ionization; (—) proton impact CX; (X) proton impact CX + ionization.

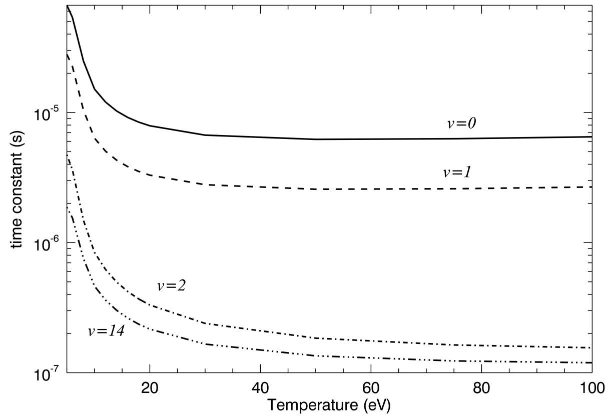


Figure 3.7: Time constants for dissociative excitation from H_2 (X $^1\Sigma_g^+$,v) versus temperature for an electron density of $n_e = 3 \times 10^{13}\text{cm}^{-3}$. Intermediate time constants between $v = 2$ and $v = 14$ have been removed for clarity.

molecules. Kinetic model of the plasma wall transition layer [53] picture molecules coming from sputtering in the walls, at the temperature and densities of the plasma we are focus in we can neglect rearrangement as source of molecules. Is then needed an input flux which maintain the molecular population constant in plasmas which has been taken into account in the molecular CR model and will be treated in section 3.2. In this case the molecular metastable population will be dominant over the "ordinary" states and they will evolve on the time scales of the input flux, that is plasma time scales.

3.1.2 Collisional-Radiative model

Collisional-radiative model are widely used in the atomic case (see for example [47] and references herein). The molecular collisional-radiative model can be done analogous to the atomic ones and its coefficients can be obtained in a similar way (see [43, 47]). However, some care must be taken with the fact that various molecular ionization stages can dissociate in the same atomic ionization stage and that new processes such dissociation must go into the balance equations. Another significative difference is the number of metastables due to the non-existance of a permanent dipole moment between vibrational states of homonuclear diatomic molecules (see 3.1.1). That makes that every vibrational level of any electronic state metastable is as well a metastable. In the H_2 molecule the ground state is multiplied by 14 metastables and the triplet metastable by 19. In the molecular picture, there is a new process that has not atomic analogy: this is dissociation. From dissociation two atomic products are created at same time. Furthermore, dissociation is associated to the other "conventional" processes as it can be produced from excitation, ionization or charge exchange.

These reasons make that is necessary to rewrite the equations for molecular collisional-radiative model and reconsider all the processes to get new molecular collisional-radiative coefficients which have no atomic analogy.

The reaction considered for the molecular collisional-radiative processes of homonuclear diatomic molecules are:

$$\text{Electronic excitation by electron impact} \quad A_2(N,v)+e \rightarrow \quad A_2(N',v')+e \tag{3.5a}$$

$$\text{Vibrational excitation by electron impact} \quad A_2(N,v)+e \rightarrow \quad A_2(N,v')+e \tag{3.5b}$$

$$\text{Ionisation by electron impact} \quad A_2(N,v)+e \rightarrow \quad A_2^+(N'',v'')+2e \tag{3.5c}$$

$$\text{Recombination} \quad A_2^+(N',v')+e \rightarrow \quad A_2(N,v) \tag{3.5d}$$

$$\text{Charge eXchange} \quad A_2(N,v)+B^+ \rightarrow \quad A_2^+(N'',v'')+B \tag{3.5e}$$

$$\text{Inverse Charge eXchange} \quad A_2^+(N'',v'')+B \rightarrow \quad A_2(N,v)+B^+ \tag{3.5f}$$

$$\text{Dissociation by excitation to dissociative state} \quad A_2(N,v)+e \rightarrow \quad A_2(N'_{diss})+e \rightarrow A+A+e \tag{3.5g}$$

$$\text{Dissociative excitation} \quad A_2(N,v)+e \rightarrow \quad A_2(N',v'_{diss})+e \rightarrow A+A+e \tag{3.5h}$$

$$\text{Dissociative ionisation} \quad A_2(N,v)+e \rightarrow \quad A_2^+(N''_{diss})+2e \rightarrow A^++A+2e \tag{3.5i}$$

$$\text{Dissociative Charge eXchange} \quad A_2(N,v)+B^+ \rightarrow \quad A^++A+B \tag{3.5j}$$

$$\text{Dissociative Inverse Charge eXchange} \quad A_2^+(N'',v'')+B \rightarrow \quad A+A+B^+ \tag{3.5k}$$

To these processes, the "standard" atomic processes such as ionization, recombination, ionization and CX should be added to complete the whole collisional-radiative picture. Dissociative processes will be treated regarding only to their final products and all dissociation going to the same products will be sum to the final dissociative coefficients

Molecular Generalized Collisonal-Radiative Theory

We define by N_σ and N_ρ as the metastable density of one molecular ion (we need two indexes to caccount for exciation prcesses); $N_{i/j}$ the "ordinary" states density of this molecular ion; $N_{\nu/\nu'}$ the one time ionized molecule metastable density; $N^{(A)}_{\mu/\mu'}$ the neutral derived atomic specie metastable density; $N^{(A)}_{i''/j''}$ the neutral derived atomic specie "ordinary" states density and $N^{(A^+)}_{\mu^+/\mu^+}$, the one-time ionized atom density. We also consider that N_H is the main neutral density, N_{H^+} is the plasma ion density and N_e is the electron density.

From the discussion in section 3.1.1 we can assume a quasi-equilibrium situation where the ordinary states population will be in equilibrium wit the metastables whose population will vary in plasma time-scales.

The continuity equations for the metastables of our molecule can be writen as:

$$\frac{\mathrm{d}N_\rho}{\mathrm{d}t} = C_{\rho j}N_j + C_{\rho\sigma}N_\sigma + Q^{\mathrm{ICX}}_{\rho\nu}N_\nu N_H + r_{\rho\nu}N_\nu N_e + \Gamma \tag{3.6}$$

where the collisional terms are explained in table 3.2 and we use the convention of summation performed over the subscripts. The collisional terms C_{xy} include all collisional excitation and deexcitation as well as spontaneous and radiative processes from level y to level x. For each level i, the total loss rate given by:

$$C_{ii} = -\sum_{j\neq i} C_{ji} - NeS_i - \sum_{\nu/\sigma} Q^{\mathrm{CX/ICX}}_i - \sum_\mu D_i \tag{3.7}$$

being $Q^{\mathrm{CX/ICX}}_i$ the losses by direct or inverse charge exchange and D_i the losses by dissociation.

Γ include the source terms from the molecular metastables. We will ignore these sources for now and will come back to them in section 3.2.

Coefficient	Units	process
C_{xy}	s^{-1}	Collisional excitation rate ($cm^3/s \times Ne$)
Q^{CX}_{xy}	$cm^3 s^{-1}$	Direct charge exchange
Q^{ICX}_{xy}	$cm^3 s^{-1}$	Inverse charge exchange
S_{xy}	$cm^3 s^{-1}$	Ionisation
r_{xy}	$cm^3 s^{-1}$	Recombination
D_{xy}	$cm^3 s^{-1}$	Dissociation

Table 3.2: Nomenclature for the collisional coefficients in the collisional radiative equations

In equation (3.6), we have assumed that no other molecules with more electrons can exist in the plasma. To follow the ADAS collisional-radiative nomenclature which considers that the recombined speciess are “children” and the ionized ones are “parents”, this molecular ionization stage is defined as the “last descendant”, the ionized molecular stages are the “parents” till the “first ancestor” (the highest ionized molecular stage we consider that can be found in the plasma). Finally the atoms are the “atomic parents” with an “atomic first ancestor” and an “atomic last descendant”.

We can now write the continuity equation for the molecular last descendant ordinary states:

$$\frac{\mathrm{d}N_i}{\mathrm{d}t} = C_{ij}N_j + C_{i\sigma}N_\sigma + r_{i\nu}N_\nu N_e + Q^{\mathrm{ICX}}_{i\nu}N_\nu N_H \tag{3.8}$$

In quasi-equilibrium, the left term of equation (3.8) is null and we can solve it for N_j:

$$N_j = -C^{-1}_{ji}C_{ij}N_\sigma - C^{-1}_{ji}r_{i\nu}N_\nu N_e - C^{-1}_{ji}Q^{\mathrm{ICX}}_{i\nu}N_\nu N_H \tag{3.9}$$

Substituting in (3.6) we get:

$$\frac{\mathrm{d}N_\rho}{\mathrm{d}t} = \mathcal{M}C_{\rho\sigma}N_\sigma + \mathcal{M}Q^{\mathrm{ICX}}_{\rho\nu}N_\nu N_H + \mathcal{M}\mathcal{R}_{\rho\nu}N_\nu N_H \tag{3.10}$$

where:

$$
\begin{aligned}
\mathcal{MC}_{\rho\sigma} &= \left[C_{\rho\sigma} - C_{\rho j}C^{-1}_{ji}C_{i\sigma}\right]/N_e && \text{MQCD} && (3.11a)\\
\mathcal{MR}_{\rho\nu} &= r_{\rho\nu} - C_{\rho j}C^{-1}_{ji}r_{i\nu} && \text{MACD} && (3.11b)\\
\mathcal{MQ}^{\mathrm{ICX}}_{\rho\nu} &= Q^{\mathrm{ICX}}_{\rho\nu} - C_{\rho j}C^{-1}_{ji}Q^{\mathrm{ICX}}_{i\nu} && \text{MCXIACD} && (3.11c)
\end{aligned}
$$

These new coefficients are the molecular effective collisional-radiative coefficients. They are respectively the molecular effective cross coupling, recombination and inverse charge exchange recombination coefficients. They are named analogous to the atomic effective coefficients [46] and the "M" stands for molecules.

Now we can write the continuity equation for the ionized molecular species:

$$
\frac{\mathrm{d}N_\nu}{\mathrm{d}t} = S_{j\nu}N_jN_e + S_{\nu\sigma}N_\sigma N_e + \mathcal{MC}_{\nu\nu'}N_{\nu'} + Q^{\mathrm{CX}}_{\nu\sigma}N_\sigma N_{H^+} + Q^{\mathrm{CX}}_{\nu j}N_jN_{H^+} + \mathcal{MQ}^{\mathrm{ICX}}_{\nu\nu^+}N_{\nu^+}N_H + \mathcal{MR}_{\nu\nu^+}N_{\nu^+}N_e \qquad (3.12)
$$

where the level ν^+ represent the metastables of the next ionized molecular specie and where we have already included the contribution of the ordinary states of this molecular ion in the recombination and inverse charge exchange. In addition, substituing the child ordinary states from equation (3.6) in this molecular parent we arrive to the molecular efective coefficients for ionization and charge exchange:

$$
\begin{aligned}
\mathcal{MS}_{\nu\sigma} &= S_{\nu\sigma} - S_{\nu j}C^{-1}_{ji}C_{i\sigma} && \text{MSCD} && (3.13a)\\
\mathcal{MQ}^{\mathrm{CX}}_{\nu\sigma} &= Q^{\mathrm{CX}}_{\nu\sigma} - Q^{\mathrm{CX}}_{\nu j}C^{-1}_{ji}C_{i\sigma} && \text{MCXCD} && (3.13b)
\end{aligned}
$$

and a cross-coupling term via recombination and inverse charge exchange and new ionization or direct charge exchange:

$$
\mathrm{MXCD}_{\nu\nu'} = -\left[S_{\nu j} + Q^{\mathrm{CX}}_{\nu j}N_{H^+}/N_e\right] \times \left[C^{-1}_{ji}Q^{\mathrm{ICX}}_{i\nu'}N_H/N_e + C^{-1}_{ji}r_{i\nu'}\right] \qquad (3.14)
$$

Note that in molecular equations all metastable and ordinary terms of every ionisation stage that is present in plasma should be counted as all of them contribute by dissociation processes to the atomic species. It is also needed to count all levels in the atomic especies as dissociation products, that makes the collisional-radiative model more complicated and computationally more difficult to deal with.

The atomic dissociation products balance equations can be writen adding the dissociation sources from the molecular species:

$$
\frac{\mathrm{d}N^{(A)}_\mu}{\mathrm{d}t} = \sum_\sigma D_{\mu\sigma}N_\sigma N_e + \sum_j D_{\mu j}N_jN_e + C_{\mu\mu'}N^{(A)}_{\mu'} + C_{\mu j''}N_{j''} + S_{\mu\mu^-}N^{(A^-)}_{\mu^-}N_e + S_{\mu j^-}N^{(A^-)}_{j^-}N_e + r_{\mu\mu^{+\prime}}N^{(A^+)}_{\mu^{+\prime}}N_e + \Gamma^{(A)}_\mu \quad (3.15)
$$

Here again, the collisional losses are included in the diagonal excitation terms $C_{\mu\mu}$. The summatory in σ indicates that is needed to sum over all the metastates of all the molecular species wich dissociate into this neutral atom and the summatory over j indicates the sum over "ordinary" states. Here is assumed ionization only to metastables and recombination only from metastables.

If we forget ionization to the last atomic descendant, assuming for the moment that there are not negative species we can try to solve the balance equation assuming equilibrium for the "ordinary" states (quasi-static equilibrium):

$$\frac{\mathrm{d}N_{i''}^{(A)}}{\mathrm{d}t} = \sum_{\sigma} D_{i''\sigma} N_{\sigma} N_e + \sum_{j} D_{i''j} N_j N_e + C_{i''\mu'} N_{\mu'} + C_{i''j''} N_{j''} + r_{i''\mu^{+\prime}} N_{\mu^{+\prime}} N_e = 0 \tag{3.16}$$

Solving, we obtain the usual atomic coefficients for excitation and recombination[47]:

$$\mathcal{C}_{\mu\mu'} = \left[C_{\mu\mu'} - C_{\mu j''} C^{-1}_{j''i''} C_{i''\mu'}\right]/N_e \quad \text{QCD} \tag{3.17a}$$

$$\mathcal{R}_{\mu\mu^{+\prime}} = r_{\mu\mu^{+\prime}} - C_{\mu j''} C^{-1}_{j''i''} r_{i''\mu^{+\prime}} \quad \text{ACD} \tag{3.17b}$$

and the dissociation effective coefficients:

$$\mathcal{PD}_{\mu\sigma} = \mathcal{D}_{\mu\sigma} - C_{\mu j''} C^{-1}_{j''i''} \mathcal{D}_{i''\sigma} \quad \text{PDCD} \tag{3.18a}$$

$$\mathcal{PAD}_{\mu\nu} = -\mathcal{D}_{\mu j} C^{-1}_{ji} Q^{\mathrm{ICX}}_{i\nu} N_H - \mathcal{D}_{\mu j} C^{-1}_{ji} r_{i\nu} N_e \quad \text{PADCD} \tag{3.18b}$$

where

$$\mathcal{D}_{\mu\sigma} = D_{\mu\sigma} - D_{\mu j} C^{-1}_{ji} C_{i\sigma} \quad \text{DCD (met)} \tag{3.19a}$$

$$\mathcal{D}_{i''\sigma} = D_{i''\sigma} - D_{i''j} C^{-1}_{ji} C_{i\sigma} \quad \text{DCD (ord)} \tag{3.19b}$$

$$\mathcal{D}_{\mu j} = D_{\mu j} - C_{\mu j''} C^{-1}_{j''i''} D_{i''j} \quad \text{DCD (mol. ord.)} \tag{3.19c}$$

Here $\mathcal{PD}$ stands for partial dissociative because the total dissociation must be summed over all the initial molecular states.

Effective PDCD dissociative coefficients can be explained as follows: dissociation can be direct from metastables or through a collisional-radiative proceses by the molecular "ordinary" states and both processes combine to give an effective ionization to one atomic states (DCD coefficients). However, the dissociation product can be formed directly or by dissociation followed by a collisional-radiative process and both combine to produce the final PDCD coefficients.

If the molecule is recombined with an electron to an "ordinary" molecular state it can decay or be excited to another state which dissociates into an atomic state. The atomic collisional radiative combination of such processes are the effective dissociation through recombination (PADCD) effective coefficients.

Finally, looking at the metastables of the ionized atom:

$$\frac{\mathrm{d}N_{\mu^+}^{(A^+)}}{\mathrm{d}t} = \sum_{\sigma} D_{\mu^+\sigma} N_{\sigma} N_e + \sum_{j} D_{\mu^+j} N_j N_e + S_{\mu^+\mu'} N_{\mu'}^{(A)} N_e + S_{\mu^+j''} N_{j''}^{(A)} N_e + C_{\mu^+\mu^{+\prime}} N_{\mu^{+\prime}}^{(A^+)} + \mathcal{R}_{\mu^+\mu^{++}} N_{\mu^{++}}^{(A^{++})} + \Gamma_{\mu^+}^{(A^+)} \tag{3.20}$$

Solving for the atomic "ordinary" states of the recombined atom we obtain the atomic effective coefficients for ionization and cross-coupling through recombination and ionization[47]:

$$\mathcal{S}_{\mu^+\mu'} = S_{\mu^+\mu'} - S_{\mu^+j''} C^{-1}_{j''i''} C_{i''\mu'} \quad \text{SCD} \tag{3.21a}$$

$$XCD_{\mu^+\mu^{+\prime}} = -N_e \left[S_{\mu^+j''} C^{-1}_{j''i''} r_{i''\mu^{+\prime}}\right] \quad \text{XCD} \tag{3.21b}$$

At the same time solving equation (3.20) for the “ordinary” molecular states we obtain the addicional terms for dissociation:

$$
\begin{aligned}
\mathcal{PDS}_{\mu^+\sigma} &= -N_e\left[S_{\mu^+j''}C^{-1}_{j''i''}D_{i''\sigma}\right] && \text{PDSCD} && (3.22a)\\
\mathcal{PADS}_{\mu^+\nu} &= -N_eS_{\mu^+j''}C^{-1}_{j''i''}D_{i''j}C^{-1}_{ji}\left[Q^{\mathrm{ICX}}_{i\nu}N_H + r_{i\nu}N_e\right] && \text{PADSCD} && (3.22b)
\end{aligned}
$$

The effective coefficient from equation (3.22a) is the contribution coming from dissociation followed by collisional radiative excitation and ionization. The effective coefficient from equation (3.22b) is the contribution from a molecular “ordinary” state that is the result of a collisional-radiative excitation from a recombined state.

These coefficients need to be obtained for all the ionization stages of the dissociation product wich can be originated from the molecules in a plasma. This is because many of the molecules can originate the same dissociation products through different dissociation paths and it is needed to deal with the whole molecular system to have complete picture (see figure 3.8).

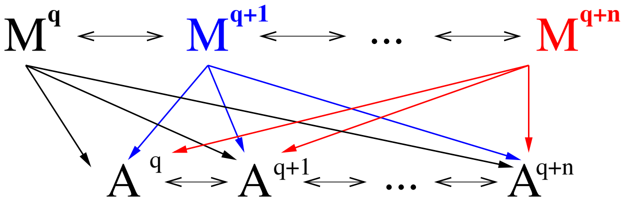


Figure 3.8: Molecular species and dissociation atomic products needed to be considered in a molecular collisional radiative calculation

Fully Statical Equilibrium Populations

Once obtained the effective coefficients, it is possible to construct the collisional matrix including all the metastables of the system:

$$
\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} N_\rho \\ N_\sigma \\ N_\nu \\ \vdots \\ N^{(A)}_{\mu} \\ N^{(A)}_{\mu'} \\ N^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} = N_e \times \begin{pmatrix}
\mathcal{MC}_{\rho\rho} & \mathcal{MC}_{\rho\sigma} & \mathcal{MR}_{\rho\nu} + \mathcal{MQ}^{\mathrm{ICX}}_{\rho\nu} & \cdots & 0 & 0 & 0 & \cdots(0) \\
\mathcal{MC}_{\sigma\rho} & \mathcal{MC}_{\sigma\sigma} & \mathcal{MR}_{\sigma\nu} + \mathcal{MQ}^{\mathrm{ICX}}_{\sigma\nu} & \cdots & 0 & 0 & 0 & \cdots(0) \\
\mathcal{MS}_{\nu\rho} + \mathcal{MQ}^{\mathrm{CX}}_{\nu\rho} & \mathcal{MS}_{\nu\sigma} + \mathcal{MQ}^{\mathrm{CX}}_{\nu\sigma} & \mathcal{MC}_{\nu\nu} + MXCD_{\nu\nu} & \cdots & 0 & 0 & 0 & \cdots(0) \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
\mathcal{TD}_{\mu\rho} & \mathcal{TD}_{\mu\sigma} & \mathcal{TD}_{\mu\nu} & \cdots & \mathcal{C}_{\mu\mu} & \mathcal{C}_{\mu\mu'} & \mathcal{R}_{\mu\mu^+} & \cdots \\
\mathcal{TD}_{\mu'\rho} & \mathcal{TD}_{\mu'\sigma} & \mathcal{TD}_{\mu'\nu} & \cdots & \mathcal{C}_{\mu'\mu} & \mathcal{C}_{\mu'\mu'} & \mathcal{R}_{\mu'\mu^+} & \cdots \\
\mathcal{TD}_{\mu^+\rho} & \mathcal{TD}_{\mu^+\sigma} & \mathcal{TD}_{\mu^+\nu} & \cdots & \mathcal{S}_{\mu^+\mu} & \mathcal{S}_{\mu^+\mu'} & \mathcal{C}_{\mu^+\mu^+} + XCD_{\mu^+\mu^+} & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
$$

$$
\times \begin{pmatrix} N_\rho \\ N_\sigma \\ N_\nu \\ \vdots \\ N^{(A)}_{\mu} \\ N^{(A)}_{\mu'} \\ N^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} + \begin{pmatrix} \Gamma_\rho \\ \Gamma_\sigma \\ \Gamma_\nu \\ \vdots \\ \Gamma^{(A)}_{\mu} \\ \Gamma^{(A)}_{\mu'} \\ \Gamma^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} \qquad (3.23)
$$

Here, we have grouped into the term $\mathcal{TD}$ all the dissociative effective coefficients that relate both states. Compressing the notation of equation (3.23) to $\frac{d}{dt}\mathbf{N} = N_e\overline{\mathbf{F}} \times \mathbf{N} + \mathbf{\Gamma}$ and setting the left-hand side to zero we obtain the *fully statical equilibrium* solution:

$$\mathbf{N} = -\frac{1}{N_e}\overline{\mathbf{F}}^{-1} \times \mathbf{\Gamma} \tag{3.24}$$

Then, given an input flux and assuming a system in equilibrium it is possible to obtain the populations of the metastables of **the whole system**. Note that in the matrix $\overline{\mathbf{F}}$ the upper right square is null (see equation (3.23))as it must be as re-arrangement of atoms to form molecules is neglected at the temperatures considered, meaning that the processes only go in one direction, needing the input flux to compensate the equilibrium. this point will be disscused in detail in section 3.2.

3.1.3 Vibrational and electronic resolutions in molecular GCR

The vibronic levels of the molecules can increase the number of states in two orders of magnitud and in extreme examples they can make the calculation computationally slow. To avoid that it is possible to "compress" the vibrational states into the electronic states dealing the electronic states as if they were "atomic" levels (see figure 3.9). This reduces the number of levels to be considered and allow a fast computation of collisional-radiative quantities. In the diatomic homonuclear molecules which are the object of this study the vibrational levels of the metastable electronic states are kept in their full resolution independently of the total resolution adopted for the rest of the "ordinary" states.

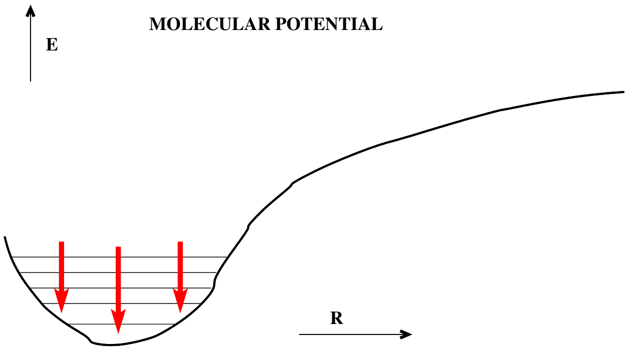


Figure 3.9: In the electronic resolution the vibrational levels of the "ordinary" electronic states are "compressed" to the electronic state.

Thus, to pass from full vibrational resolution to electronic resolution, it is needed to sum the rates over all the vibrational levels to get the electronic rates save in the case of the metastables. Details of vibrational resolution approaches are given in section 2.1.3. Then, the effective coefficients will be obtained in the electronic resolution and population can be obtained for fully statical equilibrium from equation (3.24).

Differences in the results in the two resolutions can be expected as the collisionality between vibrational levels have been reduced to the electronic levels and they are not independent any more but act in "groups" inside each electronic levels. An analysis of the behaviour of populations and effective coefficients for the H_2 system is presented in section **??**.

3.2 Source terms

The source terms come from the density flux of species of our molecular system inside the observation volume (positive) and outside it (negative). However, in a statical equilibrium situation the source term can be traslated into a stationary density of molecules inside of an observation volume which dissociates into cold atoms [52].

Therefore, it is possible to obtain the source terms corresponding to a stationary density of one or more states of the molecular system. It is possible then modify them to obtain the corresponding fluxes for the collisional-radiative matrix of equation (3.23).We can suppose then, that we have an input source term traslated in the constant set of populations of the neutral states N_ρ. Then the flux vector will be:

$$N_e \times \Gamma_\rho = N_e \times \begin{pmatrix} \Gamma_\rho \\ \mathcal{MC}_{\sigma\rho} N_\rho \\ \mathcal{MS}_{\nu\rho} N_\rho + \mathcal{MQ}^{\mathrm{CX}}_{\nu\rho} N_\rho \\ \vdots \\ \mathcal{TD}_{\mu\rho} N_\rho \\ \mathcal{TD}_{\mu'\rho} N_\rho \\ \mathcal{TD}_{\mu^+\rho} N_\rho \\ \cdots \end{pmatrix} \tag{3.25}$$

Here the collisional-radiative terms contain the direct and collisional-raditaive contributions to the populations from this source term. Other species than molecules can also be a source term, specially dissociation products which can come from physical sputtering at the same time than the molecules(see for example [53]). The total source term Γ_{tot} will be the sum of all of them.

Knowing the population of N_ρ we can extract it form the full system equation (3.23) and obtain the new system:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} N_\sigma \\ N_\nu \\ \vdots \\ N^{(A)}_\mu \\ N^{(A)}_{\mu'} \\ N^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} &= N_e \times \begin{pmatrix} \mathcal{MC}_{\sigma\sigma} & \mathcal{MR}_{\sigma\nu} + \mathcal{MQ}^{\mathrm{ICX}}_{\sigma\nu} & \cdots & 0 & 0 & 0 & \cdots (0) \\ \mathcal{MS}_{\nu\sigma} + \mathcal{MQ}^{\mathrm{CX}}_{\nu\sigma} & \mathcal{MC}_{\nu\nu} + MXCD_{\nu\nu} & \cdots & 0 & 0 & 0 & \cdots (0) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \mathcal{TD}_{\mu\sigma} & \mathcal{TD}_{\mu\nu} & \cdots & \mathcal{C}_{\mu\mu} & \mathcal{C}_{\mu\mu'} & \mathcal{R}_{\mu\mu^+} & \cdots \\ \mathcal{TD}_{\mu'\sigma} & \mathcal{TD}_{\mu'\nu} & \cdots & \mathcal{C}_{\mu'\mu} & \mathcal{C}_{\mu'\mu'} & \mathcal{R}_{\mu'\mu^+} & \cdots \\ \mathcal{TD}_{\mu^+\sigma} & \mathcal{TD}_{\mu^+\nu} & \cdots & \mathcal{S}_{\mu^+\mu} & \mathcal{S}_{\mu^+\mu'} & \mathcal{C}_{\mu^+\mu^+} + XCD_{\mu^+\mu^+} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \\ &\times \begin{pmatrix} N_\sigma \\ N_\nu \\ \vdots \\ N^{(A)}_\mu \\ N^{(A)}_{\mu'} \\ N^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} + \begin{pmatrix} \Gamma_\sigma \\ \Gamma_\nu \\ \vdots \\ \Gamma^{(A)}_\mu \\ \Gamma^{(A)}_{\mu'} \\ \Gamma^{(A^+)}_{\mu^+} \\ \cdots \end{pmatrix} \end{aligned} \tag{3.26}$$

To this equation is possible now to apply the solution (3.24) and obtain the rest of the populations.

3.3 Non-linear terms from Charge Exchange

In the case of hydrogen molecular system, if CX is considered, the following processes must be considered:

$$\text{Charge eXchange} \quad H_2 + H^+ \rightarrow \quad H_2^+ + H \tag{3.27a}$$

$$\text{Inverse Charge eXchange} \quad H_2^+ + H \rightarrow \quad H_2 + H^+ \tag{3.27b}$$

These collisions affect the density of molecules and dissociation products at the same time and create a non-linearity in the balance equations. Now, given the lower importance of CX in the collisional processes that we discussed on section 3.1.1 one can try to deal with this terms in an iterative way and after some iteration the system will eventually gain the convergence.

To solve this, it is assumed that the proton and neutral density remains constant, that it, it is not affected by charge exchange processes, during the first iteration of the population calculation. Setting $N_H^{(0)} = N_\mu^{(A)}$, $N_{H'}^{(0)} = N_{\mu'}^{(A)}$ and $N_{H^+}^{(0)} = N_{\mu^+}^{(A^+)}$ in the notation of equation (3.23), in full equilibrium the equations for the atomic hydrogen metastables will be:

$$
\begin{aligned}
0 \equiv \frac{\mathrm{d}N_H^{(0)}}{\mathrm{d}t} &= N_e\mathcal{T}\mathcal{D}_{H\rho}N_\rho + N_e\mathcal{T}\mathcal{D}_{H\sigma}N_\sigma + N_e\mathcal{T}\mathcal{D}_{H\nu}N_\nu + \cdots + N_e\mathcal{C}_{HH}N_H^{(0)} + \\
&\quad + N_e\mathcal{C}_{HH'}N_{H'}^{(0)} + N_e\mathcal{R}_{HH^+}N_{H^+}^{(0)} + \cdots \qquad (3.28a) \\
0 \equiv \frac{\mathrm{d}N_H^{(0)}}{\mathrm{d}t} &= N_e\mathcal{T}\mathcal{D}_{H^+\rho}N_\rho + N_e\mathcal{T}\mathcal{D}_{H^+\sigma}N_\sigma + N_e\mathcal{T}\mathcal{D}_{H^+\nu}N_\nu + \cdots + N_e\mathcal{S}_{H^+H}N_H^{(0)} + \\
&\quad + N_e\mathcal{S}_{H^+H'}N_{H'}^{(0)} + N_e\mathcal{C}_{H^+H^+}N_{H^+}^{(0)} + N_eXCD_{H^+H^+}N_{H^+}^{(0)} + \cdots \qquad (3.28b)
\end{aligned}
$$

which we can simplify as:

$$
\begin{aligned}
N_e\mathcal{C}_{HH}N_H^{(0)} + A &= 0 \qquad (3.29a) \\
N_e\mathcal{C}_{H^+H^+}N_{H^+}^{(0)} + B &= 0 \qquad (3.29b)
\end{aligned}
$$

where in the terms A and B are included all the collisional processes save the losses. After that the iterated populations will be:

$$
\begin{aligned}
0 \equiv \frac{\mathrm{d}N_H^{(1)}}{\mathrm{d}t} &= N_e\mathcal{C}_{HH}N_H^{(1)} + A - Q^{\mathrm{ICX}}N_{H_2^+}N_H^{(0)} + Q^{\mathrm{CX}}N_{H^+}^{(0)}N_{H_2} \qquad (3.30a) \\
0 \equiv \frac{\mathrm{d}N_{H^+}^{(1)}}{\mathrm{d}t} &= N_e\mathcal{C}_{H^+H^+}N_{H^+}^{(1)} + B + -Q^{\mathrm{CX}}N_{H^+}^{(0)}N_{H_2} + Q^{\mathrm{ICX}}N_{H_2^+}N_H^{(0)} \qquad (3.30b)
\end{aligned}
$$

Now substituting A and B from equations (3.29) the iterated populations are obtained:

$$
\begin{aligned}
N_H^{(1)} &= N_H^{(0)}\left(1 + \frac{Q^{\mathrm{ICX}})N_{H_2^+}}{\mathcal{C}_{HH}}\right) - \frac{Q^{\mathrm{CX}}N_{H^+}^{(0)}N_{H_2}}{\mathcal{C}_{HH}} \qquad (3.31a) \\
N_{H^+}^{(1)} &= N_{H^+}^{(0)}\left(1 + \frac{Q^{\mathrm{CX}}N_{H_2}}{\mathcal{C}_{H^+H^+}}\right) - \frac{Q^{\mathrm{ICX}}N_H^{(0)}N_{H_2^+}}{\mathcal{C}_{H^+H^+}} \qquad (3.31b)
\end{aligned}
$$

Then the populations of the rest of the metastable are calculated again with the new “background” proton and neutral densities and the operation is repeated as many times as necessary to achieve convergency.

This treatment will be valid if two conditions are fullfilled. First, the proton and neutral densities are not mainly driven by the CX processes; and second, CX processes are low enough to don’t affect the molecular population importantly. Otherwis, non linearities would become important and the system will not converge. In that case a solution must be search solving the complete equation system by different techniques.

Chapter 4

ADAS9xx: The molecular ADAS

The model explained in chapter 3 has been traslated to a series of fortran routines which integrate in ADAS [46] and constitute the ADAS series 9xx (ADAS9xx). At the same time, the fundamental data needed to be processed as well as the derivated data obtained as an output of the ADAS9xx have been rationally written in different formats witch allow at the same time a correct processing of the different cases and a human localization and read of possible problems.

In this chapter the ADAS9xx routines and molecular data formats are described.

4.1 Structure and Diagrams

ADAS9xx are a series of independent routines which sequentially work to provide collisional radiative coefficients and other derived quantities from the fundamental compiled data which are cross sections and rates from external sources (see chapter 2).

These data should be integrated and completed. Then they must be set up in the adequate resolution to be treated by the collisional-radiative routines and obtain the corrected effective coefficients.

In figure 4.1 can be seen the general scheme of ADAS9xx series.The fundamental molecular data, which come from external sources are compiled in a format *mdf02* file (see sections 4.3 and chapter 2) and then the routines ADAS902 and ADAS903 generate the *mdf04* format file, which has the most complete matrix available to be included inside the CR model (ADAS904) which is going to produce the derivate (collisional radiative) coefficients that can be used in plasma studies.

In the intermediate stage the format file *mdf33* with the maxwellian rates is generated from ADAS902 as is shown in the diagram 4.2. Thus, it is possible to call sequentially these routines to produce step by step the data necessary to be run by the next routine and arrive finally to the last collisional-radiative data.

The role of the different routines is summarized as follows:

- ADAS901 package obtains effective lifetimes and reads and plots the coefficients of the various processes.
- ADAS902 integrates, interpolates and extrapolates (if necessary) the existing cross sections and creates the maxwellian rate coefficients. It also creates the different resolution files.
- ADAS903 looks for the gap in the transitions and calculates them by semi-classical Impact Parameter approach in the required resolution.
- ADAS904 calculates the molecular effective coefficients, write them in the various *mdf11* and *mdf15* formats and inverts the matrix to obtain the populations.
- MDFLIBS are different tools to deal with the data stored.

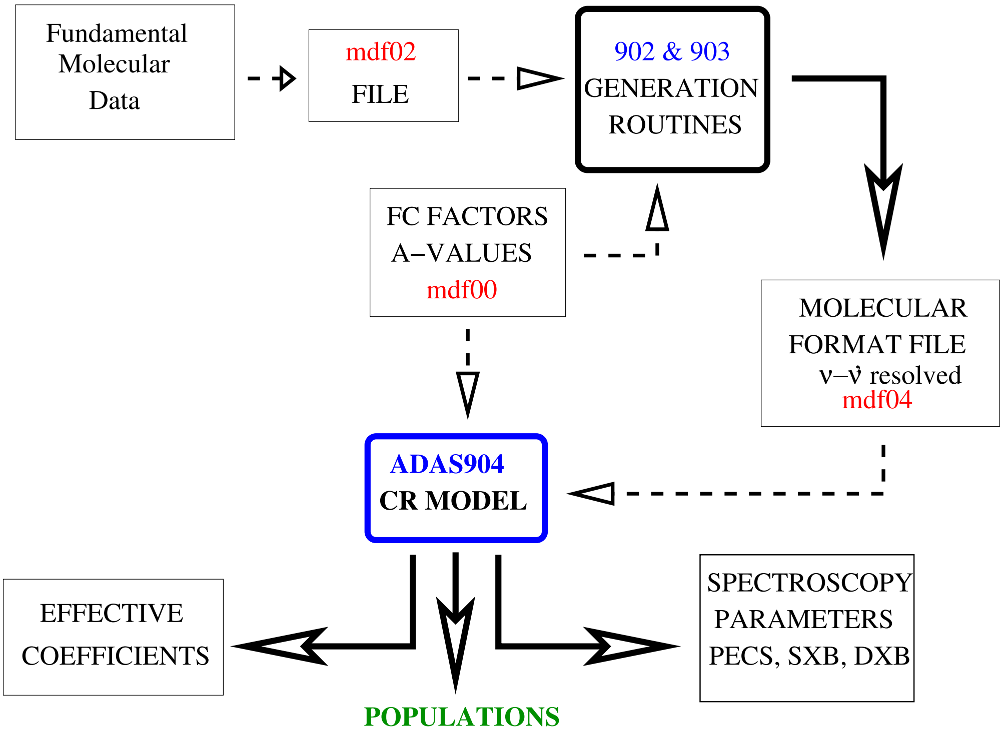


Figure 4.1: General scheme of ADAS9xx routines working.

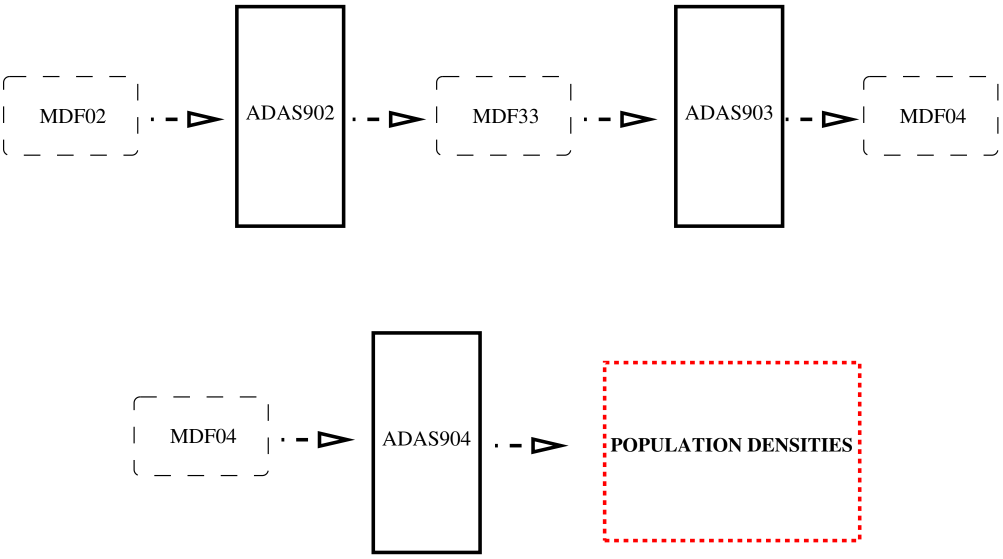


Figure 4.2: Sequential scheme of ADAS9xx routines.

Details of every of subroutines follows.

4.2 The Molecular ADAS9xx routines

4.2.1 ADAS901

This subroutine (header is given in appendix C.1) is a *multiuse* routine whose objective is to interrogate different formats and produce an output that can be use to be read in a environment which allows to make plots as IDL or MATLAB or by a shellscript in an UNIX server.

ADAS901 deals with the formats *mdf33*, *mdf34*, *mdf04*, *mdf14* and *mdf11*. All of them have been processed by at least one of ADAS9xx routines as can be seen in figure 4.2.

Case *mdf33*, *mdf34*, *mdf04* and *mdf14*

ADAS901 reads the input format data and calculates the relaxation times from the rates. Some input parameters should be given to the code in order to obtain the required results in a file called *itaus.dat*:

1. SW. '33', '04' or '11' allows the program to discriminate the format to be read.
2. PFILE. Path to the *mdf* file.
3. CATEG, MI. Category of data (1=upsilons, 2=rates or 3=non-maxwellian) and ion mass if *mdf34* or *mdf14* (0 otherwise).
4. NGRPS. Number of groups of data wanted for output.

   For each group:

   i TYP. Type of selecting processes:'ST' for states, in this case the code will look for the final states of the transition.'PR' for processes, the code will look for the indicated processes.'DS' for dissociation processes, the code will look only for dissociation processes to give a total dissociation relaxation time.

   ii NPRS, (PRS(C1,C2), C2=1,NPRS(C1)). number of processes/final states to be summed, process/final state number. In case of dissociation the last parameter is just "-3".
5. NNES. Number of densities.
6. (NE(C2), C2=1,NNES). Array of densities.
7. IENRP. Number of temperatures.
8. (ENRP(C2), C2=1,IENRP). Array of temperatures.
9. STL, STU, VL, VU. Lower and upper initial state for the transitions to be summed up. Lower and upper initial vibrational states to be summed up.

This input driver must be located in the directory where ADAS901 runs. An example of input driver is given in the figure 4.3.

The output will be given in the files "TAUS_ELEC.dat" and "TAUS_VIB.dat". Here is given a matrix of values whose columns vary in densities and rows in temperature. Groups are separated and some information about them is given as header. An example of the file is given in figure 4.4

in case of vibrational resoultion of the initial states required a new file is given called "TAUS_VIB" which is similar to the previous one but in each group the vibrational levels between VL and VU are resolved.

```
'04'
'/madas/madas/mdf33/h2/el#09_h2.dat'
2 0
5
'pr'
2 2 3
'pr'
1 13
'pr'
3 17 19 20
'ds'
1 -3
'st'
1 17
16
1.d12 2.d12 4.d12 6.d12 8.d12 1.d13 2.d13 3.d13 4.d13 6.d13 8.d13 1.d14 3.d14 5.d14 1.d15 5.d15
15
1.d0 2.d0 3.d0 4.d0 5.d0 6.d0 8.d0 10.d0 12.d0 14.d0 16.d0 18.d0 20.d0 30.d0 50.d0
1 1 0 0
```

Figure 4.3: Example of file *itaus*, input of ADAS901.

```
/GROUP  1 PROCESSES:  2  3
                 0.1000E+13 0.2000E+13 0.4000E+13 0.6000E+13 0.8000E+13 0.1000E+14 0.2000E+14 0.3000E+…
   1.000         0.4829E-07 0.2415E-07 0.1207E-07 0.8048E-08 0.6036E-08 0.4829E-08 0.2415E-08 0.1610E-…
   2.000         0.4566E-10 0.2283E-10 0.1141E-10 0.7610E-11 0.5707E-11 0.4566E-11 0.2283E-11 0.1522E-…
   3.000         0.7361E-11 0.3680E-11 0.1840E-11 0.1227E-11 0.9201E-12 0.7361E-12 0.3680E-12 0.2454E-…
   4.000         0.2229E-11 0.1115E-11 0.5573E-12 0.3716E-12 0.2787E-12 0.2229E-12 0.1115E-12 0.7431E-…
   5.000         0.9621E-12 0.4810E-12 0.2405E-12 0.1603E-12 0.1203E-12 0.9621E-13 0.4810E-13 0.3207E-…
   6.000         0.5224E-12 0.2612E-12 0.1306E-12 0.8707E-13 0.6530E-13 0.5224E-13 0.2612E-13 0.1741E-…
   8.000         0.2289E-12 0.1145E-12 0.5723E-13 0.3815E-13 0.2861E-13 0.2289E-13 0.1145E-13 0.7630E-…
   10.00         0.1338E-12 0.6690E-13 0.3345E-13 0.2230E-13 0.1672E-13 0.1338E-13 0.6690E-14 0.4460E-…
   12.00         0.9120E-13 0.4560E-13 0.2280E-13 0.1520E-13 0.1140E-13 0.9120E-14 0.4560E-14 0.3040E-…
   14.00         0.6820E-13 0.3410E-13 0.1705E-13 0.1137E-13 0.8525E-14 0.6820E-14 0.3410E-14 0.2273E-…
   16.00         0.5417E-13 0.2708E-13 0.1354E-13 0.9028E-14 0.6771E-14 0.5417E-14 0.2708E-14 0.1806E-…
   18.00         0.4485E-13 0.2242E-13 0.1121E-13 0.7474E-14 0.5606E-14 0.4485E-14 0.2242E-14 0.1495E-…
   20.00         0.3827E-13 0.1913E-13 0.9566E-14 0.6378E-14 0.4783E-14 0.3827E-14 0.1913E-14 0.1276E-…
   30.00         0.2238E-13 0.1119E-13 0.5596E-14 0.3731E-14 0.2798E-14 0.2238E-14 0.1119E-14 0.7461E-…
   50.00         0.1284E-13 0.6419E-14 0.3209E-14 0.2140E-14 0.1605E-14 0.1284E-14 0.6419E-15 0.4279E-…
-----------------------------------------
/GROUP  2 PROCESSES: 13
                 0.1000E+13 0.2000E+13 0.4000E+13 0.6000E+13 0.8000E+13 0.1000E+14 0.2000E+14 0.3000E+…
   1.000         0.4753E-03 0.2376E-03 0.1188E-03 0.7921E-04 0.5941E-04 0.4753E-04 0.2376E-04 0.1584E-…
   2.000         0.4548E-05 0.2274E-05 0.1137E-05 0.7579E-06 0.5684E-06 0.4548E-06 0.2274E-06 0.1516E-…
   3.000         0.1875E-05 0.9377E-06 0.4689E-06 0.3126E-06 0.2344E-06 0.1875E-06 0.9377E-07 0.6252E-…
   4.000         0.1189E-05 0.5943E-06 0.2972E-06 0.1981E-06 0.1486E-06 0.1189E-06 0.5943E-07 0.3962E-…
   5.000         0.8834E-06 0.4417E-06 0.2208E-06 0.1472E-06 0.1104E-06 0.8834E-07 0.4417E-07 0.2945E-…
   6.000         0.7107E-06 0.3554E-06 0.1777E-06 0.1185E-06 0.8884E-07 0.7107E-07 0.3554E-07 0.2369E-…
   8.000         0.5230E-06 0.2615E-06 0.1308E-06 0.8717E-07 0.6538E-07 0.5230E-07 0.2615E-07 0.1743E-…
   10.00         0.4216E-06 0.2108E-06 0.1054E-06 0.7026E-07 0.5270E-07 0.4216E-07 0.2108E-07 0.1405E-…
   12.00         0.3574E-06 0.1787E-06 0.8935E-07 0.5957E-07 0.4467E-07 0.3574E-07 0.1787E-07 0.1191E-…
   14.00         0.3129E-06 0.1564E-06 0.7822E-07 0.5215E-07 0.3911E-07 0.3129E-07 0.1564E-07 0.1043E-…
   16.00         0.2800E-06 0.1400E-06 0.6999E-07 0.4666E-07 0.3499E-07 0.2800E-07 0.1400E-07 0.9332E-…
   18.00         0.2545E-06 0.1273E-06 0.6363E-07 0.4242E-07 0.3181E-07 0.2545E-07 0.1273E-07 0.8484E-…
   20.00         0.2342E-06 0.1171E-06 0.5855E-07 0.3903E-07 0.2927E-07 0.2342E-07 0.1171E-07 0.7806E-…
   30.00         0.1724E-06 0.8619E-07 0.4310E-07 0.2873E-07 0.2155E-07 0.1724E-07 0.8619E-08 0.5746E-…
   50.00         0.1197E-06 0.5986E-07 0.2993E-07 0.1995E-07 0.1496E-07 0.1197E-07 0.5986E-08 0.3991E-…
-----------------------------------------
/GROUP  3 PROCESSES: 17 19 20
                 0.1000E+13 0.2000E+13 0.4000E+13 0.6000E+13 0.8000E+13 0.1000E+14 0.2000E+14 0.3000E+…
   1.000         0.1530E-04 0.7651E-05 0.3825E-05 0.2550E-05 0.1913E-05 0.1530E-05 0.7651E-06 0.5101E-…
   2.000         0.5013E-02 0.2506E-02 0.1253E-02 0.8355E-03 0.6266E-03 0.5013E-03 0.2506E-03 0.1671E-…
   3.000         0.1300E-01 0.6498E-02 0.3249E-02 0.2166E-02 0.1624E-02 0.1300E-02 0.6498E-03 0.4332E-…
   4.000         0.8071E-02 0.4035E-02 0.2018E-02 0.1345E-02 0.1009E-02 0.8071E-03 0.4035E-03 0.2690E-…
   5.000         0.6270E-02 0.3135E-02 0.1567E-02 0.1045E-02 0.7837E-03 0.6270E-03 0.3135E-03 0.2090E-…
   6.000         0.5426E-02 0.2713E-02 0.1356E-02 0.9043E-03 0.6782E-03 0.5426E-03 0.2713E-03 0.1809E-…
   8.000         0.4735E-02 0.2367E-02 0.1184E-02 0.7891E-03 0.5919E-03 0.4735E-03 0.2367E-03 0.1578E-…
   10.00         0.4541E-02 0.2271E-02 0.1135E-02 0.7569E-03 0.5677E-03 0.4541E-03 0.2271E-03 0.1514E-…
   12.00         0.4539E-02 0.2270E-02 0.1135E-02 0.7565E-03 0.5674E-03 0.4539E-03 0.2270E-03 0.1513E-…
   14.00         0.4630E-02 0.2315E-02 0.1157E-02 0.7716E-03 0.5787E-03 0.4630E-03 0.2315E-03 0.1543E-…
   16.00         0.4773E-02 0.2387E-02 0.1193E-02 0.7955E-03 0.5967E-03 0.4773E-03 0.2387E-03 0.1591E-…
   18.00         0.4950E-02 0.2475E-02 0.1238E-02 0.8251E-03 0.6188E-03 0.4950E-03 0.2475E-03 0.1650E-…
   20.00         0.5147E-02 0.2573E-02 0.1287E-02 0.8578E-03 0.6433E-03 0.5147E-03 0.2573E-03 0.1716E-…
   30.00         0.6293E-02 0.3147E-02 0.1573E-02 0.1049E-02 0.7867E-03 0.6293E-03 0.3147E-03 0.2098E-…
   50.00         0.8964E-02 0.4482E-02 0.2241E-02 0.1494E-02 0.1120E-02 0.8964E-03 0.4482E-03 0.2988E-…
-----------------------------------------
```

Figure 4.4: Example of file *TAUS_ELEC.dat*, output of ADAS901.

Case *mdf11*

Given the complexity and variety of *mdf11* files it is always good to represent the effective coefficients in a human readable way. Furthermore, sometimes could be reasonable to sum up the coefficients from the different vibrational levels of the initial electronic metastable to provide an "electronic coefficient". In the same way could be useful, for example in the ionization case to sum over all the states of the resulting species. ADAS901 when "SW" tag is switch to '11' is providing these coefficient in a readable format.

As before an input drive file must be given (see figure 4.5 for an example). It should have the following variables:

1. SW. '33', '04' or '11' allows the program to discriminate the format to be read.
2. PFILE. Path to the *mdf* file.
3. TYP(1). Set to 'TM' varies the matrix rows in molecular temperature given a different matrix for a different electronic temperature. Set to 'TE' varies in electronic temperature.
4. (PRS(1,C1), C1=1,2). Final electronic states limits for summing up.
5. (PRS(2,C1), C1=1,2). Final vibrational levels limit in the previous electronic states for summing up.
6. NTMS. Number of molecular temperatures. If bigger than 1 then:
    - (TM(C1),C1=1,NTMS). Array of molecular temperatures.
7. NNES. Number of densities.
8. (NE(C2), C2=1,NNES). Array of densities.
9. IENRP. Number of temperatures.
10. (ENRP(C2), C2=1,IENRP). Array of temperatures.
11. STL, STU, VL, VU. Lower and upper initial state for the transitions to be summed up. Lower and upper initial vibrational states to be summed up.

Output is given in file "EFF_COEFS.dat" in a format given in the figure 4.6. Here the molecular temperature is 0eV and is given in the first column.

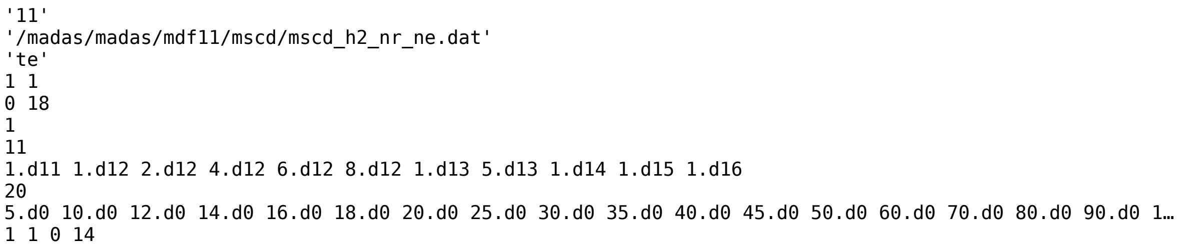
4.2.2 ADAS902

This program is the one which deals with the original fundamental data stored in *mdf02* and integrate them to give Maxwellian rate coefficient in the desired energy range. The header of the routine is given in appendix C.2.

A diagram of the structure of ADAS902 can be seen on figure 4.7. As in the previous section it is needed an input file with the parameters which will define how this program will run and the characteristics of the data read. An example of it is in figure 4.8

The parameters needed to be given in file input 902 are:

1. NPF. Number of *mdf02* files to be read.
2. PFILE(). Path for each of the *mdf02* files.
3. EI. If 'e' *mdf02* are electron impact files. If EI is 'I' *mdf02* are ion impact files.
4. MMOL, MP. Molecule mass and ion mass (0 in case of electron impact).
5. NMTE. Number of electronic temperatures desired.



```
'11'
'/madas/madas/mdf11/mscd/mscd_h2_nr_ne.dat'
'te'
1 1
0 18
1
11
1.d11 1.d12 2.d12 4.d12 6.d12 8.d12 1.d13 5.d13 1.d14 1.d15 1.d16
20
5.d0 10.d0 12.d0 14.d0 16.d0 18.d0 20.d0 25.d0 30.d0 35.d0 40.d0 45.d0 50.d0 60.d0 70.d0 80.d0 90.d0 1…
1 1 0 14
```

Figure 4.5: Example of file *itaus*, input of ADAS901 for *mdf11* format files.

```
/GROUP  1 INCLUDING: te   1  0
                           0.1000E+12 0.1000E+13 0.2000E+13 0.4000E+13 0.6000E+13 0.8000E+13 0.1000E+1…
 0.000       5.000         0.3553E-07 0.3553E-07 0.3553E-07 0.3553E-07 0.3553E-07 0.3553E-07 0.3553E-0…
 0.000       10.00         0.9152E-07 0.9152E-07 0.9152E-07 0.9152E-07 0.9152E-07 0.9152E-07 0.9151E-0…
 0.000       12.00         0.1104E-06 0.1104E-06 0.1104E-06 0.1104E-06 0.1104E-06 0.1104E-06 0.1104E-0…
 0.000       14.00         0.1273E-06 0.1273E-06 0.1273E-06 0.1273E-06 0.1273E-06 0.1273E-06 0.1273E-0…
 0.000       16.00         0.1425E-06 0.1425E-06 0.1425E-06 0.1425E-06 0.1425E-06 0.1425E-06 0.1425E-0…
 0.000       18.00         0.1564E-06 0.1564E-06 0.1564E-06 0.1564E-06 0.1564E-06 0.1564E-06 0.1564E-0…
 0.000       20.00         0.1691E-06 0.1691E-06 0.1690E-06 0.1690E-06 0.1690E-06 0.1690E-06 0.1690E-0…
 0.000       25.00         0.1966E-06 0.1966E-06 0.1966E-06 0.1966E-06 0.1966E-06 0.1966E-06 0.1966E-0…
 0.000       30.00         0.2199E-06 0.2199E-06 0.2199E-06 0.2199E-06 0.2199E-06 0.2199E-06 0.2199E-0…
 0.000       35.00         0.2402E-06 0.2402E-06 0.2402E-06 0.2402E-06 0.2402E-06 0.2402E-06 0.2402E-0…
 0.000       40.00         0.2582E-06 0.2582E-06 0.2582E-06 0.2582E-06 0.2582E-06 0.2582E-06 0.2582E-0…
 0.000       45.00         0.2745E-06 0.2745E-06 0.2745E-06 0.2745E-06 0.2745E-06 0.2745E-06 0.2745E-0…
 0.000       50.00         0.2894E-06 0.2894E-06 0.2894E-06 0.2894E-06 0.2894E-06 0.2894E-06 0.2894E-0…
 0.000       60.00         0.3162E-06 0.3162E-06 0.3162E-06 0.3162E-06 0.3162E-06 0.3162E-06 0.3162E-0…
 0.000       70.00         0.3400E-06 0.3400E-06 0.3400E-06 0.3400E-06 0.3400E-06 0.3400E-06 0.3400E-0…
 0.000       80.00         0.3616E-06 0.3616E-06 0.3616E-06 0.3616E-06 0.3616E-06 0.3616E-06 0.3616E-0…
 0.000       90.00         0.3816E-06 0.3816E-06 0.3816E-06 0.3816E-06 0.3816E-06 0.3816E-06 0.3816E-0…
 0.000       100.0         0.4002E-06 0.4002E-06 0.4002E-06 0.4002E-06 0.4002E-06 0.4002E-06 0.4002E-0…
 0.000       150.0         0.4809E-06 0.4809E-06 0.4809E-06 0.4809E-06 0.4809E-06 0.4809E-06 0.4809E-0…
 0.000       200.0         0.5492E-06 0.5492E-06 0.5492E-06 0.5492E-06 0.5491E-06 0.5491E-06 0.5491E-0…
------------------------------------------
------------------------------------------
ST = ELECTRONIC STATES; PR =  PROCESSES; DS = DISSOCIATION
```

Figure 4.6: Example of file *EFF_COEFS.dat*, output of ADAS901.

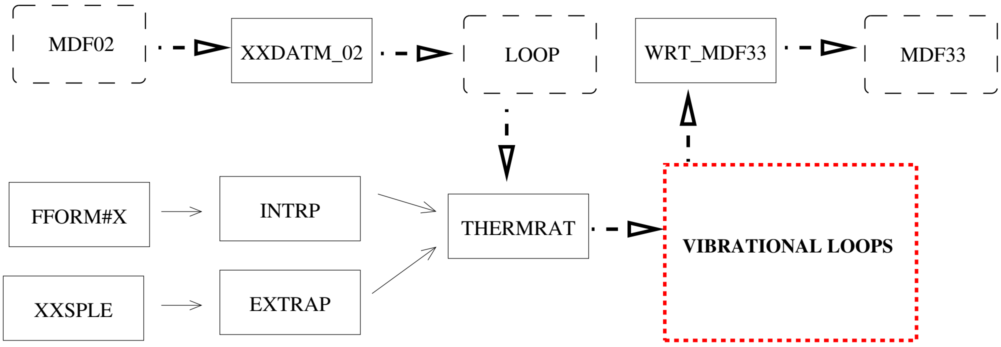


Figure 4.7: Structure of program ADAS902 for maxwellian integration of coefficients.

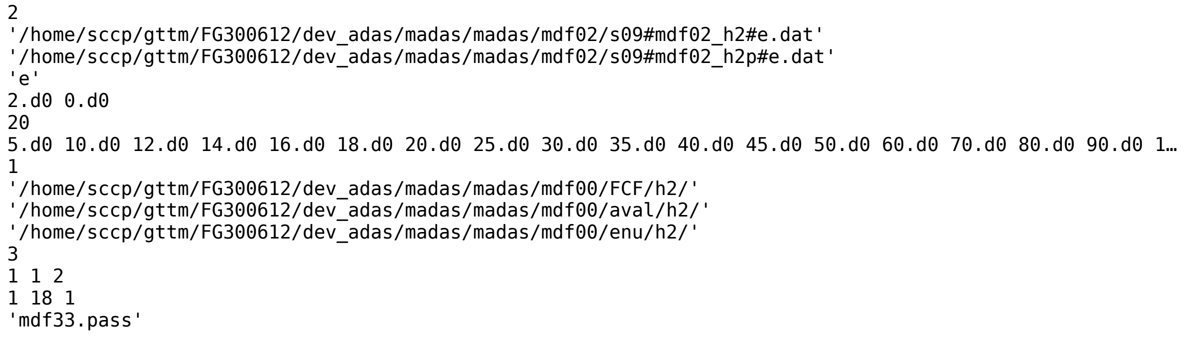
6. (TEI(C1), C1=1,NMTE). Array of electronic temperatures.
7. If EI='I' then:
   - NMTM. Number of molecular temperatures. If NMTM≠0 then
     - (TM(C2), C2=1,NMTM). array of molecular temperatures.
8. VIB. Vibrational resolution required. 1 - full vibrational resolution. 2 - electronic resolution.
9. DFILE. Directory where Franck - Condon factor are stored.
10. AVFILE. Directory where A-values are stored.
11. DENU. Directory where vibrational energies are stored.
12. IRST. Number of metastables in *mdf02* states.
13. (RST(C1,1),C1=1,IRST). Species index of each metastable (see section 4.3.2).
14. (RST(C1,2),C1=1,IRST). Electronic states index of each metastable (see section 4.3.2).
15. OFILE. Output file *mdf33* or *mdf34*.

Data are readed with reading routine *xxdatm_02.for* (header in appendix C.5.5). A double loop in data and in files is needed to avoid repeticions of data. In case of inconsistencies on the different files to be read ADAS902 displays an error message and interrupts running. Inconsistencies are different molecular symbols and different statistical weights for electronic states (all *mdf02* files should have a list of electronic states with some parameters as it is explained in section 4.3.2). A number of checks are carried out to be sure that we are dealing with the same electronic states in the different transitions in the two files. Total number of processes is obtained and the transitions parameters are filled. Finally, the resolution for each transition is kept and the double-Maxwellian flag is set up in case of ion impact collisions.

Maxwell integration

Integration of the cross section is made by a call to the subroutine *thermrat*. The header of this subroutine is on appendix C.2.6. This subroutine calculates the rates from the cross sections for electron and ion-impact collisions. The sequence of steps employed for doing that is:

1. It loops over the input energy values and gets the required energy values for Gauss-Lagrange integration.
2. It interpolates and/or extrapolates into the required energy points using central ADAS routine XXSPLE.



```
2
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf02/s09#mdf02_h2#e.dat'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf02/s09#mdf02_h2p#e.dat'
'e'
2.d0 0.d0
20
5.d0 10.d0 12.d0 14.d0 16.d0 18.d0 20.d0 25.d0 30.d0 35.d0 40.d0 45.d0 50.d0 60.d0 70.d0 80.d0 90.d0 1…
1
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/FCF/h2/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/aval/h2/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/enu/h2/'
3
1 1 2
1 18 1
'mdf33.pass'
```

Figure 4.8: Example of file *input902.dat*, input drivers for ADAS902.

3. It performs a single Maxwellian integration for electron-impact case or a double maxwellian for ion-impact case.
4. It outputs the rates to the calling program.

thermrat admits cross sections or collision strengths and interpolates using the subroutine *intrp* (whose header is in appendix C.2.4). this subroutine can use the formulae provided in *mdf02* (see 4.3.2) or a spline. Formulae are preferred as default. The formula values are obtained by the subroutine *dstform* (appendix C.2.2) which calls the needed formula number. These functions are in a library called libfform.o and are explained in section **??**.

In case that there are extrapolated points in the new energy values, subroutine *extrap* (appendix C.2.3) is called. This subroutine uses the formula whenever this is applicable. If there is no formula available, then different approaches are taken whose details are explained in section 2.3:

- Bethe model for high energy ionization and excitation.
- Spline for low energies excitation.
- Overbarrier model for high energies CX.

In the case of extrapolation for excitation at high energies, it is needed to calculate the collision strength from the dipolar approximation to obtain the Bethe formula (see section 2.3). To avoid steps and gaps between the extrapolated data and the original values the extrapolated points are normalized to the original data so a smooth continuity is obtained.

The Maxwell integration is not performed in case that the original data are given in rates.

Resolution loops

After the Maxwell integration is carried out the resolution loops are launched before writting the data in the *mdf33* format.

Firstly, in case of total cross sections ($v = -2$), if a dissociative part of cross section is listed also in *mdf02* files this is substracted from it in that way that only the bound part is conserved. These will change their vibrational number to $v = -1$ (summed cross section).

For the case of fully vibrational resolution the loop in all the states looks for the summed and total rates with $v = -1$ and $v = -2$ and uses the Franck-Condon Factors to split them in partial vibronic rates. Franck-Condon factors are stored in files of type *mdf00* format (see section 4.3) and are read by the subroutine *xxdatm_00* (see section 4.2.5). Indexes are modified accordingly to account for the new transitions.

In the case of electronic resolution the vibronic rates are summed up to give the electronic rates. However some care is needed with the metastable electronic states which must be keeped in vibrational resolution as it was said in section 3.1.3. The same procedure as in the fully vibrational case is followed with these special states.

In ADAS902 there is an special testing case in which no choice in vibrational resolution in taken and no action is taken. This is got by setting the VIB parameter to 3 in the input driver *input902.dat*.

Writing *mdf33* format files

Finally, the resulting rates are written in the output file *mdf33* or *mdf34* by the subroutine *wrt_mdf33*. The header of this routine is given on appendix C.2.7.

4.2.3 ADAS903

This program interrogates the *mdf33* format files and looks into the matrix to fill the gaps due to the lack of fundamental data with the models explained on section 2.5.2. The header of the routine is given in appendix C.3.

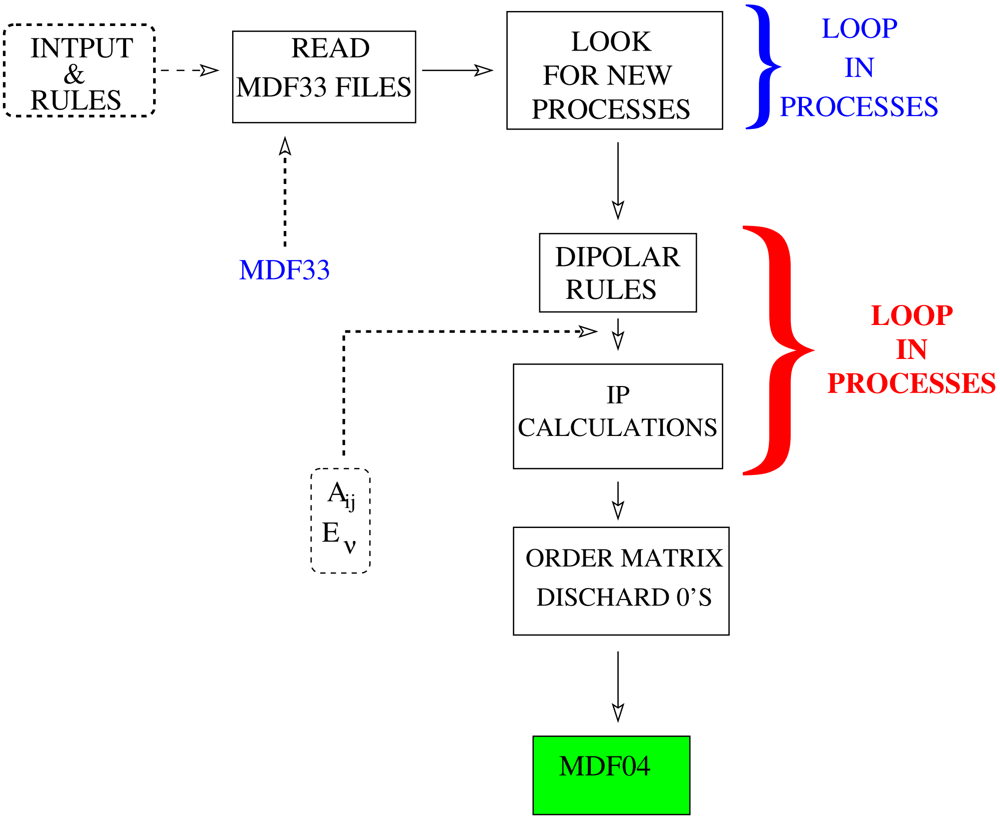


Figure 4.9: Structure of program ADAS903.

A diagram of the structure of ADAS903 can be seen on figure 4.9. The code needs an input file as before. An example of it is in figure 4.10

The parameters for the file file *input903.dat* are:

1. PFILE. Path to *mdf33* or *mdf34* file. Only one file is allowed here.
2. CATEG, MI, NE. Category of data (1 - Upsilons , 2 - Rates, 3 - reserved for others; see section 4.3.3), ion mass (null for electron impact) and number of equivalent electrons in the ground state of neutral molecule.
3. LIMIT, LIMU. Lowest and uppest limit for storage of rates. The former permits to save memory space in the case of negligible low rates compared with the dominant ones. The latter acts a security cut off of non-physical calculated values.
4. AVFILE. Directory where A-values are stored.
5. FCFILE. Directory where Franck - Condon factors are stored.
6. DENU. Directory where vibrational energies are stored.
7. VIB. Vibrational resolution required. 1 - full vibrational resolution. 2 - electronic resolution.
8. IRST. Number of metastables in *mdf33/34* file. The index number of the files is now a global number for all the species and states. It is this global index the one which must be introduced.

```
'/home/sccp/gttm/FG300612/dev_adas_pruebas/madas/pass/mdf33.pass'
2 0 2
0.d0 0.d0
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/aval/h2/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/FCF/h2/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/enu/h2/'
1
3
1 18 28
14 19 18
'mdf04.pass'
'y'
ED
3
17 29 30
1->4+4 1->4+5 1->4+5
```

Figure 4.10: Example of file *input903.dat*, input drivers for ADAS903.

9. (RST(C1),C1=1,IRST). Global index number for metastables.
10. (MXVR(C1),C1=1,IRST). Number of vibrational levels for each metastable.
11. OFILE. Path for *mdf04/01* output file.
12. ECIP_IN. If ’y’ use ECIP approximation for bound-continuum processes. Otherwise do not calculate these processes[1].
13. RULE. Rule ’ED’ (Excitation to Dissociative) signals the code the number and position of fully dissociative states. These states will be direct the electronic flux to their dissociation limits in all cases. In this case:
    - NEDISS. Number of dissociative states.
    - (SDISS(C1), C1=1, NEDISS). Dissociative states indexes.
    - (EDCH(C1), C1=1,NEDISS). Dissociation chanels of previous dissociative states.

Look for new processes

The input format file of *mdf33/34* format is read using *xdatm_33* routine (see section **??**). Then a first loop in the possible transitions between states is run in order to look for the transitions which lack. This loop is made in a different way for the two resolutions considered (electronic and fully vibrational). A new loop is needed to be carried out inside this to look for the process which cover this transition. If the process has an existing rate, this is kept and a series of parameter defining the transition are saved. Here, there is the necesity of having an array with an electronic temperature index, a molecular temperature index and a total process index. That needs memory arrays of several Gb for the fully vibrational case in order to account for al the possible transitions. To allow running the program in standard computers it has been decided to write this information into the hard disk in a temporal file to be read later by the code. The program then writes it in a binary file.

Some rules are applied here that are consistent with the molecular collisional-radiative model. They refer to that metastables are always vibrationally resolved, that ionization is always made to metastables and that recombination is produced always from metastables.

It can happen, regarding to transitions between excited states, that the proximity of the potential curves makes that some of the vibrational levels of the upper state are actually below some of the vibrational levels of the lower state. In this case, it is needed to invert the transition to be calculated to avoid negative energy difference problems.

Excitation to dissociative states are counted as dissociative transitions and the dissociation products are the ones in which the dissociative state asymptotically tends in the separated atom limit.

Finally, the transitions not taken into account before but present in the input datasets (e.g. vibrational excitation by electron attachment or inportant transitions which are dipole forbidden) are added to the matrix.

Calculation loops

Once identified and selected the processes which must be calculated ADAS903 opens new loops and read the temporal file created to calculate them.

Calculation methods are explained in section 2.5. ADAS903 retrieves the vibrational energies and Einstein coefficient in order to calculate the collision strength as it was explained in detail in section 2.5.1, where it has been proved that partial vibrational cross sections calculated from the collision strengths automatically fullfill the Franck-Condon unitarity principle. Therefore, cross sections are calculated in fully vibrational resolution and summed up if electronic resolution is required.

The subroutine employed for the bound-bound calculations is *ipmrate* which is a copy of central ADAS subroutine *iprate* where the dimensions have been increased. This subroutine uses the EIQIP approach previously explained in

---

[1] Other aproaches as Gryzinski methods[54] will be implemented in the future

section 2.5.2. Comparisons of results obtained using this approach with previous calculations are shown in section 2.3.4. Before calling this subroutine ADAS903 interrogates the mapping files *amtx_s.dat* and *amtx_t.dat*. These files are located in the A-values *mdf00* subdirectory and map the transitions rules for the singlet and triplet system. The program first verifies that upper and lower levels are form the same spin system and that the transition to be calculated is allowed. If that is correct it goes on.

For the bound-free transitions as ionizative and dissociative processes (including excitation to dissociative states), ECIP approach is taken and *r8ecip* function from central ADAS is used for the moment. However, in view that the result give a worse agreement than EIQIP ones, other methods, as Gryzinski [54] could be implemented for these transitions. The transitions rules are also checked here for the dissociative excitation processes.

Writing to *mdf04*

Finally, results are ordered in a final matrix where the gaps in the matrix which are still null are discharded. Subroutine *wrt_mdf04* (in appendix C.3.3) is used to write the results in the *mdf04* format file (see **??**) as output.

4.2.4 ADAS904

This program contains the collisional-radiative equations and produces the collisional-radiative coefficients in the *mdf11* files as well as obtains the population of the metastables. An upgrade to obtain ordinary populations and photon emission coefficients is under implementation. A diagram of the structure of ADAS904 is shown in figure 4.11. Header is given in appendix C.4.

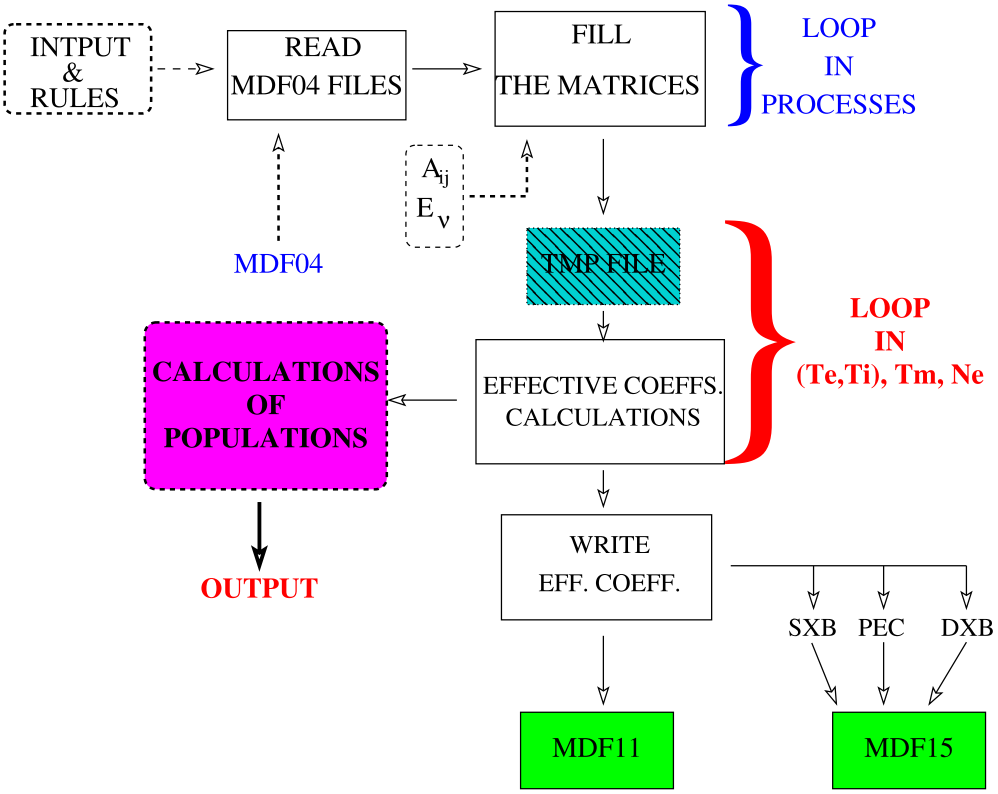


Figure 4.11: Structure of program ADAS904.

An example of input file is found in the figure 4.12.

The parameters for the input file *input904.dat* are:

```
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/'
'/home/sipp/gipp/adas/adas/'
'./res/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/aval/h2/'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf00/enu/h2/'
1
'mdf04.pass'
'e'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf38/aut/h2/aut_pp.dat'
'/home/sccp/gttm/FG300612/dev_adas/madas/madas/mdf38/pred/h2/pred.dat'
0
'n' 'y'
'N' 'N' 'N'
8
1.d11 1.d12 5.d12 1.d13 5.d13 1.d14 1.d15 1.d16
1.d12 1.d0                              NH_I ZEFF
3
5.d0 25.d0 100.d0
1
2
3
1 18 28
3
17 29 30
1 1 1 1
1 1 2 1
1 1 2 1
1
1
0
1.d0
'y'
4 5
1
2
4 5
1 0
9 1
1 1
1
1
0
0
'n' 'n' 'n'
```

Figure 4.12: Example of file *input904.dat*, input drivers for ADAS904.

1. DMADAS. Path to *mdf* format files.
2. DADAS. Path to central adas *adf* format files.
3. OPATH. Path for output file, in case of no specifications will be at current directory.
4. AVFILE. Directory where A-values are stored.
5. DENU. Directory where vibrational energies are stored.
6. NPFILES. Number of input *mdf04* files.
7. Loop in NPFILES:
   - PFILE(). Path to *mdf04* file.
   - FCLASS(). Class of previous file: 'e'→ el. impact file; 'I'→ ion impact file.
8. AUFILE. Path to the auto-ionization file to be used.
9. PRFILE. Path to the pre-dissociation file to be used.
10. MXN. Number of extrapolated n's.**Currently not in use; set to 0**.
11. DEFAULT_T, TE_EQ_TI. ('Y' OR 'N'). Use default temperature in files and use $T_e = T_i$.
12. REC, CXI, CX. ('Y' or 'N'). Include recombination, inverse CX and direct CX.
13. NNES. Number of electron densities.
14. (NE(C1), C1=1, NNES). Electron densities array.
15. NH_I, ZEFF. Initial neutral density (in cm^{-3}) and effective charge.
16. IF $T_e = T_i$ (TE_EQ_TI = 'Y') then:
    - IF there are not default temperatures (DEFAULT_T = 'N') then:
      - ⋆ IENRP. Number of electron/ion temperatures.
      - ⋆ (ENRP(C1), c1=1, IENRP). Electron/ion temperatures in eV.
      - ⋆ NTM. Number of molecule temperatures.
      - ⋆ IF NTM bigger than 1:(TM(C1), C1=1,NTM). Array for molecule temperatures in eV/amu.
17. ELSE $Te \neq T_i$ (TE_EQ_TI = 'N') then:
    - IF there are not default temperatures (DEFAULT_T = 'N') then:
      - ⋆ NTE. Number of electron/ion pairs of temperatures.
      - ⋆ (TE(C1), C1=1, NTE). Electron temperatures in eV.
      - ⋆ (TI(C1), C1=1, NTE). Ion temperatures in eV.
      - ⋆ NTM. Number of molecule temperatures.
      - ⋆ IF NTM bigger than 1:(TM(C1), C1=1,NTM). Array for molecule temperatures in eV/amu.
18. VIB. Vibrational resolution required. 1 - full vibrational resolution. 2 - electronic resolution.
19. IRST. Number of metastables of the system. The index is the same global index found in *mdf04*.
20. If IRST is bigger than 1 then: (RST(C1), C1=1, IRST). Metastable global index array. If IRST is one then the ground state (index 1) is assumed to be the only metastable.
21. NDISS. Number of dissociative states in the global index number.
22. (DISS(C1), C1=1, NDISS). Dissociative states global index array.
23. Loop in dissociative states number (NDISS):

- P11(),P12(),P21(),P22(). Dissociation products in the atomic specie and atomic state index. The asymptotic dissociation channels (F. e. b dissociates in 1 1 1 1 that is in ground state of neutral atomic hydrogen).

24. NCPOP. Number of states that will have an input flux and constant population for full equilibrium calculation. For obvious reason these must be metastables.
25. (STCPOP(C1), C1=1, NCPOP). Global index state constant population array. only molecular states.
26. (VCPOP(C1), C1=1, NCPOP). Vibrational level index constant population array.
27. (CPOP(C1), C1=1, NCPOP). Density of the constant population (for normalized results can be set to 1 or to the corresponding fraction in case of more than 1 constant population.
28. THIS_IS_H ('y' or 'n'). If this is hydrogen set to 'y' means that the non linearity of the CX processes will be treated by iteration.
29. If this is hydrogen then:
    - ASPCPOP(C1), C1=1, NCPOP+2). Atomic product global index states for constant populations.
    - NITE. Number of iterations desired.
30. Else
    - NACPOP. Number of dissociation products constant population
    - If NACPOP is bigger than 0 then
        - ⋆ ASPCPOP(C1), C1=1, NCPOP+NACPOP). Atomic product global index states states for constant populations.
        - ⋆ (STCPOP(C1), C1=1, NCPOP+NACPOP). Internal index states of atomic species for constant populations.
        - ⋆ (CPOP(C1), C1=1, NCPOP+NACPOP). Constant populations densities.
31. NATSP. Number of atomic species in the calculation.
32. (NASP(C1), C1=1, NATSP). Species index number of each atomic species.
33. (ION_ALWD(C1), C1=1, NATSP). If 1 that species can be ionized, 0 it cannot.
34. (NMAXPRD(C1), C1=1, NATSP). Maximun number of atomic states considered in each atomic species.
35. (IATMET(C1), C1=1 NATSP). Number of atomic metastables per atomic specie.
36. Loop in the number of atomic species (NATSP)
    - (ATMET(C1,), C1=1, IATMET). Index of atomic metastables in *mdf25* mapping files with central ADAS.
37. SHM. H^- global index. If this parameter is set to 0 then H^- production is not taken in account.
38. (**Under implementation**) NORDPOP. Number of ordinary populations to calculate.
39. (**Under implementation**) If NORDPOP is bigger than 0 then:
    - (**Under implementation**) (IORDPOP(C1), C1=1, NORDPOP). Global index for ordinary populations states.
40. (**Under implementation**) DOPEC,DOSXB,DODXB ('Y' or 'N') .If 'y' do calculate PEC,DXB or SXB for the specific wavelength specified after.

Before the squential working of ADAS904 is explained some concepts of its structure as the index system and temporal files usage must be explained.

The molecular and atomic indexes

Along the different routines a global index is kept after the arranging of the fundamental data by ADAS902. This index asign a unique number to molecular states independent of their species. However atomic states don't have a number in this index system. The number is given to the general ionization stage. It is only in ADAS904 where atomic states count for the collisional-radiative model and an internal index is asigned to them. This atomic index runs only for the atomic states of each of the ionization stages which must be mapped with atomic adas indexes of *adf04* format files through *mdf25* mapping files. An schem of the working of the different indexes is given on figure 4.13.

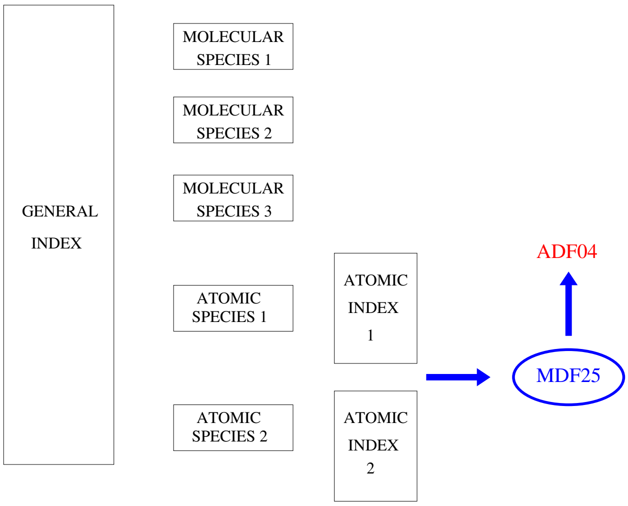


Figure 4.13: Schem of the atomic and molecular indexes on ADAS904.

Temporal files

ADAS904 is carrying out several loops in elecron denstiy, ionic and electronic temperature, molecular temperature and states indexes that combined would give arrays so large that will colapse the memory of a medium size computer. To allow the user to run this code in every scientific computer it is decided to sacrifize computer time rather than availability. In this line, temporal files are used so hard disk memory can be used fro that. There are two main temporal files:

- First of it is storing the main parameters of every transition from *mdf04* files. This is created before reading first time *mdf04* files and maintained along the running of the code in order to be used for filling the collisional matrices. It stores for every transition the transition index, cathegory of the transitions (upsilon or rates), type of the transition (dipolar, non dipolar, etc), lower electronic state index, lower vibrational index, upper electronic state index, upper vibrational index, type of process and dissociation channel. It is deleted before writting *mdf11* files.
- The second one is storing the calculated effective collisional-radiative coefficients for each temeperature-density set of values. This file stores them in form of matrix between upper and lower metastables. This file is read by the routine *wrt_mdf11* in order to write this information on the *mdf11* files. This file is deleted after *mdf11* are written.

Loop and new authomatic general index

ADAS904 starts making three nested loops in densities, electron-ion temperature pairs and molecular temperatures. Each time rate coefficients are read from *mdf04* for the selected temperatures. This is done in this way in order to save memory rather to have multidimensional arrays which would consume the memory.

After that, and depending on the resolution required a new index is authomatically created by the program. This index will include vibrational leves of metastables (or of every state if fully vibrational resolution is required) and will count for the atomic index as well. Constant populations introduced as an input are excluded. Molecular and atomic metastables flags are created and at the same time the molecular or atomic character of every indexed level is kept. What it is wanted here is to prepare the system for fill the collisional matrices and at the same time to distinguish all the "independent" states to be treated in the balance equations.

Matrices filling and quasy statical equilibrium

After the new index is created, matrices are filled subsequentially in a loop on the transitions. Collisional matrices are initialized for every temperatuture and density value and then filled. At the same time that a matrix element is filled by a value the oposite transition is filled as well if this is allowed by the decay rates and de-excitation calculated rates. Excitation, recombination, ionization, charge exchange and dissociation matrices between metastables, ordinary states, metastables to ordinary states and ordinary states to metastables are filled. Predisciation and autoionization are then taken from *mdf38* format files.

Then, the matrixes are inverted inside subroutine *mr2mcd* and the effective coefficient matrixes are obtained for every effective collisional coefficient described on chapter 3. after that the matrix is stored in a temporal file in hard disk to be read after in order to write *mdf11* files at the end of the program. MQCD, MACD, MSCD, MCXIACD and MCXCD are calculated sequentially in this way. After that, atomic rate coefficients are readed from *adf04* format file with the help of the mapping file *mdf25* using the routine *rdxxdata_04*. These arte coefficients are used to calculate dissociative effective coefficientas as PDCD, PADCD, DCD, PDSCD and PADSCD. More than one inversion of different matrices is needed to produce this coefficients (see chapter 3). Finally molecular cross coupling coefficients MXCD are calculated.

In the end atomic coefficients are read from *adf11* files with subroutine *rdxxdata11* and again using *mdf25* mapping file.

Population calculation

Once the effective coefficients have been calculated is possible to fill the matrix from equation (3.26) and invert the system as in equation (3.24).

To do that, first flux input vector is filled from the effective coefficients as in equation (3.25). Then the collisional effective matrix is filled and subsequently inverted.

If iteration for non linear terms are required (see section 3.3) they are calculated from the previous coefficients. All these population are written for every temperature and density value in the file *pops.txt*. A routine can be used later (*xxrdpop.for*) to read this file and write pouplation in the form of matrices for plotting populations.

Ordinaru populations are calculated but its writting in a file is still under implementation. PEC, SXB and DXB calculation for wavelength ranges is under implementation as well.

Closing of loops and end of the program

Loops in temperature and density are completed and then effective coefficient are wroten in the different *mdf11* files which are explained on section 4.3.5. If there is any coefficient that has not been calculated by the program by swiching off any of the variables in file *input904.dat* by the user, then these *mdf11* file will not be created. *mdf11* files are created in a new directory specified by the user. The program will end succesfully after that.

4.2.5 ADAS900 subroutines

The programs of molecular extension of ADAS are based in many subroutines that read data, write data or perform special calculations needed for the main program. These subroutines are grouped with the main program for tha one they are designed but some of them can be used by other programs and some others can be used independently. Most of the last are grouped in the *mdflibs* directory, these are oriented to the user so it can be easier to construct a molecular system which can go through the whole computing processes allowing a focus on the real physics problems.

A brief description of the different subroutines follows.

ADAS902

CHNG_PRCS . Header in appendix C.2.1. This routine change the process number to the adequate for the required resolution inside *adas902* program.

DSTFORM . Header in appendix C.2.2. This routine calls to the different fitting formulas for a set of energies and parameters.

EXTRAP . Header in appendix C.2.3. This is the extrapolation routine which applies the extrapolation formulas and estrategies discussed on section 2.3.

INTRP . Header in appendix C.2.4. This routine interpolates values of cross sections and rates by formula (calling to *dstform*) or splines.

RD_ENU . Header in appendix C.2.5. This routine reads vibrational energies from *mdf00* files. It also outputs the maximun vibrational level of any state.

THERMRAT . Header in appendix C.2.6. This routine performs the maxwellian integration discussed on 2.4 after calling subroutines *intrp* and *extrap* for the interpolation and extrapolation.

WRT_MDF33 . Header in appendix C.2.7. This routine writes the input data in *mdf33* format.

ADAS903

DGFCTR . Header in appendix C.3.1. This routine calculates degeneracy factor from equation (2.33)

IPMRATE . Header in appendix C.3.2. This routine calculates electron collisional excitation and de-excitation rate coefficients in the impact parameter approximation (EIQIP) for dipole transitions. It is an adaptation of routine EIQIP (H. P. Summers 1977) for the molecular case.

WRT_MDF04 . Header in appendix C.3.3. This routine writes the input data in *mdf04* format.

ADAS904

AUTRATE . Header in appendix C.4.1. This routine interrogates *mdf38* files to obtain auto-ionization coefficients.

GETPRD . Header in appendix C.4.2. This routine obtains the real state index for atomic dissociation products from molecular states using the *mdf25* mapping files.

MR2MCD . Header in appendix C.4.3. This routine calculates the matrix product $C_{\rho\sigma} - C_{\rho i} C_{ij}^{-1} C_{j\sigma}$ for the original input matrices C and gives the ordinary states contribution $C_{ij}^{-1} C_{j\sigma}$ to calculate the ordinary states populations and PEC, SXB and DXB coefficients.

PREDRATE . Header in appendix **??**. This routine interrogates *mdf38* files to obtain pre-dissociation coefficients.

RDXXDATA_04 . Header in appendix C.4.5. This routine returns the rate coefficients for atomic transitions from *adf04* files using the mapping files *mdf25*. It also fills the corresponding matrices accordingly.

RDXXDATA_11 . Header in appendix C.4.6. This routine returns the atomic effective coefficients ACD, SCD, QCD and XCD from the *adf11* files and fills the input matrices accordingly. It uses *mdf25* files for mapping.

WRT_MDF11 . Header in appendix C.4.7. This routine clasifies writes the data in temporal file in the different output files in *mdf11* format.

MDFLIBS

CREATE_FMT_MDF02 . Header in appendix C.5.1. This routine creates blocks for mdf02 file from blocks of columns of data in any numeric FORTRAN format. A template called **template_create_mdf02.dat** can be used for this purpose. This routine call *wrt_mdf02* for it.

FFORM_X . Different formulae for fitting the input data. A description of them is given in appendix E.

RT2UPSLN . Header in appendix C.5.2. This routine converts rates in cm^3s^{-1} to upsilon defined on equation (2.16) and viceversa.

SPCTRLBANDS . **Under implementation**. This routine will obtain the vibrational spectral bands for the input of a wavelength range or a lower and upper state. This is intended to calculate the bands for obtaining the spectral effective coefficients for them in the program *ADAS904*.

WRT_MDF02 . Header in appendix C.5.3. This routine writes fundamental data in the format *mdf02* from the input.

XXDATM_00 . Header in appendix C.5.4. This routine reads *mdf00* files and returns the Franck-Condon or the A-values for the transition given in the input parameters. It also returns the maximun vibrational values of upper and lower states.

XXDATM_02 . Header in appendix C.5.5. This routine read *mdf02* files and returns the information in the output arrays.

XXDATM_04 . Header in appendix C.5.5. This routine read *mdf02* files and returns the information in the output arrays. Due to the necessity of dealing with the difficulties of managing big arrays in adas904 routines and because the routine is destined as well for general use there are three modes of running it:

1. Read all the file at once for small matrices (less than 8500 blocks).
2. Read the matrix for only one temperature. In this case the routine will perform an spline to interpolate for the desired temperature input. In this case the paremeters of which determine the process will be written in a file that must exist before the routine is called.
3. Read all the temperatures for only one block, wich is defined by the process parameters.

The mode is switched by the input parameter IRDMD. Program *adas904* works with IRDMD=2.

XXDATM_11 . Header in appendix C.5.7. This routine read *mdf11* files and returns the information in the output arrays.

XXDATM_25 . Header in appendix C.5.8. This routine read *mdf25* mapping files and returns an output with the different equivalent indexes for the *mdf* and *adf* systems.

XXDATM_33 . Header in appendix C.5.9. This routine read *mdf33* files and returns the information in the output arrays.

XXRDPOP . Header in appendix C.5.10. This program reads the output form *ADAS904* and writes it in columns versus temperautre of density depnding on the user wishes.

4.3 MDF: The Molecular ADAS format

The molecular data in ADAS will be stored in diferent files depending of the fundamental (cross section or collision strength) or derived quantity (effective excitation coefficients, emissivities, etc) in a similar fashion as it is done in the atomic part of adas. For this new directories are created that are called *mdfxx* where *mdf* stands for "Molecular Data Format" and *xx* refers to a number. The number is required to follow the same or as similar as possible conventions as the *adf* case. Thus, for example *mdf04* will be the directory and format for electron impact thermal rates and *mdf14* is the directory for double maxwellian ion impact thermal rates as it is in the atomic case.

The molecular data is organized in a way that not unique data is treated. Instead, compilations of data are given as fundamental *mdf02* files from wich rates *mdf04* are generated and introduced as an input in the collisional-radiative modelling to created the derived quantities (see graphs in section **??**).

Here the different files at the moment in ADAS are described:

4.3.1 mdf00

In these files the energy curves and information about the process is stored as well as the calculated A-values and the Franck-Condon Factors. An example of this files can be found in appendix A.1

As different quantities are stored inside this directory it needs to be organized in subdirectories. The subdirectories are:

pot/ Here the potential in function of the internuclear distance for diatomic molecules will be stored. These will be useful to obtain the turning points for the vibrational states and the correct energy differences and threshold for the different processes. The different molecule files will be called by their nomenclature and their isotopic class, e.g. h2.dat for H2 molecule vibrational energies or hd.dat for HD molecule.

enu/ Here the vibrational energies for the different electronic states are stored. Inside every file the different iosotopes are given in different columns, in the first column is the vibrational state given. The files are inside subdirectories corresponding to their molecular specie (e.g. h2 for h2 files) and they are named following the species and electronic state in them, i.e. '*"enuSE"* where S stands for species and E for electronic state. For example:

- **h2/enu11.dat** corresponds to the vibrational energies of species 1 and electronic state 1 of h2, that is, $H_2(X^1\Sigma_g^+)$ state.

Their format is described in appendix A.

FCF/ Franck-Condon Factors are stored in files inside this subdirectory. They are two dimension tables where the columns stand for the vibrational states of the lower state and the rows for the upper state. Before this table two values give the number of states of lower and upper state. The notation of the files correspond with the species and electronic state numbers of the lower state followed by the ones of the upper state, i.e. *"FC(SL)(EL)(SU)(EU).dat"* where S stands for species, E for electronic state and U and L for upper or lower state respectively. For example:

- **h2/FC1112.dat** corresponds to the Franck-Condon Factors between electronic state 1 of species 1 and electronic state 2 of species 1, that is, between the $H_2(X^1\Sigma_g^+, v)$ vibrational states and $H_2(B^1\Sigma_g, v')$ vibrational states.

Their format is described in appendix A.

aval/ Here the A einstein coefficients are stored. They are two dimension tables where the columns stand for the vibrational states of the lower state and the rows for the upper state. Before this table two values give the number of states of lower and upper state. The notation of the files correspond with the species and electronic state numbers of the upper state followed by the ones of the lower state, i.e. *"aval(SU)(EU)(SL)(EL).dat"* where S stands for species, E for electronic state and U and L for upper or lower state respectively. For example:

- **h2/aval1211.dat** corresponds to the A-values between electronic state 2 of species 1 and electronic state 1 of species 1, that is, between the $H_2(B^1\Sigma_g, v')$ vibrational states and $H_2(X^1\Sigma_g^+, v)$ vibrational states.

Their format is the same as FCF files and is explained in appendix A.

Examples of these file are given in appendix A together with the fortran-like formatting conventions.

4.3.2 mdf02

The fundamental data, that is cross sections and collision strength, will come from the *mdf02* files. However, when no cross sections are available, maxwellian rates can also be introduced. An example of this files are given in appendix A.2

The cross sections can be ion or electron impact. Nevertheless, this two types of collision will be separated in different files that are named in different way.

The notation chosen for naming these files is *syy#mdf02_mmm#(e/i).dat*. Here:

s stands for cross section.

yy is the compilation year number. As these fundamental data must be compiled from different sources is better to care about the year of compilation that will alow after to distinguish between older or newer (and possibily more complete) compilation of data. A documentation with the information of the different year compilations will be stored.

mmm is the molecule name. There is no limit in the number of caracter for that. The hydrogen molecula will be written as *h2* while its ionized specie by *h2p*, negative hydrogen would be *h2m*, methane would be *ch4*,double ionized methane *ch4p2*, etc.

e/i separates electron collisions and ion collisions.

From here, the electron impact collisons compilation from year 2009 for Hydrogen molecule is called *s09#mdf02_h2#e.dat*. Extra information about how this compilation is made and who performed it and from wich sources should be found in the comment sections of the file. In the case that various compilations are made in the same year a new letter index can be added to the end of the year in the file name (in the last case *s09b#mdf02_h2#e.dat*, *s09c#mdf02_h2#e.dat*, etc).

The files are organized in the following way:

- The name of the molecular system and the type of collision(i.e. electron impact or ion impact) are in the top line.
- The possible species that can come from ionization or dissociation of this molecule are listed now together with their ionization and dissociation energies (usually in cm^{-1}) and the channels.
- Processes ocurring from collisions are described in simplified ascii notation and by some brief text. Each one is asigned with a number.
- The electronic states for the different species are listed with some comments when required (e.g. in case of dissiociative state). A number on each species is given to the electronic states. The united atom, spearated atom and coupled atom configurations together with the statistical weight are given in the columns next to the state index. Ionization energies and dissociation asymptotic limits are given as well.
- Data in form of collision strengths or cross sections. Each block is preceded by a set of numbers that specify the process and the initial and final state and some information about the data type, fitting formula and transition energy.
- Comments

The data stored in the files is in form of in collision strengths and cross sections depending when is more adequate to use one or the other. The variable *categ* is used to tell them apart: *categ=1* corresponds to collision strengths and *categ=2* corresponds to cross sections. The definition of collision strength have been given in equation (**??**). Another value of *categ*: *categ=3* is reserved for maxwellian rate coefficients. As it have been explained in chapter 2 the philosophy of the molecular ADAS is to store the fundamental cross sections data and derive the maxwellian rates from them, however it is possible to include maxwellian rates in *mdf02* format and use the ADAS9xx routines to produce the *mdf04* files wich will not touch these data.

Most of the data can be fitted by a formula. The formulas that are used to fit the molecular Hydrogen data have been developed by R. Janev and are presented in appendix E. Formula behaviour have been discussed in section 2.2. In the *mdf02* format files the formula number and the parameters of the formula are given. This will allow to extrapolate the data to the correct behaviour at high and low energies.

4.3.3 mdf33 and mdf34

The extrapolated and interpolated maxwellian rates coming form the integration of the cross sections of the *mdf02* files are stored in these format. *mdf33* is reserved for electron impact and *mdf34* is reserved for ion impact. An example is shown in appendix A.3.

The files are named as *mmm#nnn#rrr.dat* where:

mmm is the molecule name. There is no limit in the number of characters for that. The hydrogen molecula will be written as *h2* while its ionized specie by *h2p*, negative hydrogen would be *h2m*, methane would be *ch4*,double ionized methane *ch4p2*, etc.

nnn is the origin of the compilation. As these fundamental data may come from different sources the initials of the person wh did the job may be written.

rrr are the tag for electronic resolution (*el*), no resolution (*nr*) or vibronic resolution (*vb*). Note that the non resolution case means that no action is taken to unify the resolution in mdf33 final file and that is not a good source file to obtain a collisional radiative model existing only for debugging purposes. Sometimes (*n_r*) is used for electron resolution.

The files are organized in the following way:

1. The name of the molecule and the type of collision(i.e. electron impact or ion impact)and the molecular mass in *amu* are in the first line as a header.
2. The possible species that can become from ionization or dissociation of this molecule are listed now together with their ionization and dissociation energies (usually in cm^{-1}).
3. The electronic states are following with one number to identify both species and state. The coupled state notation, asymptotic sparated atoms configuration, statistical weight and ionization and sissociation energies (in cm^{-1}) are given in the nex columns as well.
4. Electronic or ionic temperatures are below. In ***mdf34*** case another block of temperatures with the molcular temperatures is given.
5. The number of values block come before the blocks of values. These last have one line with the parameters needed for each process (see A) and the values themselves for the temperatures arrays before. In case of molecular temperatures, the block will be subdivided in several block to account for each molecular temperature.
6. Comments.

The values can be given in Υ or rates. These are defined on section 2.4. The specific fortran-like format is given in A

4.3.4 mdf04 and mdf14

This format is reserved for the single maxwellian electron impact rates. An example of this file is given in appendix A.4 together with the fortran-like formatting conventions.

The files are named as *(el/nr/vb)#yy_mmm#ccc.dat* where:

el/nr/vb are the tag for electronic resolution (*el*), no resolution (*nr*) or vibronic resolution (*vb*). Note that the non resolution case means that no action is taken to unify the resolution in mdf33 final file and that is not a good source file to obtain a collisional radiative model existing only for debugging purposes.

yy is the compilation year number. As these fundamental data must be compiled from different sources is better to care about the year of compilation that will alow after to distinguish between older or newer (and possibly more complete) compilation of data. A documentation with the information of the different year compilations will be stored.

mmm is the molecule name. There is no limit in the number of characters for that. The hydrogen molecula will be written as *h2* while its ionized specie by *h2p*, negative hydrogen would be *h2m*, methane would be *ch4*,double ionized methane *ch4p2*, etc.

ccc are other comments relevant for this file in key letters. As l-15, for example to indicate that there is a lower limit in rates of $10^{-17}\text{cm}^3\text{s}^{-1}$.

The "simple" excitation rates to non-disociative levels are given in Υ, see equations (2.16) and (**??**), the rates can be deduced from equations (**??**) and (2.26).

Dissiociative and ionizative processes are given in rates. *mdf04* generation routines are in a way such that if the data is in collision strengths in the previous *mdf02* files then Υ will be given and viceversa.

The structure of *mdf04* and *mdf14* files is very similar to the mdf33 with the difference of that no energy difference parameter is used.

4.3.5 mdf11

Format *mdf11* correspond to the format files for the effective coefficients from metastable to metastable calculated by *ADAS904*. The coefficients are defined in section 3.1.2 and placed in the different directories. In table 4.1 are summarized the different effective coefficients.

An example of *mdf11* file is shown in appendix A.5. These file are named with the convewntion *qqqq_mmm_rr_ccc.dat* where:

qqqq is the coefficient name as in table 4.1.

mmm is the molecular species symbol as before. In this case $H_2{}^+$ will be represented as `H2^+`.

rr is the resolution. As before (*vb*) is used for vibronic resolution and (*el*) or (*nr*) for electronic one.

ccc are reserved for technical comments about the details of the calculation.

These format start with a top line with general information about the data. Symbol of molecular especies, and number of densities, electron or ion temperatures and molecular temperatures is given. At the end of this line the molecular system is specified.

Then the arrays of temperatures and densities are given in eV and cm−3 units. and then the coefficients are given in different blocks preceded by an explanatory line with lower and upper electronic state and charge of the lower state and the block number.

Data are given in matrix on temeperature(rows) and density (columns).

At the end of the file is a space reserved for comments.

4.3.6 mdf25

This format is a mapping format that relates atomic adas *adf* files with *mdf* format files. An example of this format is given on appendix A.6.

It is needed to stablish a correlation between the internal indexes of the states for atomic products of dissociation in the molecular collisional radiative code and the ones in the central *adf* system. This is done in order to collect the atomic effective coefficients from the *adf11* format files and the rates from the *adf04* files.

The file is structured as follows:

1. The number of dissociation products is given.
2. For the required coefficicients is given the path of the required *adf11* files.
3. For any of the atomic species the path for *adf04* file is given.
4. A block for any of the species come. This block starts with the number of state and the charge of this specie.
    - For every state is given the number and nomenclature of state in the molcular index and the number and nomenclature in the corresponding *adf04* file.
5. End of file is marked with a -1 and then comments are added.

One file per molecular system must exist in order to run *ADAS904* for each molecular system.

Table 4.1: Effective coefficients calculated by *ADAS904* program.

Name	Directory	Description
MQCD	mdf11/mqcd/	Molecular excitation CR coefficient.
MACD	mdf11/macd/	Molecular recombination CR coefficient.
MSCD	mdf11/mscd/	Molecular ionization CR coefficient.
MCXIACD	mdf11/mcxiacd/	Molecular inverse charge exchange CR coefficient.
MCXCD	mdf11/mcxcd/	Molecular charge exchange CR coefficient.
PDCD	mdf11/pdcd/	Partial (from a molecular specie) dissociation CR coefficient.
MXCD	mdf11/mxcd/	Molecular cross coupling (through ionization) CR coefficient.
PADCD	mdf11/padcd/	Partial (from a molecular specie) cross-coupling (through recombination) dissociation CR coefficient.
PDSCD	mdf11/pdscd/	Partial cross-coupling (through atomic ionisation) dissociation CR coefficient.
PADSCD	mdf11/padscd/	Partial (from a molecular specie) double cross-coupling (through molecular recombination and atomic ionization) dissociation CR coefficient.
SCD	adf11/scd/	Atomic ionization CR coefficient.
ACD	adf11/acd/	Atomic recombination CR coefficient.
QCD	adf11/qcd/	Atomic excitation CR coefficient.
XCD	adf11/xcd/	Atomic cross-coupling (through ionization) CR coefficient.

4.3.7 mdf38

mdf38 format files are reserved for predissociation and autoionization rates. Being these two format different it is not a unique reading routine that reads all these files.

Auto-ionization

An example of *mdf38* auto-ionization file is given in appendix A.7.1. This file have lower and upper states and lower and higher vibrational level for the auto-ionization process and is followed by the rate. If an "N" is given then the set of states of the given N are the upper state (e.g "1N5" for all the $N = 5$ levels of species 1).

Pre-dissociation

An example of *mdf38* pre-dissociation file is given in appendix A.7.2. This file have upper and lower states for pre-dissociation rates and the dissociation channel. Then the number of vibrational vlevels from where there is dissociation is preceding the pre-dissociation rates for each of this levels.

4.3.8 Not yet implemented formats (mdf15)

The status of developing of molecular ADAS code makes that some of its final features would be not yet totally defined. That correspond to the format *mdf15*.

Photon emission coefficients will be calculated by *ADAS904* for a vibrational spectral range (see section 4.2.4). These coefficient will be stored in the analogous to *adf15* files that will be similar to *mdf11* files adding the spectral range and the states involved in it. PEC will account for molecular band and they will also measure the molecular dissociation contribution to the atomic product bands allowing to separate the line features that come from the molecular contribution.

In the same format will be stored SXB and DXB coefficients taht account for the number of photons per ionizationa and dissociation respectively. Finaly line/Band powers will be stored in the same way.

4.4 The interactive user interface

The interactive graphical user interface to ADAS is impplemented in IDL. At the command line, type

```
> adas
```

to bring up the top level menu, as shown in figure 4.14. Click at 9 to bring up the series 9 menu, as shown in figure 4.15, which lists all the interactive user procedures available for ADAS molecular modelling. The first two procedures, ADAS901 and ADAS902 are interrogative on the molecular database. Later procedures arry out aspects of collisional-radiative modelling and spectral display. These are described individually in the following sub-secttions.

4.4.1 ADAS901

The interactive procedures of molecular ADAS in general operate in the same manner as the atomic/ionic ADAS procedures. There are three principal screens for data selection, specification of prrocessing required and finally output an display of results. These are called the *Input*, *Processing* and *Output* screens. Secondary screens are displayed, as appropriate, for additional more specialised selections. The *input* screen of ADAS901 is shown in figure 4.16. It is interrogative on data format *mdf02* and so the default *Data Root* of Central Data is to */home/adas/adas/mdf02*. The *Data File* list shows available datasets which currentl span only H_2 (*h2*) and H_2^+ (*h2p*). For H_2 both electron impact (*#e*) and ion impact (*#p*) data are available. Click on on a dataset and it appears in the selection window. Note the possibility of examining the comments in the dataset (*Browse Comments* button). *Cancel* returns the user to the previous screen

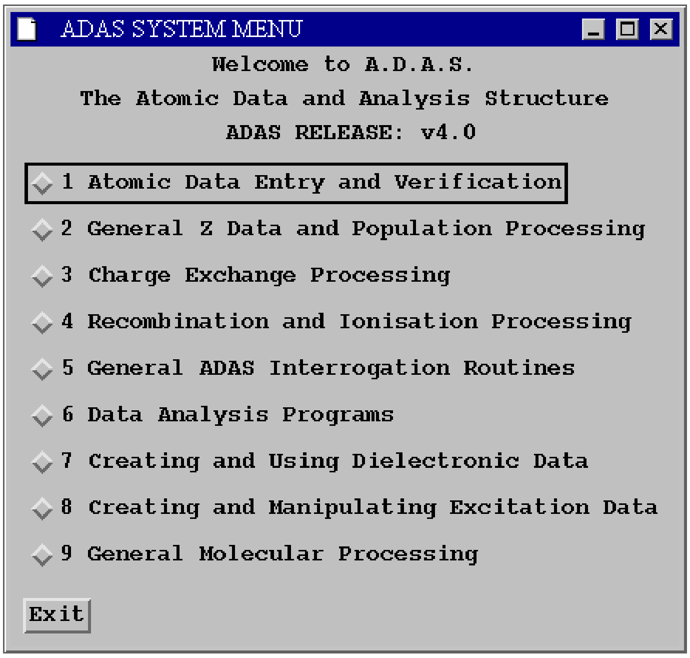


Figure 4.14: The ADAS top level menu.

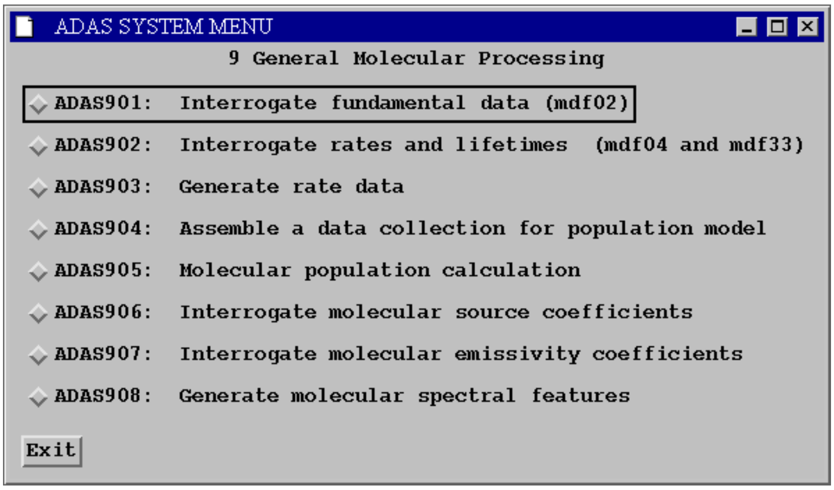


Figure 4.15: The ADAS series 9 menu.

and *Done* moves the uer forward to the *Processing* screen. These are standard ADAS usages. The processing screen is shown in figure 4.17. The H_2 system includes in principle six species. Click on *Browse Species* to see the species list in the subscreen shown at the right of figure 4.18 and some additional pathway information.. In a similar manner, *Browse States* to see the various electronic states listed in the subscreen shown at the right of figure 4.18. Note that in this example there are 150 transitions in various categories of process. *Choose Process* to examine in the drop-down list towards the top of the processing screen. According to this selection transitions become available for selection in the panel titled *Select Transition*. The permitted choices of channels, species, electronic state, vibrational state are shown in the panel for the use to make his/her choices. Finally the right hand panel allows selection of the energy or temperature range for display of the selected cross-section or rate coefficient. The *Default* button selects the energy

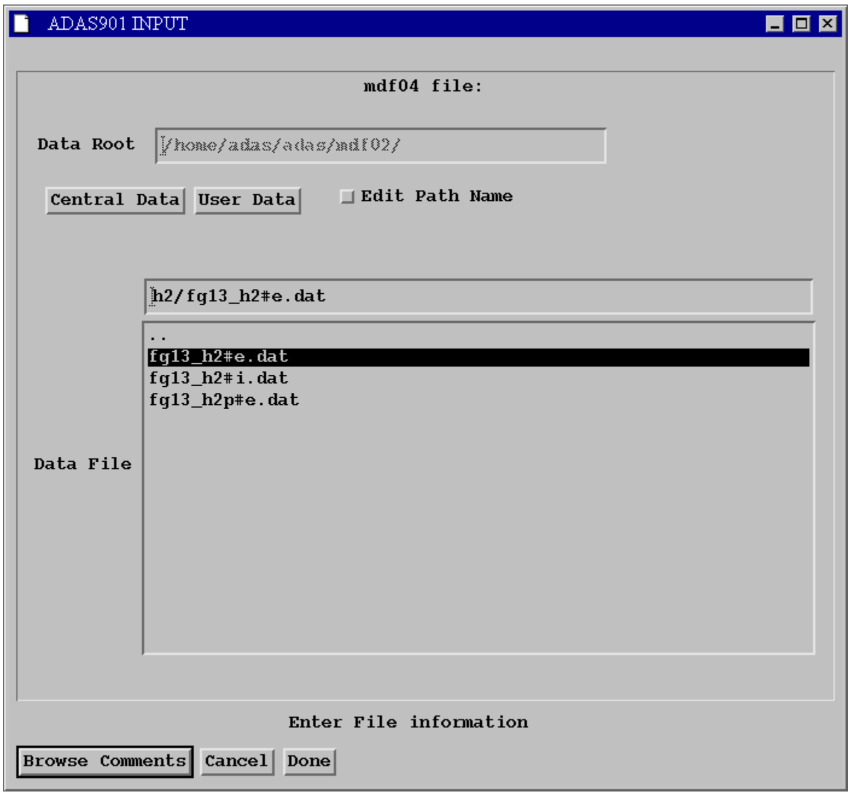
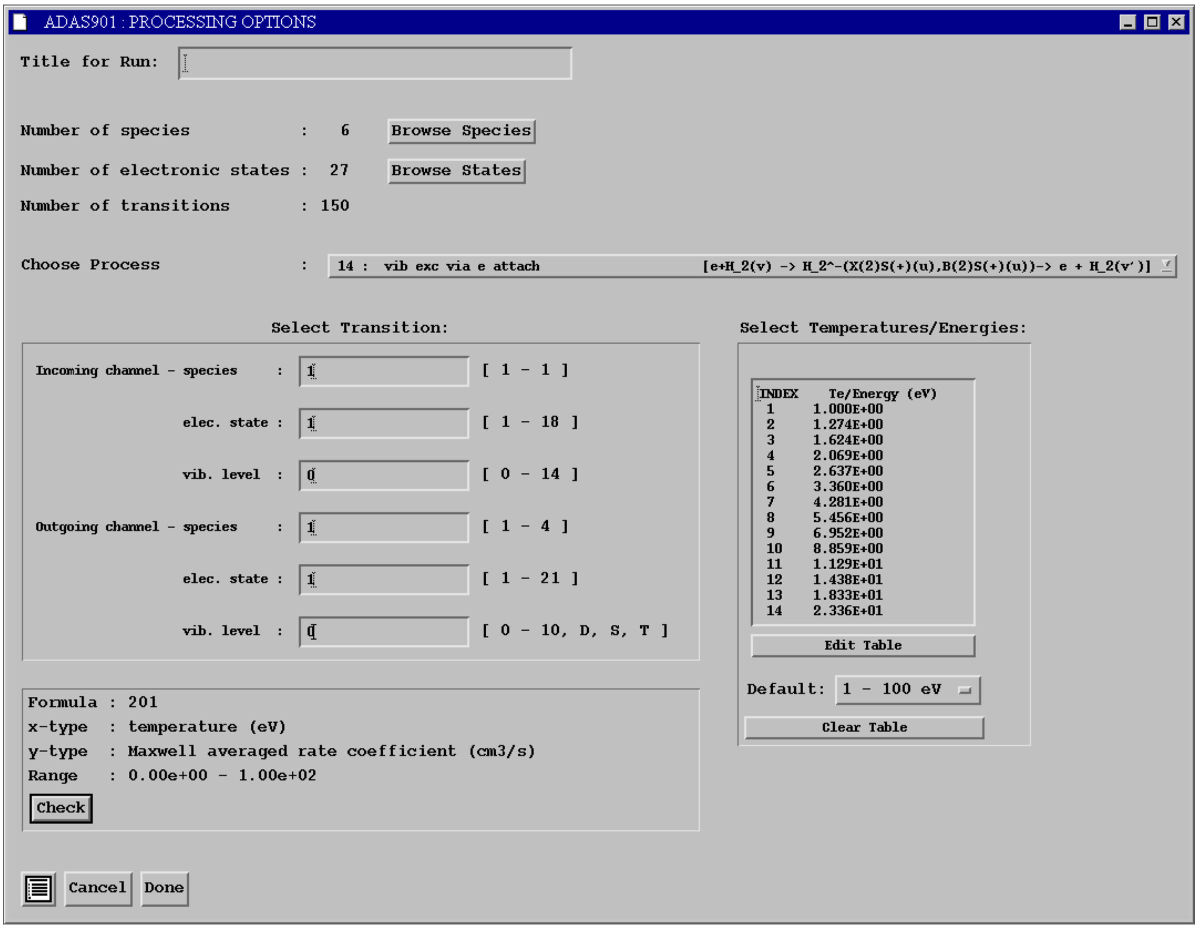


Figure 4.16: The ADAS901 input screen.

(or temperature) range of the tabulation in the source *mdf02* dataset. Summary information of the user's choices are given in the bottom panel. The *Check* button verifies existence. Click *Done* to advance to the *Output* screen.

The *Output* screen has the usual ADAS choices of entering a title for graphs, selecting graphical and/or hard copy output and explicit scaling of the output graph.



Title for Run:

Number of species : 6

Number of electronic states : 27

Number of transitions : 150

Choose Process : 14 : vib exc via e attach [e+H_2(v) -> H_2^-(X(2)S(+)(u),B(2)S(+)(u))-> e + H_2(v')]

Incoming channel - species : 1 [1 - 1]

elec. state : 1 [1 - 18]

vib. level : 0 [0 - 14]

Outgoing channel - species : 1 [1 - 4]

elec. state : 1 [1 - 21]

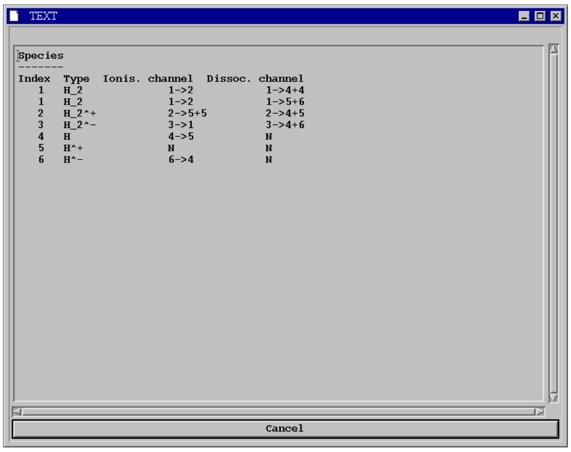
vib. level : 0 [0 - 10, D, S, T]

INDEX	Te/Energy (eV)
1	1.000E+00
2	1.274E+00
3	1.624E+00
4	2.069E+00
5	2.637E+00
6	3.360E+00
7	4.281E+00
8	5.456E+00
9	6.952E+00
10	8.859E+00
11	1.129E+01
12	1.438E+01
13	1.833E+01
14	2.336E+01

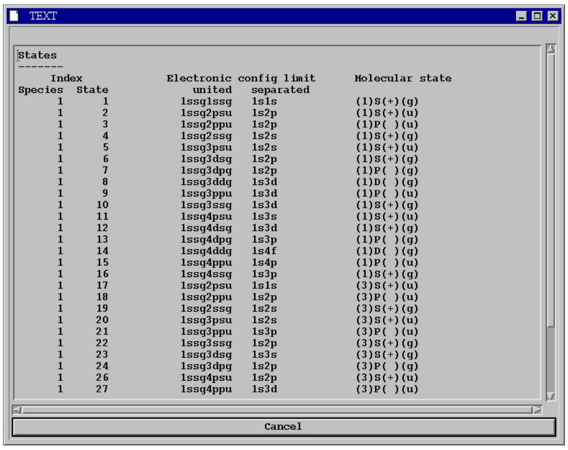
Default: 1 - 100 eV

Formula : 201
x-type : temperature (eV)
y-type : Maxwell averaged rate coefficient (cm3/s)
Range : 0.00e+00 - 1.00e+02

Figure 4.17: The ADAS901 processing screen.

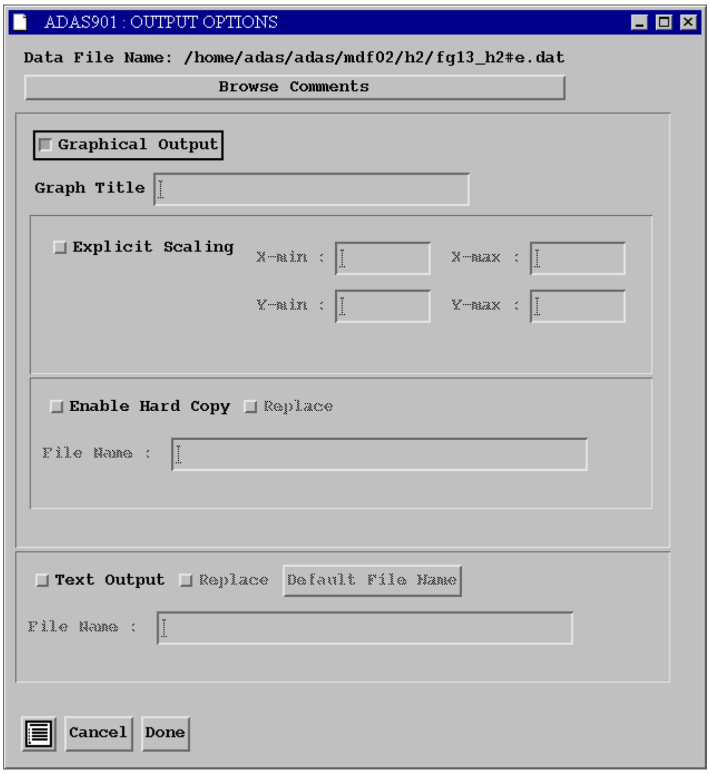


```
Species
--------
Index  Type   Ionis. channel  Dissoc. channel
   1   H_2            1->2           1->4+4
   1   H_2            1->2           1->5+6
   2   H_2^+          2->5+5         2->4+5
   3   H_2^-          3->1           3->4+6
   4   H              4->5           N
   5   H^+            N              N
   6   H^-            6->4           N
```



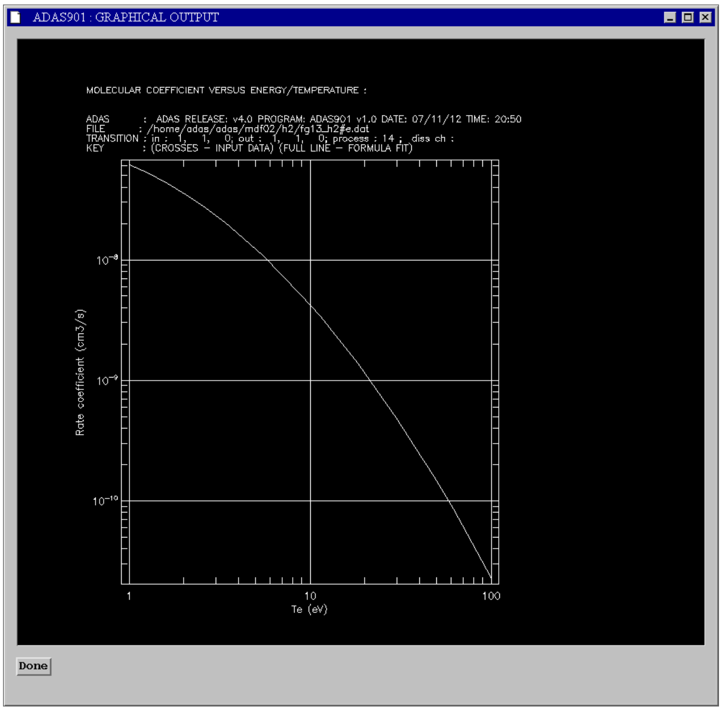
```
States
-------
      Index          Electronic config limit      Molecular state
Species   State          united   separated
       1        1       1ssg1ssg   1s1s           (1)S(+)(g)
       1        2       1ssg2psu   1s2p           (1)S(+)(u)
       1        3       1ssg2ppu   1s2p           (1)P( )(u)
       1        4       1ssg2ssg   1s2s           (1)S(+)(g)
       1        5       1ssg3psu   1s2s           (1)S(+)(u)
       1        6       1ssg3dsg   1s2p           (1)S(+)(g)
       1        7       1ssg3dpg   1s2p           (1)P( )(g)
       1        8       1ssg3ddg   1s3d           (1)D( )(g)
       1        9       1ssg3ppu   1s3d           (1)P( )(u)
       1       10       1ssg3ssg   1s3d           (1)S(+)(g)
       1       11       1ssg4psu   1s3s           (1)S(+)(u)
       1       12       1ssg4dsg   1s3d           (1)S(+)(g)
       1       13       1ssg4dpg   1s3p           (1)P( )(g)
       1       14       1ssg4ddg   1s4f           (1)D( )(g)
       1       15       1ssg4ppu   1s4p           (1)P( )(u)
       1       16       1ssg4ssg   1s3p           (1)S(+)(g)
       1       17       1ssg2psu   1s1s           (3)S(+)(u)
       1       18       1ssg2ppu   1s2p           (3)P( )(u)
       1       19       1ssg2ssg   1s2s           (3)S(+)(g)
       1       20       1ssg3psu   1s2s           (3)S(+)(u)
       1       21       1ssg3ppu   1s3p           (3)P( )(u)
       1       22       1ssg3ssg   1s2p           (3)S(+)(g)
       1       23       1ssg3dsg   1s3s           (3)S(+)(g)
       1       24       1ssg3dpg   1s2p           (3)P( )(g)
       1       26       1ssg4psu   1s2p           (3)S(+)(u)
       1       27       1ssg4ppu   1s3d           (3)P( )(u)
```

Figure 4.18:



Data File Name: /home/adas/adas/mdf02/h2/fg13_h2#e.dat

Figure 4.19: The ADAS901 output screen.



```
MOLECULAR COEFFICIENT VERSUS ENERGY/TEMPERATURE :

ADAS       :  ADAS RELEASE: v4.0 PROGRAM: ADAS901 v1.0 DATE: 07/11/12 TIME: 20:50
FILE       : /home/adas/adas/mdf02/h2/fg13_h2#e.dat
TRANSITION : in :  1,   1,   0; out :  1,   1,   0; process : 14 ;  diss ch :
KEY        : (CROSSES - INPUT DATA) (FULL LINE - FORMULA FIT)
```

Figure 4.20: The ADAS901 output graph.

Chapter 5

Prediction of spectra

A central objective of ADAS is that it connects to spectroscopic observations, although it must be recognised that historically ADAS has not been a database of spectral line tabulations and identifications. So also in this molecular extension, aspirations are restricted to spectral predictions of direct diagnostic analysis. The models developed in the previous chapters do not quite achieve that. From these latter molecular collisional-radiative models, local populations of vibronic states are obtained as functions of local plasma parameters. Observationally, line-of-sight emission of rotational-vibrational band structure is observed, which in general is resolved into component rotational transitions between vibronic states, branches, band head accumulations and so on. Also in the H_2 case, the complex spectrum is dispersed and diagnostic analysis requires and exploits the variation between components across significant spectral regions. To make this link, a number of capabilities, that is ADAS codes and *mdf* datasets, have been been implemented.

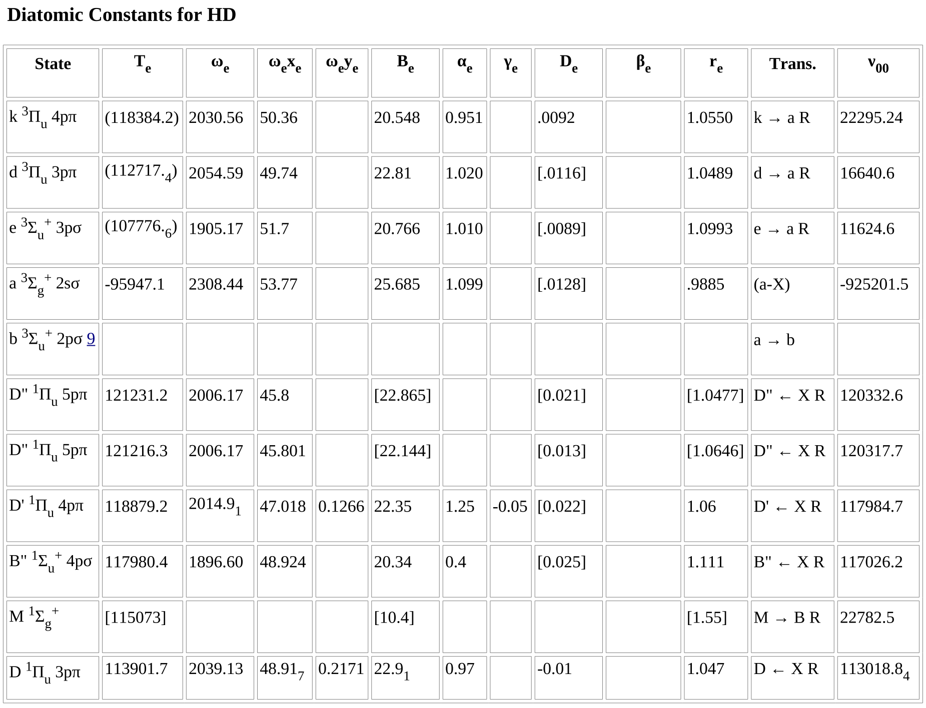
At the most basic level, it is helpful to have the molecular constants for the species (diatomics) of interest to ADAS fusion users. These are archived in an *mdf00* and are certainly not exhaustive, but go a little further than just the H_2 isotopic systems - to some light element hydrides, reflecting the light element focus at JET over many years. In attempts to analyse diatomic spectra, such as the green bands of BeD illustrated in chapter 1, we found it helpful to prepare more sophisticated and detailed band spectral predictions using the CALCAT package of Pickett [55]and to integrate its handling into the ADAS interactive IDL system. Noting that molecular ADAS has no rotational sub-population redistibutive collisional-radiative model, such sub-populations, as indicated earlier, are assumed Boltzmann at a specified rotational temperature and then relative intensities come simply from Hoenl-London factors. Nontheless, this approach does allow full simulation of molecular feature and local feature emissivity coefficients. Thereafter the preparation of feature emissivity functions follows the familiar ADAS-supported post-processing stage of plasma predictive models. Molecular ADAS delivers the derived qunatities for the spectral diagnostic analysis and post-processing above, the details of which are in the following sections.

5.1 Molecular constants

The directory */mdf00/const/* has been assigned to diatomic molecular constants, held by molecular symbol with lower case *p* used to denote the singly-charged molecular ions. The constants are simple tabulations extracted from the NIST databases [1] and refreshed periodically. The full referencing of the sources is not retained, the orginating NIST source being the reference in the various datasets. An extract is shown in figure 5.1. Such a dataset is read in FORTRAN by the subroutine *xxdatm_00c.for* and in IDL by *read_mdf00c.pro*. There is no graphical user interface. Datasets are present for the H_2, H_2^+ and the various isotopic combinations. Data are also present for BeH, CH and isotopic combinations. It is expected that this collection will increase gradually.

---

[1] http://webbook.nist.gov/chemistry/form-ser.html



Diatomic Constants for HD

State	T_e	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	γ_e	D_e	β_e	r_e	Trans.	ν_{00}
k $^3\Pi_u$ 4pπ	(118384.2)	2030.56	50.36		20.548	0.951		.0092		1.0550	k → a R	22295.24
d $^3\Pi_u$ 3pπ	(112717.$_4$)	2054.59	49.74		22.81	1.020		[.0116]		1.0489	d → a R	16640.6
e $^3\Sigma_u^+$ 3pσ	(107776.$_6$)	1905.17	51.7		20.766	1.010		[.0089]		1.0993	e → a R	11624.6
a $^3\Sigma_g^+$ 2sσ	-95947.1	2308.44	53.77		25.685	1.099		[.0128]		.9885	(a-X)	-925201.5
b $^3\Sigma_u^+$ 2pσ 9											a → b	
D" $^1\Pi_u$ 5pπ	121231.2	2006.17	45.8		[22.865]			[0.021]		[1.0477]	D" ← X R	120332.6
D" $^1\Pi_u$ 5pπ	121216.3	2006.17	45.801		[22.144]			[0.013]		[1.0646]	D" ← X R	120317.7
D' $^1\Pi_u$ 4pπ	118879.2	2014.9$_1$	47.018	0.1266	22.35	1.25	-0.05	[0.022]		1.06	D' ← X R	117984.7
B" $^1\Sigma_u^+$ 4pσ	117980.4	1896.60	48.924		20.34	0.4		[0.025]		1.111	B" ← X R	117026.2
M $^1\Sigma_g^+$	[115073]				[10.4]					[1.55]	M → B R	22782.5
D $^1\Pi_u$ 3pπ	113901.7	2039.13	48.91$_7$	0.2171	22.9$_1$	0.97		-0.01		1.047	D ← X R	113018.8$_4$

Figure 5.1: A portion of the molecular constants table for HD */mdf00/const/hd.dat*. For detailed comments, references and notes on the parameters reference should be made to NIST.

5.2 General diatomic rotational-vibrational band prediction

For molecular ADAS, **for species other than the H_2 isotopic system**, an infra-structure has been set-up based on the use of the CALCAT code [55]. The usual inputs for CALCAT are the *.int* and *.par* datasets. It has been convenient for the present purposes to combine these into a composite driver spanning sets of vibronic transtions for a molecule. These are archived in data format *mdf01* in individual molecule isotopic system sub-directories as, for example, */mdf01/beh/*. This contains individual drivers for BeH, BeD and BeT. Lower case letters are normally used, so the members are *beh,dat, bed.dat and bet.dat*. Figure 5.2 shows a portion of the BeD driver. For those familar with CALCAT inputs, there are *.int* and *.par* blocks for the sequence bands successively down the dataset with an initial index at the top of the dataset for ADAS organisational purposes. Contruction of such a driver is a matter for some care and detailed assessment of the literature. The ADAS team has received much help in this regard from Prof. G. Dubury, a molecular spectroscopy specialist [56], whose work has underpinned special studies on molecular emission at JET [1],[57]. In ADAS terms, the output from the set of wavelengths and relative emissivities from CALCAT is a feature primitive. That means, it is the equivalent of a single A-value and transition wavelength from an upper electronic state in the atomic case. It may be converted to a feature by multiplying by the relative populations of the upper emitting vibronic levels. Since the latter are referred to the metastables of the molecular system, this yields feature emissivity coefficients. Various forms of output are possible, some of which are useful mainly for immediate viewing (such as a predicted spectrum of all the component emission in a spectral range) others (such as feature emssivity coefficients themselves as a function of local plasma parameters), which are suitable for archiving. In the molecular case, there is also a need for predicted aggregated emission for lower resolution diagnostics and for plasma models. A number of additional *mdf* data formats have been created to this end, while two ADAS9XX series graphical interface codes have been prepared to assist the user. The schematic of figure 5.4 shows the computational architecture, the processing ADAS9XX codes and the relevant *mdf* data formats. For spectral processing purposes, it is convenient to have a data format for the population output from ADAS902. Following the ADAS precedent for atoms and ions, this is called *mdf24*. The rotationally resolved code ADAS904 takes as primary input a dataset of format *mdf01*. This allows the code to run CALCAT and prepare a list of wavelengths and relative intensities of interest for display. This intermediate dataset is routed to the user's */pass* directory. Also it may be displayed and/or printed via the usual ADAS form of

```
Beryllium deuteride study for JET trace tritium experiment     mdf01
   1  sig sigma                     0.000
   2  sig pi                    20037.910
  -1
   1  e=1 v=0              1        0.000
   2  e=1 v=1              1     1488.780
                  .   .  .
  14  e=2 v=6              2     8320.162
  -1
   1    8    1
   2    9    2
   3   10    3
   4   11    4
  -1
   1
beryllium deuteride 2pi-2sig       14-Oct-2003
1010  79002 494.139  0 120 -45.0 -45.0 600000 TTTTT
 013  0.0100
---
Beryllium deuteride 0-0 band  2pi-2sigma  14 Oct 2003
   16      600    3    0   1.1220000E-10   1000.000    1.000
'a'   -2   2  0   0   0   2     1    1     -1      1
      -2   1  1   1   0   2     1    1     0      1
      11     20037.68838      .05           ! E' (Band Centre)
     100     5.62479800    9.59E-8       ! Bbar"  (1sig)
     111     5.69574400    9.59E-8       ! Bbar'  (1pi)
     200    -3.1176800E-4  2.00E-10      ! DJ"  (1sig)
     211    -3.1670100E-4  2.00E-10      ! DJ'  (1pi)
     300     1.6238000E-8  2.00E-10      ! HJ"  1sig)
     311     1.5743000E-8  2.00E-10      ! HJ'  (1pi)
     400    -0.8746000E-12 2.00E-10      ! LJ"  1sig)
     411    -0.9078000E-12 2.00E-10      ! LJ'  (1pi)
   40011     2.1096000e-3  2.00e-10      !  q/2 lambda
   40111    -4.5860000e-7  2.00e-10      !  dq/2 lambda
   40211     2.6995000e-11 2.00e-10      !  hq/2 lambda
10010011     2.1592000     2.00e-10      !  Aso 2pi
 1000011     -0.801500e-2  2.00e-10      !  gamma 2pi
 1000111      0.806900e-5  2.00e-10      !  dgamma 2pi
 1000211     -2.218000e-9  2.00e-10      !  hgamma 2pi
+++
  2
beryllium deuteride 2pi-2sig       14-Oct-2003
1010  79002 494.139  0 120 -45.0 -45.0 600000 TTTTT
 013  0.0100
---
Beryllium deuteride 1-1 band  2pi-2sigma  14 Oct 2003
   16      600    3    0   1.1220000E-10   1000.000    1.000
'a'   -2   2  0   0   0   2     1    1     -1      1
      -2   1  1   1   0   2     1    1     0      1
      11     20054.1000      .05           ! E' (Band Centre)
     100     5.49863790    9.59E-8       ! Bbar"  (1sig)
                   .   .  .
1000111      0.753600e-5  2.00e-10      !  dgamma 2pi
 1000211     -2.043000e-9  2.00e-10      !  hgamma 2pi
+++
  3
                   .   .  .

 -1
C------------------------------------------------------------------
C
C   Compiler:  Allan Whiteford
C   Date    :  14 Oct. 2003
C
C------------------------------------------------------------------
```

Figure 5.2: ADAS driver of format */mdf01* prepared for a study of the 0-0, 1-1, 2-2 and 3-3 sequence band structure of BeD $^2\Pi -^2\Sigma$ emission.

output screen. An illustration is shown in figure 5.2. There is an optional *mdf24* secondary input dataset to ADAS904, whose presence modifies the behaviour and options on the processing screen.

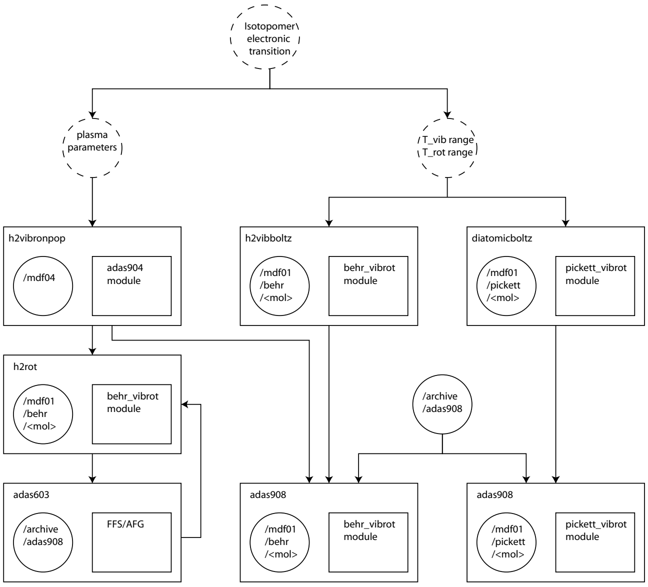


Figure 5.3: Schematic of molecular spectral emission processing

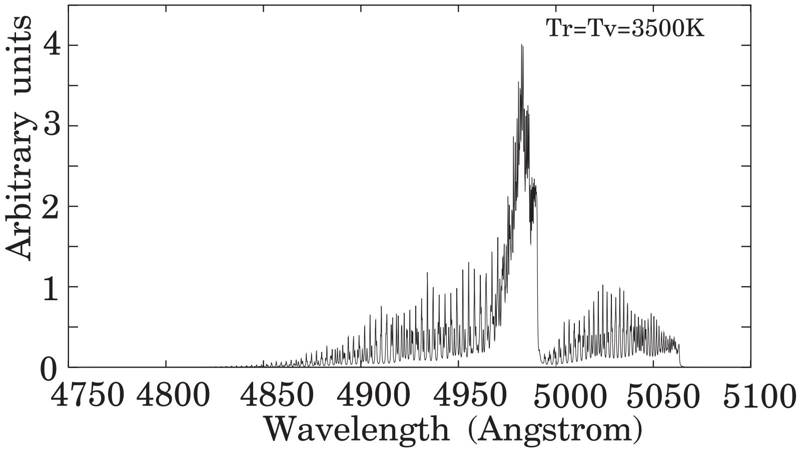


Figure 5.4: Predicted sequence band relative emission for *BeD* ($A\ ^2\Pi - X\ ^2\Sigma$) in the spectral range 4850-5100Å at speciified rotational and vibrational temperatures.

5.3 H_2 system rotational-vibrational band prediction

Because of the light masses of the nuclei of H_2 system, the Pickett code described in the previous section is less suited to this case. A dedicated predictive code has been prepared for H_2 system bands and for comparison with experimental data. This code is designed to act as an interface between the relatively complex, but rotationally unresolved vibronic population model and the highly detailed, rotationally resolved observed spectral bands. A number of issues must be considered. The term values of the vibrating rotor are usually written as

$$\begin{aligned} T_{v,J} &= G(v) + f_v(J) \\ &= \omega_e(v+1/2) - \omega_e x_e(v+1/2)^2 + \omega_e y_e(v+1/2)^3 + \ldots \\ &\quad + B_v J(J+1) - D_v J^2(J+1)^2 + H_v J^3(J+1)^3 + \ldots \end{aligned} \tag{5.1}$$

where

$$\begin{aligned} B_v &= B_e - \alpha_e(v+1/2) + \beta_e(v+1/2)^2 + \ldots \\ D_v &= D_e - \gamma_e(v+1/2) + \ldots \end{aligned} \tag{5.2}$$

The above polynomical expansions (usually only to second order in $J(J+1)$ and with the B_v coefficient only to first order in v), for the rotational energies as a function of vibrational state (such as from the NIST tabulations of format *mdf00c*) are insufficiently precise. Many experimental studies of, for example the Fulcher bands, have led to more exact estimates of each rotational state and it is these which need to be incorporated, as tabulations. Only when such tabulations are not available is it appropriate to revert to the cruder polynomial fits of equations 5.1 and 5.2. Secondly, we must be concerned with the estimated relative intensities of rotational band components in terms of rotational temperature. Representation of the rotational sub-state populations of each vibrational upper state in terms of a Boltzmann rotational temperature is misleading. The short radiative lifetime of the upper electronic state means that the relative rotational sub-state populations are essentially frozen as they were formed from the precursor rovibronic state. It may be assumed that that is either the ground $X\ ^1\Sigma$ or the metastable $a\ ^3\Sigma$ or a combination of both. Evidently the B_v coefficient for a particular upper vibrational state must be a weighted average over precursor vibrational populations multiplied by the appropriate Frank-Condon factors [2]. For upper ordinary state k, in vibrational sub-state v', the modified B_v coefficient is given by

$$\bar{B}'_{k,v'} = \left[\sum_{v_g} B_{g,v_g} F^{k,v'}_{gv_g} N_{g,v_g} + \sum_{v_m} B_{m,v_m} F^{k,v'}_{mv_m} N_{m,v_m}\right] \Big/ \left[\sum_{v_g} N_{g,v_g} + \sum_{v_m} N_{m,v_m}\right] \tag{5.3}$$

The vibronic levels of the upper ordinary state are labelled k, v', the ground state as g, v_g and the metastable as m, v_m. The Fs are the Franck-Condon factors. N_{g,v_g} is the population of the state g, v_g and N_{m,v_m} that of the state m, v_m. These populations are determined by the collisional-radiative model. More simply, they can be specified as Boltzmann relative populations. Finally the rotational populations of the upper emitting state, assuming a rotational temperature T_r for the ground and metastable population distributions, are

$$N_{k,v',J} = \omega_J exp(-\bar{B}'_{k,v''} J(J+1)/kT_r) N_{k,v'} / \sum_J \omega_J exp(-\bar{B}'_{k,v'} J(J+1)/kT_r) \tag{5.4}$$

This is more usually expressed as a modified rotational temperature for the upper vibrational state as

$$N_{k,v',J} = \omega_J exp(-\bar{B}'_{k,v''} J(J+1)/kT'_r) N_{k,v'} / \sum_J \omega_J exp(-B'_{k,v'} J(J+1)/kT'_r) \tag{5.5}$$

where $T'_r = B'_{k,v'} T_r / \bar{B}'_{k,v'}$. The line strengths for the radiative transitions are the Hönl-London factors given, for example by Herzberg [**?**], for the various P, Q and R branches. In practical application, note must be taken of nuclear spin and associated permutation symmetry constraints. H_2 has total nuclear spin quantum number 0 or 1 (so called para- and ortho- forms). This combined with requirement that the whole wavefunction must be antisymmetric, determines the alternating so called 'weak' and 'strong' rotational line character of the successive members of the rotational band series members. The D_2 case of spin 1 bosons results in different weighting of the alternating 'weak' and 'strong'

---

[2] When using Franck-Condon factors to resolve A-values for a $k', v' \rightarrow k'', v''$ transition from the unresolved electronic $A_{k' \rightarrow k''}$, consistency requires that there be an $A_{k',v' \rightarrow k''\epsilon}$ representing loss to the k'' continuum, so that $\sum_{v''} A_{k',v' \rightarrow k''v''} + A_{k',v' \rightarrow k''\epsilon} = A_{k' \rightarrow k''}$. There is also a corresponding $F^{k',v'}_{k''\epsilon}$ so that $\sum_{v''} F^{k',v'}_{k''v''} + F^{k',v'}_{k''\epsilon} = 1$. $F^{k',v'}_{k''\epsilon}$ is very small for low v' but not negligible for large v'.

members. T_2 is as H_2 again, while the mixed isotopic combinations have no nuclear symmetry constraints. These aspects must be taken into account in the spectral simulation model [**?**] [**?**]. Following Brown & Carrington [**?**], using the full Hund's case (a) quantal representation, the electronic orbital wave function $psi_{\eta\Lambda}$, vibrational wave function ψ_v, electron spin wave function $\psi_{S,\Sigma}$ and rotational wav function $\psi_{J,\Omega,M}$ under space-fixed inversion (E^*) behaviour

$$\begin{aligned} E^*\psi_{\eta\Lambda^s}\psi_v\psi_{S,\Sigma}\psi_{J,\Omega,M} &= (-1)^{\Lambda+s+S-\Sigma+J-\Omega}\psi_{\eta-\Lambda^s}\psi_v\psi_{S,-\Sigma}\psi_{J,-\Omega,M} \\ &= (-1)^{J+s-S}\psi_{\eta-\Lambda^s}\psi_v\psi_{S,-\Sigma}\psi_{J,-\Omega,M} \end{aligned} \tag{5.6}$$

s is even for Σ^+ and higher Λ states and odd for Σ^-. For Hund's case (b) this becomes

$$E^*\psi_{\eta\Lambda^s}\psi_v\psi_{N,\Lambda,S,J,M} = (-1)^{N+s}\psi_{\eta-\Lambda^s}\psi_v\psi_{N,-\Lambda,S,J,M} \tag{5.7}$$

Introduce the nuclear permutation operator, P for the homonuclear case, recognise that $PE^* = E^*P$ corresponds to inversion in the molecular-fixed axis system and introduce the nuclear spin wave function ψ_{I_1,I_2,I_T}. Then for case (a)

$$\begin{aligned} P\psi_{\eta\Lambda^s_t}\psi_v\psi_{S,\Sigma}\psi_{J,\Omega,M}\psi_{I_1,I_2,I_T} &= (-1)^{t+\Lambda+s+S-\Sigma+J-\Omega+I_T-I_1-I_2}\psi_{\eta-\Lambda^s_t}\psi_v\psi_{S,-\Sigma}\psi_{J,-\Omega,M}\psi_{I_1,I_2,I_T} \\ &= (-1)^{t+J+s-S+I_T-I_1-I_2}\psi_{\eta-\Lambda^s}\psi_v\psi_{S,-\Sigma}\psi_{J,-\Omega,M}\psi_{I_1,I_2,I_T} \end{aligned} \tag{5.8}$$

The exponent t is even for g states and odd for u states. For case (b)

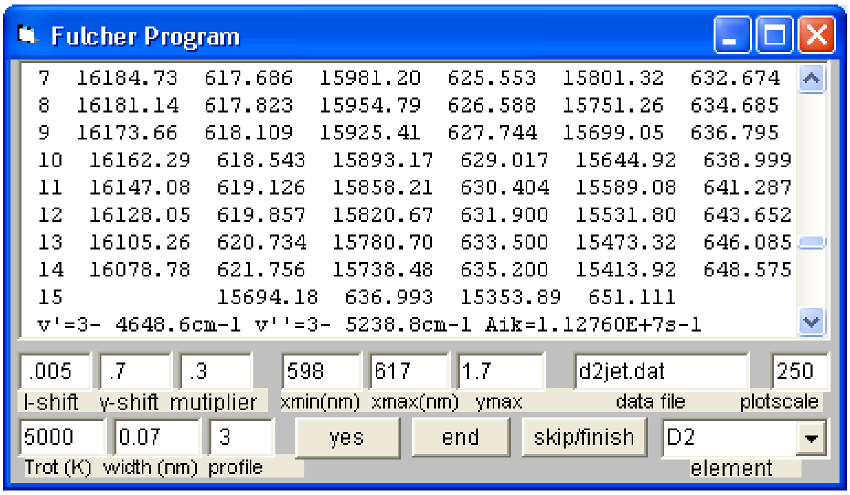
$$P\psi_{\eta\Lambda^s}\psi_v\psi_{N,\Lambda,S,J,M}\psi_{I_1,I_2,I_T} = (-1)^{N+s+t+I_T-I_1-I_2}\psi_{\eta-\Lambda^s}\psi_v\psi_{N,-\Lambda,S,J,M}\psi_{I_1,I_2,I_T} \tag{5.9}$$

For homo-nuclear H_2 (spin 1/2 fermions), $I_1 = I_2 = 1/2$. The symmetric nuclear state (*ortho*, $I_T = 1$) has nuclear spin weight $(I+1)(2I+1) = 3$ and the rest of the wavefunction must be odd to nuclear permutation for full antisymmetry. The antisymmetric nuclear state (*para*, $I_T = 0$) has nuclear spin weight $I(2I+1) = 1$ and the rest of the wavefunction to nuclear permutation must be even for full antisymmetry.For homo-nuclear D_2 (spin 1 bosons), $I_1 = I_2 = 1$. The symmetric nuclear state (*ortho*, $I_T = 2$) has nuclear spin weight $(I+1)(2I+1) = 6$ and the rest of the wavefunction must be even to nuclear permutation for full symmetry. The antisymmetric nuclear state (*para*, $I_T = 0$) has nuclear spin weight $I(2I+1) = 3$ and the rest of the wavefunction to nuclear permutation must be odd for full symmetry. T_2 with spin 1/2 fermions is at for H_2.

The heter-nuclear isotopomers, HD, HT and DT, in ground vibrational states, have a fluctuating non-vanishing dipole moment due to the separation between the centroid of the electron cloud and the centre of mass. This implies radiative transition probabilities between ground vibrational states and infra-red line emission!!!

The calculation and display is handled by an interactive control screen which is illustrated in figure 5.3. This allows isotopic selection, rotational temperature selection , comparative experimental data selection together with scaling, wavelength scale displacements and resolution.

Figure 5.3 illustrates the resulting spectral display in which an experimental spectrum is also shown in blue for comparison. The figure is of a portion of the Fulcher bands in the vsisble spectral region. A second figure 5.4 shows a simulation of the Lyman bands in the UV and an experimental spectrum for comparison.



```
7  16184.73  617.686  15981.20  625.553  15801.32  632.674
8  16181.14  617.823  15954.79  626.588  15751.26  634.685
9  16173.66  618.109  15925.41  627.744  15699.05  636.795
10  16162.29  618.543  15893.17  629.017  15644.92  638.999
11  16147.08  619.126  15858.21  630.404  15589.08  641.287
12  16128.05  619.857  15820.67  631.900  15531.80  643.652
13  16105.26  620.734  15780.70  633.500  15473.32  646.085
14  16078.78  621.756  15738.48  635.200  15413.92  648.575
15                 15694.18  636.993  15353.89  651.111
v'=3- 4648.6cm-1 v''=3- 5238.8cm-1 Aik=1.12760E+7s-1
```

l-shift: .005
y-shift: .7
mutiplier: .3
xmin(nm): 598
xmax(nm): 617
ymax: 1.7
data file: d2jet.dat
plotscale: 250
Trot (K): 5000
width (nm): 0.07
profile: 3
element: D2

Figure 5.5: Control screen for interactive D_2 isotopomer Fulcher band prediction and experimental result display.

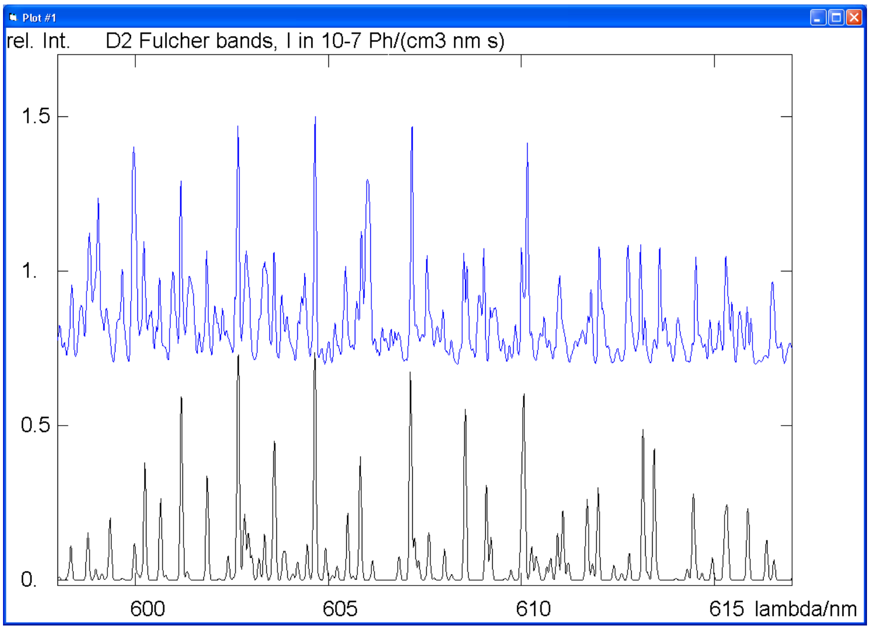


Figure 5.6: D_2 isotopomer Fulcher band prediction and experimental comparison

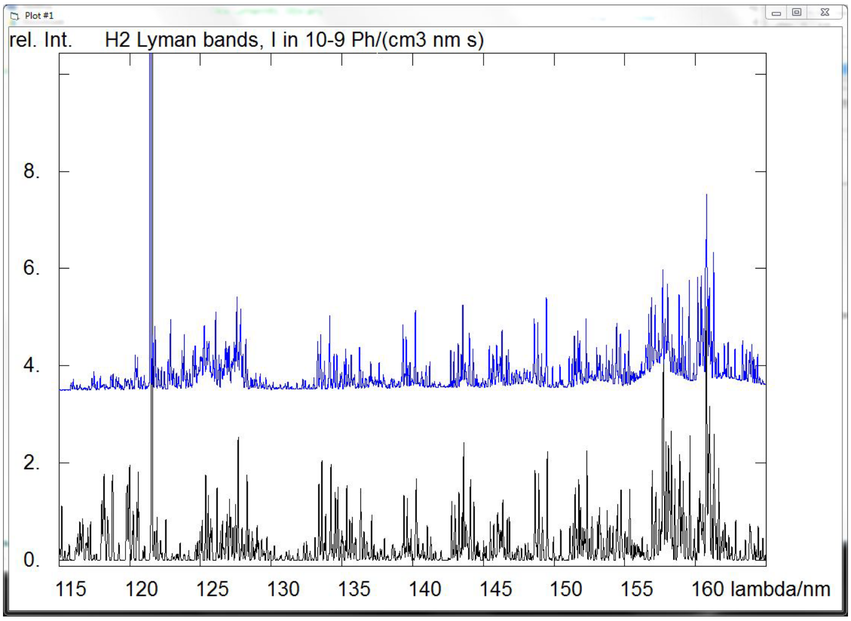


Figure 5.7: H_2 isotopomer Lyman band prediction and experimental comparison. Note the presence of HI Lα in the experimental spectrum and an esstimate of it in the theoretical spectrum

5.4 ADAS908

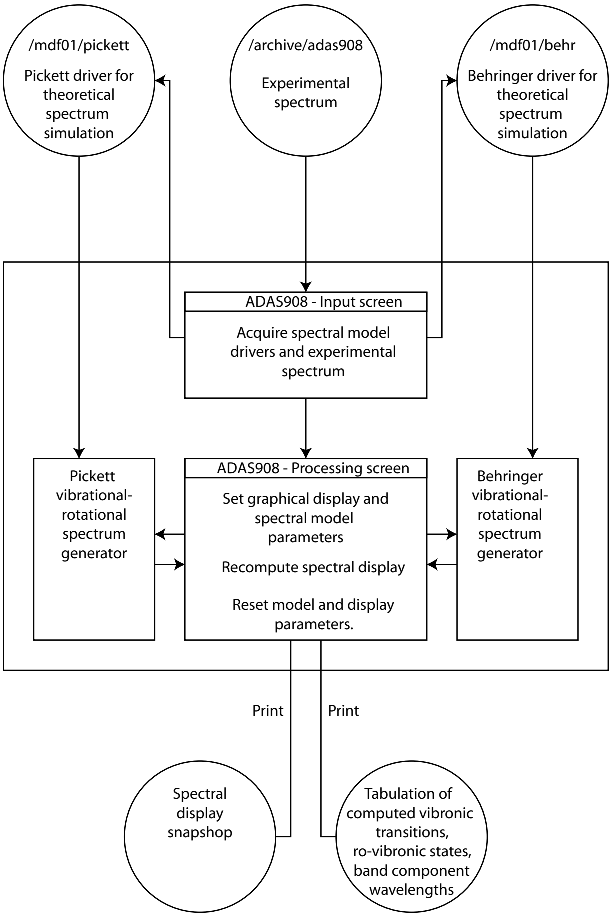
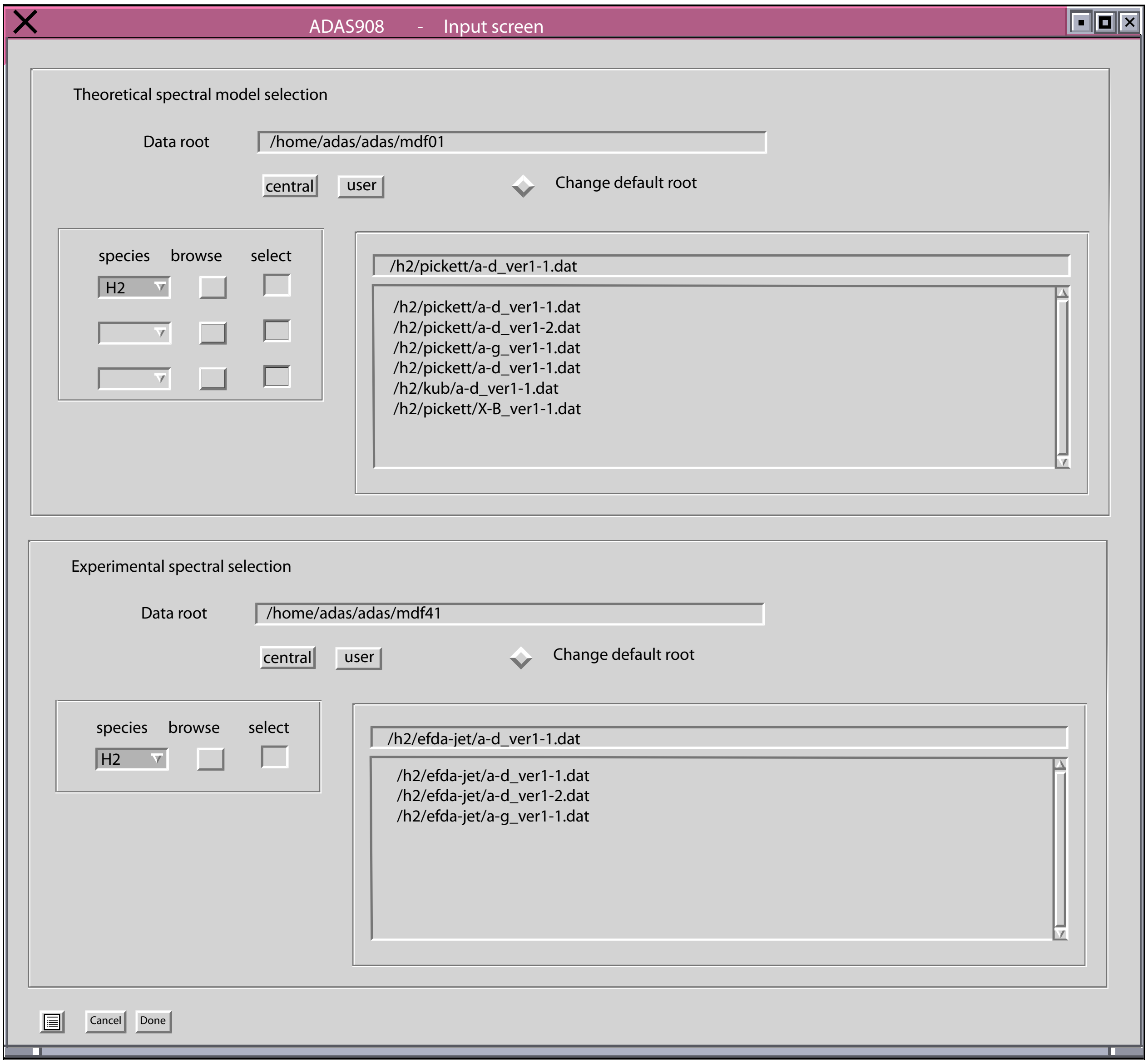


Figure 5.8: Schematic of ADAS908 and related *mdfxx* datasets used



Theoretical spectral model selection

Data root /home/adas/adas/mdf01

species H2

/h2/pickett/a-d_ver1-1.dat

/h2/pickett/a-d_ver1-1.dat
/h2/pickett/a-d_ver1-2.dat
/h2/pickett/a-g_ver1-1.dat
/h2/pickett/a-d_ver1-1.dat
/h2/kub/a-d_ver1-1.dat
/h2/pickett/X-B_ver1-1.dat

Experimental spectral selection

Data root /home/adas/adas/mdf41

species H2

/h2/efda-jet/a-d_ver1-1.dat

/h2/efda-jet/a-d_ver1-1.dat
/h2/efda-jet/a-d_ver1-2.dat
/h2/efda-jet/a-g_ver1-1.dat

Figure 5.9: The input screen for ADAS908

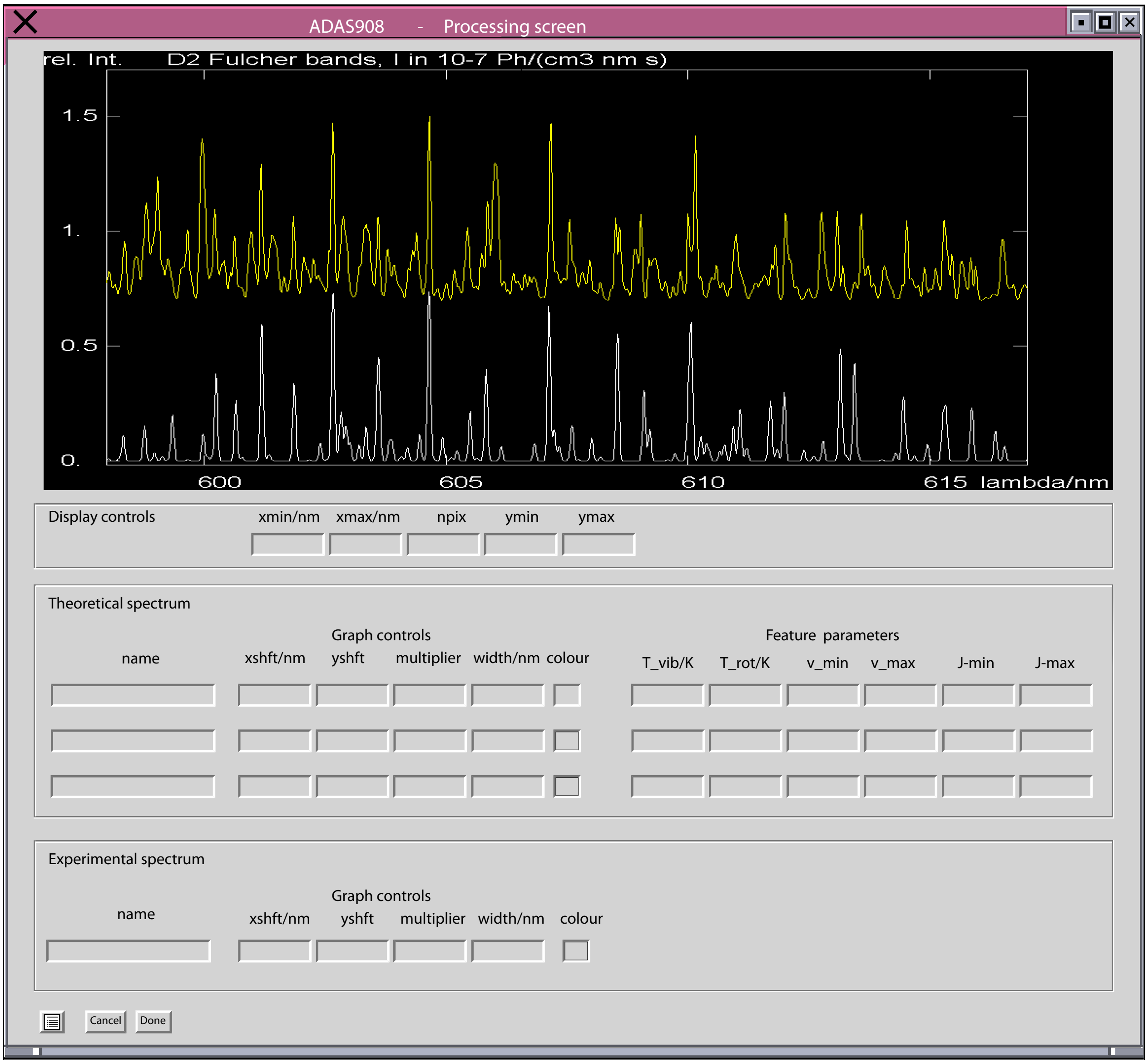


Figure 5.10: The processing screen for ADAS908

Chapter 6

Results

As seen in previous chapter the molecular Collisonal-Radiative model allow to get populations for a big variety of boundary and initial conditions. Looking into real plasma situations, the population calculations from molecules obtained by this model cal help to resolve the problem of particule flux in the divertor [**?**, **?**, **?**]. Measuring the band spectra, molecular rovibrational temperature and concentration in divertor plasmas can be reproduced. As seen on chapter 5 the molecular population of upper levels as well as the spectral effective coefficients as PEC (in implementation) can be the input for the rovibrational band prediction codes as the one showed in section 5.3. Molecules in the divertor contribute importantly to the neutral flux compiting with charge exchange (CX) [52] and making a significant contribution for fuelling: Pospiesczcyk *et al.*[**?**] report 70% of the total photon flux originating from molecular sources. Molecular collisional-radiative effective coefficients can help to the plasma wall interaction models as [53] to study the contribution from the molecules desorbed form the wall.

These situations can be handled by the model presented here. In this chapter, first results illustrating the capabilities of the model are presented, compared and analyzed.

6.1 Plasma Initial conditions and molecular set up

For our standard input settings it has been chosen plasma conditions similar to Tore Supra experiment made on 2001 by Escarguel *et al.* [52]:

Neutral density	$n_H = 10^{12}\mathrm{cm}^{-3}$
Effective charge	$Z_{eff} = 1.0$
Ion density	$n_i = Z_{eff} * n_e$
Ion temperature	$T_i = T_e$
Electron temperature	$T_e = 5 - 100\mathrm{eV}$
Electron density	$n_e = 10^{11} - 10^{16}\mathrm{cm}^{-3}$

The electron temperatures and densities have been chosen in order to well cover the possible low temperature plasmas in the divertor inside the possibilities of our model.

A set of 27 electronic states for the H_2 molecule and 3 for the $H_2{}^+$ ion have been considered and are shown in table 2.1 that is reproduced in this chapter in table 6.1 for clarity. Of these, 16 are singlets (para-hydrogen states) and 11 triplets (ortho-hydrogen states). The dissociative states are the $\mathrm{b}\,{}^3\Sigma_u^+$ of H_2 and $2p\sigma_u$ and $2p\pi_u$ of $H_2{}^+$.

The two dissociative states absorb all the excitation from the $H_2{}^+$ ion. Obviously, this excitation to dissociative states ends on dissociation processes and thus is accounted as dissociation.

Dissociative recombination processes produce excited hydrogen atoms that should decay to the ground state. However although some branching ratio are available under certains conditions [11] and new calculations have been done

For H_2							
State	Separated atom config.	Asymptotic levels	coupled config.	$(wt-1)/2$	$E_{\mathrm{min}}\mathrm{cm}^{-1}$	$E_{\mathrm{diss}}\mathrm{cm}^{-1}$	Comments
X	$1s\sigma_g 1s\sigma_g$	H(1s) + H(1s)	$^1\Sigma_g^+$	0.0	0.0	38292.98	ground state
B	$1s\sigma_g 2p\sigma_u$	H(1s) + H(2p)	$^1\Sigma_u^+$	0.0	91691.69	120595.97	
C	$1s\sigma_g 2p\pi_u$	H(1s) + H(2p)	$^1\Pi_u$	0.5	100101.80	120595.97	
EF	$1s\sigma_g 2s\sigma_g$	H(1s) + H(2s)	$^1\Sigma_g^+$	0.0	100146.88	120595.97	
B′	$1s\sigma_g 3p\sigma_u$	H(1s) + H(2s)	$^1\Sigma_u^+$	0.0	111640.12	120595.97	
GK	$1s\sigma_g 3d\sigma_g$	H(1s) + H(2p)	$^1\Sigma_g^+$	0.0	112223.18	120595.97	
I	$1s\sigma_g 3d\pi_g$	H(1s) + H(2p)	$^1\Pi_g$	0.5	113017.64	122442.16	potential barrier
J	$1s\sigma_g 3d\delta_g$	H(1s) + H(3d)	$^1\Delta_g$	0.5	113443.18	135837.26	
D	$1s\sigma_g 3p\pi_u$	H(1s) + H(3d)	$^1\Pi_u$	0.5	113934.45	135837.26	
$\mathrm{H\bar{H}}$	$1s\sigma_g 3s\sigma_g$	H(1s) + H(3d)	$^1\Sigma_g^+$	0.0	114020.67	135837.26	
$\mathrm{B''\bar{B}}$	$1s\sigma_g 4p\sigma_u$	H(1s) + H(3s)	$^1\Sigma_u^+$	0.0	117958.11	135837.26	
P	$1s\sigma_g 4d\sigma_g$	H(1s) + H(3d)	$^1\Sigma_g^+$	0.0	118422.44	135837.26	
R	$1s\sigma_g 4d\pi_g$	H(1s) + H(3p)	$^1\Pi_g$	0.5	118514.31	135837.26	
S	$1s\sigma_g 4d\delta_g$	H(1s) + H(4f)	$^1\Delta_g$	0.5	118703.93	141171.72	
D′	$1s\sigma_g 4p\pi_u$	H(1s) + H(4p)	$^1\Pi_u$	0.5	118910.00	141171.72	
O	$1s\sigma_g 4s\sigma_g$	H(1s) + H(3p)	$^1\Sigma_g^+$	0.0	118954.12	135837.26	
b	$1s\sigma_g 2p\sigma_u$	H(1s) + H(1s)	$^3\Sigma_u^+$	1.0	66178.12	66178.12	dissociative state
c	$1s\sigma_g 2p\pi_u$	H(1s) + H(2p)	$^3\Pi_u$	2.5	95888.20	120595.97	triplet metastable
a	$1s\sigma_g 2s\sigma_g$	H(1s) + H(2s)	$^3\Sigma_g^+$	1.0	95977.76	120595.97	
e	$1s\sigma_g 3p\sigma_u$	H(1s) + H(2s)	$^3\Sigma_u^+$	1.0	107766.65	120595.97	
d	$1s\sigma_g 3p\pi_u$	H(1s) + H(3p)	$^3\Pi_u$	2.5	112750.43	135837.26	
h	$1s\sigma_g 3s\sigma_g$	H(1s) + H(2p)	$^3\Sigma_g^+$	1.0	112787.69	123870.60	potential barrier
g	$1s\sigma_g 3d\sigma_g$	H(1s) + H(3s)	$^3\Sigma_g^+$	1.0	112937.71	135837.26	
i	$1s\sigma_g 3d\pi_g$	H(1s) + H(2p)	$^3\Pi_g$	2.5	113006.18	123897.40	potential barrier
f	$1s\sigma_g 4p\sigma_u$	H(1s) + H(2p)	$^3\Sigma_u^+$	1.0	116631.81	131018.27	potential barrier
k	$1s\sigma_g 4p\pi_u$	H(1s) + H(3d)	$^3\Pi_u$	2.5	118418.65	135837.26	
r	$1s\sigma_g 4d\pi_g$	H(1s) + H(3d)	$^3\Pi_g$	2.5	118509.87	135837.26	
For ${H_2}^+$							
X	$1s\sigma_g$	H(1s) + H^+	$^2\Sigma_g^+$	0.5	124418.00	148030.30	ground state
$2p\sigma_u$	$2p\sigma_u$	H(1s) + H^+	$^2\Sigma_u^+$	0.5	274666.12	274666.12	dissiociative state
$2p\pi_u$	$2p\pi_u$	H(2s) + H^+	$^2\Pi_u$	0.5	318289.02	318289.02	dissiociative state

Table 6.1: Parameters of the states of H_2 taken in account. wt is the statistical weight, E_{min} is the energy of the potential minimum, E_{diss} is the asymptotic dissociative energy for this potential.

up to $n = 5$ by quantum defect theory [**?**]. Experimental validations and new calculations are ongoing to confirm these data. At this stage, we have assumed that these processes produce atoms in its ground state.

Spontaneous decay to the dissociative triplet b state is considered here and it is one of the mechanisms which makes dissociation dependent on density [25].

Ionization from $H_2{}^+$ is considered as a dissociative process. However, the dissociation channel is giving two protons and two electrons as dissociation products.

Ion impact processes are considered in some of the calculations. The processes included on those calculations will be detailed when presenting the specific results.

Calculations are presented here in increasing order of complexity and compared between them so a better understanding of complex molecular system is achieved. Differences between electronic and fully vibrational resolutions is also evaluated and analyzed in the next sections.

6.2 Electron Impact results

These calculations have been performed with only electron impact processes. These results are important to see the influence of CX processes in the molecular model. The simplest calculations can serve as a reference to check the influence of the different grades of complexity in the initial conditions of molecules.

6.2.1 Electron impact normalized to vibrational ground level input in electronic resolution

The first and simplest calculation has been made using a normalized input in the $v = 0$ vibrational level of $H_2(X\,^1\Sigma_g^+)$ ground vibrational state in order to serve as a reference for future calculations. That is equivalent to the asumption that H_2 is produced only in this vibrational level. Electronic resolution is used for this calculation.

In the figure 6.1, the sum of the MQCD for all vibrational levels of the transitions $H_2(X\,^1\Sigma_g^+) \rightarrow H_2(c\,^3\Pi_u)$ are plotted in function of electron temperature and electron density. These coefficients have a strong variation with temperature but almost no variation with density due to the small rates that account for transition between the singlet and the triplet systems in the H_2 molecule.

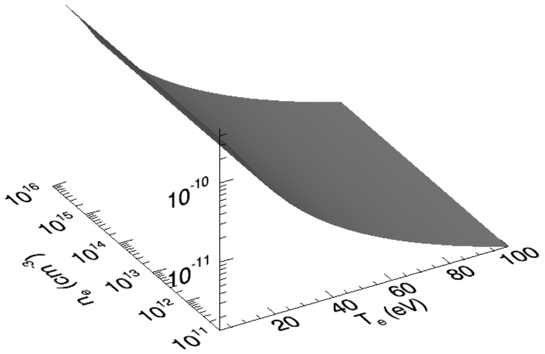


Figure 6.1: Sum on all the vibrational levels of MQCD coefficients for the $H_2(X\,^1\Sigma_g^+) \rightarrow H_2(c\,^3\Pi_u)$ transitions. The MQCD coefficients are in cm^3s^{-1}.

The collisional-radiative effect can be seen in figure 6.2 where the excitation MQCD coefficients from $H_2(X\,^1\Sigma_g^+, v = 0) \rightarrow H_2(X\,^1\Sigma_g^+, v')$ are given. Here it is possible to see how these effective coefficients are strongly influenciated by the indirect populating through excitation and decay. These coefficients have also a strong variation at higher densities. This latter effect comes due to the high competence of cascade excitation and ionization and dissociation processes at higher temperatures as can be seen on figures 6.3 and 6.4 where vibrationally summed MSCD $H_2(X\,^1\Sigma_g^+)$ $\rightarrow H_2{}^+(X\,^2\Sigma_g^+)$ and PDCD $H_2(X\,^1\Sigma_g^+) \rightarrow H + H(H^+)$ coefficients are shown respectively.

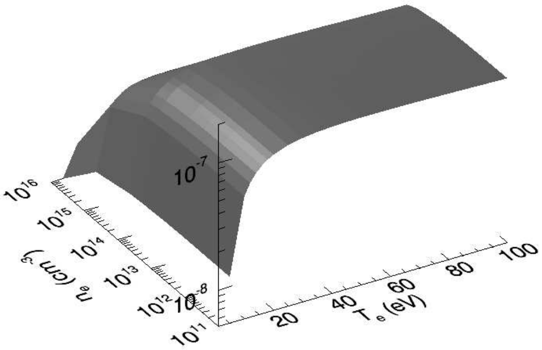


Figure 6.2: Sum on all the vibrational levels of MQCD coefficients for the $H_2(X\,^1\Sigma_g^+, v = 0) \rightarrow H_2(c\,^1\Sigma_g^+, v')$ transitions. The MQCD coefficients are in cm^3s^{-1}.

The MSCD coefficients are also changing at higher densities growing in importance. At higher densities the direct ionization is increasingly important as many more high energy tail electron from the maxwellian distribution are impinging on the molecules and causing it.

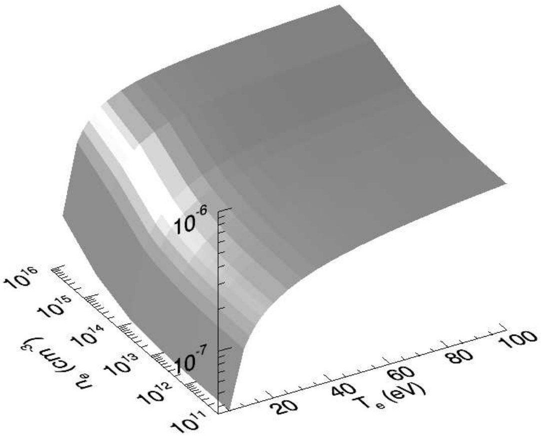


Figure 6.3: Sum on all the vibrational levels of MSCD coefficients for the $H_2(X\,^1\Sigma_g^+) \rightarrow H_2{}^+(X\,^2\Sigma_g^+)$ transitions. The MSCD coefficients are in cm^3s^{-1}.

Dissociation processes in turn can happen inside every electronic state by excitation to continuum of any other electronic state. That makes dissociation to be a more "direct" process and depend only weakly on density as is appreciated in figure 6.4.

Population of vibrational levels of ground sate of H_2 for different temperatures are shown in figure 6.5. It is possible to see here how ionization and dissociation make the population to fall steeply at electron densities higher that $10^{14}cm^{-3}$. The populations fall smoothly with temperature as it can be seen at figure 6.6.

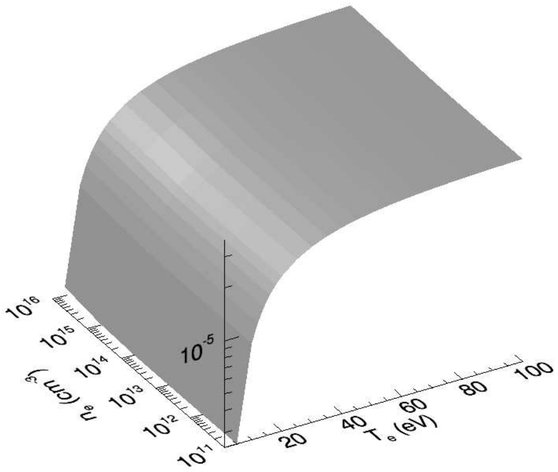


Figure 6.4: Sum on all the initial vibrational levels of PDCD coefficients for the process $H_2(X\,^1\Sigma_g^+) \rightarrow H + H(H^+)$, where at least one of the products is an H atom. The PDCD coefficients are in cm^3s^{-1}.

In the graphs 6.5 and 6.6 the population of vibrational levels have the same variation as they are not coupled between themselves due to the transitions between them are forbidden. The relative populations are shown in a bar diagram in figure 6.7 for $T_e = 25$eV and $n_e = 10^{12}$cm^{-3}. It is not surprising that $v = 14$ peaks over the immediate lower vibrational values if we look for the lower excitation rates from this level compared with the others. That can be easily seen on formula number form=13 for excitation in appendix E which depends on the energy difference at the turning point as can see in the schem of figure 6.8. When the minimum of the higher potential is displaced, that makes that the energy difference is increased and then the probability of transtions decreases.

These calculations will make the starting point to compare the influence of the calculation with fully vibrational resolution or the introduction of ion impact modeling.

6.2.2 Electron impact normalized to vibrational ground level input in fully vibrational resolution

This calculation is the equivalent to the previous one in fully vibrational resolution. As before, there is an input of H_2 molecules in their lowest vibrational level of ground state and the population will be normalized to that.

As seen on figure 6.9 the MQCD effective coefficients for excitation from all the vibrational levels of ground state have a similar shape as in the electronic resolution. These coefficients, when compared with the electronic ones are lower in a factor ~ 2 as can be seen in figure 6.10. That can owe to the fact that more channels are open now and which can diffuse the population flux to the other metastables.

Population of the vibrational states of ground state are shown in figure 6.11. These relative populations are higher than the ones from the electronic resolution calculation that have been shown in figure 6.5. A plaussible explanation can be found looking again at the difference on the effective coefficients shown in figure 6.10. Again, more decaying channels are open to the vibrational states allowing part of the flux that was previously dissociating or ionizing to decay on the vibrational levels of the ground state making being that enogh for their population to grow. This is also seen in the fact that the population fall less steeply in the present case.

The population of the higher vibrational levels seem to be crossing at $T_e = 5$eV in the figure 6.11. In a closer look at electron density of $n_e = 10^{12}$cm^{-3} shown in figure 6.12 can be appreciated that the populations from $v = 9$ to $v = 14$ are very similar with a small peak at $v = 10$. This peculiarity is not present at higher temperatures which is indicative of a low energy process. At low energies there is a process that add to other losses, that is dissociative electron attachment.

Dissociative electron attachment cross sections are plotted in figure 6.13 for a very narrow range of energies around

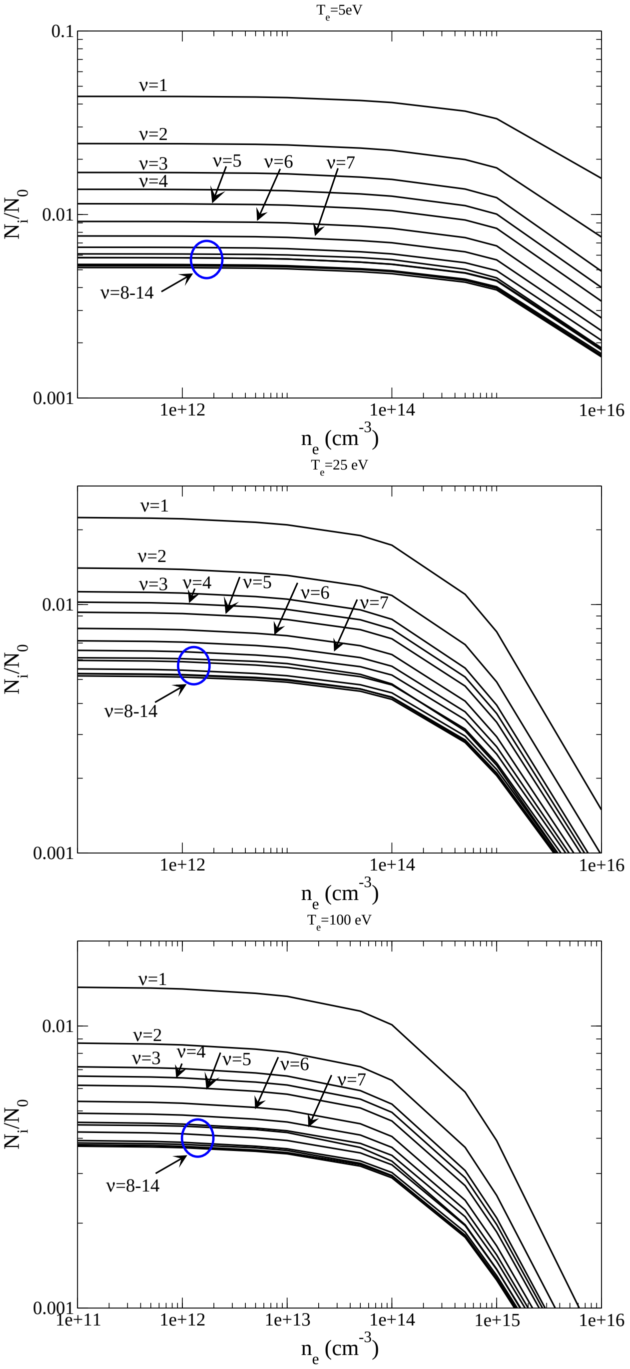


Figure 6.5: Population of the vibrational levels of ground state of H_2 molecule normalized to ground level $\nu = 0$.Top: $T_e = 5$eV; middle: $T_e = 25$eV; Bottom: $T_e = 100$eV.

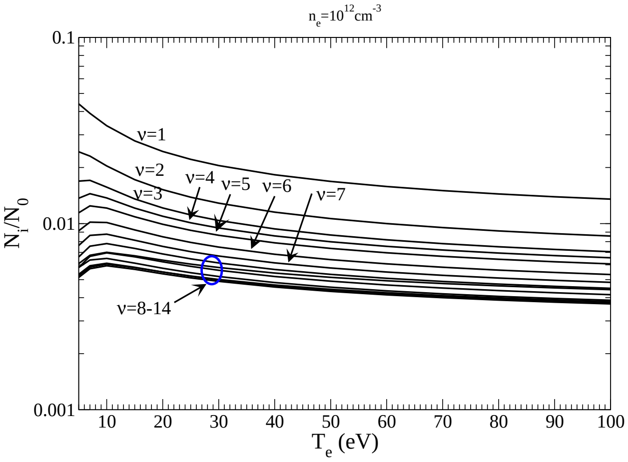


Figure 6.6: Variation of H_2 ground state vibrational levels populations with temperature for an elctron density of 10^{12}cm^{-3}. The population are normalized to the ground vibrational level $\nu = 0$.

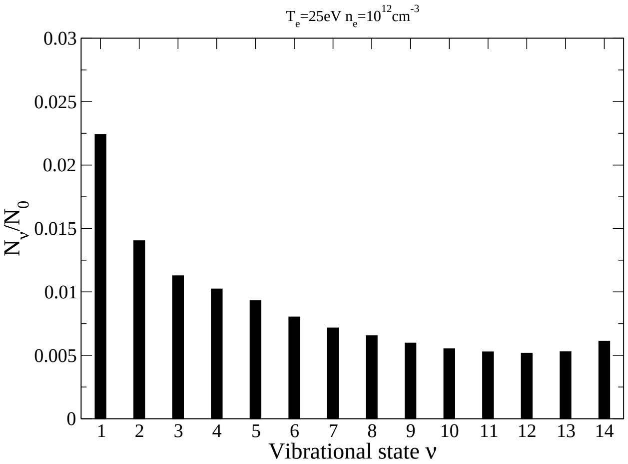


Figure 6.7: Relative population of vibrational levels from the ground state of H_2 normalized to $\nu = 0$ level for $T_e = 25$eV and $n_e = 10^{12}$cm^{-3}.

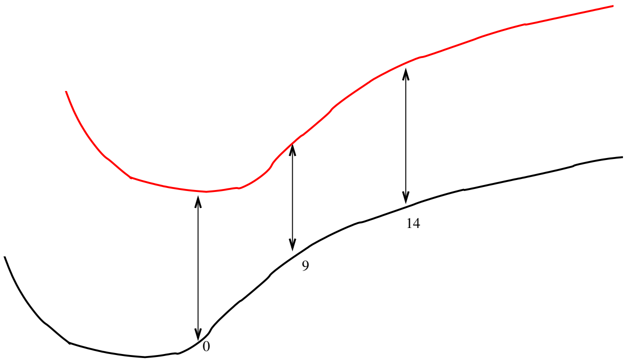


Figure 6.8: Schem where the energy difference of two generic potentials with repect of the vibrational turning points of the lower one are shown.

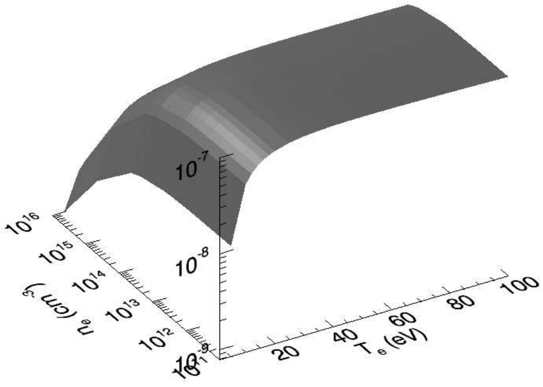


Figure 6.9: Sum on all the vibrational levels of MQCD coefficients for the $H_2(X\,^1\Sigma_g^+, v = 0) \rightarrow H_2(X\,^1\Sigma_g^+, v')$ transitions. The MQCD coefficients are in cm^3s^{-1}.

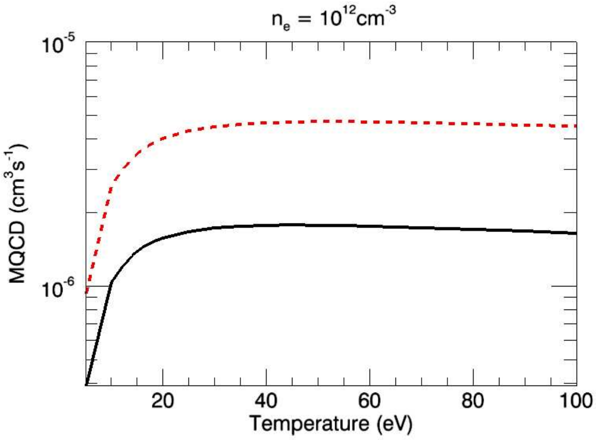


Figure 6.10: Sum on all the vibrational levels of MQCD coefficients for all the excitation departing form all the $H_2(X\,^1\Sigma_g^+, v)$ levels for an electron density $n_e = 10^{12}cm^{-3}$. (—) Fully vibrational resolution; (– –) Electronic resolution.

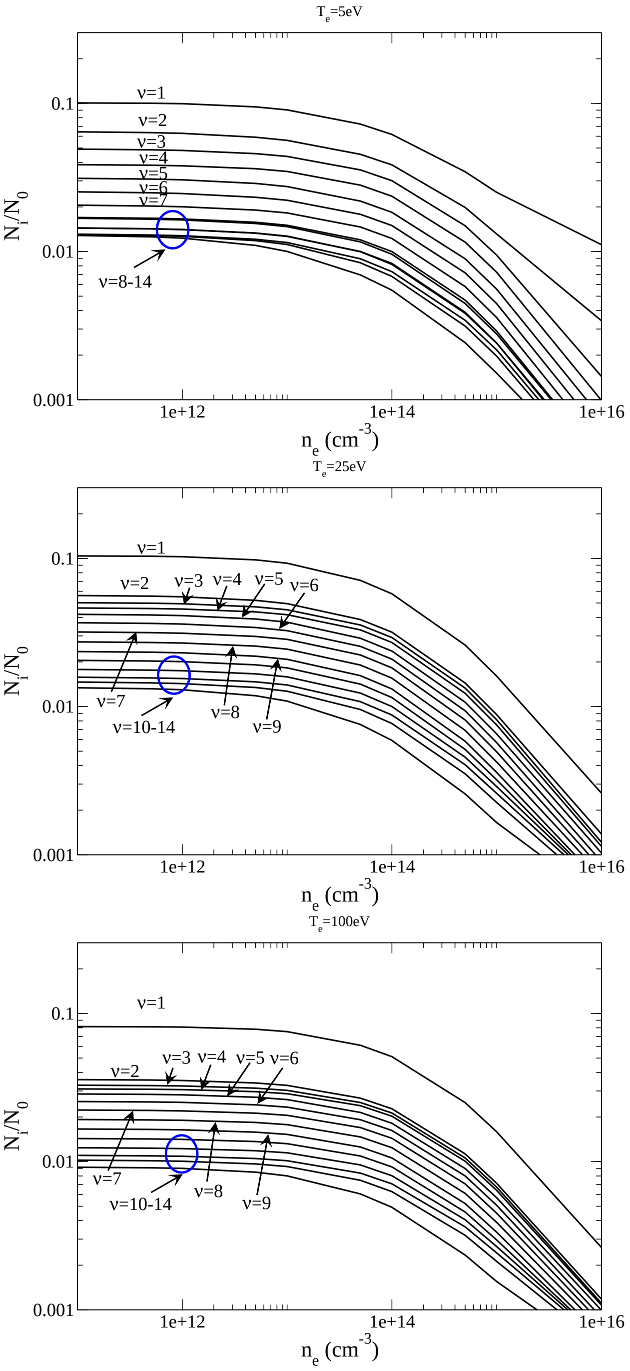


Figure 6.11: Population of the vibrational levels of ground state of H_2 molecule normalized to ground level $\nu = 0$ in fully vibrational resolution.Top: $T_e = 5$eV; middle: $T_e = 25$eV; Bottom: $T_e = 100$eV.

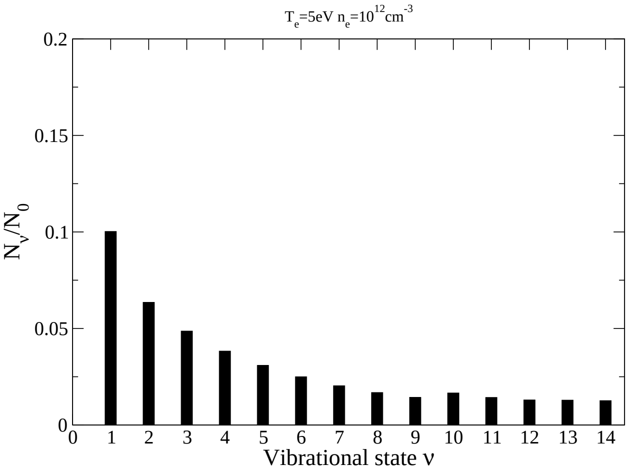


Figure 6.12: Relative population of vibrational levels from the ground state of H_2 normalized to $v = 0$ level for $T_e = 5$eV and $n_e = 10^{12}$cm^{-3} and fully vibrational resolution calculation.

5 eV. These values are from the fitting formula “form=11” given in appendix E which has been recommended in [11]. The initial vibrational level $v = 10$ has the lowest cross section driving to this higher population after the collisional radiative model. The explanation to this low cross section rest in the discontinuity in the energy difference of $v = 9$ and $v = 10$ levels with repect to the ground state of $H_2{}^-$: while $v = 9$ has the lowest of the positive energy differences producing an endotermic process, $v \geq 10$ are over this potential and the electron attachment is endothermic. That invalidates the local resonance theory [?] used to calculate the first 10 levels (till $v = 9$) and non-local theory must be used. These calculations (local and non-local) are all given in formula “form=11”, and it is not possible with the information available in the literature at the present to know if this effect is physical, or is a consequence of a lack of precision of the calculations. We do not expect that the change in population would be big in any case and a more linear result may reduce a bit $v = 10$ leveling it with the populations of their neighbour vibrational levels.

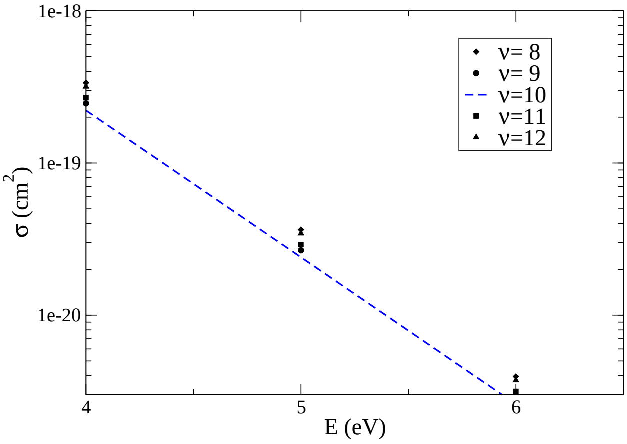


Figure 6.13: Cross sections for dissociative electron attachment for the process $e + H_2(X\,^1\Sigma_g^+; v) \rightarrow H_2^-(X\,^2\Sigma_u^+) \rightarrow H^- + H(1s)$ for $v = 8 - 12$.

6.2.3 Sawada and Fujimoto CR model

When making collisional-radiative calculations it is useful to compare with previous attemps of modelling similar systems. The most important study of molecular H_2 system made previously has been done by Sawada and Fujimoto (1995) [25] and their results are widely used by plasma modelers now. In this section, the similarities and main differences of the model presented here with Sawada and Fujimoto results will be discussed and analyzed.

Our effective coefficients defined on chapter 3 are different than those defined in reference [25] which consider dissociation paths in the ionization coefficients while we put all dissociation paths in dissociation coefficients. We do not think the that those coefficients could be comparable. We believe that the coefficient defined here have the advantage the final metastable state populations can be obtained from them only by multiplication and that the user can be sure that not a process that ends in this state has been forgoten in the way.

It is still possible to make comparisons of populations in order to compare the influence of the molecular data in both calculations. To do that we have switched off all the bound-free calculations performed by ECIP approximation but kept the rest of bound-bound new calculations. The authors of [25] use different molecular data than the new revised data presented in chapter 2 and in many cases the lack of calculated processes is approximated by hydrogen atoms transitions. For excitation between excited levels these authors use either cross sections from atomic hydrogen or similar approachs as in section 2.5.2 which are not detailed. Ionization from excited levels is taken from a different approach resulting in the cross section of excitation to one repulsive Rydberg state as they assume that the molecule is first excited to it and ionizes in its way to dissociation. For dissociative excitation these authors use the sum of the cross sections for production of all excited levels.

It is clear from the provious paragraph that due to the differences on the molecular data not a good agrement between the results of both models may be expected. In spite of this we can try to compare the populations of the levels of the ground state for low temperatures where the high levels do not play a role. In [25] it is proposed a model for vibrational excitation of vibrational levels through electron attachment and indirect collisional-radiative excitation through B and D states. The authors of reference [25] have only cross sections for electron attachment for the first $v = 0-5$ levels for 6 and 8 eV and extrapolate the rest. In our case we have maxwellian rates for $v \rightarrow v' = 0 \rightarrow 0-10$ in a variety of energies for this process. We have as well cross sections for excitation from al the vibrational levels of ground state to B and C form fitting formulas of appendix E. Otherwise than in reference [25] where electron attachment is taken as dominant for low temperatures, we have not assumed than neither of the direct or indirect processes are dominant for 5eV. The comparison can be seen on figure 6.14, population of lower vibrational levels are most steeply decreasing in the case of Sawada and Fujimoto calculation meaning that the indirect (through the higher electronic states) has no influence while in our case it is a smooth tendency to a constant population a little bellow 0.05 times the ground population reflecting the influence of indirect processes for which we have new updated cross sections.

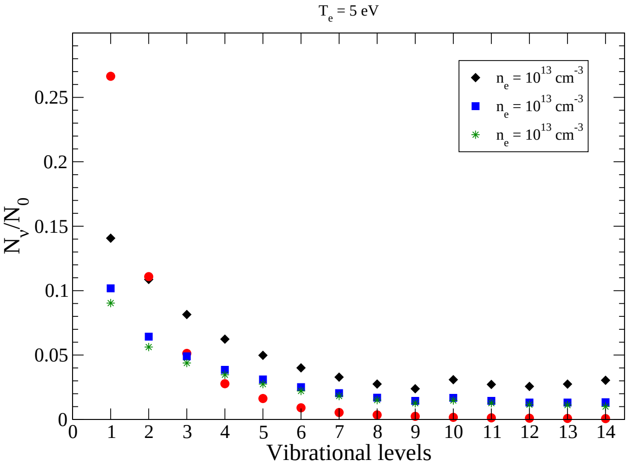


Figure 6.14: Relative population of vibrational levels for ground state. It is assumed that the molecular gorund vibrational level is the only populated as source term. (◆) calculations with only bound-free processes from $v = 0$; (■) calculations with bound free processes from metastables obtained with ECIP approximation; ✳ fully vibrational calculations including all processes; (●) Results from [25]. No information on density is given from [25].

It is needed to stress that this calculation is not complete as it has only the bound-free data available from external sources. In fact, if we include our ECIP calculation to complete bound-free processes from metastables only (blue squares in figure 6.14), the losses from dissociation and ionization processes make the ground state populations sensibly decrease. In figure 6.14 are shown the populations obtained for a complete calculation where all the bound-free process from excited states are counted. That latter results show only a little decrease from the previous ones from which we can infer that loses due to bionization and excitation from excited states are not big at that low electron temperature.

If we go to higher temperatures the absence of enough loses to depopulate the states is making the populations constant with electron density. Sawada and Fujimoto made a calculation in which they created a representative vibrational level and they approximated the ionization rates as 10 times higher of that from the ground level. We have compared their model with our full vibrational calculation for electron temperatures of 20 and 100 eV in figure 6.15. We obtain similar behaviour for the population of vibrational levels. Individual character of the levels are more important as higher densities require a more detailed collisional-radiative picture, making the fully vibrational collisional radiative model from ADAS9xx population decay faster.

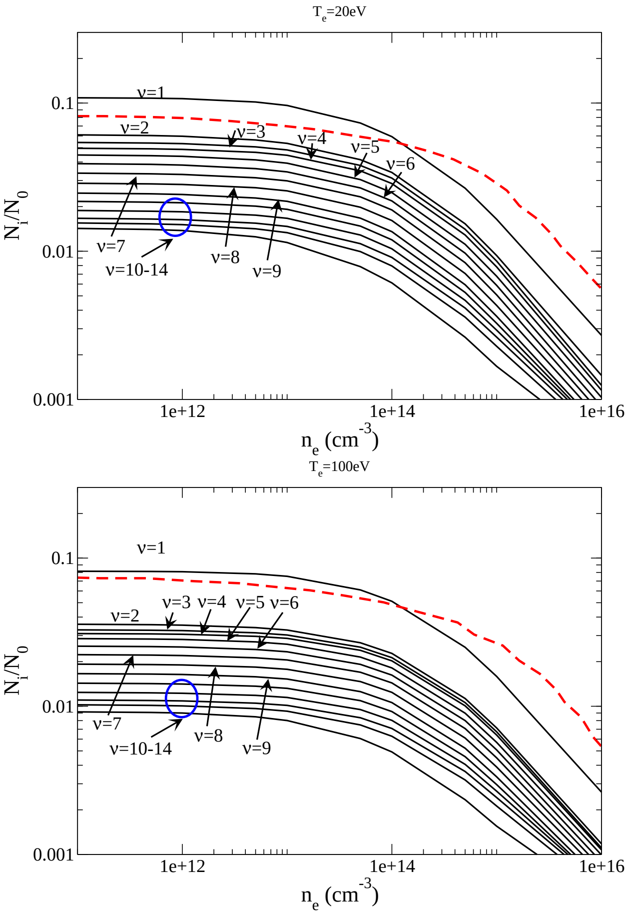


Figure 6.15: Relative population of vibrational levels from the ground state of H_2 normalized to $v = 0$ level for $T_e = 20$eV and $T_e = 100eV$ and fully vibrational resolution calculation.(– –) Representative vibrational level from [25].

6.3 Electron and ion impact

Calculations using charge exchange data have been performed. As shown in chapter 3 (see graph 3.6) charge exchange rates are about one order of magnitude lower than the corresponding electron impact ionization and it is not expected to have an important contribution in the model. However, the inverse charge exchange process from equation (3.5f):

$$A_2^+(N'', v'') + B \rightarrow A_2(N, v) + B^+ \tag{6.1}$$

has not counterpart on the electron impact data as recombineation is mainly dissociative being non-dissociative recombination negligible. It is then opened a new channel from H_2^+ to H_2 that was not possible before. In figure 6.16 the poputlation for a CX calculation are shown. The new losses due to CX make them much lower than in the only electron impact case (shown in dashed lines) but here the population also suffer sligh variation with density making the mixing at low densities. At higher densities when electron impact processes are dominant the populations recover their behaviour.

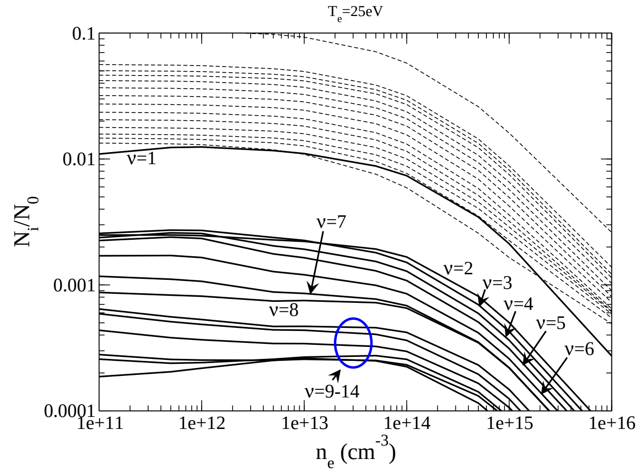


Figure 6.16: Relative population of the vibrational levels of the ground state of H_2 normalized to the $\nu = 0$ level population for $T_e = 25$eV in a fully vibrational resolution calculation using CX data. The dashed lines are shown the population of the same calculation without the CX data.

In figure 6.17 the effective excitation coefficient from all vibrational levels of ground state to every other metastable vibrational level (including ground state) are compared with the same effective coefficients for the only electron impact excitation ata an electron density of $n_e = 10^{12}\text{cm}^{-3}$. Ion impact excitation is clearly making effective excitation more diffuse as opens channels which were closed before due to the Franck-Condon factors. Studies to get a full detailed interporetation of these results are ongoing.

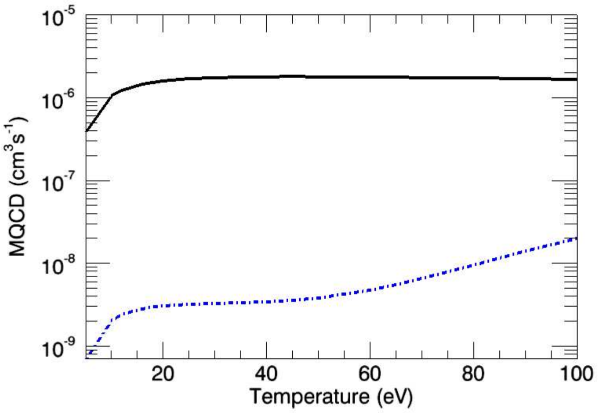


Figure 6.17: Sum on all the vibrational levels of MQCD coefficients for all the excitation departing form all the $H_2(X\,^1\Sigma_g^+, \nu)$ levels for an electron density $n_e = 10^{12}\text{cm}^{-3}$. (—) Fully vibrational resolution electron impact; (–· –) Fully vibrational resolution electron and ion impact.

In figure 6.18 are compared the effective dissociation coefficients. Effective dissociation has been enhanced due to the contribution from dissociative CX and ionization from ion impact. The increasing is small comparing with the excitation because here are the direct processes which dominate and CX rates are one order of magnitude lower than the electron impact ones. In the excitation the new channels opened make the coefficients to be sensibly different.

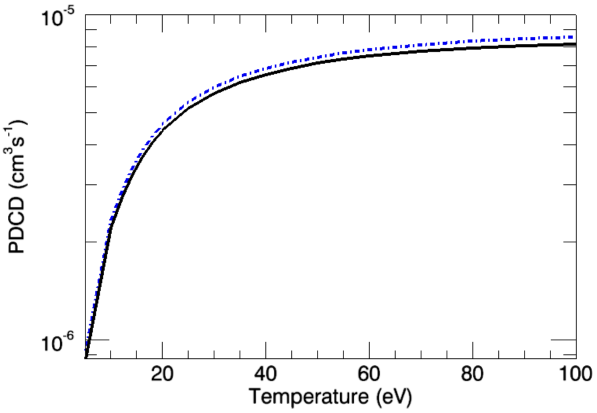


Figure 6.18: Sum of effective dissociation coefficients on all vibrational levels from H_2 ground state to produce H atoms for an electron density of $ne = 10^{12}\mathrm{cm}^{-3}$. (—) Fully vibrational resolution electron impact; (–· –) Fully vibrational resolution electron and ion impact.

Finally, in figure 6.19 are the MQCD coefficients for vibrational excitation from $v = 0$ in ground state. These are an order of magnitude smaller than the only electron impact calculations (figure 6.9) coherently with what is shown in figure 6.17. However, the behaviour in electron density[1] and temperature is the same.

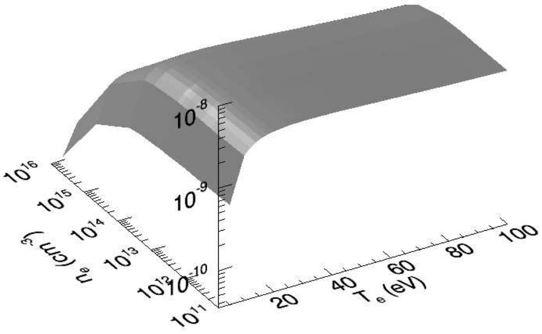


Figure 6.19: Sum on all the vibrational levels of MQCD coefficients for the $H_2(X\,^1\Sigma_g^+, v = 0) \rightarrow H_2(X\,^1\Sigma_g^+, v')$ transitions for a fully vibronic transition with electron and ion impact. The MQCD coefficients are in $\mathrm{cm}^3\mathrm{s}^{-1}$.

6.4 Conclusions

In this chapter, some results concerning H_2 system for our molecular-collisional radiative hev been presented. These results are intended to be a reference starting point for future studies on the checking and optimizing of the code.

It is striking how important is the accuracy of the data. Some key data can be fundamental at some energies to obtain the vibrational metastable populations as has been shown in figure 6.13 and the dicussion about how DA

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[1] The corresponding ion density is $n_i = Z_{eff} n_e$.

cross sections inaccuracies from different calculations can affect the final relative populations. New studies must be performed for the cases of excited states populations but preliminary results (not shown here) give similar relative populations to the observation of the molecular expectra in plasmas for the upper electronic state vibrational levels of Fulcher band (triplet d) and Lymann-alpha band (singlet B). However, accurate data will be always desiderable.

Ion impact data have been for first time included inside the collisional radiative model for H_2. The main difference with the atomic case where thermalized charge exchange and excitation is negligible at these temperatures compared with electron impact processes is on the high values of the ion impact rates that make the populations change and disorganize the equilibrium imposed by the Franck-Condon coupling in the electron impact case as it has been explained on the section 6.3. New studies of the excited states populations must be carried out in order to understand the consecuences of the new excitation coefficients.

Light from the dissociation products coming from molecules can be predicted as well with the help of this model and for example the H_α line structure could be defined. There are needed more dissociation data in order to make that accurately. Some efforts on dissociative recombination are being done by theoriticians and are expected to be used in CR calculations soon.

In order to test all these results an exhaustive and careful comparison with experimental results may be performed and real plasma situation need to be moedelled with the help of the tools presented in this reports. It may be that new plasma experiments need to be done in order to understand the behaviour of the molecules in plasmas.

These future directions will be discussed on chapter 7.

Chapter 7

Future directions for molecular models and ADAS series 9

7.1 Checking in the experimental plasma

7.2 The molecular challenge. ADAS9xx: a general molecular software

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Appendix A

MDF data formats

A.1 *mdf00*: general parameter information files and potentials curves

A.1.1 potentials

A.1.2 vibrational energies

The data sets provide the bound vibrational energies of the electronic states of the molecule.

Molecule	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	h2	high

Data lines:	*format:*
A,(B(L),L=1,6)	3X,A2,6(4X,A8)
DO J=1, MAXV1+1	
V, (C(L),L=1,6)	3X,I2,6(4X,F8.5)
repeat	

variable identification:

A	dummy variable
B	isotope formula
MAXV1	maximun quantum number of bound vibrational levels
V	vibrational number
B()	vibrational energy

```
 v       H2          D2          T2          HD          HT          DT
 0    14.28369    14.24153    14.22277    14.26445    14.25733    14.23263
 1    14.55861    14.44064    14.38703    14.50526    14.48530    14.41528
 2    14.80724    14.62860    14.54433    14.72769    14.69741    14.58896
 3    15.02398    14.80155    14.69294    14.92549    14.88791    14.75088
 4    15.22392    14.95710    14.83024    15.10416    15.05906    14.89799
 5    15.41254    15.10272    14.95584    15.27534    15.22269    15.03365
 6    15.50981*   15.24335    15.07568    15.43569    15.37749    15.16488
 7    15.55331*   15.37680    15.19198    15.50689*   15.50581*   15.29061
 8    15.58570*   15.50317    15.30364    15.54470*   15.52268*   15.41069
 9    15.59569*   15.50341*   15.41081    15.58167*   15.54151*   15.50207*
10    15.63686*   15.53442*   15.50057*   15.58505*   15.57647*   15.52440*
```

11	15.67683*	15.56487*	15.51287*	15.61775*	15.61064*	15.53042*
12	15.71565*	15.59474*	15.52599*	15.65292*	15.64399*	15.55832*
13	15.74249*	15.62153*	15.55104*	15.68720*	15.65706*	15.58574*
14	15.75336*	15.62400*	15.57572*	15.72063*	15.67655*	15.61265*
15	15.78999*	15.65266*	15.60000*	15.72189*	15.70834*	15.63158*
16	15.82557*	15.68073*	15.60969*	15.75323*	15.73939*	15.63905*
17	15.86009*	15.70822*	15.62386*	15.78503*	15.76973*	15.66496*
18	15.88156	15.73160*	15.64732*	15.81603*	15.78029*	15.69039*
19	15.89358*	15.73516*	15.67039*	15.84561	15.79934*	15.71534*
20	15.92602*	15.76156*	15.69307*	15.84624*	15.82826*	15.73174*
21	15.95741*	15.78742*	15.70102*	15.87567*	15.85647*	15.73983*
22	15.98773*	15.81275*	15.71538*	15.90432*	15.88399*	15.76387*
23	15.99964	15.83290*	15.73732*	15.93219*	15.89128	15.78747*
24	16.01692*	15.83755*	15.75889*	15.95464	15.91082*	15.81062*
25	16.04477*	15.86183*	15.78011*	15.95928*	15.93695*	15.82459*
26	16.07033*	15.88559*	15.78656*	15.98555*	15.96238*	15.83333*
27	16.08644	15.90884*	15.80097*	16.01099*	15.98710*	15.85561*
28	16.10106	15.92455	15.82149*	16.03541*	15.98822	15.87745*
29	16.12322	15.93156*	15.84165*	16.04500	16.01107*	15.89886*
30	16.14477	15.95376*	15.86146*	16.05915*	16.03420*	15.90951
31	16.16545	15.97543*	15.86602*	16.08095*	16.05608*	15.91984*
32	16.18626	15.99655*	15.88092*	16.09947	16.06611	15.94038*
33	16.20742	16.00502	15.90004*	16.11399	16.07844*	15.96048*
34	16.22866	16.01710*	15.91881*	16.13067	16.09769*	15.98014*
35	16.24982	16.03701*	15.93724*	16.14916	16.11465	15.98543
36	16.27083	16.05608*	15.93879	16.16760	16.13006	15.99935*
37	16.29167	16.06924*	15.95531*	16.18588	16.14651	16.01807*
38	16.31233	16.07579	15.97303*	16.20418	16.16380	16.03625*
39	16.33276	16.09238	15.99039*	16.22253	16.18118	16.04986
40	16.35295	16.10755	16.00389	16.24087	16.19850	16.05401*
41	16.37289	16.12093	16.00738*	16.25913	16.21581	16.07071*
42	16.39255	16.13478	16.02397*	16.27729	16.23311	16.08587
43	16.41194	16.14957	16.04012*	16.29531	16.25037	16.09687
44	16.43104	16.16457	16.05562*	16.31318	16.26754	16.10746
45	16.44983	16.17954	16.05917	16.33089	16.28460	16.12092
46	16.46832	16.19452	16.07093*	16.34841	16.30154	16.13455
47	16.48651	16.20952	16.08482	16.36575	16.31835	16.14794
48	16.50438	16.22453	16.09606	16.38288	16.33501	16.16139
49	16.52194	16.23950	16.10531	16.39981	16.35150	16.17501
50	16.53918	16.25443	16.11674	16.41653	16.36781	16.18871
51	16.55611	16.26929	16.12890	16.43303	16.38395	16.20243
52	16.57273	16.28407	16.14091	16.44930	16.39991	16.21614
53	16.58904	16.29876	16.15292	16.46534	16.41568	16.22984
54	16.60503	16.31334	16.16505	16.48115	16.43126	16.24351
55	16.62073	16.32781	16.17728	16.49673	16.44663	16.25713
56	16.63612	16.34217	16.18953	16.51207	16.46180	16.27069
57	16.65121	16.35640	16.20181	16.52718	16.47676	16.28418
58	16.66601	16.37050	16.21408	16.54205	16.49152	16.29759
59	16.68051	16.38447	16.22635	16.55669	16.50607	16.31093
60	16.69473	16.39829	16.23859	16.57110	16.52041	16.32417
61	16.70867	16.41198	16.25079	16.58526	16.53454	16.33731
62	16.72233	16.42552	16.26296	16.59920	16.54846	16.35035
63	16.73571	16.43891	16.27507	16.61291	16.56218	16.36328
64	16.74882	16.45215	16.28713	16.62639	16.57568	16.37610
65	16.76167	16.46524	16.29912	16.63964	16.58898	16.38881
66	16.77426	16.47817	16.31104	16.65268	16.60207	16.40140
67	16.78659	16.49095	16.32289	16.66549	16.61496	16.41388

68	16.79866	16.50357	16.33467	16.67808	16.62765	16.42623
69	16.81046	16.51604	16.34637	16.69045	16.64013	16.43845
70	16.82197	16.52834	16.35798	16.70261	16.65242	16.45056
71	16.83308	16.54049	16.36949	16.71456	16.66451	16.46253
72		16.55248	16.38092	16.72630	16.67640	16.47437
73		16.56432	16.39226	16.73784	16.68810	16.48609
74		16.57600	16.40351	16.74917	16.69961	16.49768
75		16.58752	16.41466	16.76031	16.71093	16.50914
76		16.59890	16.42571	16.77125	16.72207	16.52046
77		16.61011	16.43667	16.78200	16.73303	16.53165
78		16.62118	16.44752	16.79256	16.74380	16.54271
79		16.63209	16.45827	16.80292	16.75440	16.55365
80		16.64286	16.46891	16.81307	16.76482	16.56445
81		16.65347	16.47946	16.82300	16.77507	16.57512
82		16.66394	16.48990	16.83261	16.78514	16.58566
83		16.67426	16.50024		16.79505	16.59607
84		16.68443	16.51047		16.80478	16.60636
85		16.69446	16.52060		16.81433	16.61651
86		16.70435	16.53062		16.82367	16.62654
87		16.71410	16.54053		16.83272	16.63645
88		16.72372	16.55035			16.64623
89		16.73319	16.56005			16.65589
90		16.74253	16.56965			16.66542
91		16.75174	16.57915			16.67483
92		16.76081	16.58855			16.68412
93		16.76976	16.59784			16.69329
94		16.77857	16.60703			16.70234
95		16.78726	16.61612			16.71128
96		16.79581	16.62511			16.72010
97		16.80424	16.63399			16.72880
98		16.81253	16.64278			16.73740
99		16.82068	16.65147			16.74588
100		16.82863	16.66005			16.75424
101		16.83629	16.66854			16.76250
102			16.67693			16.77065
103			16.68523			16.77869
104			16.69343			16.78663
105			16.70153			16.79446
106			16.70954			16.80218
107			16.71746			16.80979
108			16.72529			16.81728
109			16.73302			16.82464
110			16.74067			16.83180
111			16.74822			16.83864
112			16.75569			
113			16.76307			
114			16.77036			
115			16.77757			
116			16.78469			
117			16.79172			
118			16.79867			
119			16.80553			
120			16.81230			
121			16.81897			
122			16.82554			
123			16.83194			
124			16.83806			

A.1.3 Franck-Condon Factors

The data sets provide the Franck-Condon Factors for transition between the first excited states.

Molecule	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	h2	high

Data lines:	*format:*
MAXV1,MAXV2	I2,1X,I2
DO J=1, MAXV2+1	
(FC(K,J),K=1,MAXV1+1)	2X,100(G11.4,1X)
repeat	

variable identification:

MAXV1,MAXV2	maximun quantum number of bound vibrational levels of lower and upper states
FC(,)	Franck-Condon Factors

```
14 36
  4.4078e-003 3.0756e-002 9.7816e-002 1.8819e-001 2.4296e-001 2.1920e-001 1.3870e-001...
  1.5463e-002 7.5353e-002 1.4239e-001 1.1605e-001 2.0045e-002 2.0896e-002 1.4928e-001...
  3.1530e-002 1.0445e-001 1.0195e-001 1.2613e-002 3.1826e-002 1.1140e-001 4.5886e-002...
  4.8910e-002 1.0595e-001 3.9175e-002 9.1123e-003 8.2701e-002 3.0488e-002 2.0441e-002...
  6.4044e-002 8.5702e-002 3.9075e-003 4.7372e-002 5.0176e-002 3.5875e-003 7.5337e-002...
  7.4739e-002 5.6661e-002 3.0991e-003 6.2243e-002 6.9083e-003 4.2821e-002 3.3599e-002...
  8.0309e-002 2.9885e-002 2.0148e-002 4.5896e-002 3.2545e-003 5.3454e-002 8.6061e-005...
  8.1145e-002 1.1223e-002 3.7366e-002 2.0051e-002 2.3962e-002 2.7545e-002 1.7892e-002...
  7.8247e-002 1.8528e-003 4.5581e-002 3.2455e-003 3.9526e-002 3.8091e-003 3.9348e-002...
  7.2782e-002 1.5481e-004 4.3784e-002 4.9572e-004 3.8360e-002 1.6500e-003 3.5151e-002...
  6.5827e-002 3.4811e-003 3.5289e-002 7.4719e-003 2.5653e-002 1.3795e-002 1.6197e-002...
  5.8247e-002 9.2858e-003 2.4302e-002 1.7381e-002 1.1380e-002 2.5749e-002 2.2180e-003...
  5.0670e-002 1.5636e-002 1.4081e-002 2.5163e-002 2.2761e-003 2.9389e-002 9.1328e-004...
  4.3502e-002 2.1310e-002 6.4169e-003 2.8614e-002 6.5644e-005 2.4717e-002 8.2918e-003...
  3.6971e-002 2.5690e-002 1.8407e-003 2.7786e-002 3.0899e-003 1.5935e-002 1.6862e-002...
  3.1181e-002 2.8589e-002 7.6490e-005 2.3914e-002 8.5265e-003 7.4566e-003 2.1519e-002...
  2.6149e-002 3.0083e-002 4.5990e-004 1.8530e-002 1.3901e-002 1.9266e-003 2.1001e-002...
  2.1840e-002 3.0388e-002 2.2366e-003 1.2942e-002 1.7700e-002 1.1501e-005 1.6706e-002...
  1.8192e-002 2.9763e-002 4.7321e-003 8.0320e-003 1.9373e-002 1.0427e-003 1.0929e-002...
  1.5127e-002 2.8467e-002 7.4238e-003 4.2586e-003 1.9056e-002 3.8004e-003 5.6378e-003...
  1.2568e-002 2.6727e-002 9.9534e-003 1.7448e-003 1.7245e-002 7.0867e-003 1.9613e-003...
  1.0441e-002 2.4729e-002 1.2107e-002 3.9554e-004 1.4543e-002 1.0017e-002 2.1408e-004...
  8.6773e-003 2.2614e-002 1.3781e-002 2.5060e-009 1.1496e-002 1.2091e-002 1.4983e-004...
  7.2173e-003 2.0486e-002 1.4950e-002 3.0693e-004 8.5226e-003 1.3139e-002 1.2515e-003...
  6.0095e-003 1.8416e-002 1.5640e-002 1.0725e-003 5.8951e-003 1.3223e-002 2.9541e-003...
  5.0097e-003 1.6450e-002 1.5902e-002 2.0860e-003 3.7560e-003 1.2532e-002 4.7775e-003...
  4.1808e-003 1.4612e-002 1.5798e-002 3.1789e-003 2.1478e-003 1.1301e-002 6.3807e-003...
  3.4916e-003 1.2913e-002 1.5392e-002 4.2250e-003 1.0448e-003 9.7611e-003 7.5655e-003...
  2.9161e-003 1.1350e-002 1.4739e-002 5.1340e-003 3.7957e-004 8.1084e-003 8.2524e-003...
  2.4322e-003 9.9141e-003 1.3881e-002 5.8424e-003 6.4219e-005 6.4907e-003 8.4456e-003...
  2.0207e-003 8.5864e-003 1.2844e-002 6.3037e-003 3.7268e-006 5.0084e-003 8.1985e-003...
  1.6644e-003 7.3395e-003 1.1633e-002 6.4757e-003 1.0390e-004 3.7188e-003 7.5841e-003...
  1.3467e-003 6.1346e-003 1.0220e-002 6.3078e-003 2.7420e-004 2.6447e-003 6.6706e-003...
  1.0488e-003 4.9113e-003 8.5310e-003 5.7205e-003 4.2677e-004 1.7802e-003 5.4983e-003...
  7.4690e-004 3.5748e-003 6.4163e-003 4.5827e-003 4.7442e-004 1.0948e-003 4.0553e-003...
  4.1040e-004 1.9935e-003 3.6574e-003 2.7225e-003 3.3999e-004 5.3430e-004 2.2696e-003...
```

```
  1.1429e-004 5.5874e-004 1.0348e-003 7.8397e-004 1.0547e-004 1.4055e-004 6.3624e-004...
```

A.1.4 A-values

The data sets provide the A-values for transition between the first excited states.

Molecule	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	h2	high

Data lines:	*format:*
MAXV1,MAXV2	I2,1X,I2
DO J=1, MAXV2+1	
(AVAL(K,J),K=1,MAXV1+1)	2X,100(G11.4,1X)
repeat	

variable identification:

MAXV1,MAXV2	maximun quantum number of bound vibrational levels of lower and upper states
FC(,)	Franck-Condon Factors

```
14 36
  8.9713e+006 6.1697e+007 1.9152e+008 3.5577e+008 4.3815e+008 3.7204e+008 2.1812e+008...
  3.1551e+007 1.5195e+008 2.8153e+008 2.2314e+008 3.7505e+007 3.5420e+007 2.4004e+008...
  6.4382e+007 2.1128e+008 2.0296e+008 2.4664e+007 5.9051e+007 1.9872e+008 7.8613e+007...
  9.9828e+007 2.1459e+008 7.8245e+007 1.7809e+007 1.5713e+008 5.6383e+007 3.4164e+007...
  1.3055e+008 1.7351e+008 7.7304e+006 9.3701e+007 9.6916e+007 6.3714e+006 1.3298e+008...
  1.5205e+008 1.1443e+008 6.4138e+006 1.2397e+008 1.3572e+007 8.0205e+007 6.1499e+007...
  1.6298e+008 6.0012e+007 4.1195e+007 9.1774e+007 6.3464e+006 1.0210e+008 2.1478e+005...
  1.6421e+008 2.2246e+007 7.6226e+007 4.0089e+007 4.7409e+007 5.3420e+007 3.2907e+007...
  1.5784e+008 3.5056e+006 9.2793e+007 6.3930e+006 7.8737e+007 7.5134e+006 7.4244e+007...
  1.4629e+008 3.9954e+005 8.8874e+007 1.0828e+006 7.6722e+007 3.2109e+006 6.7448e+007...
  1.3180e+008 7.4386e+006 7.1317e+007 1.5469e+007 5.1371e+007 2.7282e+007 3.1520e+007...
  1.1615e+008 1.9378e+007 4.8798e+007 3.5718e+007 2.2713e+007 5.1270e+007 4.3925e+006...
  1.0062e+008 3.2267e+007 2.7996e+007 5.1504e+007 4.4537e+006 5.8762e+007 1.7704e+006...
  8.6006e+007 4.3644e+007 1.2536e+007 5.8357e+007 1.6507e+005 4.9523e+007 1.6379e+007...
  7.2773e+007 5.2293e+007 3.4461e+006 5.6442e+007 6.4918e+006 3.1911e+007 3.3546e+007...
  6.1106e+007 5.7881e+007 9.8893e+004 4.8343e+007 1.7670e+007 1.4854e+007 4.3001e+007...
  5.1020e+007 6.0605e+007 1.0896e+006 3.7231e+007 2.8637e+007 3.7604e+006 4.2074e+007...
  4.2430e+007 6.0931e+007 4.8503e+006 2.5794e+007 3.6309e+007 1.2259e+004 3.3489e+007...
  3.5191e+007 5.9409e+007 9.9950e+006 1.5827e+007 3.9586e+007 2.2503e+006 2.1870e+007...
  2.9139e+007 5.6573e+007 1.5463e+007 8.2425e+006 3.8775e+007 7.9745e+006 1.1213e+007...
  2.4110e+007 5.2888e+007 2.0536e+007 3.2635e+006 3.4927e+007 1.4727e+007 3.8344e+006...
  1.9947e+007 4.8728e+007 2.4796e+007 6.6883e+005 2.9295e+007 2.0699e+007 3.8247e+005...
  1.6511e+007 4.4378e+007 2.8052e+007 5.7139e+003 2.3010e+007 2.4876e+007 3.5454e+005...
  1.3679e+007 4.0040e+007 3.0267e+007 7.4646e+005 1.6926e+007 2.6926e+007 2.6887e+006...
  1.1345e+007 3.5853e+007 3.1507e+007 2.3859e+006 1.1592e+007 2.6994e+007 6.2246e+006...
  9.4216e+006 3.1903e+007 3.1888e+007 4.4927e+006 7.2884e+006 2.5480e+007 9.9774e+006...
  7.8334e+006 2.8234e+007 3.1545e+007 6.7263e+006 4.0878e+006 2.2880e+007 1.3251e+007...
  6.5186e+006 2.4861e+007 3.0611e+007 8.8353e+006 1.9254e+006 1.9673e+007 1.5645e+007...
  5.4252e+006 2.1778e+007 2.9200e+007 1.0643e+007 6.5382e+005 1.6260e+007 1.7004e+007...
  4.5098e+006 1.8960e+007 2.7403e+007 1.2029e+007 8.5928e+004 1.2945e+007 1.7345e+007...
  3.7351e+006 1.6370e+007 2.5272e+007 1.2905e+007 2.3139e+004 9.9267e+006 1.6785e+007...
  3.0675e+006 1.3953e+007 2.2819e+007 1.3194e+007 2.7072e+005 7.3200e+006 1.5481e+007...
  2.4754e+006 1.1631e+007 1.9992e+007 1.2800e+007 6.4302e+005 5.1661e+006 1.3577e+007...
  1.9234e+006 9.2906e+006 1.6647e+007 1.1570e+007 9.6079e+005 3.4486e+006 1.1161e+007...
  1.3671e+006 6.7497e+006 1.2496e+007 9.2440e+006 1.0462e+006 2.1034e+006 8.2129e+006...
  7.5021e+005 3.7590e+006 7.1131e+006 5.4821e+006 7.4178e+005 1.0196e+006 4.5888e+006...
```

```
  2.0881e+005 1.0530e+006 2.0114e+006 1.5774e+006 2.2917e+005 2.6733e+005 1.2854e+006...
```

A.2 mdf02

Fundamental data collections.

Molecule	*projectile*	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	H,H^+,e	h2	high

```
Data lines:                                                        format:
(RPARAM(IND_R,L),L=1,15)                  A2,1X,A2,2X,A2,7X,A2,9X,A2,2X,A2,
                                                  2X,A2,4X,A6,6X,A7,2X,A7,
                                              2X,A8,2X,A6,2X,A8,2X,A13,2X,A2
DO L=1,INT(NUMER(IND_R)/7)
     (TPARAM(IND_R,7*(L-1)+I), I=1,7)                      60X,7(2X,F10.4)
repeat
DO L=1,INT(NUMER(IND_R)/7)
     (SPARAM(IND_R,7*(L-1)+I), I=1,7)                      60X,7(2X,F10.4)
repeat
IF(PAR(IND_R).GT.0) THEN
     DO L=1,INT(PAR(IND_R)/6)
(PARVAL(IND_R,6*(L-1)+I), I=1,6)                           62X,6(1X,F11.4)
```

variable identification:

RPARAM	paramter defining each of the processes
IND_R	index of processes
NUMER	number of values.
PAR	number of formula parameters
TPARAM	Tabulated temperatures of energies
SPARAM	Tabulated cross sections or collision strengths
PARVAL	Tabulated formula parameter values

```
H_2        / electron impact                                                   mdf
/
species
/-------
/ ind_s   identity   e-config    e-coupling   ch_ion   bwno_i       ch_dis     bwno_d
/ -----   --------   --------    ----------   ------   ------       ------     ------
   1       H_2        dia-ua      dia-term     1->2    124418.       1->4+4    36117.00
   1       H_2        dia-ua      dia-term     1->2    124418.       1->5+6    36117.00
```

```
   2       H_2^+      dia-ua      dia-term     2->5+5    5386.      2->4+5    21380.21
   3       H_2^-      dia-ua      dia-term     3->1         0.      3->4+6    00000.00
   4       H          atm         atm-term     4->5    109691.      N         00000.00
   5       H^+        atm         atm-term     N            0.      N         00000.00
   6       H^-        atm         atm-term     6->4       427.      N         00000.00
/
process
/-------
/
/ind_p                               path                                      description
/-----      ---------------------------------------------------------     ---------------------
   1        e+H_2(^+q)(N,v)  -> e + H_2(+q)*(N',v')                        excitation
  11        e+H_2(N,v) -> e + H_2*(N',v')                                  vib resolved exc.
  12        e+H_2(N) -> e + H_2*(N)                                        vib unresolved exc.                       /
  13        e+H_2(N,v) -> e + H_2*(N,v**) -> e + H(1s) + H(nl)             diss. exc.                                /
  14        e+H_2(v) -> H_2^-(X(2)S(+)(u),B(2)S(+)(u))-> e + H_2(v')       vib exc via e attach
  15                                                                       others
   2        e+H_2+ -> H_2                                                  recombination                             /
  21        H+H_2+(N,v) -> H+ + H_2(N',v')                                 vib resolved inverse CX
  22        H+H_2+(N)   -> H+ + H_2(N)                                     vib unresolved inverse CX
  23        e+H_2+(N,v) -> H_2(N',v')                                      vib resolved recombination
  24        e+H_2+(N) -> H_2(N')                                           vib unresolved recombination
  25        e+H_2+ -> H_2** -> H + H                                       dissociative recombination
   3        e+H_2(N,v) -> e + e + H_2+(2)                                  ionization                                /
  31        e+H_2(N,v) -> e + e + H_2+(N',v')                              vib resolved ion.                         /
  32        e+H_2(N)   -> e + e + H_2+(N')                                 vib unresolved ion.                       /
  33        e+H_2(N,v) -> e + e + H_2+(N',v'**) ->  e + H + H+             dissociative ion.                         /
  34        H_2(N**,v**) -> H_2+ (N',v') + e                               autoionizacion
  35                                                                       others
   4        e+H_2(N,v)  ->(e + H_2(d)* ->)e + H(1s) + H(nl)                dissociation ( or exc. to dissociative)   /
  41        e+H_2(N,v)  -> e + H_2(d)* -> e + H(1s) + H(nl)                vib resolved diss.                        /
  42        e+H_2(N)  -> e + H_2(d)* -> e + H(1s) + H(nl)                  vib unresolved diss.                      /
  43        e+H_2(N;v) -> H_2-(S(+)(u/g) -> H- + H(1s)                     dis. el. attachment and H- production     /
  44        e+H_2(X;v) -> H_2-(X(2)S(+)(u/g) -> e + H(1s) + H(1s)          dis. el. attachment                       /
  45        e+H_2(X;v) -> H_2-(B(2)S(+)(u/g) -> e + H(1s) + H(1s)          dis. el. attachment                       /
  46                                                                       others
   5        H^+ + H_2 -> H(1s) + H_2^+                                     direct CX
  51        H^+ + H_2(N,v) -> H(1s) + H_2^+(N',v')                         vib resolved direct CX
  52        H^+ + H_2(N) -> H(1s) + H_2^+(N')                              vib unresolved direct CX
```

```
  53       H^+ + H_2(N,v) -> H(1s) + H + H^+                          dissiociative CX
  54       H^+ + H_2(v) -> H(1s) + H^+ + H^+ + e                      transfer ion.
  55                                                                  others
   6       H2^+ H                                                     heavy particle impact
  61       H2(N,v) + H+ -> H2(N',v') + H+                             excitation by ion impact
  62       H2^+(N,v) + H -> H2^+(N',v') + H                           excitation by neutral impact
  63       H2(N,v) + H+ -> H + H                                      dissociation by ion impact
  64       H2+(N,v) + H -> H+ + H                                     dissociation by neutral impact
  65       H+ + H_2(N,v) -> H+ + H_2+(N',v')                          ionization by ion impact              /
  66       H + H_2+(N,v) -> H + (H_2++)                               ionization by neutral impact           /
  67       H+ +H_2(N,v) -> H+ + H_2+(N',v'**) ->  H + H + H+          dissociative ion. by ion impact
  68       H+H_2(N,v) -> H + H_2+(N',v'**) ->  H + H + H+             dissociative ion. by neutral impact
  69                                                                  others
/
/
states
/------
/ ind_s   ind_e    e-con-ua  e-con-sa  coupled state   (wt.-1)/2     wno     wno_d             coments
/ -----   ------   --------  --------   -----------    ---------     ---      ---      -------------------------------
    1       1      1ssg1ssg    1s1s     (1)S(+)(g)        0.0         0.0   38292.98   ground state X
    1       2      1ssg2psu    1s2p     (1)S(+)(u)        0.0    91691.69  120595.97   B
    1       3      1ssg2ppu    1s2p     (1)P( )(u)        0.5   100101.80  120595.97   C
    1       4      1ssg2ssg    1s2s     (1)S(+)(g)        0.0   100146.88  120595.97   EF
    1       5      1ssg3psu    1s2s     (1)S(+)(u)        0.0   111640.12  120595.97   B'
    1       6      1ssg3dsg    1s2p     (1)S(+)(g)        0.0   112223.18  120595.97   GK
    1       7      1ssg3dpg    1s2p     (1)P( )(g)        0.5   113017.64  122442.16   I (potential barrier)
    1       8      1ssg3ddg    1s3d     (1)D( )(g)        0.5   113443.18  135837.26   J
    1       9      1ssg3ppu    1s3d     (1)P( )(u)        0.5   113934.45  135837.26   D
    1      10      1ssg3ssg    1s3d     (1)S(+)(g)        0.0   114020.67  135837.26   HH
    1      11      1ssg4psu    1s3s     (1)S(+)(u)        0.0   117958.11  135837.26   B''B
    1      12      1ssg4dsg    1s3d     (1)S(+)(g)        0.0   118422.44  135837.26   P
    1      13      1ssg4dpg    1s3p     (1)P( )(g)        0.5   118514.31  135837.26   R
    1      14      1ssg4ddg    1s4f     (1)D( )(g)        0.5   118703.93  141171.72   S
    1      15      1ssg4ppu    1s4p     (1)P( )(u)        0.5   118910.00  141171.72   D'
    1      16      1ssg4ssg    1s3p     (1)S(+)(g)        0.0   118954.12  135837.26   O
    1      17      1ssg2psu    1s1s     (3)S(+)(u)        1.0    66178.12   66178.12   dissiociative state b (vertical DE)
    1      18      1ssg2ppu    1s2p     (3)P( )(u)        2.5    95888.20  120595.97   metastable state c
    1      19      1ssg2ssg    1s2s     (3)S(+)(g)        1.0    95977.76  120595.97   a
    1      20      1ssg3psu    1s2s     (3)S(+)(u)        1.0   107766.65  120595.97   e
```

```
   1      21      1ssg3ppu    1s3p      (3)P( )(u)          2.5     112750.43  135837.26   d
   1      22      1ssg3ssg    1s2p      (3)S(+)(g)          1.0     112787.69  123870.60   h (potential barrier)
   1      23      1ssg3dsg    1s3s      (3)S(+)(g)          1.0     112937.71  135837.26   g
   1      24      1ssg3dpg    1s2p      (3)P( )(g)          2.5     113006.18  123897.40   i (potential barrier)
   1      26      1ssg4psu    1s2p      (3)S(+)(u)          1.0     116631.81  131018.27   f (potential barrier)
   1      27      1ssg4ppu    1s3d      (3)P( )(u)          2.5     118418.65  135837.26   k
   1      29      1ssg4dpg    1s3d      (3)P( )(g)          2.5     118509.87  135837.26   r
   2       1      1ssg                  (2)S(+)(g)          0.5     124418.00  148030.30
   2       2      2psu        1s        (2)S(+)(u)          0.5     274666.12  274666.12   dissiociative state 2psu (vertical...
   2       3      2ppu        2s        (2)P( )(u)          0.5     318289.02  318289.02   dissiociative state 2ppu (vertical...
   4       1                  1s        (2)S                0.5     148030.30  148030.30
   5       1                                                0.0                            ion H^+
/  3       1                            (2)S(+)(u)          0.5
/  3       2                            (2)S(+)(g)          0.5                            dissiociative state B
/
values
/ch_in           ind_p       ch_out      ch_dis                     parameters & values
/-----          ------       ------      ------                     -------------------
s   e   v                    s   e   v
1   1   0       14           1   1   0               categ=3  tcode=1  form=201  par=6   numer=28  DE=0.0000e+00  EX
                                                         te=   1.000       1.200       1.400       1.600       1.800       2.0...
                                                               2.400       2.600       2.800       3.000       4.000       5.0...
                                                               7.000       8.000       9.000       10.00       15.00       20....
                                                               40.00       50.00       60.00       70.00       80.00       90....
                                                        omg=  0.6124E-07  0.5456E-07  0.4877E-07  0.4380E-07  0.3953E-07  0.35...
                                                              0.2989E-07  0.2746E-07  0.2531E-07  0.2341E-07  0.1650E-07  0.12...
                                                              0.7480E-08  0.6063E-08  0.5004E-08  0.4191E-08  0.2019E-08  0.11...
                                                              0.2487E-09  0.1444E-09  0.9086E-10  0.6057E-10  0.4218E-10  0.30...
```

A.3 mdf33 and mdf34

Maxwellian rates collection.

Molecule	*projectile*	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	e	mdf33/h2	high
H_2	H_2,H_2^+	H,H^+	mdf34/h2	high

```
Data lines:                                                                    format:
read temperatures
NMTE, NMTM                                                               '/',1X,2(I2,1X)
(TEI(C2),C2=1, NMTE)                                                       8(1X,G12.4)
IF(NMTM.GT.1) THEN
    (TM(C2),C2=1, NMTM)                                                    8(1X,G12.4)
ENDIF
INDR                                                                                I4
DO C4=1, INDR
    C1, CATEGF(C1), TCODE(C1),
    SL(C1),V1(C1),SU(C1),V2(C1),
     PRCS(C1), DE(C1), DCH(C1)                       '/',I4,3(2X,I2),3(1X,I2),2X,
                                                                 I2,3X,F10.4,2X,A6
    DO C3=1,NMTM              (TRAT(C2,C3,C1), C2=1, NMTE)                 8(1X,G12.4)
    repeat
repeat
```

variable identification:

NMTE,NMTM	Electron and molecule number of temperature values
TEI	Electron/ion temperature array
TM	Molecule tempertature array
INDR	Number of processes
CATEGF	1=upsilons values; 2=rates (cm^3/s); 3=others.
TCODE	1=dipole trensition; 2= non-dipole, non-spin change; 3=spin change; 4=others
SL,V1	Lower specie and lower vibrational index
SU,V2	Upper specie and lower vibrational index
PRCS	Process index
DE	trasition energy
DCH	dissociation channel
TRAT	Transition rates array.

```
H_2         2.0000
H_2                                  1->2      124418.00        1->4+4     36117.00
H_2                                  1->2      124418.00        1->5+6     36117.00
H_2^+                                2->5+5      5386.00        2->4+5     21380.21
H_2^-                                3->1           0.00        3->4+6         0.00
H                                    4->5      109691.00        N              0.00
H^+                                  N              0.00        N              0.00
H^-                                  6->4         427.00        N              0.00
-1
   1    1   1     (1)S(+)(g)    1s1s    0.0          0.00   38292.98
   2    1   2     (1)S(+)(u)    1s2p    0.0      91691.69  120595.97
   3    1   3     (1)P( )(u)    1s2p    0.5     100101.80  120595.97
   4    1   4     (1)S(+)(g)    1s2s    0.0     100146.88  120595.97
   5    1   5     (1)S(+)(u)    1s2s    0.0     111640.12  120595.97
   6    1   6     (1)S(+)(g)    1s2p    0.0     112223.18  120595.97
   7    1   7     (1)P( )(g)    1s2p    0.5     113017.64  122442.16
```

```
   8    1   8     (1)D( )(g)    1s3d    0.5    113443.18  135837.26
   9    1   9     (1)P( )(u)    1s3d    0.5    113934.45  135837.26
  10    1  10     (1)S(+)(g)    1s3d    0.0    114020.67  135837.26
  11    1  11     (1)S(+)(u)    1s3s    0.0    117958.11  135837.26
  12    1  12     (1)S(+)(g)    1s3d    0.0    118422.44  135837.26
  13    1  13     (1)P( )(g)    1s3p    0.5    118514.31  135837.26
  14    1  14     (1)D( )(g)    1s4f    0.5    118703.93  141171.72
  15    1  15     (1)P( )(u)    1s4p    0.5    118910.00  141171.72
  16    1  16     (1)S(+)(g)    1s3p    0.0    118954.12  135837.26
  17    1  17     (3)S(+)(u)    1s1s    1.0     66178.12   66178.12
  18    1  18     (3)P( )(u)    1s2p    2.5     95888.20  120595.97
  19    1  19     (3)S(+)(g)    1s2s    1.0     95977.76  120595.97
  20    1  20     (3)S(+)(u)    1s2s    1.0    107766.65  120595.97
  21    1  21     (3)P( )(u)    1s3p    2.5    112750.43  135837.26
  22    1  22     (3)S(+)(g)    1s2p    1.0    112787.69  123870.60
  23    1  23     (3)S(+)(g)    1s3s    1.0    112937.71  135837.26
  24    1  24     (3)P( )(g)    1s2p    2.5    113006.18  123897.40
  25    1  26     (3)S(+)(u)    1s2p    1.0    116631.81  131018.27
  26    1  27     (3)P( )(u)    1s3d    2.5    118418.65  135837.26
  27    1  29     (3)P( )(g)    1s3d    2.5    118509.87  135837.26
  28    2   1     (2)S(+)(g)            0.5    124418.00  148030.30
  29    2   2     (2)S(+)(u)    1s      0.5    274666.12  274666.12
  30    2   3     (2)P( )(u)    2s      0.5    318289.02  318289.02
  31    4   1     (2)S          1s      0.5    148030.30  148030.30
  32    5   1                           0.0         0.00       0.00
-1
/ 20  1
    5.000        10.00        12.00        14.00        16.00        18.00        20.0...
    30.00        35.00        40.00        45.00        50.00        60.00        70.0...
    90.00        100.0        150.0        200.0
-1
 262
/   1   2   1   1  0  1  0  14       0.0000
   0.1224E-07   0.4191E-08   0.3046E-08   0.2298E-08   0.1784E-08   0.1417E-08   0.114...
   0.4829E-09   0.3402E-09   0.2487E-09   0.1873E-09   0.1444E-09   0.9086E-10   0.605...
   0.3041E-10   0.2255E-10   0.6721E-11   0.2686E-11
-1
```

A.4 mdf04

Molecule	*projectile*	*Members*	*lybrary*	*Quality*
H_2	H_2,H_2^+	e	mdf04/h2	high
H_2	H_2,H_2^+	H,H^+	mdf14/h2	high

```
Data lines:                                                          format:
read temperatures
NMTE, NMTM                                                           '/',1X,2(I2,1X)
(TEI(C2),C2=1, NMTE)                                                 8(1X,G12.4)
IF(NMTM.GT.1) THEN
    (TM(C2),C2=1, NMTM)                                              8(1X,G12.4)
ENDIF
INDR                                                                 I4
DO C4=1, INDR
    C1, CATEGF(C1), TCODE(C1),
    SL(C1),V1(C1),SU(C1),V2(C1),
     PRCS(C1),DCH(C1)                     1X,I6,3(2X,I2),3(1X,I2),2X,I2,5X,A6
    DO C3=1,NMTM          (TRAT(C2,C3,C1), C2=1, NMTE)               8(1X,G12.4)
    repeat
repeat
```

variable identification:

NMTE,NMTM	Electron and molecule number of temperature values
TEI	Electron/ion temperature array
TM	Molecule tempertature array
INDR	Number of processes
CATEGF	1=upsilons values; 2=rates (cm^3/s); 3=others.
TCODE	1=dipole trensition; 2= non-dipole, non-spin change; 3=spin change; 4=others
SL,V1	Lower specie and lower vibrational index
SU,V2	Upper specie and lower vibrational index
PRCS	Process index
DCH	dissociation channel
TRAT	Transition rates array.

```
H_2         2.0000
H_2                               1->2     124418.00          1->4+4     36117.00
H_2                               1->2     124418.00          1->5+6     36117.00
H_2^+                             2->5+5     5386.00          2->4+5     21380.21
H_2^-                             3->1          0.00          3->4+6         0.00
H                                 4->5     109691.00          N              0.00
H^+                               N             0.00          N              0.00
H^-                               6->4        427.00          N              0.00
-1
   1    1   1    (1)S(+)(g)    1s1s    0.0         0.00   38292.98
   2    1   2    (1)S(+)(u)    1s2p    0.0     91691.69  120595.97
   3    1   3    (1)P( )(u)    1s2p    0.5    100101.80  120595.97
   4    1   4    (1)S(+)(g)    1s2s    0.0    100146.88  120595.97
   5    1   5    (1)S(+)(u)    1s2s    0.0    111640.12  120595.97
   6    1   6    (1)S(+)(g)    1s2p    0.0    112223.18  120595.97
   7    1   7    (1)P( )(g)    1s2p    0.5    113017.64  122442.16
   8    1   8    (1)D( )(g)    1s3d    0.5    113443.18  135837.26
   9    1   9    (1)P( )(u)    1s3d    0.5    113934.45  135837.26
  10    1  10    (1)S(+)(g)    1s3d    0.0    114020.67  135837.26
  11    1  11    (1)S(+)(u)    1s3s    0.0    117958.11  135837.26
```

```
  12    1  12     (1)S(+)(g)    1s3d    0.0    118422.44  135837.26
  13    1  13     (1)P( )(g)    1s3p    0.5    118514.31  135837.26
  14    1  14     (1)D( )(g)    1s4f    0.5    118703.93  141171.72
  15    1  15     (1)P( )(u)    1s4p    0.5    118910.00  141171.72
  16    1  16     (1)S(+)(g)    1s3p    0.0    118954.12  135837.26
  17    1  17     (3)S(+)(u)    1s1s    1.0     66178.12   66178.12
  18    1  18     (3)P( )(u)    1s2p    2.5     95888.20  120595.97
  19    1  19     (3)S(+)(g)    1s2s    1.0     95977.76  120595.97
  20    1  20     (3)S(+)(u)    1s2s    1.0    107766.65  120595.97
  21    1  21     (3)P( )(u)    1s3p    2.5    112750.43  135837.26
  22    1  22     (3)S(+)(g)    1s2p    1.0    112787.69  123870.60
  23    1  23     (3)S(+)(g)    1s3s    1.0    112937.71  135837.26
  24    1  24     (3)P( )(g)    1s2p    2.5    113006.18  123897.40
  25    1  26     (3)S(+)(u)    1s2p    1.0    116631.81  131018.27
  26    1  27     (3)P( )(u)    1s3d    2.5    118418.65  135837.26
  27    1  29     (3)P( )(g)    1s3d    2.5    118509.87  135837.26
  28    2   1     (2)S(+)(g)            0.5    124418.00  148030.30
  29    2   2     (2)S(+)(u)    1s      0.5    274666.12  274666.12
  30    2   3     (2)P( )(u)    2s      0.5    318289.02  318289.02
  31    4   1     (2)S          1s      0.5    148030.30  148030.30
  32    5   1                           0.0         0.00       0.00
-1
/ 20  1
    5.000        10.00        12.00        14.00        16.00        18.00        20.0...
    30.00        35.00        40.00        45.00        50.00        60.00        70.0...
    90.00        100.0        150.0        200.0
-1
  1434
/     1   2   3   1  0  2 -1  12
   0.5205E-08   0.2000E-07   0.2460E-07   0.2833E-07   0.3133E-07   0.3376E-07   0.357...
   0.4126E-07   0.4252E-07   0.4326E-07   0.4364E-07   0.4381E-07   0.4371E-07   0.433...
   0.4217E-07   0.4154E-07   0.3851E-07   0.3602E-07
-1
```

A.5 mdf11

Molecular species	*type*	*lybrary*
H_2	mqcd, mscd, pdcd,pdscd	mdf11/mqcd, mdf11/mscd, mdf11/pdcd, mdf11/pdscd
H_2^+	mqcd, mscd, pdcd,pdscd	mdf11/mqcd, mdf11/mscd, mdf11/pdcd, mdf11/pdscd

Data lines:	*format:*
DO C1=1, NBLCK	
SLMST, VLMST, IZ, SUMST,VUMST, N	17X,I2,14X,I2,4X,F4.2,13X,I2,14X,I2,10X,I3
DO C2=1,NNES	
DO C3=1, NMTM	
(CF(C2,C4,C3), C4=1, NMTE)	1X,30(G12.5,1X)
repeat	
repeat	
repeat	

variable identification:

SLMST,VLMST	Lower metastables electronic state and vibrational level
SUMST,VUMST	Upper metastables electronic state and vibrational level
IZ	Charge of initial state
NNES	Number of electron densities
NMTM	Number of molecular temperaturesprocesses
NMTE	Number of electron/ion temperatures
CF	Matrix of coefficients

```
    H_2            10  14    1  /H_2
1    1190
--------------------------------------------------------------------------------
   5.0000        7.0000        10.000        15.000        20.000        25.000        30.000        40.000        50.000        60.000...
  0.10000E+12   0.50000E+12   0.10000E+13   0.50000E+13   0.10000E+14   0.50000E+14   0.10000E+15   0.50000E+15   0.10000E+16   0.10000...
--------------------------------------------------------------------------------
-----/L. EL. ST.= 1 /L. VIB. ST.= 0 /Z=0.00 /U. EL. ST.= 1 /U. VIB. ST.= 1 /IBLCK =    1
  0.15018E-08   0.31111E-08   0.52774E-08   0.76150E-08   0.95157E-08   0.10469E-07   0.11048E-07   0.11612E-07   0.11777E-07   0.11763...
  0.15010E-08   0.31074E-08   0.52662E-08   0.75906E-08   0.94772E-08   0.10422E-07   0.10993E-07   0.11549E-07   0.11711E-07   0.11695...
  0.15001E-08   0.31029E-08   0.52530E-08   0.75630E-08   0.94345E-08   0.10369E-07   0.10935E-07   0.11483E-07   0.11641E-07   0.11624...
  0.14931E-08   0.30722E-08   0.51716E-08   0.74097E-08   0.92117E-08   0.10108E-07   0.10647E-07   0.11168E-07   0.11315E-07   0.11295...
  0.14856E-08   0.30432E-08   0.51041E-08   0.72962E-08   0.90532E-08   0.99250E-08   0.10449E-07   0.10951E-07   0.11090E-07   0.11068...
  0.14496E-08   0.29306E-08   0.48626E-08   0.68772E-08   0.84434E-08   0.91965E-08   0.96343E-08   0.10030E-07   0.10116E-07   0.10068...
```

```
  0.14262E-08  0.28584E-08  0.46919E-08  0.65413E-08  0.79436E-08  0.85875E-08  0.89466E-08  0.92456E-08  0.92823E-08  0.92112...
  0.13375E-08  0.25291E-08  0.38585E-08  0.49090E-08  0.56658E-08  0.59021E-08  0.59898E-08  0.59844E-08  0.58891E-08  0.57695...
  0.12634E-08  0.22532E-08  0.32207E-08  0.38055E-08  0.42663E-08  0.43428E-08  0.43393E-08  0.42529E-08  0.41394E-08  0.40274...
  0.74045E-09  0.90968E-09  0.95355E-09  0.78805E-09  0.92880E-09  0.90104E-09  0.87434E-09  0.82855E-09  0.79138E-09  0.76048...
```

A.6 mdf25

```
 3
acd    adf11/acd93/acd93_h.dat
scd    adf11/scd93/scd93_h.dat
qcd
xcd
 4 adf04/adas#1/ha00_ls#h0.dat
 5
 6
 9  0.0
 1 1s  1  1S1
 2 2s  2  2S1
 3 2p  3  2P1
 4 3s  4  3S1
 5 3p  5  3P1
 6 3d  6  3D1
 7 4s  7  4S1
 8 4p  8  4P1
 9 4d  9  4D1
 1   1.0
 1  -1.0
-1
C-----------------------------------------------------------------------
C
C        MAPPING OF ATOMIC LEVELS WITH ADF04 FILES
C
C        AFTER THE FILE NAMES THE NUMBER OF STATES PER SPECIE AND
C        IONCHARGE ARE PROVIDED. THEN FOR EACH PRODUCT LEVEL THE
C        THE ADF04 EQUIVALENT LEVEL AND CONFIGURATION SHOULD BE PROVIDED
C
C------------------------------------------------------------------------
```

A.7 mdf38

Auto-ionization and pre-dissociation files

A.7.1 Auto-ionization

Data lines:	*format:*
S1,E1,S2,E2,V1,V2,AR	4(1X,I2),1X,2(I3,1X),G12.4
repeat	

variable identification:

S1,E1	Lower species and electronic state index
S2,E2	Upper species and electronic state index
V1, V2	Lower and upper vibrational level
AR	Auto-ionization rate

```
  1  9  2  1   7   0 7.4e4
  1 15  2  1   4   0 1.4e7
  1 15  2  1   5   1 1.0e7
  1 15  2  1   6   2 6.3e8
  1 15  2  1   7   3 2.1e9
  1 15  2  1   8   3 6.3e8
  1N5   2  1   2   0 2.2e9
  1N5   2  1   3   0 5.7e7
  1N5   2  1   4   1 7.6e8
  1N5   2  1   5   2 1.1e9
  1N6   2  1   2   0 1.3e9
  1N6   2  1   3   1 4.0e9
  1N6   2  1   4   2 8.5e9
  1N6   2  1   5   3 1.5e10
-1
C----------------------------------------------------------
C       AUTOIONIZAZION RATES FROM
C       DEHMER & CHUPKA JCP 65 (1976) 2243
C
C
C----------------------------------------------------------
```

A.7.2 Pre-dissociation

Data lines: *format:*
SU, EU, SD(RD), ED(RD), DCH(RD), VUM,
(PR(C1,RD+1), C1=1, VUM+1) 4(I2,1X),A6,1X,I3,1X,100(1X,F10.4)
repeat

variable identification:

SU,EU	initial species and electronic state
SD,ED	final molecular species and electronic state
DCH	dissociation channel
VUM	number of vibrational levels to account for rates
PR	pre-dissociation rates

```
1  5  1  1 1->4+4   8  5.3600e+00 1.5700e+01 1.6700e+01 4.8700e+01 2.0800e+02 5.1700e+03 9.2200e+05 2.4100e+06 7.0900e+06
1  9  1  1 1->4+4  17  2.0600e+00 4.6600e+00 6.0200e+00 1.2600e+01 7.7300e+02 6.2300e+03 2.3700e+05 1.1900e+06 1.1300e+07 3.12...
-1

C-------------------------------------------------------------
C
C        PREDISSOCIATION RATES FROM
C        M. GLASS-MAUJEAN AD&NDT 30, 301-311 (1984)
C        D-X PREDISOCIATION IS ONLY GIVEN FOR THE FIRST 15 VIBRONIC
C        LEVELS SO THE LAST TWO ARE EQUAL 0.0 DUE TO THE LACK OF DATA
C
C        AUTHOR: F. GUZMAN 06/02/2012
C
C-------------------------------------------------------------
```

Appendix B

IDL procedures

Appendix C

FORTRAN subroutines

C.1 ADAS901

```
      PROGRAM ADAS901

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 PROGRAM: ADAS901 **********************
C
C  PURPOSE: CALCULATE THE COLLISION TIME CONSTANTS AND COEFFS USING
C     THE RATES STORED IN MDF33, MDF04 AND MDF11 FORMATS.
C
C  ORIGINAL NAME: GETTAUS
C
C  VERSION:  1.0
C
C     PROGRAM:
C
C     (I*4)  C#         = COUNTERS
C     (I*4)  IUNT10     = PARAMETER = INPUT UNIT FOR DATA
C     (I*4)  IUNIT      = PARAMETER = INPUT UNIT FOR PARAMETERS
C     (I*4)  OUNIT      = PARAMETER = OUTPUT UNIT FOR DATA IN MDF04/MDF14
C                         FORMAT
C     (C*80) PFILE      = PATH TO INPUT DATA SET FILE READ FROM FORTRAN
C     (I*2)  CATEG      = REQUIRED CATEGORY OF COLLISIONAL TRANSITIONS
C                             1 -> UPSILON
C                             2 -> RATES (CM3/S)
C                             3 -> OTHER N0N MAXWELLIAN
C     (R*8)  MI         = PROJECTILE MASS (IF ION IMPACT, 0 OTHERWISE)
C     (I*4)  NGRPS      = NUMBER OF GROUPS OF PROCESSES TOGETHER TO GET A
C                         TAU
C     (I*4)  NPRS()     = NUMBER OF PROCESSES PER GROUP
C     (I*4)  PRS(,)     = PROCESS NUMBER TO BE INCLUDED IN ANY GROUP
C     (I*4)  NNES       = NUMBER OF DENSITIES
C     (R*8)  NE()       = DENSITIES ARRAY
C     (I*4)  STL        = LOWER LIMIT INITIAL STATE TO ACCOUNT FOR
C     (I*4)  STU        = UPPER LIMIT INITIAL STATE TO ACCOUNT FOR
C     (I*4)  VL         = LOWER LIMIT VIBRQTIONAL INITIAL STATE TO
```

```
C                          ACCOUNT FOR
C      (I*4)  VU         = UPPER LIMIT VIBRATIONAL INITIAL STATE TO
C                          ACCOUNT FOR
C      (C*10)  MSYMB     = MOLECULAR SYMBOL
C      (R*8)   MMOL      = TOTAL MOLECULAR MASS
C      (I*4)   NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C      (I*4)   ELIM      = LIMIT OF THE NUMBER OF TRANSITION TO
C                           READ AT THE SAME TIME
C      (C*10)  SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C      (C*6)   CH_ION()  = IONISATION CHANNELS
C      (C*6)   CH_DIS(,) = DISSOCIATION CHANNELS
C      (R*8)   BWNO_I()  = IONISATION ENERGY
C                          (MEASURED FROM LOWEST ELECTRONIC STATE
C                           MINIMUM) (cm^-1)
C      (R*8)   BWNO_D(,) = DISSOCIATION ENERGY
C                          (MEASURED FROM LOWEST ELECTRONIC STATE
C                           MINIMUM) (cm^-1)
C      (I*4)   INDS()    = INDEX OF SPECIES
C      (I*4)   INDE()    = INDEX OF ELECTRONIC STATE
C      (C*10)  COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC
C                          CONFIGURATION
C      (R*8)   WT()      = STATISTICAL WEIGHT
C      (C*10)  WNO()     = BOUND ENERGY OF STATES
C                          (MEASURED FROM LOWEST ELECTRONIC STATE
C                           MINIMUM) (cm^-1)
C      (R*8)   WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                          (MEASURED FROM LOWEST ELECTRONIC STATE
C                           MINIMUM) (cm^-1)
C      (I*3)   NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C      (I*3)   NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C      (R*8)   TEI()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                          PARTICLES(ELECTRON/IONS) (eV)
C      (R*8)   TM()      = ARRAY OF TEMPERATURES FOR TARGET
C                          PARTICLES(MOLECULES) (eV)
C      (I*4)   INDR      = NUMBER OF TRANSITIONS
C      (I*2)   CATEGF()  = CATEGORY OF COLLISIONAL TRANSITIONS
C                            1 -> UPSILON
C                            2 -> RATES (CM3/S)
C                            3 -> OTHER NON MAXWELLIAN
C      (I*4)   TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
C                                  1 = DIPOLE
C                                  2 = NON-DIPOLE, NON SPIN CHANGE
C                                  3 = SPIN CHANGE
C                                  4 = OTHER (AMBIGUOUS)
C      (I*4)   PRCS()    = PROCESS NUMBER
C      (I*4)   SU()      = UPPER STATE INDEX OF A TRANSITION
C      (I*4)   SL()      = LOWER STATE INDEX OF A TRANSITION
C      (I*4)   V1()      = INITIAL STATE VIBRATIONAL INDEX
C      (I*4)   V2()      = FINAL STATE VIBRATIONAL INDEX
C      (R*8)   DE()      = TRANSITION/THRESHOLD ENERGY FOR A PROCESS
C      (C*6)   DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C      (R*8)   TRAT(,,)  = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                           FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                           SECOND INDEX OVER MOLECULAR TEMPERATURES
C                           THIRD INDEX RUNS OVER TRANSITIONS
C                          IN CASE THAT NMTE=0 ONLY FIRST AND THIRD INDEX
C                          FILLED
```

```
C     (L)     LSETX     = VARIABLE TO SET THE KNOTS OF SPLINE
C                         .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                         .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                         ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                          RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                          TO USE IT AGAIN FOR THE SAME KNOTS)
C     (I*4)   IOPT      = SPLINE END POINT CURVATURE/GRADIENT OPTION
C                             1 => DDY1 = 0, DDYN = 0
C                             4 => DY1 = 0 , DDYN = 0
C                         OTHER OPTION AVAILABLE WITH NEGATIVE
C                         DERIVATIVE AND NO CURVATURE. NOW IOPT WILL
C                         BE SET TO IOPT=1
C     (R*8)   XIN()     = INTERNAL SPLINE INDEPENDENT VARIABLE
C     (R*8)   YIN()     = INTERNAL SPLINE DEPENDENT VARIABLE
C     (R*8)   XOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   YOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   DY()      = DERIVATIVES AT SPLINE KNOTS
C     (I3)    IENRP     = NUMBER OF ENERGIES TO INTERPOLATE
C     (R*8)   ENRP()    = ARRAY OF INTERPOLATION ENERGIES REQUIRED
C     (L)     LINTRP()  = INTERPOLATION INDEX
C                         .TRUE.  => POINT INTERPOLATED
C                         .FALSE. => POINT EXTRAPOLATED
C     (R*8)   SRAT(,)   = SUM OF THE MAXWELLIAN RATES IN EACH GROUP OF
C                         PROCESSES
C     (R*8)   SRATV(,,) = SUM OF THE MAXWELLIAN RATES IN EACH VIBRATIONAL
C                         STATE
C     (R*8)   TAU(,,)   = TIME CONSTANT ARRAY
C                         1ST INDEX -> PROCESSES GROUP NUMBER
C                         2ND INDEX -> DENSITY
C                         3RD INDEX -> INTERPOLATED ENERGY
C     (R*8)   TAUV(,,)  = TIME CONSTANT ARRAY
C                         1ST INDEX -> PROCESSES GROUP NUMBER
C                         2ND INDEX -> DENSITY
C                         3RD INDEX -> INTERPOLATED ENERGY
C                         4TH INDEX -> INITIAL VIB STATE
C     (C*2)   TYP()     = GROUPING TYPE
C                          'ST' LOOKING AT STATES
C                          'PR' LOOKING AT PROCESSES
C                          'DS' LOOKING AT DISSOCIATION PROCESSES
C     (I*4)   STORE     = STORE THE TYP VARIABLE
C     (C*4)  ECONSA()   = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C     (C*2)   SW        = '33' READ FROM MDF33/34; '04' READS FROM MDF04/14
C     (L)     NOTMP     = .TRUE. TMPFILE ALREADY WRITEN (DO NOT WRITE IT)
C     (I*1)   IRDMD     = SWITCH THE MODE OF READING MDF04
C                          1: READ ALL AT ONCE FOR SMALL MATRICES (LESS
C                             THAN 8500 ELEMENTS)
C                          2: READ THE MATRIX FOR ONLY ONE TEMPERATURE
C                          3: READ ALL TEMPERATURES FOR ONE PROCESS
C     (I*4)   STI       = STATE INDEX AND NUMBER OF STATES
C     (I*4)   NSP       = NUMBER OF SPECIES
C     (R*8)   RAT_ONET  = MATRIX FOR ONE TEMPERATURE
C     (R*8)   TEO, TMO  =  ELECTRON/ION/MOLECULE DESIRED TEMPERATURES (MDF04)
C     (I*4)   NBLCK     = NUMBER OF BLOCKS OF THE FILE (MDF11)
C     (I*4)   NTMS      = WISHED NUMBER OF MOLECULAR TEMPERATURES (MDF11)
C     (R*8)   TMI()     = MOLECULAR TEMPERATURES FROM MDF11 FILE
C     (R*8)   TE()      = ELECTRON TEMPERATURES FROM MDF11 FILE
```

```
C     (R*8)   TI()      = ION TEMPERATURES FROM MDF11 FILE
C     (I*4)   INBLCK    =  NUMBER OF BLOCK TO BE READ
C     (I*4)   NDEN      = NUMBER OF DENSITIES ON MDF11 FILE
C     (R*6)   NEO()     = DENSITIES READ FROM MDF11 FILE
C     (I*4)   TIEQTE    = 1 TI = TE, 0 OTHERWISE
C     (R*8)   IZ        = ION/MOLECULE CHARGE
C     (R*8)   ECF(,,)   = EFFECTIVE COEFFICIENT FROM MDF11
C     (C*13)  FILEN     = OUTPUT FILE NAME
C
C
C ROUTINES:
C         ROUTINE    SOURCE    BRIEF DESCRIPTION
C         ------------------------------------------------------------
C         R8FUN1     ADAS      EXTERNAL FUNCTION FOR NEEDED FOR
C                              XXSPLE THAT ONLY RETURNS ARGUMENT
C         XXSPLE     ADAS      INTERPOLATES USING CUBIC SPLINES
C         I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C         XXDATM_33  MADAS     FETCH DATA FROM INPUT MDF33 FORMAT
C         XXDATM_04  MADAS     FETCH DATA FROM MDF04 FORMAT FILES
C         XXDATM_11  MADAS     FETCH DATA FROM MDF11 FORMAT FILES
C
C
C     AUTHOR: F. GUZMN
C
C  VERSION  : 1.0
C  DATE     : 22/06/2011
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C  VERSION  : 1.1
C  DATE     : 06/07/2011
C  MODIFIED : F. Guzman
C     - changed to calculated taus of reaction to specific states and
C       to dissociation. That can be chosen at the input
C
C  VERSION  : 2.0
C  DATE     : 24/04/2012
C  MODIFIED : F. Guzman
C     - changed to read time coefficients from mdf11 files.
C       CHANGED NAME TO ADAS901
C
C-----------------------------------------------------------------------
```

C.2 ADAS902

```
      PROGRAM ADAS902

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 PROGRAM: ADAS902 **********************
C
C  PURPOSE: TO CREATE MDF33 FILES FROM MDF02 ONES.
C
C     IN THIS WAY THE DATA FROM MDF02 FILES THAT COULD BE IN COLLISION
C     STRENGTHS OR CROSS SECTIONS IS INTEGRATED IN A SINGLE OR DOUBLE
C     MAXWELL BY THE USE OF THERMRAT. AFTER THAT THE DATA ARE ORGANIZED
C     AND WRITED IN A MDF33 FILE. THIS WOULD BE READY TO USE IN CR
C     MODELS.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                      C
C     MARCH 2011                                                       C
C                                                                      C
C     THIS ROUTINE IS MADE IN FORTRAN AND WILL BE DESIGNED TO BE RUN  C
C     IN FORTRAN. IT IS EXPECTED TO BE LATER MODIFIED TO BE CALLED    C
C     FROM IDL PROGRAMS                                                C
C                                                                      C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C  ORIGINAL NAME: ADAS902
C
C
C
C
C  PROGRAM:
C
C     (I*4)  IUNT10   = PARAMETER = INPUT UNIT FOR DATA
C     (I*4)  IUNIT    = PARAMETER = INPUT UNIT FOR PARAMETERS
C     (I*4)  OUNIT    = PARAMETER = OUTPUT UNIT FOR DATA IN MDF04/MDF14 FORMAT
C     (I*4)  MDT      = PARAMETER = MAX NUMBER OF INPUT DATA IN MDF02
C                       FILES
C     (I*4)  MNME     = PARAMETER = MAX NUMBER OF DESIRED TEMPERATURES
C     (I*4)  MNMTE    = PARAMETER = MAX NUMBER OF DESIRED MOLECULAR
C                       TEMPERATURES
C     (I*4)  MDP      = PARAMETER = MAX NUMBER OF FORMULA PARAMETERS IN
C                       INPUT DATA IN MDF02 FILES
C     (I*4)  MNS      = PARAMETER = MAX NUMBER OF SPECIES IN DIFFERENT
C                       MDF02 FILES
C     (I*4)  MNF      = PARAMETER = MAX NUMBER OF INPUT DATA FILES
C     (I*4)  NCEST    = PARAMETER = MAX TOTAL NUMBER OF PROCESSES
C     (I*4)  MNE      = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C     (I*4)  MNV      = PARAMETER = MAX NUMBER OF VIBRATIONAL STATES
C     (I*4)  NCEST    = PARAMETER = MAX NUMBER OF TRANSITIONS
C
C
C     (I*4)  C#       = COUNTERS
C     (C*80) PFILE()  = PATH TO INPUT DATA SET FILE READ FROM FORTRAN
```

```
C     (I*4)  NPF      = NUMBER OF MDF02 FILES TO BE INCLUDED
C     (C*1)  EI       = 'E' ELECTRON IMPACT TYPE DATA
C                       'I' ION IMPACT TYPE DATA
C     (R*8)  TEI()    = ARRAY OF DESIRED TEMPERATURES FOR COLLISIONING
C                       PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)  TM()     = ARRAY OF DESIRED TEMPERATURES FOR TARGET
C                       PARTICLES(MOLECULES) (eV)
C     (R*8)  MMOL     = TOTAL MOLECULAR MASS
C     (R*8)  MP       = PROJECTILE MASS (ASSUMED 0 IN THE ELECTRON
C                       IMPACT CASE)
C     (I*3)  NME      = NUMBER OF INPUT ENERGIES
C     (I*3)  NMTE     = NUMBER OF ELECTRON/ION TEMPERATURES
C     (I*3)  NMTM     = NUMBER OF MOLECULAR TEMPERATURES
C     (C*10) MSYMB    = MOLECULAR SYMBOL
C     (I*4)  ATNUM    = NUMBER OF ATOMS IN THE MOLECULE
C     (C*2)  ATSYMB   = ATOMIC SYMBOLS IN THE MOLECULE
C     (I*4)  IND_S()  = MAX. INDEX OF SPECIES THAT IS DIFFERENT MOLECULES,
C                       ATOMS AND THEIR IONS PER FILE
C     (I*4)  IND_SF   = MAX. TOTAL INDEX OF SPECIES
C     (C*10) SYMBS()  = ARRAY OF THE SYMBOLS FOR EACH IND_S
C     (C*10) SYMBSI(,)= ARRAY OF THE SYMBOLS FOR EACH IND_S
C     (C*10) SYMBSF() = FINAL ARRAY OF THE SYMBOLS FOR EACH IND_S
C     (C*6)  CH_ION() = IONISATION CHANNELS
C     (C*6)  CH_IONI(,)= IONISATION CHANNELS
C     (C*6)  CH_IONF()= FINAL ARRAY OF IONISATION CHANNELS
C     (R*8)  BWNO_I() = IONISATION ENERGY
C                       (MEASURED FROM LOWEST ELECTRONIC STATE
C                        MINIMUM) (cm^-1)
C     (R*8)  BWNO_II(,)= IONISATION ENERGY
C     (R*8)  BWNO_IF()= FINAL ARRAY OF IONISATION ENERGY
C     (C*6)  CH_DIS(,)= DISSOCIATION CHANNELS
C     (C*6)  CH_DISI(,,)= DISSOCIATION CHANNELS
C     (C*6)  CH_DISF(,)=FINAL ARRAY OF DISSOCIATION CHANNELS
C     (R*8)  BWNO_D(,)= DISSOCIATION ENERGY
C                       (MEASURED FROM LOWEST ELECTRONIC STATE
C                        MINIMUM) (cm^-1)
C     (R*8)  BWNO_DI(,,)= DISSOCIATION ENERGY
C     (R*8)  BWNO_DF(,)=FINAL ARRAY OF DISSOCIATION ENERGY
C     (I*4)  NDIS()   = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C     (R*8)  WNO(,)   = BOUND ENERGY OF STATES
C                       (MEASURED FROM LOWEST ELECTRONIC STATE
C                        MINIMUM) (cm^-1) (SAME AS WNOI AND WNOF)
C     (R*8)  WNOD(,)  = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                       (MEASURED FROM LOWEST ELECTRONIC STATE
C                        MINIMUM) (cm^-1) (SAME AS WNOI AND WNOF)
C     (I*4)  NDISI(,) = NUMBER OF DISSOTIATION CHANNELS PER SPECIE PER FILE
C     (I*4)  NDISF()  = FINAL NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C     (I*4)  IND_P()  = MAX, INDEX OF ELECTRON IMPACT PROCESSES BETWEEN
C                       DIFFERENT SPECIES
C     (C*60) PATH_P() = PATH OF THE DIFFERENTS PROCESS IN IND_P
C     (C*40) DESC_P() = DESCRIPTION OF THE DIFFERENT PROCESS IN IND_P
C     (I*4)  IND_E()  = MAX. INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (I*4)  IND_EI(,)= MAX. INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (I*4)  IND_EF() = MAX. TOTAL INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (C*8)  ECONUA() = ELECTRONIC CONFIGURATION IN THE UNITED ATOMS
C                       LIMIT
C     (C*4)  ECONSA() = ELECTRONIC CONFIGURATION IN THE SEPARATED
```

```
C                         ATOMS LIMIT
C      (C*10) COUPSTA()= COUPLED MOLECULAR STATE ELECTRONIC CONFIGURATION
C      (C*10) COUPSTAI()= COUPLED MOLECULAR STATE ELECTRONIC CONFIGURATION
C      (C*10) COUPSTAF()=FINAL ARRAY OF  COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C      (R*8)  WT(,)    = STATISTICAL WEIGHT (AS WTF)
C      (C*15) RPARAM(,)= PARAMETERS FOR EACH REACTION VALUES,
C                         ARRAY(IND_R,20)
C      (I*4)  IND_R    = MAX. NUMBER OF REACTIONS
C      (R*8)  TPARAM(,)= TEMPERATURES ARRAY FOR DATA
C      (R*8)  SPARAM(,)= CROSS SECTION DATA ARRAY
C      (R*8)  PARVAL(,)= PARAMETERS ARRAY FOR FITTING FORMULA
C      (R*8)  EPARAM() = TRANSITION ENERGY PARAMETER
C      (C*145)CMMT()   = COMMENTS ON THE INPUT FILE (100 LINES)
C      (I*4)  IERR     = ERROR RETURN CODE.
C      (I*2)  CATEG()  = CATEGORY OF COLLISIONAL TRANSITIONS
C                           1 -> COLLISION STRENGTH (OMG TABULATIONS)
C                           2 -> CROSS SECTIONS (Erel (ev/AMU) AND SIG(CM2))
C                           3 -> MAXWELL AVERAGED (cm3/s)
C      (I*2)  CATEGF() = CATEGORY OF COLLISIONAL TRANSITIONS (FINAL ARRAY)
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER NON MAXWELLIAN
C      (L)    DM       = .TRUE. FOR DOUBLE MAXWELLIAN INTEGRATION
C                         (DEFAULT FOR ION COLLISIONS)
C                         IN THIS CASE THE ARRAY WITH MOLECULAR TEMPERATURES
C                         WILL BE RELEVANT.
C      (R*8)  OMG()    = ARRAY OF COLLISION STRENGTHS FOR INPUT
C      (R*8)  ELE()    = ARRAY OF ENERGIES FOR COLLISION STRENGTH (eV)
C      (I*3)  FORM()   = FITTING FORMULA NUMBER
C      (I*3)  IPAR()   = NUMBER OF PARAMETERS FROM FORM
C      (I*3)  IPARF()  = NUMBER OF PARAMETERS FROM FORM (FINAL LOOP)
C      (R*8)  PAR(,)   = ARRAY OF FITTING FORMULA PARAMETERS
C      (R*8)  DE()     = TRANSITION/THRESHOLD ENERGY FOR A PROCESS
C      (R*8)  DEF()    = FINAL ARRAY FOR TRANSITION/THRESHOLD ENERGY FOR A
c                         PROCESS
C      (I*3)  PROCESS/F= PROCESS NUMBER FROM MDF02
C      (R*8)  W        = STATISTICAL WEIGTH FROM THE FINAL STATE
C      (L)    FR_INT   = FORMULA INTERPOLATING.
C                          .TRUE. USE FORMULA WHENEVER EXIST(DEFAULT)
C                          .FALSE. INTERPOLATE BY SPLINE
C      (L)    FR_EXT   = FORMULA EXTRAPOLATING.
C                          .TRUE. USE FORMULA WHENEVER EXIST(DEFAULT)
C                          .FALSE. EXTRAPOLATE BY SPLINE
C      (C*2)  PIMPCT   = TYPE OF PROCESS:
C                           CX = CHARGE EXCHANGE
C                           EX = EXCITATION
C                           IO = IONIZATION
C                           RC = RECOMBINATION
C                           DISSOSIATION PROCESSES ARE INCLUDED BEFORE AS THEIR
C                           PRIMARY PROCESS IS ALWAYS ONE OF THESE.
C      (R*8) TRAT(,)   = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                          FIRST INDEX RUN OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                         IN CASE THAT NMTE=0 ONLY FIRST ELEMENT FILLED
C      (R*8) TRATI(,,) = MATRIX OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                          HERE THRD ELEMENT RUNS OVER NUMBER OF STATES
```

```
C     (R*8) TRATF(,,) = FINAL MATRIX OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                        HERE THRD ELEMENT RUNS OVER NUMBER OF STATES
C     (I*4) INDX()    = ARRAY OF SEVERAL INDEXES
C     (I*4) CEST      = PROCESSES COUNTER
C     (I*4) CESTF     = PROCESSES COUNTER
C     (I*4) VIB       = 1 -> TAKE VIBRONIC RESOLUTION WHEREEVER POSSIBLE,
C                            BY FC FACTORS
C                       2 -> ONLY ELECTRONIC RESOLUTION
C                       3 -> OBTAIN THE RATES ONLY FROM THE DATA ON THE FILE
C     (I*4) S1()      = INITIAL STATE SPECIE INDEX (AS S1F)
C     (I*4) E1()      = INITIAL STATE ELECTRONIC INDEX (AS E1F)
C     (I*4) V1()      = INITIAL STATE VIBRATIONAL INDEX (AS V1F)
C     (I*4) S2()      = FINAL STATE SPECIE INDEX (AS S2F)
C     (I*4) E2()      = FINAL STATE ELECTRONIC INDEX (AS E2F)
C     (I*4) V2()      = FINAL STATE VIBRATIONAL INDEX (AS V2F)
C     (R*8) FC(,)     = ARRAY WITH THE FC FACTORS FOR THE VIB STATES
C     (I*4) MAXV1     = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                       STATE E1
C     (I*4) MAXV2     = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                       STATE E2
C     (R*8) OMGT()    = COLLISION STRENGTHS ARRAY INPUT OF THERMRAT
C     (R*8) ELET()    = ENERGIES  ARRAY INPUT OF THERMRAT
C     (R*8) PART()    = FITTING FORMULA PARAMETERS INPUT OF THERMRAT
C     (L)   FLAGS     = FLAG TO USE IN THE LOOPS OF ELECTRONIC RESOLUTION
C     (I*2) UPSRT()   = TYPE OF OUTPUT FROM THEMRAT
C                         1 => UPSILONS
C                         2 => RATES (CM3/S)
C     (I*4) FXPH      = FIRST EXTRAPOLATED POINT AT HIGH ENERGIES
C                         (0 NO POINTS EXTRAPOLATED AT HIGH ENERGIES)
C     (I*4) LXPL      = LAST EXTRAPOLATED POINT AT LOW ENERGIES
C                         (0 NO POINTS EXTRAPOLATED AT LOW ENERGIES)
C     (C*100)OFILE    = NAME OF THE OUTPUT FILE
C     (I*4) TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
C                                 1 = DIPOLE
C                                 2 = NON-DIPOLE, NON SPIN CHANGE
C                                 3 = SPIN CHANGE
C                                 4 = OTHER (AMBIGUOUS)
C     (I*4) TCODEF()  = FINAL ARRAY OF TCODE()
C     (R*8) ENU#()    = ARRAY WITH THE EIGENVALUES FROM 1 TO MAXV1+1
C     (R*8) ENUC(,)  = ARRAY WITH THE ENERGY DIFFERENCE FOR THE VIB
C                       RESOLUTION
C     (L)   LSETX     = VARIABLE TO SET THE KNOTS OF SPLINE
C                       .TRUE.  => SPLINE PRESET FOR THESE KNOTS
C                       .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                                 (I.E. THEY WERE SET IN A PREVIOUS CALL )
C                       ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                        RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                        TO USE IT AGAIN FOR THE SAME KNOTS)
C     (L)   LPASS       = LOGARITHMIC CONVERSION
C                        .TRUE. => DO NOT CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C                        .FALSE.=> CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C     (L)   LINTRP()    = INTERPOLATION INDEX
C                        .TRUE.  => POINT INTERPOLATED
C                        .FALSE. => POINT EXTRAPOLATED
C     (R*8) TR()        = INTERPOLATED ARRAY OF CATEG=3 VALUES
```

```
C     (C*3) TDATA      = CHARACTER FOR CATEG, INPUT OF INTRP
C     (C*6) DCH,DCHF() = DISSICIATION CHANNEL STRING FOR EACH PROCESS
C     (C*80)DFILE      = FCF DIRECTORY
C     (C*80)DENU       = ENU DIRECTORY
C     (L)   VDFLAG(,)  = LOGICAL FLAG FOR IDENTIFY DISSOCIATIVE EXCITATION
C     (L)   VTFLAG(,)  = LOGICAL FLAG FOR IDENTIFY TOTAL EXCITATION
C     (L)   VFLAG(,)   = .TRUE. THE CROSS SECTION HAS BEEN REST FOR THIS
C                         STATE
C     (I*4) NM2(,)     = TRANSITION NUMBER FOR TOTAL EXCITATION
C     (I*4) NM3(,)     = TRANSITION NUMBER FOR DISSOCIATIVE EXCITATION
C     (I*4) NTRAN      = TO GET TRANSITION NUMBER
C     (R*8) TRIN       = RATE TO INPUT IN RT2UPSLN
C     (L)   RSTFLG     = FLAG FOR METASTABLES
C     (I*4) IRST       = COUNTER OF THE NUMBER OF ALWAYS RESOLVED STATES
C     (I*4) RST(,)     = ALWAYS RESOLVED STATES MATRIX
C     (I*4) IN_E(,)    = INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (C*1) COUPS1     = UPPER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (C*1) COUPS2     = LOWER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (C*80)AVFILE    = A-VALUES DIRECTORY
C
C
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          I4FCTN     ADAS      RETURNS CHARACTER STRING AS AN INTEGER.
C          XXDATM_02  MADAS     READS MDF02 FILES AND RETURNS VALUES
C          THERMRAT   ADAS902   CALCULATES THERMAL RATE COEFFICIENTS
C          XXDATM_00  ADAS902   READS AND RETURN FC FACTORS
C          INTRP      ADAS902   INTERPOLATE DATA BY FORMULA OR BY SPLINE
C          RT2UPSLN   MADAS     CONVERTS CM3/S <-> UPSILON
C          WRT_MDF33  MADAS     CREATE A MDF33 FORMAT FILE
C
C
C     AUTHOR: F. GUZMN
C
C   VERSION  :  1.0
C   DATE     : 31/03/2011
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  : 1.1
C   DATE     :    26/05/2011
C   MODIFIED : F.GUZMAN
C               to prepare for isotopes reading (dfile and variables)
C
C   VERSION  : 1.2
C   DATE     : 22/09/2011
C   MODIFIED : F. GUZMN
C     included the new matrix WNOD(,) that accounts for the
C     electronic asymptotic energy needed after and writing to mdf33
C
```

```
C   VERSION  : 1.3
C   DATE     : 27/09/2011
C   MODIFIED : F. GUZMN
C     included removal of dissociative excitation cross section from
C     the total cross section when these are included, otherwise they
C     treated as non dissociative
C
C   VERSION  : 1.4
C   DATE     : 10/10/2011
C   MODIFIED : F. GUZMN
C     included separate atom configuration to account to dissociation
C     products.
C
C   VERSION  : 1.5
C   DATE     : 14/11/2011
C   MODIFIED : F. GUZMN
C     included vibronic resolution for metastables in vib=2
C
C   VERSION  : 1.6
C   DATE     : 14/11/2011
C   MODIFIED : F. GUZMN
C     uses chng_proc to change process in case of vib modification
C
C VERSION  : 1.7
C DATE     : 21/04/2012
C MODIFIED : F. GUZMN
C     included the new matrix IN_E to account for electronic
C     index independently
C
C VERSION  : 2.0
C DATE     : 22/04/2012
C MODIFIED : F. GUZMN
C     ignore upper states than the ones in the list
C
C VERSION  : 2.1
C DATE     : 24/07/2012
C MODIFIED : F. GUZMN
C     prepared for extrapolation using bethe formula in extrap.for
C
C
C-----------------------------------------------------------------------
```

C.2.1 chng_prcs.for

```
      SUBROUTINE CHNG_PRCS( VIB, PRCS, PRCSF)
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: WRITE_MDF33 *******************
C
C     PURPOSE: CHANGE PROCESS VALUE TO THE CORRECT ONE
C
C  INPUT:
C
C     (I*4) VIB       = 1 -> TAKE VIBRONIC RESOLUTION WHEREEVER POSSIBLE,
C                            BY FC FACTORS
C                       2 -> ONLY ELECTRONIC RESOLUTION
C     (I*3)  PRCS     = PROCESS NUMBER FROM MDF02
C
C     OUTPUT:
C
C     (I*3)  PRCSF     = CHANGED PROCESS NUMBER
C
C     AUTHOR: F. GUZMN
C
C  VERSION  : 1.0
C  DATE     : 23/01/2012
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C-----------------------------------------------------------------------
```

C.2.2 dstform.for

```
      SUBROUTINE  DSTFORM(FORM,IOUTPUT,IPAR,IENER,DE,W,PAR,ELE,FFORM)

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ******************** FORTRAN77 SUBROUTINE: DSTFORM  *****************
C
C  PURPOSE: SELECTS THE FITTING FORMULA FOR
C            A SET OF MOLECULAR DATA
C
C     INPUT:
C     FORM   (I3)      :FITTING FORMULA NUMBER
C     IOUTPUT(I3)      :KIND OF OUTPUT: 0 OMG ARRAY; 1 SIGMAS
C     IPAR   (I3)      :NUMBER OF PARAMETERS FROM FORM
C     IENER  (I3)      :NUMBER OF ENERGIES TO TO GET VALUES FOR
C     DE     (R*8)     :TRANSITION, THRESHOLD OR IONIZATION ENERGY
C     W      (R*8)     :STATISTICAL WEIGTH FROM THE FINAL STATE
C     PAR    (R*8)()   :ARRAY OF FITTING FORMULA PARAMETERS
C     OUTPUT:
C
C     ELXTRP(R*8)()    :ARRAY OF REQUIRED ENERGIES
C     FFORM(R*8) ()     :ARRAY OF VALUES FOR REQUIRED ENERGIES
C
C ROUTINES:
C     ROUTINE    SOURCE    BRIEF DESCRIPTION
C     -------------------------------------------------------------
C     FFORM_x    ADAS9XX   FITTING F0RMULA x
C
C
C     AUTHOR: F. GUZMN
C
C  VERSION  : 1.0
C  DATE     : 09/2010
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C-----------------------------------------------------------------------
C
C
```

C.2.3 extrap.for

```
      SUBROUTINE EXTRAP ( HL    , AVFILE,
     &                    S1    , E1    , V1    , S2    ,
     &                    E2    , V2    , COUPS1, COUPS2,
     &                    FORM  , IPAR  , IENERO, DE    ,
     &                    W     , PAR   , ENERO , TDATA ,
     &                    UPTE  , UPTSIG, PIMPCT, SPL   ,
     &                    SIGO
     &                   )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: EXTRAP *********************
C
C     PURPOSE: SELECTS THE CROSS SECTION ASYMPTOTIC BEHAVIOUR DEPENDING
C               ON THE INPUT OF THE PARAMETERS OF THE DATA
C
C     INPUT:
C
C     HL    (I2)       :VARIABLE FOR HIGH/LOW ENERGY EXTRAPOLATION
C                       0 -> LOW ENERGY EXTRAPOLATION
C                       1 -> HIGH ENERGY EXTRAPOLATION
C                       3 -> HIGH ENERGY FORMULA EXTRAPOLATION
C                       4 -> LOW ENERGY FORMULA EXTRAPOLATION
C     FORM  (I3)       :FITTING FORMULA NUMBER
C     IPAR  (I3)       :NUMBER OF PARAMETERS FROM FORM
C     PAR   (R*8)()    :ARRAY OF FITTING FORMULA PARAMETERS
C     IENERO(I3)       :NUMBER OF ENERGIES TO EXTRAPOLATE
C     ENERO (R*8)()    :ARRAY OF EXTRAPOLATION ENERGIES REQUIRED
C     DE    (R*8)      :TRANSITION, THRESHOLD OR IONIZATION ENERGY
C     W     (R*8)      :STATISTICAL WEIGTH FROM THE FINAL STATE
C     UPTE  (R*8)()    :THE LAST TWO ENERGY INTERPOLATED POINTS TO NORMALIZE
C                       IN INVERSE ORDER
C     UPTSIG(R*8)()    :THE LAST SIGMA(OMG) INTERPOLATED POINTS TO NORMALIZE
C                       IN INVERSE ORDER
C     TDATA (C*3)      :TYPE OF DATA IN OMG'S OR CROSS SECTIONS
C     PIMPCT(C*2)      :TYPE OF PROCESS:
C                        CX = CHARGE EXCHANGE
C                        EX = EXCITATION
C                        IO = IONIZATION
C                        RC = RECOMBINATION
C                        DISSOSIATION PROCESSES ARE INCLUDED BEFORE AS THEIR
C                        PRIMARY PROCESS IS ALWAYS ONE OF THESE.
C     S1(I*4)          :INITIAL STATE SPECIE INDEX (AS S1F)
C     E1(I*4)          :INITIAL STATE ELECTRONIC INDEX (AS E1F)
C     V1(I*4)          :INITIAL STATE VIBRATIONAL INDEX (AS V1F)
C     S2(I*4)          :FINAL STATE SPECIE INDEX (AS S2F)
C     E2(I*4)          :FINAL STATE ELECTRONIC INDEX (AS E2F)
C     V2(I*4)          :FINAL STATE VIBRATIONAL INDEX (AS V2F)
C
C     OUTPUT:
C
C     SIGO  (R*8)()    :ARRAY OF EXTRAPOLATED SIGMAS(OMG) FOR THE REQUIRED
```

```
C                         ENERGIES
C     SPL   (L)       :SWITCH TO THE SPLINE EXTRAPOLATION
C
C     INTERNAL:
C
C     A     (R*8)     :FIRST PARAMETER FOR BETHE NORMALIZATION
C     B     (R*8)     :SECOND PARAMETER FOR BETHE NORMALIZATION
C     LXTRP (R*8)()   :LOG OF ENERGIES FOR BETHE EXTRAPOLATION
C     ELXTRP(R*8)()   :ARRAY OF EXTRAPOLATED ENERGIES
C     SIGXTRP(R*8)()   :ARRAY OF EXTRAPOLATED SIGMAS(OMG)
C     DIFF  (R*8)     :DIFFERENCE BETWEEN THE EXTRAPOLATED FORMULA DATA
C                       AND NUMERICAL DATA
C     IOUTPUT(I3)     :KIND OF OUTPUT: 0 OMG ARRAY; 1 SIGMAS
C     AVAL(,)(R*8)    :A VALUES FOR VIB-VIB TRANSITIONS
C     AVAL_T(R*8)     :SUMMATION OF AVAL FOR EL-EL TRANSITIONS
C     AVAL_L()(R*8)   :SUM OF AVAL FOR THE UPPER EL. STATE.
C     AVAL_U()(R*8)   :SUM OF AVAL FOR THE LOWER EL. STATE
C     G(R*8)          :MOLECULAR DEGENERACY FACTOR
C     VUMAX(I*4)      :HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        UPPER STATE
C     VLMAX(I*4)      :HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        LOWER STATE
C     AF(R*8)         :A-FACTOR (COLL SRTENGTH F=AF*CONST/DE)
C     IERR(I*4)       :'1' ERROR ON OUTPUT FROM SUBROUTINE
C     BTHNRM          :NORMALIZATION CONSTANT FOR BETHE EXCITATION
C                       EXTRAPOLATION
C
C ROUTINES:
C     ROUTINE    SOURCE    BRIEF DESCRIPTION
C     -------------------------------------------------------------
C     DSTFORM    ADAS9XX   SELECTS THE FITTING FORMULA FOR
C                          A SET OF MOLECULAR DATA
C     I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C     DGFCTR     MADAS     CALCULATES THE DEGENERACY FACTOR FOR MO
C     XXDATM_00  MADAS     READS AND RETURN FC FACTORS AND A-VAL
C
C
C
C
C     AUTHOR: F.GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 09/2010
C  MODIFIED : F.GUZMAN
C             FIRST VERSION
C
C  VERSION  : 2.0
C  DATE     : 24/07/2012
C  MODIFIED : F.GUZMAN
C             - Added extrapolation w/o formula by bethe formula,
C               always normalized to previous results.
C
C  VERSION  : 2.1
C  DATE     : 24/10/2012
C  MODIFIED : F.GUZMAN
C             - corrected B formula for Bethe ionization,
C             - safety sigma>0 condition imposed in CX and Bethe.
```

```
C             - spline is taken in case smooth condition is not fullfilled
C             - omega is corrected for bethe ionization.
C
C-----------------------------------------------------------------------
```

C.2.4 intrp.for

```
      SUBROUTINE INTRP ( FRT_INT, TDATA, IENRP, ENRP,
     &                   FORM   , DE   , W    ,
     &                   IPAR   , PAR  ,
     &                   NME    , ELE  , OMG  ,
     &                   LSETX  , LPASS,
     &                   SIGP   , LINTRP, IERR
     &                 )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: INTRP *********************
C
C     PURPOSE: INTERPOLATE DATA BY FORMULA OR BY SPLINE TO
C              PERFORM MAXWELL INTEGRATION
C
C     INPUT:
C
C     FR_INT (L)         :FORMULA INTERPOLATING.
C                        .TRUE. USE FORMULA WHENEVER EXIST(DEFAULT)
C                        .FALSE. INTERPOLATE BY SPLINE
C     TDATA  (C*3)       :TYPE OF DATA IN OMG'S OR CROSS SECTIONS
C     IENRP  (I3)        :NUMBER OF ENERGIES TO INTERPOLATE
C     ENRP   (R*8) ()    :ARRAY OF INTERPOLATION ENERGIES REQUIRED
C     FORM   (I3)        :FITTING FORMULA NUMBER
C     DE     (R*8)       :TRANSITION, THRESHOLD OR IONIZATION ENERGY
C     W      (R*8)       :STATISTICAL WEIGTH FROM THE FINAL STATE
C     IPAR   (I3)        :NUMBER OF PARAMETERS FROM FORM
C     PAR    (R*8) ()    :ARRAY OF FITTING FORMULA PARAMETERS
C     NME    (I*3)       :NUMBER OF ENERGIES
C     OMG    (R*8) ()    :ARRAY OF COLLISION STRENGTHS FOR INPUT
C     ELE    (R*8) ()    :ARRAY OF ENERGIES FOR COLLISION STRENGTH (eV)
C     LSETX  (L)         :VARIABLE TO SET THE KNOTS OF SPLINE
C                        .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                        .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                        ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                         RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                         TO USE IT AGAIN FOR THE SAME KNOTS)
C     LPASS  (L)         :LOGARITHMIC CONVERSION
C                        .TRUE. => DO NOT CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C                        .FALSE.=> CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C
C     OUTPUT:
C
C     SIGP   (R*8) ()    :ARRAY OF INTERPOLATED SIGMAS(OMG)
C     LINTRP (L)   ()    :INTERPOLATION INDEX
C                        .TRUE.  => POINT INTERPOLATED
C                        .FALSE. => POINT EXTRAPOLATED
C     IERR()             : ERROR FLAG FOR ENERGY POINTS
C
C
```

```
C     INTERNAL:
C
C     INDx   (I*4)       :MULTIUSE INDEX
C     IOPT   (I*4)       :SPLINE END POINT CURVATURE/GRADIENT OPTION
C                             1 => DDY1 = 0, DDYN = 0
C                             4 => DY1 = 0 , DDYN = 0
C                         OTHER OPTION AVAILABLE WITH NEGATIVE
C                         DERIVATIVE AND NO CURVATURE. NOW IOPT WILL
C                         BE SET TO IOPT=4
C     XIN    (R*8) ()    :INTERNAL SPLINE INDEPENDENT VARIABLE
C     YIN    (R*8) ()    :INTERNAL SPLINE DEPENDENT VARIABLE
C     XOUT   (R*8) ()    :INTERNAL OUTPUT SPLINE VARIABLE
C     YOUT   (R*8) ()    :INTERNAL OUTPUT SPLINE VARIABLE
C     DY     (R*8) ()    :DERIVATIVES AT SPLINE KNOTS
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          -------------------------------------------------------------
C          DSTFORM    ADAS9XX   SELECTS THE FITTING FORMULA FOR
C                               A SET OF MOLECULAR DATA
C          XXSPLE     ADAS      INTERPOLATES USING CUBIC SPLINES
C          R8FUN1     ADAS      EXTERNAL FUNCTION FOR NEEDED FOR
C                               XXSPLE THAT ONLY RETURNS ARGUMENT
C
C     AUTHOR: F. GUZMN
C
C   VERSION  : 1.0
C   DATE     : 26/10/2010
C   MODIFIED : F.GUZMAN
C              FIRST VERSION
C
C   VERSION  : 1.1
C   DATE     : 23/06/2011
C   MODIFIED : F.GUZMAN
C     corrected interpolation under threshold when rates may not be zero
C
C   VERSION  : 1.2
C   DATE     : 13/07/2011
C   MODIFIED : F.GUZMAN
C      control of NaN from formulas. Go to spline in this situation
C
C
C   VERSION  : 1.3
C   DATE     : 15/10/2012
C   MODIFIED : F.GUZMAN
C      ioutput only is 1 or 0 now. using tdata for separate rates from sigmas
C
C  -----------------------------------------------------------------------
```

C.2.5 rd_enu.for

```
      SUBROUTINE RD_ENU( S1, E1, MAXV1, MSYMB, DENU, ENU, ERROR)

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 FUNCTION: RD_ENU    ********************
C
C  PURPOSE: THIS FUNCTION READS THE EIGENVALUES OF THE VIBRATIONAL
C           LEVELS FROM THE FILES IN MDF00
C
C  ORIGINAL NAME: RD_ENU
C
C
C
C
C
C INPUT:
C
C     (I*4) S1      = INITIAL STATE SPECIE INDEX
C     (I*4) E1      = INITIAL STATE ELECTRONIC INDEX
C     (C*80)DENU    = DIRECTORY WITH ENUS
C     (C*10) MSYMB    = MOLECULAR SYMBOL
C
C OUTPUT
C
C     (R*8) ENU()   = ARRAY WITH THE EIGENVALUES FROM 1 TO MAXV1+1
C     (I*4) MAXV1   = MAX. QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                     STATE E1 TO READ
C
C
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          XXRMWS      ADAS     REMOVES ALL BLANKS IN INPUT STRING
C          I4UNIT      ADAS     FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C  AUTHOR: F. GUZMN
C
C   VERSION  : 1.0
C   DATE     : 29-03-2011
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  : 1.1
C   DATE     : 26/05/2011
C   MODIFIED : F. GUZMAN
C     - TO INCLUDE ALL ISOTOPES
C
C   VERSION  : 1.2
C   DATE     : 05/10/2011
```

```
C   MODIFIED : F. GUZMAN
C     - the maximal vib state MAXV1 is now an output from the program
C
C   VERSION  : 1.3
C   DATE     : 26/10/2011
C   MODIFIED : F. GUZMAN
C              Added an error status for output.
C-----------------------------------------------------------------------
```

C.2.6 thermrat.for

```
      SUBROUTINE THERMRAT(  AVFILE,
     &                      EI    , CATEG  , DM    ,
     &                      MMOL  , MP     ,
     &                      OMG   , ELE    ,
     &                      TEI   , TM     ,
     &                      FORM  , IPAR   , PAR   ,
     &                      DE    , PROCESS, W     ,
     &                      NME   , NMTE   , NMTM  ,
     &                      FR_INT, FR_EXT , PIMPCT,
     &                      S1    , E1     , V1    ,
     &                      S2    , E2     , V2    ,
     &                      COUPS1, COUPS2 ,
     &                      TRAT  ,
     &                      UPSRT ,
     &                      FXPH  , LXPL
     &                   )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: THERMRAT *******************
C
C     PURPOSE: CALCULATES THE RATES FROM THE CROSS SECTIONS (OMEGAS)
C              FOR ELECTRON AND ION IMPACT COLLISIONS.
C              PATH: 1) LOOP OVER REQUIRED ENERGY RATES AND GET
C                       REQUIRED ENERGY VALUES FOR GAUSS LAGRANGE
C                       INTEGRATION
C                    2) INTERPOLATION AND EXTRAPOLATION OF VALUES
C                    3) SINGLE MAXWELLIAN INTEGRATION FOR E-IMPACT AND
C                       DOUBLE THERMAL INTEGRATION FOR I-IMPACT.
C                    4) OUTPUT OF RATES
C
C     INPUT:
C
C     EI     (C*2)       :ELECTRON/ION COLLISION SWITCHER
C                        'e'= ELECTRON COLLISIONS
C                        'I'= ION COLLISIONS
C     CATEG  (I*2)       : CATEGORY OF COLLISIONAL TRANSITIONS
C                         1 -> COLLISION STRENGTH (OMG TABULATIONS)
C                         2 -> CROSS SECTIONS (Erel (ev/AMU) AND SIG(CM2))
C                         3 -> MAXWELL AVERAGED COLLISON STRENGTH (T(K) AND
C                              UPSILONS)
C     DM     (L)         :.TRUE. FOR DOUBLE MAXWELLIAN INTEGRATION
C                        (DEFAULT FOR ION COLLISIONS)
C                         IN THIS CASE THE ARRAY WITH MOLECULAR TEMPERATURES
C                         WILL BE RELEVANT.
C     MMOL   (R*8)       :TOTAL MOLECULAR MASS
C     MP     (R*8)       :PROJECTILE MASS
C     OMG    (R*8) ()    :ARRAY OF COLLISION STRENGTHS FOR INPUT
C     ELE    (R*8) ()    :ARRAY OF ENERGIES FOR COLLISION STRENGTH (eV)
C     TEI    (R*8) ()    :ARRAY OF DESIRED TEMPERATURES FOR COLLISIONING
C                        PARTICLES(ELECTRON/IONS) (eV)
C     TM     (R*8) ()    :ARRAY OF DESIRED TEMPERATURES FOR TARGET
```

```
C                          PARTICLES(MOLECULES) (eV)
C     FORM   (I3)         :FITTING FORMULA NUMBER
C     IPAR   (I3)         :NUMBER OF PARAMETERS FROM FORM
C     PAR    (R*8) ()     :ARRAY OF FITTING FORMULA PARAMETERS
C     DE     (R*8)        :TRANSITION/THRESHOLD ENERGY FOR THE PROCESS
C     PROCESS(I*3)        :PROCESS NUMBER FROM MDF02
C     W      (R*8)        :STATISTICAL WEIGTH FROM THE FINAL STATE
C     NME    (I*3)        :NUMBER OF ENERGIES
C     NMTE   (I*3)        :NUMBER OF ELECTRON/ION TEMPERATURES
C     NMTM   (I*3)        :NUMBER OF MOLECULAR TEMPERATURES
C     FR_INT (L)          :FORMULA INTERPOLATING.
C                         .TRUE. USE FORMULA WHENEVER EXIST(DEFAULT)
C                         .FALSE. INTERPOLATE BY SPLINE
C     FR_EXT (L)          :FORMULA EXTRAPOLATING.
C                         .TRUE. USE FORMULA WHENEVER EXIST(DEFAULT)
C                         .FALSE. EXTRAPOLATE BY SPLINE
C     PIMPCT (C*2)        :TYPE OF PROCESS:
C                          CX = CHARGE EXCHANGE
C                          EX = EXCITATION
C                          IO = IONIZATION
C                          RC = RECOMBINATION
C                          DISSOSIATION PROCESSES ARE INCLUDED BEFORE AS THEIR
C                          PRIMARY PROCESS IS ALWAYS ONE OF THESE.
C     S1     (I*4)        :INITIAL STATE SPECIE INDEX (AS S1F)
C     E1     (I*4)        :INITIAL STATE ELECTRONIC INDEX (AS E1F)
C     V1     (I*4)        :INITIAL STATE VIBRATIONAL INDEX (AS V1F)
C     S2     (I*4)        :FINAL STATE SPECIE INDEX (AS S2F)
C     E2     (I*4)        :FINAL STATE ELECTRONIC INDEX (AS E2F)
C     V2     (I*4)        :FINAL STATE VIBRATIONAL INDEX (AS V2F)
C     COUPS1 (C*1)        :UPPER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                           (S FOR SIGMA, P FOR PI, ETC)
C     COUPS2 (C*1)        :LOWER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                           (S FOR SIGMA, P FOR PI, ETC)
C     AVFILE (C*80)       :A-VALUES DIRECTORY

C
C     OUTPUT:
C
C     TRAT   (R*8) (,)    :ARRAY OF MAXWELLIAN RATES FOR INPUT ENERGY VALUES
C     PIMPCT (C*2)        :TYPE OF PROCESS:
C                          CX = CHARGE EXCHANGE
C                          EX = EXCITATION
C                          IO = IONIZATION
C                          DISSOSIATION PROCESSES ARE INCLUDED BEFORE AS THEIR
C                          PRIMARY PROCESS IS ALWAYS ONE OF THESE.
C     UPSRT  (I*2)        :TYPE OF OUTPUT
C                          1 => UPSILONS
C                          2 => RATES (CM3/S)
C     FXPH   (I*4)        :FIRST EXTRAPOLATED POINT AT HIGH ENERGIES
C                          (0 NO POINTS EXTRAPOLATED AT HIGH ENERGIES)
C     LXPL   (I*4)        :LAST EXTRAPOLATED POINT AT LOW ENERGIES
C                          (0 NO POINTS EXTRAPOLATED AT LOW ENERGIES)
C
C
C     INTERNAL:
C
C     INDx   (I*4)        :MULTIUSE INDEX
```

```
C     TDATA  (C*3)       :CHARACTER FOR CATEG, INPUT OF EXTRAP
C     ETH    (R*8)       :THRESHOLD ENERGY FOR THE PROCESS
C     IENRX  (I*3)       :NUMBER OF ENERGIES TO INTERPOLATE AND EXTRAPOLATE
C     ENRX   (R*8) ()    :ARRAY OF ENERGIES TO INTERPOLATE AND EXTRAPOLATE
C     OMGX   (R*8) ()    :INTERPOLATED COLL. STRENGTHS (X SECTIONS)
C     HEX    (R*8) ()    :ARRAY OF HIGH ENERGIES TO EXTRAPOLATE
C     LEX    (R*8) ()    :ARRAY OF LOW ENERGIES TO EXTRAPOLATE
C     LSETX  (L)         :VARIABLE TO SET THE KNOTS OF SPLINE
C                        .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                        .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                                  (I.E. THEY WERE SET IN A PREVIOUS CALL )
C                        ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                         RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                         TO USE IT AGAIN FOR THE SAME KNOTS)
C     LPASS  (L)         :LOGARITHMIC CONVERSION
C                        .TRUE. => DO NOT CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C                        .FALSE.=> CONVERT INTO LOG FOR
C                                  ENERGIES AND X-SECTS. FOR SPLINE
C     LINTRP (L)   ()    :INTERPOLATION INDEX
C                        .TRUE.  => POINT INTERPOLATED
C                        .FALSE. => POINT EXTRAPOLATED
C     UPTE   (R*8) ()    :THE LAST TWO ENERGY INTERPOLATED POINTS TO NORMALIZE
C     UPTSIG (R*8) ()    :THE LAST SIGMA(OMG) INTERPOLATED POINTS TO NORMALIZE
C     SPL    (L)         :SWITCH TO THE SPLINE EXTRAPOLATION
C     HXOMG  (R*8) ()    :ARRAY OF EXTRAPOLATED SIGMAS(OMG) FOR THE REQUIRED
C                         HIGH ENERGIES
C     LXOMG  (R*8) ()    :ARRAY OF EXTRAPOLATED SIGMAS(OMG) FOR THE REQUIRED
C                         LOW ENERGIES
C     NXPH   (I*3)       :NUMBER OF EXTRAPOLATED POINTS AT HIGH ENERGIES
C     NXPL   (I*3)       :NUMBER OF EXTRAPOLATED POINTS AT LOW ENERGIES
C     HL     (I*2)       :VARIABLE FOR HIGH/LOW ENERGY EXTRAPOLATION
C                         0 -> LOW ENERGY EXTRAPOLATION
C                         1 -> HIGH ENERGY EXTRAPOLATION
C                         3 -> HIGH ENERGY FORMULA EXTRAPOLATION
C                         4 -> LOW ENERGY FORMULA EXTRAPOLATION
C     VINTx  (R*8)       :INTEGRATION VARIABLES
C     MT     (R*8)       :TOTAL MASS (AMU)
C     REDM   (R*8)       :REDUCED MASS (AMU)
C     TAU    (R*8)       :REDUECED EFFECTIVE TEMPERATURE
C     IERR   (I*3)       : ARRAY FOR WRONG FORMULA VALUES FROM INTRP
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          -------------------------------------------------------------
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          EXTRAP     ADAS9XX   EXTRAPOLATES THE OMG OR CROSS SECTION VALUES
C          INTRP      ADAS9XX   INTERPOLATE DATA BY FORMULA OR BY SPLINE
C
C     AUTHOR: F. GUZMN
C
C   VERSION  : 1.0
C   DATE     : 9/11/2009
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  : 1.1
```

```
C   DATE     : 24/07/2012
C   MODIFIED : F. GUZMAN
C             - prepared for Bethe formula in excitation in extrap subrrout.
C
C   VERSION  : 1.2
C   DATE     : 24/10/2012
C   MODIFIED : F. GUZMAN
C             - new condition for extrapolation in case all points are
C               extrapolated in intrp.for.
C             - lpass=.false.
C
C   VERSION  : 1.3
C   DATE     : 25/10/2012
C   MODIFIED : F. GUZMAN
C             - corrected last point of non extrapolated energies for
C               normalization, now they come from original vales not
C               interpolated ones that can change.
C
C  ----------------------------------------------------------------------
```

C.2.7 wrt_mdf33.for

```
      SUBROUTINE WRT_MDF33( OUNIT  , OFILE , MMOL  ,
     &                      INDS   , NDIS  , IN_E  , INDE  ,
     &                      MSYMB  , SYMBS , CH_ION,
     &                      BWNO_I , CH_DIS, BWNO_D,
     &                      COUPSTA, WT    , ECONSA,
     &                      WNO    , WNOD  ,
     &                      INDR   , TCODE , PRCS  ,
     &                      CATEGF , DCH   ,
     &                      S1     , E1    , V1    ,
     &                      S2     , E2    , V2    ,
     &                      NMTE   , NMTM  , DE    ,
     &                      TEI    , TM    , TRAT
     &                     )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: WRITE_MDF33 *******************
C
C     PURPOSE: CREATE A MDF04 FORMAT FILE
C
C  INPUT:
C
C
C     (I*2)   OUNIT     = UNIT WHERE THE OUTPUT WILL BE WRITTEN
C     (C*10)  MSYMB     = MOLECULAR SYMBOL
C     (C*100) OFILE     = NAME OF THE OUTPUT FILE
C     (R*8)   MMOL      = TOTAL MOLECULAR MASS
C     (I*4)   INDS      = MAX. TOTAL INDEX OF SPECIES
C     (I*4)   IN_E(,)   = INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (C*10)  SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (C*6)   CH_ION()  = IONISATION CHANNELS
C     (R*8)   BWNO_I()  = IONISATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (C*6)   CH_DIS(,) = DISSOCIATION CHANNELS
C     (R*8)   BWNO_D(,) = DISSOCIATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*4)   NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C     (I*4)   INDE()    = MAX. INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (C*10)  COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C     (R*8)   WT(,)     = STATISTICAL WEIGHT
C     (R*8)   WNO()     = BOUND ENERGY OF STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)   WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*4)   INDR      = MAX NUMBER OF TRANSITIONS TO WRITE
C     (I*4)   TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
```

```
C                                 1 = DIPOLE
C                                 2 = NON-DIPOLE, NON SPIN CHANGE
C                                 3 = SPIN CHANGE
C                                 4 = OTHER (AMBIGUOUS)
C     (I*4)   PRCS()    = PROCESS NUMBER
C     (I*2)   CATEGF()  = CATEGORY OF COLLISIONAL TRANSITIONS (FINAL ARRAY)
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER NON MAXWELLIAN
C     (I*4)   S1()      = INITIAL STATE SPECIE INDEX
C     (I*4)   E1()      = INITIAL STATE ELECTRONIC INDEX
C     (I*4)   V1()      = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)   S2()      = FINAL STATE SPECIE INDEX
C     (I*4)   E2()      = FINAL STATE ELECTRONIC INDEX
C     (I*4)   V2()      = FINAL STATE VIBRATIONAL INDEX
C     (I*3)   NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C     (I*3)   NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C     (R*8)   TEI()     = ARRAY OF DESIRED TEMPERATURES FOR COLLISIONING
C                         PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)   TM()      = ARRAY OF DESIRED TEMPERATURES FOR TARGET
C                         PARTICLES(MOLECULES) (eV)
C     (R*8)   TRAT(,)   = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                          FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                          THIRD INDEX RUNS OVER TRANSITIONS
C                         IN CASE THAT NMTE=0 ONLY FIRST ELEMENT FILLED
C     (R*8)   DE()      = TRANSITION/THRESHOLD ENERGY FOR A PROCESS
C     (C*6)   DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (C*4)  ECONSA()   = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C
C INTERNAL:
C
C     (I*1)   SPRTR     = PARAMETER = SEPARATRIX (=-1)
C     (I*4)   MNE       = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C
C     (I*4)   C#        = COUNTERS
C     (I*4)   CTOT      = TOTAL NUMBER OF STATES
C     (R*8)   WM12      = (WT-1)/2
C
C
C     AUTHOR: F. GUZMN
C
C  VERSION  : 1.0
C  DATE     : 31/03/2011
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C  VERSION  : 1.1
C  DATE     : 17/05/2011
C  MODIFIED : F. GUZMAN
C     - writes number of temperatures NMTE and
C     NMTM before temperatures
C     - writes INDR before the list of processes
C
C  VERSION  : 1.2
C  DATE     : 31/05/2011
```

```
C  MODIFIED : F. GUZMAN
C     -  included process number for writing in mdf33
C
C  VERSION  : 1.3
C  DATE     : 22/09/2011
C  MODIFIED : F. GUZMN
C    - included the new matrix WNOD(,) that accounts for the
C     electronic asymptotic energy needed after
C
C   VERSION  : 1.4
C   DATE     : 10/10/2011
C   MODIFIED : F. GUZMN
C     included separate atom configuration to account to dissociation
C     products.
C
C VERSION  : 1.5
C DATE     : 21/04/2012
C MODIFIED : F. GUZMN
C     included the new matrix IN_E to account for electronic
C     index independently
C
C
C
C-----------------------------------------------------------------------
```

C.3 ADAS903

```
      PROGRAM ADAS903

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 PROGRAM: ADAS903 *********************
C
C  PURPOSE:
C
C     TO COMPLETE MDF33 FORMAT FILES WITH THE LACKING REACTIONS TO CREATE
C     THE MDF04 FILES READY FOR THE USE FOR A COLLISIONAL RADIATIVE
C     MODEL.
C
C     TO CALCULATE RATES EXCITED-EXCITED IPRATE (EIQIP) IS USED. FOR
C     IONIZATION ECIP WILL BE USED.
C
C     A FUTURE OPCION TO GRYZINSKI OR OTHER CALCULATION WILL BE PROVIDED
C
C     MDF33 FORMAT FILES ARE THE MAXWELLIAN RATES FROM MDF02 CROSS SECTION
C     FILES. HERE THESE VALUES WILL BE UNIFORMIZED TO WORK IN UPSILON OR
C     RATES AS DESIRED IN INPUT
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                     C
C     MAY 2011                                                        C
C                                                                     C
C     THIS ROUTINE IS MADE IN FORTRAN AND WILL BE DESIGNED TO BE RUN  C
C     IN FORTRAN. IT IS EXPECTED TO BE LATER MODIFIED TO BE CALLED    C
C     FROM IDL PROGRAMS                                               C
C                                                                     C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C  ORIGINAL NAME: ADAS903
C
C
C  PROGRAM:
C
C     (I*4)  IUNT10   = PARAMETER = INPUT UNIT FOR DATA
C     (I*4)  IUNIT    = PARAMETER = INPUT UNIT FOR PARAMETERS
C     (I*4)  OUNIT    = PARAMETER = OUTPUT UNIT FOR DATA IN MDF04/MDF14 FORMAT
C     (I*4)  IAUNIT   = PARAMETER = INPUT UNIT FOR A-VALUES RULES
C     (I*4)  NCEST    = PARAMETER = MAX NUMBER OF TRANSITIONS
C     (I*4)  NSP      = PARAMETER = MAX NUMBER OF SPECIES
C     (I*4)  NST      = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C     (R*8)  ME       = PARAMETER = ELECTRON MASS (g)
C     (R*8)  RYEV     = PARAMETER = RYDBERG ENERGY (eV)
C     (R*8)  EV2K     = PARAMETER = FACTOR TO CONVERT EV->K
C
C     (I*4)  C#       = COUNTERS
C     (C*80) PFILE    = PATH TO INPUT DATA SET FILE READ FROM FORTRAN
C     (I*2)  CATEG    = REQUIRED CATEGORY OF COLLISIONAL TRANSITIONS
C                             1 -> UPSILON
```

```
C                            2 -> RATES (CM3/S)
C                            3 -> OTHER NON MAXWELLIAN
C      (I*2)  CATEG(I,F)()= CATEGORY OF OUTPUT COLLISIONAL TRANSITIONS
C                            1 -> UPSILON
C                            2 -> RATES (CM3/S)
C                            3 -> OTHER NON MAXWELLIAN
C      (R*8)  MI        = PROJECTILE MASS (IF ION IMPACT, 0 OTHERWISE)
C      (C*10) MSYMB     = MOLECULAR SYMBOL
C      (R*8)  MMOL      = TOTAL MOLECULAR MASS
C      (I*4)  NSPC      = NUMBER OF SPECIES
C      (I*4)  STI       = NUMBER OF STATES
C      (R*8)  MU        = REDUCED MASS
C      (I*4)  NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C      (C*10) SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C      (C*6)  CH_ION()  = IONISATION CHANNELS
C      (C*6)  CH_DIS(,)= DISSOCIATION CHANNELS
C      (R*8)  BWNO_I()  = IONISATION ENERGY
C                           (MEASURED FROM LOWEST ELECTRONIC STATE
C                            MINIMUM) (cm^-1)
C      (R*8)  BWNO_D(,)= DISSOCIATION ENERGY
C                           (MEASURED FROM LOWEST ELECTRONIC STATE
C                            MINIMUM) (cm^-1)
C      (I*4)  INDS()    = INDEX OF SPECIES
C      (I*4)  INDE()    = INDEX OF ELECTRONIC STATE
C      (C*10) COUPSTA()= COUPLED MOLECULAR STATE ELECTRONIC
C                           CONFIGURATION
C      (R*8)  WT()      = STATISTICAL WEIGHT
C      (C*10) WNO()     = BOUND ENERGY OF STATES
C                           (MEASURED FROM LOWEST ELECTRONIC STATE
C                            MINIMUM) (cm^-1)
C      (R*8)  WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                           (MEASURED FROM LOWEST ELECTRONIC STATE
C                            MINIMUM) (cm^-1)
C      (I*3)  NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C      (I*3)  NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C      (R*8)  TEI()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                           PARTICLES(ELECTRON/IONS) (eV)
C      (R*8)  TM()      = ARRAY OF TEMPERATURES FOR TARGET
C                           PARTICLES(MOLECULES) (eV)
C      (R*8)  TAU()     = ARRAY OF REDUCED TEMPERATURES FOR A DOUBLE
C                          MAXWELLIAN
C      (I*4)  INDR      = NUMBER OF TRANSITIONS
C      (I*4)  TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
C                                  1 = DIPOLE
C                                  2 = NON-DIPOLE, NON SPIN CHANGE
C                                  3 = SPIN CHANGE
C                                  4 = OTHER (AMBIGUOUS)
C      (I*4)  PRCS()    = PROCESS NUMBER
C      (I*4)  SU()      = UPPER STATE INDEX OF A TRANSITION
C      (I*4)  SL()      = LOWER STATE INDEX OF A TRANSITION
C      (I*4)  V1()      = INITIAL STATE VIBRATIONAL INDEX
C      (I*4)  V2()      = FINAL STATE VIBRATIONAL INDEX
C      (I*4)  VL()      = LOWER STATE VIBRATIONAL INDEX
C      (I*4)  VU()      = UPPER STATE VIBRATIONAL INDEX
C      (R*8)  DE()      = TRANSITION/THRESHOLD ENERGY FOR A PROCESS
C      (C*6)  DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C      (R*8)  TRAT(,,) = ARRAY OF MAXWELLIAN RATES OUTPUT FROM XXDATM_33
```

```
C                          FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                          THIRD INDEX RUNS OVER TRANSITIONS
C                         IN CASE THAT NMTE=0 ONLY FIRST AND THIRD INDEX
C                         FILLED
C     (R*8)  QRAT(,) =  ARRAY OF MAXWELLIAN RATES, INDEX OF ELECTRONIC
C                        TEMPERATURE AND DENSITY AS IN TRAT
C     (R*8)  QRATF(,,)= FINAL ARRAY OF MAXWELLIAN RATES, INDEX AS IN TRAT
C     (L)    PFLAG    = FLAG FOR THE ORIGINAL PROCESSES CONSIDERED
C     (L)    PFFLAG() = FLAG FOR THE FINAL PROCESSES CONSIDERED
C     (I*4)  NTCEST   = TOTAL NUMBER OF PROCESSES THAT WILL BE CONSIDERED
C     (I*4)  NFCEST   = FINAL NUMBER OF PROCESSES THAT WILL BE CONSIDERED
C     (I*4)  ISL      = LOWER SPECIES INDEX OF A TRANSITION
C                       (RUNS OVER TOTAL INDEX)
C     (I*4)  ISU      = UPPER SPECIES INDEX OF A TRANSITION
C                       (RUNS OVER TOTAL INDEX)
C     (I*4)  IEL      = LOWER ELECTRONIC STATE INDEX OF A
C                        TRANSITION (RUNS OVER TOTAL INDEX)
C     (I*4)  IEU      = UPPER ELECTRONIC STATE INDEX OF A
C                       TRANSITION (RUNS OVER TOTAL INDEX)
C     (I*4)  SLL      = LOWER STATES OF TRANSITIONS
C     (I*4)  SUU      = UPPER STATES OF TRANSITIONS
C     (I*4)  VL       = LOWER VIB INDEXES OF TRANSITIONS
C     (I*4)  VU       = UPPER VIB INDEXES OF TRANSITIONS
C     (R*8)  IWTL     = LOWER ELECTRONIC STATE STATISTICAL WEIGTH
C                       (RUNS OVER TOTAL INDEX)
C     (R*8)  IWTU     = UPPER ELECTRONIC STATE STATISTICAL WEIGTH
C     (R*8)  IWNOL    = LOWER ENERGY OF STATE
C     (I*4)  M        = NUMBER OF TABULAR VALUES OF COLLISION STRENGTH
C     (R*8)  IZ()     = ION CHARGE
C     (R*8)  ZI       = ION CHARGE
C     (C*80) AVFILE   = A-VALUES DIRECTORY
C     (C*100)FILE1    = CHARACTER FOR OBTAINING DIPOLAR RULES FILES
C     (C*100)DPFILE#  = DIPOLE RULES FOR #-GLET
C     (I*1)  MTPU     = SPIN MULTIPLICITY OF UPPER STATE
C     (I*1)  MTPL     = SPIN MULTIPLICITY OF LOWER STATE
C     (I*4)  NSS      = NUMBER OF ELEMENTS OF THE MATRIX IN DIPOLE RULES
C                        FILE
C     (I*4)  IST()    = STATE NUMBER FOR EACH ROW/COLUMN IN DIPOLE RULES
C                        FILE
C     (I*1)  IDP(,)   = DIPOLE RULES FOR EACH PAIR OF STATES
C                        0 -> NOT ALOWED 1-> ALLOWED
C     (I*2)  IUP      = UPPER STATE COLUMN IN DIPOLE RULES FILE
C     (I*2)  JDW      = LOWER STATE ROW IN DIPOLE RULES FILE
C     (R*8)  AVIJ(,)  = ARRAY WITH THE A-VALUES FOR THE VIB STATES
C     (R*8)  AIJ      = A-VALUE FOR TRANSITION
C     (R*8)  EI,EJ    = RYDBERG ENERGIES OF STATES TO INPUT IN IPMRATE
C     (I*4)  MAXV     = HIGHEST QUANTUM NUMBER READ FROM ENU FILE
C     (I*4)  MAXVU,VUMAX
C                     = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        STATE UP
C     (I*4)  MAXVL, VLMAX
C                     = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        STATE LOW
C     (C*80) DENU     = ENU DIRECTORY
C     (R*8)  IENU()   = ARRAY WITH THE EIGENVALUES FROM 1 TO MAXV1+1
C                        FOR THE UPPER (I) STATE
```

```
C     (R*8)  JENU()   = ARRAY WITH THE EIGENVALUES FROM 1 TO MAXV1+1
C                        FOR THE LOWER (J) STATE
C     (R*8)  ENUU()   = ARRAY WITH THE VIB EIGENVALUES OF THE UPPER STATE
C     (R*8)  ENUL()   = ARRAY WITH THE VIB EIGENVALUES OF THE LOWER STATE
C     (I*4)  VIB      = 1 -> TAKE VIBRONIC RESOLUTION WHEREEVER POSSIBLE,
C                            BY FC FACTORS
C                       2 -> ONLY ELECTRONIC RESOLUTION
C                       3 -> OBTAIN THE RATES ONLY FROM THE DATA ON THE FILE
C     (I*4)  IRST     = COUNTER OF THE NUMBER OF ALWAYS RESOLVED STATES
C     (I*4)  RST()    = ALWAYS RESOLVED STATES
C     (I*4)  MXVR()   = MAXIMUN RESOLVED VIBRATIONAL LEVEL FOR THE ALWAYS
C                        RESOLVED STATES
C     (I*4)  IERR     = ERROR RETURN CODE.
C     (C*1)  LMBDU    = UPPER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (C*1)  LMBDL    = LOWER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (R*8)  T()      = ELECTRON TEMPERATURES (DEGS. K)
C     (R*8)  OMEG()   = COLLISION STRENGTHS (DUMB)
C     (R*8)  DMB      = DUMB VARIABLE
C     (R*8)  QI()     = IPMRATE COLLISIONAL EXCITATION RATE COEFFICIENTS
C     (R*8)  QJ()     = IPMRATE COLLISIONAL DEEXCITATION RATE COEFFICIENTS.
C     (L)    RINDFLAG = FLAG TO MARK THE PROCESS THAT HAVE BEEN READ
C     (I*1)  MOL()    = 1 IS A  MOLECULE; 0 IS AN ION OR ATOM
C     (L)    RSTFLG   = FLAG FOR METASTABLES
C     (L)    CORRIDFLG= FLAG FOR CORRECTION OF BOUND IONIZATION
C     (I*4)  VLL(,)   = ARRAY TO COVER THE RESOLVES LOWER VIBRATIONAL
C                        STATES IN THE CASE VIB=2
C     (R*8)  G        = MOLECULAR DEGENERACY FACTOR
C     (I*4)  NE       = NUMBER OF EQUIVALENT ELECTRONS IN THE GROUND STATE
C     (R*8)  ZETA     = NUMBER OF EQUIVALENT ELECTRON IN THE SHELL
C     (I*4)  NDI      = NUMBER OF DISSOCIATIVE EXCITATION AND IONIZATION
C                        TRANSITIONS
C     (L)    QFLG     = FLAG FOR METASTABLE CALCULATION OF EXCITATION
C     (L)    DIFLG    = FLAG FOR DISSOCIATIVE PROCESSES CALCULATION
C     (L)    QIFLG    = FLAG FOR METASTABLE CALCULATION OF IONIZATION
C     (I*4)  NEDISS   = NUMBER OF DISSOCIATIVE STATES IN THE SPECIE
C     (I*4)  SDISS()  = INDEX NUMBER OF THE DISSOCIATIVE STATES
C     (C*6)  EDCH()   = DISSOCIATION CHANNEL OF THE DISS STATE
C     (R*8)  XI       = EFFECTIVE IONISATION POTENTIAL FOR SHELL.
C                        UNITS: RYD
C     (C*2)  RULE     = SETS THE TYPE OF RULES ARE GOING TO BE READ:
C                        'ED' -> EXCITATION TO DISSOCIATION
C                        'ID' -> IONIZATION TO DISSOCIATION
C     (R*8)  EM       = PROTON ELECTRON MASS RATIO.
C     (R*8)  FC(,)    = ARRAY WITH THE FC FACTORS FOR THE VIB STATES
C     (C*80) FCFILE   = FCF DIRECTORY
C     (C*100)OFILE    = NAME OF THE OUTPUT FILE
C     (L)    INVFLG   = FLAG FOR INVERT PROCESSES WHEN UPPER VIB STATES
C                        ARE UNDER LOWER VIB STATES
C     (R*8)  TST      = TESTING VARIABLE FOR AVIJ TO DISCHARD NOT
C                       CALCULATED FCF
C     (L)    LDSFLG   = FLAG FOR LOWER DISSOCIATIVE STATES
C     (R*8)  LIMIT    = LOW LIMIT VALUE FOR STORAGE OF RATES
C     (R*8)  LIMU     = UPPER SAFE LIMIT VALUE FOR STORAGE OF RATES
C     (L)    IONFREE  = THIS VARIABLE ALLOWS IONIZATION ONLY TO
C                       METASTABLES (.TRUE.)
```

```
C     (L*4)  EDFLG    = .TRUE. EXCITATION ALLOWED FOR DISS EXCITATION.
C                       .FALSE. EXCITATION DIPOLAR FORBIDDEN
C     (C*1)  ECIP_IN  = 'y' USE ECIP FOR BOUND-CONTINUUM PROCESSES
C     (L*4)  ECIPFLG  = 'FALSE' ECIP NOT ALLOWED FROM NON-METASTABLES
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          XXDATM_00  MADAS     READS AND RETURN FC FACTORS
C          XXDATM_33  MADAS     FETCH DATA FROM INPUT MDF33 FORMAT
C          XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C          RD_ENU     MADAS     READS VIBRATIONAL ENERGIES FROM MDF00
C          I4FCTN     ADAS      RETURNS CHARACTER STRING AS AN INTEGER.
C          R8CONST    ADAS      RETURNS THE FUNDAMENTAL CONSTANT
C                                CORRESPONDING TO 'KEY'.C
C          DGFCTR     MADAS     CALCULATES THE DEGENERACY FACTOR FOR MO
C          RT2UPSLN   MADAS     CONVERTS FROM CM3/2 TO UPSILON OR VICEVERSA
C          R8ECIP     ADAS      CALUCLATES THE SHELL CONTRIBUTION TO THE
C                                IONISATION RATE COEFFICIENT IN THE ECIP
C                                APPROXIMATION OF BURGESS.
C          IPMRATE    MADAS     CALCULATES ELECTRON COLLISIONAL EXCITATION
C                                AND DEEXCITATION RATE
C          WRT_MDF04  MADAS     CREATE A MDF04 FORMAT FILE
C
C
C
C     AUTHOR: F. GUZMN
C
C   VERSION  :  1.0
C   DATE     : 27/10/2011
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  :  1.1
C   DATE     : 11/11/2011
C   MODIFIED : F. GUZMAN
C              end of debugging
C
C
C   VERSION  :  2.0
C   DATE     : 17/11/2011
C   MODIFIED : F. GUZMAN
C              changed to writing the matrix in binary files in order to
C              cope with the memory
C
C
C   VERSION  :  2.1
C   DATE     : 16/01/2012
C   MODIFIED : F. GUZMAN
C              introduced ionization only to metastables can be assumed
C              eliminated rule ID and other superfluous variables
C
C
C   VERSION  :  2.2
```

```
C   DATE     : 18/04/2012
C   MODIFIED : F. GUZMAN
C              introduced dipolar rules for dissociative excitation so
C              it is possibel only if it is dipole allowed
C
C
C   VERSION  :  2.3
C   DATE     : 05/05/2012
C   MODIFIED : F. GUZMAN
C              in case that ionization is exothermic there is no way of
C              calculating with ecip, so no calculayion is performed.
C
C
C-----------------------------------------------------------------------
```

C.3.1 dgfctr.for

```
      SUBROUTINE DGFCTR ( LMBDU, LMBDL, G)

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 PROGRAM: ADAS902 **********************
C
C  PURPOSE:  CALCULATES THE DEGENERACY FACTOR g FOR MOLECULAR ORBITALS
C
C
C     INPUT:
C
C     (C*1)  LMBDU      = UPPER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (C*1)  LMBDP      = LOWER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C
C     OUTPUT:
C
C     (R*8)  G          = DEGENERACY FACTOR
C
C     INTERNAL:
C     (C*1)  LMBD       = SPECTROSCOPIC ELECTRONIC LEVEL
C     (R*8)  KU,KL,K    = NUMERICAL ANGULAR MOMENTUM
C     (R*8)  DLTAPLUS   = KRONEKER DELTA: delta_(0,lmbdu+lmbdl)
C     (R*8)  DLTA       = KRONEKER DELTA: delta_(0,lmbdu)
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 15/09/2011
C
C
C-----------------------------------------------------------------------
C
```

C.3.2 ipmrate.for

```
      SUBROUTINE IPMRATE(IZ,EM,WI,EI,WJ,EJ,M,AJI,EPS,
     &                  OMEG,N,T,RAT,QI,QJ)
       IMPLICIT REAL*8(A-H,O-Z)
C-----------------------------------------------------------------------
C
C  ***************** fortran77 program: ipmrate.for ********************
C
C  Purpose:
C   CALCULATES ELECTRON COLLISIONAL EXCITATION AND DEEXCITATION RATE
C   COEFFICIENTS FOR DIPOLE TRANSITIONS IN THE IMPACT PARAMETER
C   APPROXIMATION (BURGESS AND SUMMERS,1976,MON.NOT.R.AST.SOC.,174,345)
C   OPTIONALLY A SET OF INCIDENT ELECTRON ENERGIES AND COLLISION STRENGT
C   MAY BE PROVIDED, IN WHICH CASE THE IMPACT PARAMETER THEORY IS USED T
C   CALCULATE THE COLLISION STRENGTHS AT HIGH ENERGY WITH VALUES SCALED
C   THE HIGHEST ENERGY INPUT COLLISION STRENGTH.
C   EITHER THE ABSORPTION OSCILLATOR STRENGTH OR THE EINSTEIN COEFFICIEN
C   MUST BE PROVIDED, THE OTHER BEING COMPUTED.
C
C  ARGUMENTS
C   IZ,WI,EI,WJ,EJ,M,AJI,EPS(20),OMEG(20),N,T(50),RAT,QI(50),QJ(50)
C
C  SUBROUTINES
C   EIQIP,XIP,YIP,ZERO1
C
C  INPUT
C       IZ=ION CHARGE
C       EM=PROTON ELECTRON MASS RATIO.
C       TRANSITION NAME TAKES THE FORM
C          ELECTRON TRANS.(COLS 11-15), ANGULAR TRANS.(COLS 21-40)
C       WI=STATISTICAL WEIGHT OF STATE I
C       EI=BINDING ENERGY OF STATE I (RYDBERGS)
C       WJ=STATISTICAL WEIGHT OF STATE J
C       EJ=BINDING ENERGY OF STATE J (RYDBERGS)
C       M=NUMBER OF TABULAR VALUES OF COLLISION STRENGTH
C       FIJ=ABSORPTION OSCILLATOR STRENGTH FOR TRANSITION
C       AJI=EINSTEIN COEFFICIENT FOR TRANSITION
C       EPS(K)=INCIDENT ELECTRON ENERGIES (RYDBERGS)
C       OMEG(K)=COLLISION STRENGTHS
C       N=NUMBER OF ELECTRON TEMPERATURES
C       T(I)=ELECTRON TEMPERATURES (DEGS. K)
C
C  OUTPUT
C   RAT=RATIO OF OMEG(M) TO I.P. OMEGA.
C   QI(I)=COLLISIONAL EXCITATION RATE COEFFICIENTS
C   QJ(I)=COLLISIONAL DEEXCITATION RATE COEFFICIENTS.
C
C  AUTHOR
C   HUGH SUMMERS     1977/5/20
C
C  COMMENTS
C   I IS THE LOWER LEVEL OF THE TRANSITION.
C   M MAY BE ZERO, IN WHICH CASE NO EPS AND OMEG VALUES ARE REQUIRED.
C   UNDERFLOW IS NOT TRAPPED. THIS MAY BE ACHEIVED IN IBM FORTRAN WITH T
C
```

```
C-----------------------------------------------------------------------
C
C  ADAS804 version - original version H P Summers 20-05-1977.
C
C  VERSION  : 1.1
C  DATE     : 10-03-2010
C  MODIFIED : rtin O'Mullane
C             - First ADAS version in CVS.
C
C  VERSION  : 2.0
C  DATE     : 12-10-2011
C  MODIFIED : Francisco Guzman
C             - included EM to account for proton impact in EIQQIP
C             - changed name to ipmrate and located in adas903 directory
C
C  VERSION  : 2.1
C  DATE     : 11-11-2011
C  MODIFIED : Francisco Guzman
C             - changed dimension of EPS, OMG QI, QJ and T arrays to
C               avoid core dumps
C             - removed not used array A(50)
C
C-----------------------------------------------------------------------
```

C.3.3 wrt_mdf04.for

```
      SUBROUTINE WRT_MDF04( OUNIT  , OFILE ,
     &                      IUNIT  , IFILE ,
     &                      MMOL   , NSPC  , STI    ,
     &                      INDS   , NDIS  , INDE   ,
     &                      MSYMB  , SYMBS , CH_ION,
     &                      BWNO_I , CH_DIS, BWNO_D,
     &                      COUPSTA, WT    , ECONSA,
     &                      WNO    , WNOD  ,
     &                      INDR   ,
     &                      NMTE   , NMTM  ,
     &                      TEI    , TM
     &                     )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: WRITE_MDF04 *******************
C
C     PURPOSE: CREATE A MDF04 FORMAT FILE
C
C  INPUT:
C
C
C     (I*2)   OUNIT     = UNIT WHERE THE OUTPUT WILL BE WRITTEN
C     (C*10)  MSYMB     = MOLECULAR SYMBOL
C     (C*100) OFILE     = NAME OF THE OUTPUT FILE
C     (I*2)   IUNIT     = UNIT FROM THE INPUT BINARY FILE
C     (c*100) IFILE     = NAME OF INPUT BINARY FILE
C     (R*8)   MMOL      = TOTAL MOLECULAR MASS
C     (I*4)   NSPC      = NUMBER OF SPECIES
C     (I*4)   STI       = NUMBER OF STATES
C     (I*4)   INDS()    = INDEX OF SPECIES
C     (C*10)  SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (C*6)   CH_ION()  = IONISATION CHANNELS
C     (R*8)   BWNO_I()  = IONISATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (C*6)   CH_DIS(,) = DISSOCIATION CHANNELS
C     (R*8)   BWNO_D(,) = DISSOCIATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*4)   NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C     (I*4)   INDE()    = MAX. INDEX OF ELECTRONIC STATE FOR EACH IND_S
C     (C*10)  COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C     (R*8)   WT(,)     = STATISTICAL WEIGHT
C     (R*8)   WNO()     = BOUND ENERGY OF STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)   WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
```

```
C     (I*4)   INDR      = MAX NUMBER OF TRANSITIONS TO WRITE
C     (I*3)   NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C     (I*3)   NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C     (R*8)   TEI()     = ARRAY OF DESIRED TEMPERATURES FOR COLLISIONING
C                         PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)   TM()      = ARRAY OF DESIRED TEMPERATURES FOR TARGET
C                         PARTICLES(MOLECULES) (eV)
C     (C*6)   DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (C*4)  ECONSA()   = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C
C INTERNAL:
C
C     (I*4)   TCODE     = ELECTRONIC TRANSITION SUBCATHEGORY
C                                 1 = DIPOLE
C                                 2 = NON-DIPOLE, NON SPIN CHANGE
C                                 3 = SPIN CHANGE
C                                 4 = OTHER (AMBIGUOUS)
C     (I*4)   PRCS      = PROCESS NUMBER
C     (I*2)   CATEGF    = CATEGORY OF COLLISIONAL TRANSITIONS (FINAL ARRAY)
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER NON MAXWELLIAN
C     (I*4)   S1        = INITIAL STATE SPECIE INDEX
C     (I*4)   E1        = INITIAL STATE ELECTRONIC INDEX
C     (I*4)   V1        = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)   S2        = FINAL STATE SPECIE INDEX
C     (I*4)   E2        = FINAL STATE ELECTRONIC INDEX
C     (I*4)   V2        = FINAL STATE VIBRATIONAL INDEX
C     (R*8)   TRAT(,)   = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                          FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                         IN CASE THAT NMTM=0 ONLY FIRST ELEMENT FILLED
C     (I*1)   SPRTR     = PARAMETER = SEPARATRIX (=-1)
C     (I*4)   MNE       = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C
C     (I*4)   C#        = COUNTERS
C     (I*4)   CTOT      = TOTAL NUMBER OF STATES
C     (R*8)   WM12      = (WT-1)/2
C
C
C     AUTHOR: F. GUZMN
C
C  VERSION  : 2.0
C  DATE     : 31/03/2011
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C             CREATED FROM WRT_MDF04 REMOVING THE ARRAY OF ENERGY
C              DIFFERENCE: DE
C
C   VERSION  : 3.0
C   DATE     : 17/11/2011
C   MODIFIED : F. GUZMAN
C              changed to read the matrix from binary files in order to
c              cope with the memory
C
C-----------------------------------------------------------------------
```

C.4 ADAS904

```
      PROGRAM ADAS904

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 PROGRAM: ADAS904 *********************
C
C  PURPOSE:
C
C     TO CALCULATE LOW LEVEL POPULATION FOR MOLECULES AND THEIR ATOMIC
C     PRODUCTS. MDF04 FILES ARE USED AS A SOURCE DATA TO COMPLETE THE
C     MATRIX. COEFFICIENTS ARE CONSTRUCTED USING ELECTRON, ION AND ATOM
C     IMPACT DATA AND THE TRANSITIONS PRESENT IN MDF04 ARE CONSIDERED.
C
C     IONIZATION, RECOMBINATION AND DISSOCIATIVE PARTIAL AND TOTAL
C     COLLISIONAL RADIATIVE COEFFICIENTS ARE GIVEN AS OUTPUT AS WELL AS
C     POPULATIONS
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                      C
C     2011                                                         C
C                                                                      C
C     THIS ROUTINE IS MADE IN FORTRAN AND WILL BE DESIGNED TO BE RUN  C
C     IN FORTRAN. IT IS EXPECTED TO BE LATER MODIFIED TO BE CALLED    C
C     FROM IDL PROGRAMS                                                C
C                                                                      C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C  ORIGINAL NAME: ADAS904
C
C
C  PROGRAM:
C
C     (I*4)  IUNIT    = PARAMETER = INPUT UNIT FOR PARAMETERS
C     (I*4)  TMPUNIT  = PARAMETER = UNIT FOR TEMPORAL FILE IN CASE IRDMD=2
C     (I*4)  NMF      = PARAMETER = MAX NUMBER OF INPUT DATA FILES
C     (I*4)  MNT      = PARAMETER = MAX NUMBER OF DESIRED TEMPERATURES
C     (I*4)  NST      = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C     (I*4)  MNV      = PARAMETER = MAX NUMBER OF VIB STATES
C     (I*4)  NMMST    = PARAMETER = MAX NUMBER OF MOL. METASTABLE STATES
C     (I*4)  NMOST    = PARAMETER = MAX NUMBER OF MOL. ORDINARY STATES
C     (I*4)  NMAST    = PARAMETER = MAX NUMBER OF ATOMIC ORDINARY STATES
C     (I*4)  NMAMST   = PARAMETER = MAX NUMBER OF ATOMIC METASTABLES
C     (I*4)  NMMI     = PARAMETER = MAX NUMBER OF MOLECULAR IONS
C     (I*4)  ELIM     = PARAMETER = DIMENSION OF OUTPUT ARRAYS OF
C                                    XXDATAM_04
C     (R*8)  RYEV     = PARAMETER = RYDBERG ENERGY (eV)
C     (I*4)  NMSP     = PARAMETER = MAX TOTAL NUMBER OF SPECIES
C     (I*4)  IRDMD    = PARAMETER = SWITCH THE MODE OF READING MDF04. IN THIS
C                                    PROGRAM ITS VALUE IS SET TO 2 TO READ
C                                    MATRIX FOR ONE TEMPERATURE
C     (I*4)  TMPCFF   = PARAMETER = TEMP FILE UNIT WHERE THE COEFS ARE WRITEN
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C     (I*4)  TMPPOP   = PARAMETER = OUTPUT FILE UNIT FOR POPULATION RESULTS
C     (I*4)  NDMET    = PARAMETER = MAX. NUMBER OF METASTABLES ALLOWED
C                        FOR THE ATOMIC PARENT INDEX (REQUIRED FOR ADF04)
C     (I*4)  NCF      = PARAMETER =  NUMBER OF COEFFICIENTS
C
C     (I*4)  C#       = COUNTERS
C     (C*80) DMADAS   = MADAS/MADAS/ PATH
C     (C*80) DADAS    = CENTRAL ADAS PATH
C     (C*80) AVFILE   = A-VALUES DIRECTORY
C     (C*80) PFILE()  = PATH TO INPUT DATA SET FILE READ FROM FORTRAN
C     (C*80) AUFILE   = AUTOIONISATION FILE PATH
C     (C*80) PRFILE   = PREDISSOCIATION FILE PATH
C     (I*4)  NPFILES  = NUMBER OF MDF04 FILES TO BE INCLUDED
C     (I*4)  FUNIT()  = UNIT FILE WHERE ALLOCATED INPUT DATA FILES
C                        (FROM 41 ON)
C     (C*1)  FCLASS() = DATA CLASS OF THE FILE:
C                          'E' ELECTRON IMPACT
C                          'I' ION IMPACT
C     (C*1)  DEFAULT_T= IF 'Y' USES DEFAULT TEMPERATURES FROM FILES
C     (C*1)  TE_EQ_TI = IF 'Y' SETS TI=TE AND TOGETHER WITH DEFAULT
C                        USES TEMPERATURES FROM ELECTRON IMPACT FILES
C     (I*4)  IENRP    = NUMBER OF ENERGIES TO INTERPOLATE
C     (R*8)  ENRP()   = ARRAY OF INTERPOLATION ENERGIES REQUIRED
C     (I*3)  NMTM     = NUMBER OF MOLECULAR TEMPERATURES FROM DATA FILES
C     (I*3)  NMTE     = NUMBER OF ELECTRON AND ION TEMPERATURES FROM
C                        DATA FILES
C     (R*8)  TE()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                        ELECTRON (eV)
C     (R*8)  TI()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                        IONS/ATOMS (eV)
C     (R*8)  TM()     = ARRAY OF TEMPERATURES FOR TARGET
C                        PARTICLES(MOLECULES) (eV)
C     (R*8)  TEO, TMO = ELECTRON/ION/MOLECULE DESIRED
C                        TEMPERATURES
C     (R*8)  TAU      = REDUCED(ION IMPACT) OR ELECTRONIC TEMPERATURE
C     (I*4)  NNES     = NUMBER OF DENSITIES (MAX MNT)
C     (I*4)  NTE      = NUMBER OF DESIRED ELECTRON/ION TEMPERATURES
C     (I*4)  NTM      = NUMBER OF DESIRED MOLECULAR TEMPERATURES
C     (R*8)  NE()     = DENSITIES ARRAY
C     (L*4)  NOTMP    = .TRUE. TMPFILE ALREADY WRITEN (DO NOT WRITE IT)
C     (I*4)  ITEI,ITM = INDEX OF THE ELECTRON/ION/MOLECULE DESIRED
C                        TEMPERATURES
C     (R*8)  TEI()    = ARRAY OF TEMPERATURES FOR COLLISIONING
C                        PARTICLES(ELECTRON/IONS) (eV)
C     (C*2)  SRCH     = NEEDED FOR XXDATM_04 BUT OF NO EFFECT IN THIS
C                        PROGRAM
C     (C*10) MSYMB    = MOLECULAR SYMBOL
C     (C*10) SYMBS()  = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (R*8)  MMOL     = TOTAL MOLECULAR MASS
C     (R*8)  MP       = PROJECTILE MASS (ASSUMED 0 IN THE ELECTRON
C                       IMPACT CASE)
C     (R*8)  MT       = TOTAL MASS
C     (C*6)  CH_ION() = IONISATION CHANNELS
C     (R*8)  BWNO_I() = IONISATION ENERGY
C                        (MEASURED FROM LOWEST ELECTRONIC STATE
C                         MINIMUM) (cm^-1)
C     (C*6)  CH_DIS(,)= DISSOCIATION CHANNELS
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C     (R*8)  BWNO_D(,)= DISSOCIATION ENERGY
C                        (MEASURED FROM LOWEST ELECTRONIC STATE
C                         MINIMUM) (cm^-1)
C     (I*4)  STI      = STATE INDEX AND NUMBER OF STATES FROM DATA FILES
C     (I*4)  NSP      = NUMBER OF SPECIES FROM DATA FILES
C     (I*4)  INDS()   = INDEX OF SPECIES
C     (I*4)  INDE()   = INDEX OF ELECTRONIC STATE
C     (C*10) COUPSTA()= COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C     (C*4)  ECONSA() = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C     (R*8)  WT()     = STATISTICAL WEIGHT
C     (C*10) WNO()    = BOUND ENERGY OF STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)  WNOD()   = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C     (I*4)  INDR     = NUMBER OF TRANSITIONS
C     (I*4)  INDRF    = TOTAL NUMBER OF TRANSITIONS IF THERE ARE
C                        SEVERAL INPUT FILES
C     (I*4)  CATEGF() = CATEGORY OF COLLISIONAL TRANSITIONS
C                         1 -> UPSILON
C                         2 -> RATES (CM3/S)
C                         3 -> OTHER NON MAXWELLIAN
C     (I*4)  TCODE()  = ELECTRONIC TRANSITION SUBCATHEGORY
C                               1 = DIPOLE
C                               2 = NON-DIPOLE, NON SPIN CHANGE
C                               3 = SPIN CHANGE
C                               4 = OTHER (AMBIGUOUS)
C     (I*4)  SU()     = UPPER STATE INDEX OF A TRANSITION
C     (I*4)  SL()     = LOWER STATE INDEX OF A TRANSITION
C     (I*4)  V1()     = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)  V2()     = FINAL STATE VIBRATIONAL INDEX
C     (I*4)  SAU      = READ UPPER SPECIE INDEX OF AN AUTOINISING TRANSITION
C     (I*4)  SAU      = READ UPPER ELEC. INDEX OF AN AUTOINISING TRANSITION
C     (I*4)  VAU      = READ FINAL STATE VIBRATIONAL INDEX OF AN AUTOINISING
C                        TRANSITION
C     (I*4)  VU1/VL1  = V2()/V1() + 1 VIB INDEX
C     (I*4)  PRCS()   = PROCESS NUMBER
C     (C*6)  DCH()    = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (C*6)  DCH()    = DISSOCIATION CHANNEL STRING FOR PREDISSOCIATION
C                       PROCESSES
C     (R*8)  TRAT(,,) = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                        NOT IN USE HERE
C     (R*8)  RAT_ONET(,,,,) = VIB RATES FOR ONE TEMPERATURE
C     (L*4)  DEF_TA/B = .TRUE. -> DEFAULT TEMPERATURES
C     (L*4)  LINTRP()  = INTERPOLATION INDEX
C                        .TRUE.  => POINT INTERPOLATED
C                        .FALSE. => POINT EXTRAPOLATED
C     (L*4)  TITE      = .TRUE. -> TI=TE
C     (I*4)  VIB       = 1 -> TAKE VIBRONIC RESOLUTION WHEREEVER POSSIBLE,
C                             BY FC FACTORS
C                        2 -> ONLY ELECTRONIC RESOLUTION
C                        3 -> OBTAIN THE RATES ONLY FROM THE DATA ON THE FILE
C     (I*4)  IRST     = NUMBER OF ALWAYS RESOLVED MOLECULAR ELECTRONIC STATES
C                        (METASTABLES)
C     (I*4)  RST()    = INDEX OF ALWAYS RESOLVED MOLECULAR ELECTRONIC STATES
C                        (METASTABLES)
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C     (I*4)  VUMAX    = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        UPPER STATE
C     (I*4)  VLMAX    = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                        LOWER STATE
C     (C*80) DENU     = ENU DIRECTORY
C     (R*8)  ENU()    = ARRAY WITH THE EIGENVALUES FROM 1 TO MAXV1+1
C                        FOR THE UPPER (I) STATE
C     (I*4)  MOL()    = 1 IS A  MOLECULE; 0 IS AN ION OR ATOM, INDEX: SPECIES
C     (R*8)  IZ()     = ION/MOLECULE CHARGE
C     (L)    RSTFLGU  = FLAG FOR UPPER METASTABLES
C     (L)    RSTFLGL  = FLAG FOR LOWER METASTABLES
C     (L)    VBINDF   = FLAG TO ASSIGN INDEXES ONLY ONCE
C     (R*8)  MC_RS(,,)= METASTABLES COLLISIONAL MATRIX
C     (R*8)  MC_IS(,,)= ORDINARY STATES <-  METASTABLES COLL. MATRIX
C     (R*8)  MC_RJ(,,)= METASTABLES <- ORDINARY STATES COLL. MATRIX
C     (R*8)  MC_IJ(,,)= ORDINARY STATES COLL. MATRIX
C     (R*8)  QI_RN(,,)= INVERSE CX TO METASTABLES COLL. MATRIX
C     (R*8)  QI_IN(,,)= INVERSE CX TO ORDINARY ST. COLL. MATRIX
C     (R*8)  MQ_NS(,,)= CX FROM METASTABLE COLL. MATRIX
C     (R*8)  MQ_NJ(,,)= CX FROM ORDINARY ST. COLL MATRIX
C     (R*8)  MR_RN(,,)= RECOMBINATION TO METASTABLES COLL. MATRIX
C     (R*8)  MR_IN(,,)= RECOMBINATION TO ORDINARY ST. COLL. MATRIX
C     (R*8)  MS_NS(,,)= IONIZATION FROM METASTABLES COLL. MATRIX
C     (R*8)  MS_NJ(,,)= IONIZATION FROM ORDINARY ST. COLL. MATRIX
C     (R*8)  D_MS(,,) = METASTABLES DISSOCIATION TO METASTABLES
C                        COLL. MATRIX
C     (R*8)  D_IPPS(,,)= METASTABLES DISSOCIATION TO ORDINARY ST.
C                        COLL. MATRIX.
C     (R*8)  D_MJ(,,) = ORDINARY ST. DISSOCIATION TO METASTABLES
C                        COLL. MATRIX
C     (R*8)  D_IPPJ(,,)= ORDINARY ST. DISSOCIATION TO ORDINARY ST.
C                        COLL. MATRIX
C     (L)    ARSTFLGU1/2= FLAGS FOR ATOMIC METASTABLES (PRODUCT 1 OR 2)
C     (R*8)  AVAL(,)  = A VALUES FOR VIB-VIB TRANSITIONS
C     (R*8)  AVAL_T   = SUMMATION OF AVAL FOR EL-EL TRANSITIONS
C     (R*8)  AVAL_L() = SUM OF AVAL FOR THE UPPER EL. STATE.
C     (R*8)  AVAL_U() = SUM OF AVAL FOR THE LOWER EL. STATE
C     (I*4)  EXN()    = HIGH N'S OF EXTRAPOLATED ELECTRONIC/VIBRONIC
C                        STATES
C     (I*4)  EXV      = NUMBER OF COUNTED VIBRATIONAL STATES PER
C                        EXTRAPOLATED N
C     (I*4)  MXN      = NUMBER OF EXTRAPOLATED NS
C     (I*4)  NMST()   = REAL NUMBER OF METASTABLES PER MOL. SPECIE
C     (I*4)  NOST()   = REAL NUMBER OF ORDINARY ST. PER MOL. SPECIE
C     (R*8)  ZEFF     = EFFECTIVE CHARGE OF PLASMA
C     (I*4)  NCPOP    = NUMBER OF MOLECULAR CONSTANT POPULATIONS
C     (I*4)  STCPOP() = STATE INDEX WITH CONSTANT POPULATION
C     (I*4)  VCPOP()  = VIBRATIONAL INDEX WITH CONSTANT POPULATION
C     (R*8)  CPOP()   = ARRAY WITH THE DENSITIES OF THE CNSTNT POP.
C     (C*1)  THIS_IS_H= IF 'y' SWITCHES ON THE SPECIAL FEATURES FOR
C                        H2 MOLECULAR MODEL (ITERATIONS)
C     (L*4)  TIH      = .TRUE. IF THIS_IS_H=='y'
C     (I*4)  NACPOP   = NUMBER OF ATOMIC CONSTANT POPULATIONS
C     (I*4)  ASPCPOP()= SPECIE INDEX NUMBER FOR CONSTANT POPULATIONS
C     (I*4)  NITE     = NUMBER OF ITERATIONS
C     (I*4)  IT       = ITERATION INDEX
C     (I*4)  NATSP    = NUMBER OF ATOMIC SPECIES
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C     (I*4)  NASP()   = ATOMIC SPECIE INDEX OVER NATSP
C     (I*4)  ION_ALWD()= IF '1' THEN IS POSSIBLE IONISATION FROM IT.
C                        IF '0' IONISATION NOT POSSIBLE (I.E. BARE ION)
C     (I*4)  NMAXPRD()= MAX. NUMBER OF ATOMIC PRODUCTS LEVELS
C     (I*4)  IATMET() = NUMBER OF METASTABLES PER ATOMIC SPECIE
C     (I*4)  ATMET(,) = METASTABLE PER ATOMIC SPECIE IN LEVEL INDEX
C     (I*4)  CN       = COUNTER FOR DEFAULT TEMPERATURES
C     (I*4)  IRM()    = INDR FOR DATA FILE READ
C     (I*4)  NMOLSP   = NUMBER OF MOLECULAR SPECIES
C     (I*4)  IERR     = '1' ERROR ON OUTPUT FROM SUBROUTINE
C     (L*4)  CPOPFLG  = CONSTANT POPULATION FLAG
C     (I*4)  SNMST()  = ELECTRONIC STATE INDEX FOR MOLECULAR METASTABLE
C     (I*4)  VNMST()  = VIB STATE INDEX FOR MOLECULAR METASTABLE
C     (I*4)  NMOLST   = TOTAL NUMBER OF MOLECULAR STATES
C     (I*4)  VBM(,)   = INDEX OF METASTABLE FOR SPECIE
C                        (1ST DIM=STATE, 2ND DIM=VIB INDEX)
C     (I*4)  VBOM(,)  = INDEX OF ORDINARY ST. FOR SPECIE
C                        (1ST DIM=STATE, 2ND DIM=VIB INDEX)
C     (I*4)  VBMU(,)  = INDEX OF ATOMIC METASTABLES
C                        (1ST DIM= AT. SPECIE, 2ND DIM= AT. METAST)
C     (I*4)  VBIPP(,) = INDEX OF ORDINARY AT. STATES
C                        (1ST DIM= AT. SPECIE, 2ND DIM= AT. STATE)
C     (I*4)  NMMPOP   = TOTAL NUMBER OF POPULATION OF METASTABLES TO SOLVE
C     (I*4)  SPOP()   = OUTPUTS ORIGINAL STATE TO NEW STATE INDEX
C     (I*4)  VPOP()   = OUTPUTS VIB STATE TO NEW STATE INDEX
C     (I*4)  N_INDS() = SPECIE INDEX FOR THE SOLVING METASTABLES GROUP
C     (I*4)  NSTAT    = TOTAL NUMBER OF ATOMIC STATES
C     (I*4)  NATM     = NUMBER OF ATOMIC METASTABLES
C     (I*4)  SNATM()  = ELECTRONIC STATE INDEX FOR ATOMIC METASTABLE
C     (I*4)  VNATM()  = VIB STATE INDEX FOR ATOMIC METASTABLE
C     (I*4)  NOSTAT   = NUMBER OF ORDINARY ATOMIC STATES
C     (R*8)  NHP_I()  = INITIAL DENSITY OF PROTONS
C     (R*8)  NHP      = CORRECTED (AFTER ITERATION) DENSITY OF PROTONS
C     (R*8)  NH_I     = INITIAL DENSITY OF NEUTRALS
C     (R*8)  NH       = CORRECTED (AFTER ITERATION) DENSITY OF NEUTRALS
C     (I*4)  IR()     = INDEX FOR READ TRANSITION
C     (I*4)  SP1,SP2  = NUMBER OF ATOMIC SPECIE OF BOTH PRODUCTS IN
C                       DISSOCIATION PROCESSES
C     (I*4)  NUM1,NUM2= NUMBER OF ATOMIC INDEX FOR SPECIES SP1/SP2
C     (I*4)  PRD_11/21= SPECIES INDEX OF DISSOCIATION PRODUCTS
C     (I*4)  PRD_12/22= STATE INDEX OF THE DISSOCIATION PRODUCTS
C     (I*4)  NFLG     = N LEVEL NUMBER EXTRAPOLATED
C     (R*8)  AR       = AUTOIONISATION RATE
C     (R*8)  PR(,)    = PREDISSOCIATION RATE
C     (I*4)  RD       = NUMBER OF PREDISSOCIATIONS TRANSITIONS
C                       FROM THE INITIAL STATE
C     (R*8)  CIJ(,)   = GENERAL COLLISIONAL MATRIX FOR CALCULATIONS
C     (I*4)  NDLEV    = NUMBER OF ENERGY LEVELS FOR INTPUT IN
C                       MR2MCD
C     (R*8)  CRS(,)   = GENERAL METASTABLES COLL MATRIX FOR CALCULATIONS
C     (R*8)  CIS(,)   = GENERAL METASTABLES -> ORD. STATES  COLL MATRIX
C                       FOR CALCULATIONS
C     (R*8)  CRJ(,)   = GENERAL ORD. ST. -> METASTABLES COLL MATRIX
C                       FOR CALCULATIONS
C     (R*8)  CDCRS(,) = MATRIX OF CR EFFECTIVE COEFFICIENTS
C     (R*8)  MQCD(,,) = MQCD MATRIX
C     (C*1)  REC      = 'Y' RECOMBINATION ALLOWED
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C      (L*4)  RECFLG   = FLAG TO ALLOW RECOMBINATION
C      (R*8)  MACD(,,) = MACD MATRIX
C      (R*8)  MSCD(,,) = MSCD MATRIX
C      (C*1)  CXI      = 'Y' INVERSE CX ALLOWED
C      (L*4)  CXIFLG   = FLAG FOR ALLOWED INVERSE CX
C      (R*8)  CXIACD(,,)= MCXIACD MATRIX
C      (C*1)  CX       = 'Y' CX ALLOWED
C      (L*4)  CXFLG    = FLAG FOR ALLOWED CX
C      (R*8)  MCXCD(,,)= MCXCD MATRIX
C      (R*8)  CMJPP(,,)= MATRIX ATOMIC METASTABLES-ORDINARY LEVELS TRANSITIONS
C      (R*8)  CIPPM(,,)= MATRIX ATOMIC ORDINARY-METASTABLES LEVELS TRANSITIONS
C      (R*8)  CIPPJPP(,,)= ATOMIC ORDINARY LEVELS TRANSITION MATRIX
C      (R*8)  SMPJPP(,,)= ATOMIC MATRIX ORDINARY LEVELS-> METASTABLES IONIS.
C      (R*8)  SMPM(,,) = ATOMIC METASTABLE LEVELS IONIS. MATRIX
C      (R*8)  RIPPMP(,,)= MATRIX ATOMIC METASTABLES-ORDINARY LEVELS REC.
C      (R*8)  CMM(,)   = ATOMIC METASTABLE-METASTABLE DIAGONAL TERMS
C      (R*8)  AC_IPPJPP(,)= ATOMIC COLLISIONAL MATRIX FOR ORDINARY STATES
C      (R*8)  AC_MJPP(,)= ATOMIC COLLISIONAL MATRIX FOR METASTABLES -> O. ST.
C      (R*8)  AC_IPPM(,)= ATOMIC COLLISIONAL MATRIX FOR METAST. -> ORD. STATES
C      (R*8)  AS_MPJPP(,)= ATOMIC ION. MATRIX FOR ORDINARY ST. -> METASTABLES
C      (R*8)  AC_MM()  = ATOMIC METASTABLE-METASTABLE DIAGONAL TERMS ARRAY
C      (R*8)  DCRS(,)  = MATRIX DISSOCIATION MET-MET
C      (R*8)  DCRJ(,)  = MATRIX DISSOCIATION ORD->MET
C      (R*8)  DCDCRS(,)= MATRIX EFF. COEFF. DISSOCIATION MET-MET
C      (R*8)  DCDMS(,,)= GENERAL MATRIX DISS. EFF. COEFF. MET-MET
C      (R*8)  DDCRS(,) = MATRIX FOR MET->ORD.ST. DISSOCIATION
C      (R*8)  DPCRS(,) = MATRIX FOR MET->MET EFF COEFF OF DISSOCIATION
C      (R*8)  DDCRJ(,) = MATRIX FOR ORD. ST. -> ORD. ST. DISSOCIATION
C      (R*8)  DCDIPPS(,,)= GENERAL MATRIX FOR DISS. EFF COEFF MET->ORD. ST
C      (R*8)  DDCDCRS(,)= MATRIX FOR DISS. EFF COEFF MET->ORD. ST
C      (R*8)  PDCD(,,) = PDCD EFFECTIVE COEFFICIENT MATRIX
C      (R*8)  CJIMO(,) = INVERSE CJI MATRIX FOR MOLEC. ORD STATES
C      (L*4)  LSOLVE   = .TRUE. SOLVE THE MATRIX EQUATION
C                        .FALSE. INVERTS THE MATRIX
C      (R*8)  DUM()    = DUMMY ARGUMENT TO 'XXMINV'. DIMENSION: NMOST
C      (R*8)  DINT     = DUMMY ARGUMENT TO 'XXMINV'.
C      (R*8)  MIC_JI(,,)=  INVERSE MATRIX OF ORDINARY STATES
C      (R*8)  SUMI/J/K = SUMMATORY OVER INDEXES
C      (R*8)  MXCD(,,) = MXCD EFFECTIVE COEFFICIENT MATRIX
C      (R*8)  DCDMJ(,) = MATRIX OF DISS. EFFECTIVE COEFFICIENTS MET->MET
C      (R*8)  PXDCD(,,)= PXDCD EFFECTIVE COEFFICIENTS MATRIX
C      (R*8)  CJPPIPP_IN(,)= INVERSE CJI MATRIX FOR AT. ORD. STATES
C      (R*8)  DUMA()   = DUMMY ARGUMENT TO 'XXMINV'. DIMENSION: NMAST
C      (R*8)  DXCD(,)  = DXCD EFFECTIVE COEFFICIENT MATRIX
C      (R*8)  PXSDCD(,,)= PXSDCD EFFECTIVE COEFFICIENTS MATRIX
C      (R*8)  ACD(,,)  = MATRIX ACD COEFFICIENTS FOR THE DIFFERENT
C                         ATOMIC SPECIES
C      (R*8)  SCD(,,)  = MATRIX SCD COEFFICIENTS FOR THE DIFFERENT
C                         ATOMIC SPECIES
C      (R*8)  QCD(,,)  = MATRIX QCD COEFFICIENTS FOR THE DIFFERENT
C                         ATOMIC SPECIES
C      (R*8)  XCD(,,)  = MATRIX ACD COEFFICIENTS FOR THE DIFFERENT
C                         ATOMIC SPECIES
C      (I*4)  NODATA() = '1' ADFFILE DOES NOT EXIST
C      (I*4)  NODATA11(,)= '1' ADF11 FILE DOES NOT EXIST
C      (R*8)  AACD(,)  = MATRIX FOR THE ATOMIC EFFECTIVE ACD COEFFICIENTS
C      (R*8)  ASCD(,)  = MATRIX FOR THE ATOMIC EFFECTIVE SCD COEFFICIENTS
```

```
C     (R*8)  AQCD(,)  = MATRIX FOR THE ATOMIC EFFECTIVE ACD COEFFICIENTS
C     (R*8)  AXCD(,)  = MATRIX FOR THE ATOMIC EFFECTIVE SCD COEFFICIENTS
C     (R*8)  GARR()   = ARRAY WITH THE FLUX CONTRIBUTION TO THE POPULATIONS
C     (R*8)  FMAT(,)  = COLLISIONAL MATRIX TO CALCULATE POPULATIONS
C     (I*4)  NDMAX    = NUMBER OF TOTAL POPULATION LEVELS
C     (R*8)  POP()    = ARRAY WITH THE SOLUTION OF THE POPULATIONS
C     (R*8)  FHMAT    = COLLISIONAL VALUE FOR SOLVING HYDROGEN POPULATION
C     (R*8)  FHPMAT   = COLLISIONAL VALUE FOR SOLVING PROTONS POPULATION
C     (R*8)  NH_TMP   = TEMPORAL VALUE OF HYDROGEN DENSITY
C     (R*8)  NHE()    = ITERATION BY ITERATION VALUE OF HYDROGEN DENSITY
C     (R*8)  NHPE(,)  = ITERATION BY TITERATION VALUE OF IONIC DENSITY
C                        (2ND DIM: DENSITY INDEX)
C     (I*4)  OUNIT()  = OUTPUT UNIT FOR MDF11 FILES
C     (C*80) OPATH    = OUTPUT DIRECTORY
C     (I*4)  SB()     = SPECIE TOTAL INDEX
C     (I*4)  NF       = NUMBER OF FILES READ
C     (R*8)  DE       = TRANSITION ENERGY DIFFERENCE
C     (I*4)  SAT/SAT5 = ATOMIC STATE TOTAL INDEX
C     (R*8)  ANUM     = DIAGONAL TERMS FOR ITERATION IN NEUTRALS AND PROTONS
C     (I*4)  NDISS    = NUMBER OF DISSOCIATIVE STATES
C     (I*4)  DISS()   = DISSOCIATIVE STATES INDEX
C     (I*4)  P11,12,21,22()= INDEX OF PRODUCTS FROM DISSOCIATIVE STATE
C     (I*4)  DSNUM    = DISSOCIATION INDEX
C     (L*4)  DSFLG    = DISSOCIATIO FLAG
C     (I*4)  A,B      = VIB VALUES TO DISCRIMINATE IN RAT
C     (I*4)  SHM      = NEGATIVE H SPECIE INDEX
C     (L*4)  HM       = IF H- EXIST DISSOCIATION TO IT IS ALLOWED
C     (C*1)  LMBDU    = UPPER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (C*1)  LMBDL    = LOWER STATE SPECTROSCOPIC ELECTRONIC LEVEL
C                         (S FOR SIGMA, P FOR PI, ETC)
C     (R*8)  G        = MOLECULAR DEGENERACY FACTOR
C     (R*8)  FJS(,)   = EFFECTIVE CONTRIBUTION TO MOLECULAR POPULATIONS
C     (R*8)  QFJS(,,) = EFFECTIVE CONTRIBUTION TO MOLECULAR EXCITED
C                        POPULATIONS
C     (R*8)  AFJS(,,) = EFFECTIVE CONTRIBUTION TO MOLECULAR RECOMBINED
C                        POPULATIONS
C     (R*8)  ICXFJS(,,)= EFFECTIVE CONTRIBUTION TO MOLECULAR ICX
C                        POPULATIONS
C     (R*8)  CXFJS(,,)= EFFECTIVE CONTRIBUTION TO MOLECULAR CX
C                        POPULATIONS
C     (I*4)  NORDPOP  = NUMBER OF ORDINARY STATES TO OUTPUT POPULATION
C     (I*4)  IORDPOP()= ORDINARY STATES FOR OUTPUT POPULATION
C     (C*1)  DOPEC    = 'Y' CALCULATE PECS
C     (C*1)  DOSXB    = 'Y' CALCULATE SXB
C     (C*1)  DODXB    = 'Y' CALCULATE DXB
C     (L*4)  LPEC     = .TRUE.  CALCULATE PECS
C     (L*4)  LSXB     = .TRUE.  CALCULATE SXB
C     (L*4)  LDXB     = .TRUE.  CALCULATE DXB
C     (C*6)  INPT     = 'LAMBDA' WAVELENGTH RANGE
C     (R*8)  LMIN,LMAX= WAVELENGTHS LIMITS FOR BAND CALCULATIONS
C     (I*4)  STLIM()  = STATE LIMITS FOR BAND CALCULATIONS
C     (C*2)  STWLN    = 'ST' OR 'WL' SWITCH FOR BAND LOOKING
C     (I*4)  IBAND    = NUMBER OF BANDS INSIDE SPECTRAL RANGE
C     (I*4)  NBAND(,) = UPPER AND LOWER STATES OF THE BANDS INSIDE
C                        SPECTRAL RANGE
C     (R*8)  LINE(,,) = WAVELENGHT FOR VIB LINES PER BAND.
```

```
C     (R*8)  LSIG(,,) = SIGN OF ENERGY DIFFERENCE, IN CASE THAT
C                         LOWER VIBRATIONAL LEVEL IS HIGGER THAN THE
C                         UPPER LEVEL.
C     (L*4) LOUTBND() = LOWER WAVELENGTH OF BAND UNDER THE GIVEN LIMIT
C     (L*4) UOUTBND() = UPPER WAVELENGTH OF BAND OVER THE GIVEN LIMIT
C     (R*8) SORDPOP(,)= ARRAY WITH ORDINARY STATES POPULATION
C     (R*8) SFJSN     = EXCITATION TERM FJS SUMMED OVER VIB. STATES
C     (R*8) PEC(,)    = PHOTO EMISSION COEFF. FOR MOL. BANDS
C     (R*8) SXB(,)    = SXB FOR MOLECULAR BANDS
C     (R*8) DXB(,)    = DXB FOR MOLECULAR BANDS
C     (R*8) DXB1(,)   = DXB FOR PARTIAL PDCD DISSOCIATION PROCESSES
C     (R*8) DXB2(,)   = DXB FOR PARTIAL PXDCD DISSOCIATION PROCESSES
C     (R*8) DXB3(,)   = DXB FOR PARTIAL DXCD DISSOCIATION PROCESSES
C     (R*8) DXB4(,)   = DXB FOR PARTIAL PXSDCD DISSOCIATION PROCESSES
C     (I*4) IU        = VARIABLE FOR SWITCH BETWEEN VIB CASES
C
C     (I*4)  MCLASS   = MOLECULAR COEFFICIENT CLASS
C     MCLASS                      EFF COEF.
C
C       1                          MQCD
C       2                          MACD
C       3                          MSCD
C       4                          MCXIACD
C       5                          MCXCD
C       6                          PDCD
C       7                          MXCD
C       8                          PXDCD
C       9                          DXCD
C      10                          PXSDCD
C
C
C
C
C==================================================================
C     NOTE : THE MATRICES WILL NOT MAKE MORE THAN 0.5GB AS THEY ARE
C     CURRENTLY DEFINED
C==================================================================
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT      ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          XXDATM_04   MADAS     FETCH DATA FROM MDF04 FORMAT FILES
c          RT2UPSLN    MADAS     CONVERTS FROM CM3/2 TO UPSILON OR VICEVERSA
C          MOLSTATUS   MADAS     TO GET THE MOLECULARITY AND Z FROM SPECIES
C          RD_ENU      MADAS     READS VIBRATIONAL ENERGIES FROM MDF00
C          R8CONST     ADAS      RETURNS THE FUNDAMENTAL CONSTANT
C                                 CORRESPONDING TO 'KEY'.
C          XXDATM_00   MADAS     READS AND RETURN FC FACTORS AND A-VAL
C          GETPRD      MADAS     OBTAINS THE REAL PRODUCT NUMBER IN THE
C                                 ATOMIC INDEX
C          AUTRATE     MADAS     FECH AUTOIONISATION RATES FROM FILES
C          PREDRATE    MADAS     FECH PREDISSOCIATION RATES FROM FILES
C          MR2MCD      MADAS     CONSTRUCTS THE COLLISIONAL-RADIATIVE
C                                 COEFFICIENTS MATRIX
C          RDXXDATA_04 MADAS     RETURNS THE ATOMIC RATE COEFFICIENTS MATRICES
C                                 FROM ADF04 FILES
```

```
C          XXMINV      ADAS      BOTH INVERTS A MATRIX AND SOLVES A SET
C                                 OF SIMULTANEOUS LINEAR EQUATIONS.
C          RDXXDATA_11 MADAS     RETURNS THE ATOMIC EFFECTIVE ADF11
C                                 COEFFICIENTS TO BE USED FOR MCR MODEL
C          WRT_MDF11   MADAS     TO CREATE THE MDF11 FORMAT FILES
C          DGFCTR      MADAS     CALCULATES THE DEGENERACY FACTOR FOR MO
C          SPCTRLBNDS  MADAS     TO OBTAIN THE ENERGY LEVELS AND WAVELENGTH
C                                MOLECULAR BANDS
C
C
C
C     AUTHOR: F. GUZMN
C
C   VERSION  :  1.0
C   DATE     : 22/03/2012
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  :  1.1
C   DATE     : 23/04/2012
C   MODIFIED : F. GUZMAN
C              FULLY DEBUGGED VERSION -  WORKING VERSION
C
C   VERSION  :  1.2
C   DATE     : 25/04/2012
C   MODIFIED : F. GUZMAN
C              included molecular degeneracy factor correction to A-val
c               with routine dgfctr
C
C   VERSION  :  1.3
C   DATE     : 27/04/2012
C   MODIFIED : F. GUZMAN
C              introduced dissociation channel for predissociation products
C              and rationalized autoionization
C
C
C   VERSION  :  1.4
C   DATE     : 01/05/2012
C   MODIFIED : F. GUZMAN
C              introduced dissociation from decay to dissociative state.
C              now spontaneous decay to dissociative is counted as
C              dissociation. The rate is A-val/ne and counts to the
C              effective coefficient.
C
C-----------------------------------------------------------------------
C
```

C.4.1 autrate.for

```
      SUBROUTINE AUTRATE(IFILE, SL, EL, VL, S2, E2, V2, AR, NFLG, IERR)
      IMPLICIT NONE

CC-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: AUTRATE *******************
C
C  PURPOSE: FECH AUTOIONISATION RATES FROM FILES
C
C
C     INPUT:
C
C     (C*80) IFILE  = INPUT FILE
C     (I*4)  SL     = LOWER SPECIE INDEX OF A TRANSITION
C     (I*4)  EL     = LOWER ELECTRONIC INDEX OF A TRANSITION
C     (I*4)  VL     = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)  NFLG   = IF NFLG IS 0 THEN USE SL FOR FETCHING
C                      IF N THEN USE N = N
C
C     OUTPUT:
C
C     (R*8)  AR     = AUTOIONISATION RATE
C     (I*4)  S2     = READ UPPER SPECIE INDEX OF A TRANSITION
C     (I*4)  E2     = READ UPPER ELCTRONIC INDEX OF A TRANSITION
C     (I*4)  V2     = READ FINAL STATE VIBRATIONAL INDEX
C     (I*1)  IERR   = ERROR STATUS
C
C     INTERNAL:
C
C     (C*100)CLINE  = FILE LINE STORAGE
C     (I*4)  S1     = READ LOWER SPECIE INDEX OF A TRANSITION
C     (I*4)  S1     = READ LOWER ELECTRONIC INDEX OF A TRANSITION
C     (I*4)  V1     = READ INITIAL STATE VIBRATIONAL INDEX
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 03/02/2012
C                 FIRST VERSION
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.1
C     DATE      : 27/04/2012
C                 corrected to read specie and electronic index absolute
C                  values.
C
C-----------------------------------------------------------------------
```

C.4.2 getprd.for

```
      SUBROUTINE GETPRD(DMADAS, MSYMB  ,
     &                  CH_DIS, ECONSA ,
     &                  SU    , MOL    , NATSP,
     &                  INDS  , INDE   , DCH  ,
     &                  NASP  , NMAXPRD, ATMET,
     &                  SP1   , SP2    ,
     &                  NUM1  , NUM2
     &                  )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: MR2MCD ********************
C
C  PURPOSE: OBTAINS THE REAL PRODUCT NUMBER IN THE ATOMIC INDEX
C
C
C     INPUT:
C
C     (C*80) DMADAS   = MADAS/MADAS/ PATH
C     (C*10) MSYMB    = MOLECULAR SYMBOL
C     (C*6)  CH_DIS(,)= DISSOCIATION CHANNELS
C     (C*4)  ECONSA() = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                        ATOMS LIMIT
C     (I*4)  SU       = UPPER STATE INDEX OF A TRANSITION
C     (I*4)  MOL()    = 1 IS A  MOLECULE; 0 IS AN ION OR AN ATOM
C     (I*4)  NATSP    = TOTAL NUMBER OF ATOMIC SPECIES
C     (I*4)  INDS()   = INDEX OF SPECIES
C     (I*4)  INDE()   = INDEX OF ELECTRONIC STATE
C     (C*6)  DCH      = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (I*4)  NASP()   = NUMBER OF TOTAL SPECIE OF EACH ATOMIC SPECIE
C     (I*4)  NMAXPRD  = MAX. NUMBER OF ATOMIC PRODUCTS LEVELS
C     (I*4)  ATMET(,) = ATOMIC METASTABLE INDEX FOR EACH ATOMIC SPECIE
C
C     OUTPUT:
C
C     (I*4)  SP1,SP2  = NUMBER OF ATOMIC SPECIE OF BOTH PRODUCTS
C     (I*4)  NUM1,NUM2= NUMBER OF ATOMIC INDEX FOR SPECIES S1/S2
C
C     INTERNAL:
C
C     (I*4)  C#       = COUNTERS
C     (I*4)  NA       = NUMBER OF ATOMIC SPECIES IN FILE
C     (I*4)  IASP()   = MADAS SPECIE NUMBER FOR EACH SPECIE IN FILE
C     (C*80) ATFLS()  = ADF04 PATH FOR EACH ATOMIC SPECIE
C                        (FROM ADAS DIRECTORY)
C     (I*4)  ATST()   = NUMBER OF ATOMIC STATES TO BE READ PER SPECIE
C     (R*8)  IZST()   = ION CHARGE OF EACH SPECIE
C     (I*4)  IMADAS(,)= NUMBER OF STATE IN THE MDF FILES
C     (C*2)  CMADAS(,)= CONFIGURATION FROM SEP. AT. CONF.
C     (I*4)  IADF04(,)= NUMBER OF STATE IN ADF04 FILE
C     (C*18) CADF04(,)= CONFIGURATION STRING IN ADF04 FILE
C     (L)    ADFFLG   = .TRUE. FOUND ADF04 FILE INDEX
C     (I*4)  IERR     = ERROR VAR
```

```
C     (C*80) TFILE()  = PATH FOR ADF11 FILES
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4FCTN     ADAS      RETURNS CHARACTER STRING AS AN INTEGER.
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          XXDATM_25  MADAS     TO FETCH DATA FROM MAPPING FILES MDF25
C
C
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 09/02/2012
C                 FIRST VERSION
C
C
C     VERSION   : 1.1
C     DATE      : 15/02/2012
C     MODIFIED  : F. GUZMAN
C     - restructured so numbering is get from mapping mdf25
C
C
C
C-----------------------------------------------------------------------
```

C.4.3 mr2mcd.for

```
      SUBROUTINE MR2MCD( NDLEV , NMOST ,
     &                   NMMST1, NMMST2,
     &                   CRS   , CIJ   ,
     &                   CRJ   , CIS   ,
     &                   CDCRS , FJS
     &                  )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: MR2MCD *********************
C
C  PURPOSE: CONSTRUCTS THE COLLISIONAL-RADIATIVE COEFFICIENTS MATRIX FROM
C           THE INPUT MATRICES. FOR GENERAL USE
C
C
C     INPUT:
C
C     (I*4)   NDLEV       = NUMBER OF ENERGY LEVELS
C     (I*4)   NMOST       = DIMENSION OF ORDINARY STATES
C     (I*4)   NMMST1      = DIMENSION OF RECEIVING METASTABLES
C     (I*4)   NMMST2      = DIMENSION OF DONNING METASTABLES
C     (R*8)   CRS(,)      = MATRIX OF METASTABLES
C     (R*8)   CRJ(,)      = MATRIX OF METASTABLES-LEVELS RATES
C     (R*8)   CIS(,)      = MATRIX OF LEVELS-METASTABLES RATES
C     (R*8)   CIJ(,)      = MATRIX OF RATES BETWEEN NO-METASTABLES
C
C     OUTPUT:
C
C     (R*8)   CDCRS(,)    = MATRIX OF CR COEFFICIENTS
C     (R*8)   FJS(,)      = EFFECTIVE CONTRIBUTION TO EXCITED POPULATIONS
C
C     INTERNAL:
C
C     (I*4)   IC#         = COUNTERS
C     (R*8)   CIJMO(,)    = INVERSE OF CIJ MATRIX
C     (L)     LSOLVE      = .FALSE. => 'XXMINV' ONLY INVERTS MATRIX.
C     (R*8)   DUM()       = DUMMY ARGUMENT TO 'XXMINV'.
C                            DIMENSION: NMOST
C     (R*8)   DINT        = DUMMY ARGUMENT TO 'XXMINV'.
C     (R*8)   CD32        = RESULT MATRIX AFTER MULTIPLICATION
C     (R*8)   CD12        = RESULT MATRIX AFTER MULTIPLICATION
C
C
C ROUTINES:
C         ROUTINE    SOURCE    BRIEF DESCRIPTION
C         -------------------------------------------------------
C         XXMINV     ADAS      BOTH INVERTS A MATRIX AND SOLVES A SET
C                              OF SIMULTANEOUS LINEAR EQUATIONS.
C         I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C
C     AUTHOR: F. GUZMN
C
```

```
C     VERSION   : 1.0
C     DATE      : 21/12/2011
C                 FIRST VERSION
C
C     VERSION   : 1.1
C     DATE      : 08/02/2012
C     MODIFIED  : F. GUZMAN
C     - changed to accept matrices with dimensions higher than number of
C        metastables, changed call to xxmino to a call to xxminv
C
C     VERSION   : 1.2
C     DATE      : 08/02/2012
C     MODIFIED  ; F. GUZMAN
C     - added possibility of rectangular metastables matrices to allow
C        dissociation calculations
C
C     VERSION   : 2.0
C     DATE      : 26/07/2012
C     MODIFIED  ; F. GUZMAN
C     - added effective contribution to ordinary states populations in
C        order to prepare for PECs and SXB and DXB calculations.
C
C-----------------------------------------------------------------------
```

C.4.4 predrate.for

```
      SUBROUTINE PREDRATE(IFILE, S1, E1, VUM, PR, RD, DCH, IERR)
      IMPLICIT NONE

C
C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: AUTRATE ********************
C
C  PURPOSE: FECH PREDISSOCIATION RATES FROM FILES
C
C
C     INPUT:
C
C     (C*80) IFILE     = INPUT FILE
C     (I*2)  S1        = INITIAL SPECIE TO BE READ
C     (I*2)  E1        = INITIAL ELEC. STATE TO BE READ
C
C     OUTPUT:
C
C     (I*1)  IERR      = ERROR STATUS
C     (I*3)  VUM       = NUMBER OF VIB LEVEL OF HIGHER STATE READ
C     (R*8)  PR()      = PREDISSOCIATION RATES ARRAY
C     (I*4)  RD        = NUMBER OF PREDISSOCIATIONS TRANSITIONS
C                          FROM THE INITIAL STATE
C
C     INTERNAL:
C
C     PARAMETER = MNV = MAX. NUMBER OF VIB STATES
C     C#               = COUNTERS
C     (C*100)CLINE     = FILE LINE STORAGE
C     (I*4)  SU        = HIGHER INITIAL SPECIE READ
C     (I*4)  EU        = HIGHER INITIAL ELECTR. STATE READ
C     (I*4)  SD()      = LOWER FINAL SPECIE READ
C     (I*4)  ED()      = LOWER FINAL ELEC. STATE READ
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 08/02/2012
C                FIRST VERSION
C
C     VERSION   : 1.1
C     DATE      : 27/04/2012
C                introduced dissociation channels and specie and electronic
c                index reading instead of state (which is relative)
C
C-----------------------------------------------------------------------
```

C.4.5 rdxxdata_04.for

```
      SUBROUTINE RDXXDATA_04( DMADAS, DADAS  , MSYMB ,
     &                        NMAXPRD,
     &                        NATSP , NASP   ,
     &                        IATMET, ATMET  ,
     &                        TE    , NE     ,
     &                        CMJPP , CIPPJPP, CIPPM ,
     &                        SMPJPP, SMPM   , RIPPMP,
     &                        CMM   , NODATA
     &                       )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: RDXXDATA_04 ****************
C
C  PURPOSE: RETURNS THE ATOMIC RATE COEFFICIENTS MATRICES FROM THE
C           ATOMIC DATA IN ADF04 FILES
C
C
C     INPUT:
C
C     (C*80)  DMADAS   = MADAS/MADAS/ PATH
C     (C*80)  DADAS    = CENTRAL ADAS PATH
C     (C*10)  MSYMB    = MOLECULAR SYMBOL
C     (I*4)   DIMTRN   = DIMENSION OF THE ATOMIC MATRIX (ORD. LEVELS)
C     (I*4)   NMAXPRD()= MAX. NUMBER OF ATOMIC PRODUCTS LEVELS
C     (I*4)   NATSP    = TOTAL NUMBER OF ATOMIC SPECIES
C     (I*4)   NASP()   = NUMBER OF TOTAL SPECIE OF EACH ATOMIC SPECIE
C     (I*4)   IATMET() = NUMBER OF METASTABLES PER ATOMIC SPECIE
C     (I*4)   ATMET(,) = METASTABLE PER ATOMIC SPECIE IN LEVEL INDEX
C     (R*8)   TE       = INPUT TEMPERATURE (eV)
C     (R*8)   NE       = INPUT DENSITY (CM-3)
C
C     OUTPUT:
C
C     (R*8)   CMJPP(,,)= MATRIX METASTABLES-ORDINARY LEVELS TRANSITIONS
C     (R*8)   CIPPM(,,)= MATRIX ORDINARY-METASTABLES LEVELS TRANSITIONS
C     (R*8)   CIPPJPP(,,)= ORDINARY LEVELS TRANSITION MATRIX
C     (R*8)   SMPJPP(,,)= MATRIX ORDINARY LEVELS-> METASTABLES IONIS.
C     (R*8)   SMPM(,,) = METASTABLE LEVELS IONIS. MATRIX
C     (R*8)   RIPPMP(,,)= MATRIX METASTABLES-ORDINARY LEVELS REC.
C     (R*8)   CMM(,)   = METASTABLE-METASTABLE DIAGONAL TERMS
C     (L)     NODATA() = .FALSE. MATRIX FILLED FOR THIS ATOMIC SPECIE
C                        .TRUE. NO LEVELS TO FILL -> NO FILE ->
C                         -> NO ORDINARY LEVELS
C
C     INTERNAL:
C
C     (I*4)   IUNIT    = PARAMETER = UNIT TO WHICH INPUT FILE IS ALLOCATED
C     (R.8)   EV2K     = PARAMETER = EV TO K CONVERSION (SOURCE NIST)
C     (I*4)   NDLEV    = PARAMETER = MAXIMUM NUMBER OF LEVELS THAT
C                         CAN BE READ
C     (I*4)   NDTRN    = PARAMETER = MAX. NUMBER OF TRANSITIONS THAT
C                        CAN BE READ =  DIMTRN*DIMTRN
```

```
C     (I*4)   NDMET    = PARAMETER = MAX. NUMBER OF METASTABLES ALLOWED
C                        FOR THE PARENT INDEX (REQUIRED FOR XXDATA_04)
C     (I*4)   NDQDN    = PARAMETER = MAX. NUMBER OF N-SHELLS FOR QUANTUM
C                        DEFECTS (REQUIRED FOR XXDATA_04)
C     (I*4)   NVMAX    = PARAMETER = MAX. NUMBER OF TEMPERATURES THAT
C                         CAN BE READ IN (REQUIRED FOR XXDATA_04).
C     (R*8)   RYEV     = PARAMETER = RYDBERG ENERGY (eV)
C
C     (I*4)   C#       = COUNTERS
C     (C*3)   TITLED   = ELEMENT SYMBOL.
C     (I*4)   IZ       = RECOMBINED ION CHARGE READ (OUTPUT XXDATA_04)
C     (I*4)   IZ0      =         NUCLEAR CHARGE READ (OUTPUT XXDATA_04)
C     (I*4)   IZ1      = RECOMBINING ION CHARGE READ (OUTPUT XXDATA_04)
C     (R*8)   BWNO     = IONISATION POTENTIAL (CM-1) OF LOWEST PARENT
C                         (OUTPUT XXDATA_04)
C     (I*4)   NPL      = NUMBER OF PARENTS ON FIRST LINE AND USED
C                         IN LEVEL ASIGNEMENTS (OUTPUT XXDATA_04)
C     (R*8)   BWNOA()  = IONISATION POTENTIAL (CM-1) OF PARENTS
C                         (OUTPUT XXDATA_04)
C     (L)     LBSETA() = (OUTPUT XXDATA_04)
C                         .TRUE.  - PARENT WEIGHT SET FOR BWNOA()
C                         .FALSE. - PARENT WEIGHT NOT SET FOR BWNOA()
C     (R*8)   PRTWTA() = PARENT WEIGHT FOR BWNOA()
C     (C*9)   CPRTA()  = PARENT NAME IN BRACKETS
C     (I*4)   IL       = INPUT DATA FILE: NUMBER OF ENERGY LEVELS
C                         (OUTPUT XXDATA_04)
C     (R*8)   QDORB()  = QUANTUM DEFECTS FOR ORBITALS
C                         1ST DIM: IMDEX FOR NL ORBITAL (cf i4idfl.for)
C                         (OUTPUT XXDATA_04)
C     (L*4)   LQDORB() = (OUTPUT XXDATA_04)
C                         .TRUE.  => SOURCE DATA AVAILABLE FOR QD.
C                         .FALSE. => SOURCE DATA NOT AVAILABLE QD.=0.0
C     (R*8)   QDN()    = QUANTUM DEFECT FOR N-SHELLS.  NON-ZERO ONLY
C                         FOR ADF04 FILES WITH ORBITAL ENERGY DATA
C                         1st. DIM: N-SHELL (1<=n<=ndqdn)
C                         (OUTPUT XXDATA_04)
C     (I*4)   IORB     = INPUT DATA FILE: NUMBER OF ORBITAL ENERGIES
C                         (OUTPUT XXDATA_04)
C     (I*4)   IA()     = ENERGY LEVEL INDEX NUMBER (OUTPUT XXDATA_04)
C     (C*18)  CSTRGA() = NOMENCLATURE/CONFIGURATION FOR LEVEL 'IA()'
C                         (OUTPUT XXDATA_04)
C     (I*4)   ISA()    = MULTIPLICITY FOR LEVEL 'IA()' (OUTPUT XXDATA_04)
C                         NOTE: (ISA-1)/2 = QUANTUM NUMBER (S)
C     (I*4)   ILA()    = QUANTUM NUMBER (L) FOR LEVEL 'IA()'
C                         (OUTPUT XXDATA_04)
C     (R*8)   XJA()    = QUANTUM NUMBER (J-VALUE) FOR LEVEL 'IA()'
C                         (OUTPUT XXDATA_04)
C                         NOTE: (2*XJA)+1 = STATISTICAL WEIGHT
C     (R*8)   WA()     = ENERGY RELATIVE TO LEVEL 1 (CM-1) FOR LEVEL
C                             'IA()' (OUTPUT XXDATA_04)
C     (C*1)   CPLA()   = CHAR. SPECIFYING 1st PARENT FOR LEVEL 'IA()'
C                         INTEGER - PARENT IN BWNOA() LIST
C                         'blank' - PARENT BWNOA(1)
C                         'x'   - DO NOT ASSIGN A PARENT
C                       (OUTPUT XXDATA_04)
C     (I*4)   NPLA()   = No. OF PARENT/ZETA CONTRIBUTIONS TO IONIS.
C                         OF LEVEL (OUTPUT XXDATA_04)
```

```
C     (I*4)   IPLA(,)  = PARENT INDEX FOR CONTRIBUTIONS TO IONIS.
C                         OF LEVEL (OUTPUT XXDATA_04)
C                         1st DIMENSION: PARENT INDEX
C                         2nd DIMENSION: LEVEL INDEX
C     (I*4)   ZPLA(,)  = EFF. ZETA PARAM. FOR CONTRIBUTIONS TO IONIS.
C                         OF LEVEL (OUTPUT XXDATA_04)
C                          1st DIMENSION: PARENT INDEX
C                          2nd DIMENSION: LEVEL INDEX
C     (I*4)   NV       = INPUT DATA FILE: NUMBER OF GAMMA/TEMPERATURE
C                         PAIRS FOR A GIVEN TRANSITION.
C                         (OUTPUT XXDATA_04)
C     (R*8)   SCEF()   = INPUT DATA FILE: ELECTRON TEMPERATURES (K)
C                         (NOTE: Te=Tp=Th IS ASSUMED) (OUTPUT XXDATA_04)
C     (I*4)   ITRAN    = INPUT DATA FILE: NUMBER OF TRANSITIONS
C                         (OUTPUT XXDATA_04)
C     (I*4)   MAXLEV   = HIGHEST INDEX LEVEL IN READ TRANSITIONS
C                         (OUTPUT XXDATA_04)
C     (C*1)   TCODE()  = TRANSITION: DATA TYPE POINTER: (OUTPUT XXDATA_04)
C                           ' ','1','2','3' => ELEC. IMPACT TRANS.
C                           'p','P' => PROTON   IMPACT   TRANSITION
C                           'h','H' => CHARGE EXCHANGE   RECOMBINATION
C                           'r','R' => FREE     ELECTRON RECOMBINATION
C                           'i','I' => COLL. IONIS. FROM LOWER STAGE ION
C                           's','S' => IONISATION FROM CURRENT ION
C                           'l','L' => L-LINE FOR UNRESOLVED DR EMISSIVITY
C     (I*4)   I1A()    = TRANSITION LOWER ENERGY LEVEL INDEX (CASE ' ' & 'p')
C                         OR SIGNED PARENT INDEX (CASE 'h','r','s' & 'i')
C                         (OUTPUT XXDATA_04)
C     (I*4)   I2A()    = TRANSITION UPPER ENERGY LEVEL INDEX (CASE ' ' & 'p')
C                       OR CAPTURING LEVEL INDEX (CASE 'h','r','s' & 'i')
C                       (OUTPUT XXDATA_04)
C     (R*8)   AVAL()   = TRANSITION A-VALUE (SEC-1)        (CASE ' ')
C                              NEUTRAL BEAM ENERGY      (CASE 'h')
C                              NOT USED             (CASE 'p','r' & 'i')
C                         (OUTPUT XXDATA_04)
C     (R*8)   SCOM(,)  = TRANSITION UPSILON VALUES   (CASE ' ' & 'p')
C                         RATE COEFFT.(CM3 SEC-1)(CASE 'h','r' & 'i')
C                         SCALED RATE COEFFT.(CM3 SEC-1)(CASE 's')
C                         1st DIMENSION - TEMPERATURE 'scef()'
C                         2nd DIMENSION - TRANSITION NUMBER
C                         (OUTPUT XXDATA_04)
C     (R*8)   BETH()   = TRANSITION 1st BETHE COEFFICIENT (case ' ','1','2')
C                         (OUTPUT XXDATA_04)
C     (I*4)   IADFTYP  = ADF04 TYPE: 1=OMEGA, 3=UPSILON, 4=NON-MAXWL.
C                         (OUTPUT XXDATA_04)
C     (L*4)   LPRN     = .TRUE.  => MULTIPLE PARENT DATA ON 1st LINE
C                      = .FALSE. => MULTIPLE PARENT DATA NOT PRESENT
C                         (OUTPUT XXDATA_04)
C     (L*4)   LCPL     = .TRUE.  => PARENT ASSIGNMENT ON LEVEL LINES
C                      = .FALSE. => PARENT ASSIGNMENT NOT PRESENT
C                        (OUTPUT XXDATA_04)
C     (L*4)   LORB     = .TRUE.  => ORBITAL DATA ON LEVEL TERMINATOR
C                      = .FALSE. => ORBITAL DATA NOT PRESENT
C                         (OUTPUT XXDATA_04)
C     (L*4)   LBETH    = .TRUE.  => BETHE DATA ON E-TRANSITION LINES
C                      = .FALSE. => BETHE DATA NOT PRESENT
C                         (OUTPUT XXDATA_04)
```

```
C     (L*4)   LETYP    = .TRUE.  => e- EXCITATION TRANSITIONS PRESENT
C                          (OUTPUT XXDATA_04)
C     (L*4)   LPTYP    = .TRUE.  => p- EXCITATION TRANSITIONS PRESENT
C                          (OUTPUT XXDATA_04)
C     (L*4)   LRTYP    = .TRUE.  => RECOMBINATION TRANSITIONS PRESENT
C                          (OUTPUT XXDATA_04)
C     (L*4)   LHTYP    = .TRUE.  => CX TRANSITIONS PRESENT (OUTPUT XXDATA_04)
C     (L*4)   LITYP    = .TRUE.  => IONIS. TRANS. FROM Z-1 ION PRESENT
C                          (OUTPUT XXDATA_04)
C     (L*4)   LSTYP    = .TRUE.  => IONIS. TRANS. FROM CURRENT ION PRESENT
C                          (OUTPUT XXDATA_04)
C     (L*4)   LLTYP    = .TRUE.  => 'l'-LINE FOR UNRESOLVED DR EMISSIVITY
C                          (OUTPUT XXDATA_04)
C     (I*4)   ITIEACTN = INPUT FOR XXDATA_04
C                          1 RETURN DATA EVEN IF SOME LEVELS ARE UNTIED.
C                          0 DEFAULT BEHAVIOUR - TERMINATE IF UNTIED
C                            LEVELS ARE PRESENT.
C                          ON OUTPUT 1 IF UNTIED LEVELS PRESENT
C                                    0 FOR NO UNTIED LEVELS.
C     (L*4)   LTIED()  = .TRUE.  => SPECIFIED LEVEL TIED
C                      = .FALSE. => SPECIFIED LEVEL IS UNTIED
C                          DIMENSION => LEVEL INDEX
C     (I*4)   I1AEQV() = EQUIVALENT LOWER LEVEL TRANSITIONS IN
C                          MOLECULAR LEVELS INDEX
C     (I*4)   I2AEQV() = EQUIVALENT LOWER LEVEL TRANSITIONS IN
C                          MOLECULAR LEVELS INDEX
C     (I*4)   NA       = NUMBER OF ATOMIC SPECIES IN FILE
C     (I*4)   IASP()   = MADAS SPECIE NUMBER FOR EACH SPECIE IN FILE
C     (C*80)  ATFLS()  = ADF04 PATH FOR EACH ATOMIC SPECIE
C                          (FROM ADAS DIRECTORY)
C     (I*4)   ATST()   = NUMBER OF ATOMIC STATES TO BE READ PER SPECIE
C     (R*8)   IZST()   = ION CHARGE OF EACH SPECIE
C     (I*4)   IMADAS(,)= NUMBER OF STATE IN THE MDF FILES
C     (C*2)   CMADAS(,)= CONFIGURATION FROM SEP. AT. CONF.
C     (I*4)   IADF04(,)= NUMBER OF STATE IN ADF04 FILE
C     (C*18)  CADF04(,)= CONFIGURATION STRING IN ADF04 FILE
C     (C*80)  ADFFILE  = ATFLS(I) FILE WITHOUT BLANKS
C     (C*100) IFILE    = FILE NAME FOR MDF25 WITH BLANKS
C     (C*100) FFILE    = FILE NAME FOR MDF25 WITHOUT BLANKS
C     (I*4)   LENGTH   = STRING LENGTH
C     (I*4)   IOPT     = SPLINE END POINT CURVATURE/GRADIENT OPTION
C                              1 => DDY1 = 0, DDYN = 0
C                              4 => DY1 = 0 , DDYN = 0
C                          OTHER OPTION AVAILABLE WITH NEGATIVE
C                          DERIVATIVE AND NO CURVATURE. NOW IOPT WILL
C                          BE SET TO IOPT=1
C     (R*8)   XIN()    = INTERNAL SPLINE INDEPENDENT VARIABLE
C     (R*8)   YIN()    = INTERNAL SPLINE DEPENDENT VARIABLE
C     (R*8)   XOUT()   = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   YOUT()   = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   DY()     = DERIVATIVES AT SPLINE KNOTS
C     (L)     LSETX    = VARIABLE TO SET THE KNOTS OF SPLINE
C                        .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                        .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                        ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                         RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                         TO USE IT AGAIN FOR THE SAME KNOTS)
```

```
C     (L)     LINTRP() = INTERPOLATION INDEX
C                        .TRUE.  => POINT INTERPOLATED
C                        .FALSE. => POINT EXTRAPOLATED
C     (R*8)   WT()     = STATISTICAL WEIGHT
C     (R*8)   WTU()    = UPPER STATE STATISTICAL WEIGHT
C     (R*8)   RATINT   = INTERPLATED RATE (CM3/S)
C     (L)     AMTFLG1/2= FLAG FOR METASTABLES IN UPPER AND LOWER LEVEL
C     (R*8)   DE       = LEVELS ENERGY DIFFERENCE
C     (L) I1FLG,I2FLG  = ACCOUNTS FOR CORRECTLY READ VALUES.
C     (C*80)  TFILE()   = PATH FOR ADF11 FILES
C
C
C
C ROUTINES:
C         ROUTINE    SOURCE    BRIEF DESCRIPTION
C         ------------------------------------------------------------
C         XXDATM_25  MADAS     TO FETCH DATA FROM MAPPING FILES MDF25
C         XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C         XXDATA_04  ADAS      TO FETCH DATA FROM AN ADF04 DATA SET
C                               AND DETECT ITS MAIN CHARACTERISTICS.
C         XXSPLE     ADAS      INTERPOLATES USING CUBIC SPLINES
C         R8FUN1     ADAS      EXTERNAL FUNCTION FOR NEEDED FOR
C                               XXSPLE THAT ONLY RETURNS ARGUMENT
C         RT2UPSLN   MADAS     CONVERTS FROM CM3/2 TO UPSILON OR VICEVERSA
C         I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C         R8CONST    ADAS      RETURNS THE FUNDAMENTAL CONSTANT
C                               CORRESPONDING TO 'KEY'.
C         LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN STRING
C
C
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 16/02/2012
C                 FIRST VERSION
C
C     VERSION   : 1.1
C     DATE      : 20/02/2012
c     MODIFIED  : F. GUZMAN
C                 - corrected of tcode and added ionis. to read values
C
C     VERSION   : 1.2
C     DATE      : 10/03/2012
c     MODIFIED  : F. GUZMAN
C                 - added diagonal terms array for atomic qcd
C
C     VERSION   : 1.3
C     DATE      : 30/04/2012
c     MODIFIED  : F. GUZMAN
C                 - changed dimensions to fix nmast
C                 - set lsetx to .true. as there are multiple calls to
C                    xxsple
C
C     VERSION   : 1.4
C     DATE      : 01/05/2012
c     MODIFIED  : F. GUZMAN
```

```
C                 - corrected the filling of diagonal terms
C                 - fixed bugs and created inverse terms in met-ord. filling
C
C
C-----------------------------------------------------------------------
```

C.4.6 rdxxdata_11.for

```
      SUBROUTINE RDXXDATA_11( DMADAS, DADAS, MSYMB,
     &                        NATSP , NASP ,
     &                        IATMET, ATMET,
     &                        TE    , NE   ,
     &                        ACD   , SCD  , QCD  , XCD,
     &                        NODATA
     &                       )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: RDXXDATA_11 ****************
C
C  PURPOSE: RETURNS THE ATOMIC EFFECTIVE ADF11 COEFFICIENTS TO BE USED
C           FOR MOLECULAR CR MODEL
C
C              CLASS INDEX    TYPE      GCR DATA CONTENT
C              -----------    ----      ----------------
C                  1          acd       recombination coeffts
C                  2          scd       ionisation coeffts
C                  3          ccd       CX recombination coeffts
C                  4          prb       recomb/brems power coeffts
C                  5          prc       CX power coeffts
C                  6          qcd       base meta. coupl. coeffts
C                  7          xcd       parent meta. coupl. coeffts
C                  8          plt       low level line power coeffts
C                  9          pls       represent. line power coefft
C                 10          zcd       effective charge
C                 11          ycd       effective squared charge
C                 12          ecd       effective ionisation potential
C
C     INPUT:
C
C     (C*80) DMADAS    = MADAS/MADAS/ PATH
C     (C*80) DADAS     = CENTRAL ADAS PATH
C     (C*10) MSYMB     = MOLECULAR SYMBOLC
C     (I*4)  NATSP     = TOTAL NUMBER OF ATOMIC SPECIES
C     (I*4)  NASP()    = NUMBER OF TOTAL SPECIE OF EACH ATOMIC SPECIE
C     (I*4)  IATMET()  = NUMBER OF METASTABLES PER ATOMIC SPECIE
C     (I*4)  ATMET(,)  = METASTABLE PER ATOMIC SPECIE IN LEVEL INDEX
C     (R*8)  TE        = INPUT TEMPERATURE (eV)
C     (R*8)  NE        = INPUT DENSITY (CM-3)
C
C     OUTPUT:
C
C     (R*8)  ACD(,,)   = MATRIX ACD COEFFICIENTS FOR THE DIFFERENT
C                          ATOMIC SPECIES
C     (R*8)  SCD(,,)   = MATRIX SCD COEFFICIENTS FOR THE DIFFERENT
C                          ATOMIC SPECIES
C     (R*8)  QCD(,,)   = MATRIX QCD COEFFICIENTS FOR THE DIFFERENT
C                          ATOMIC SPECIES
C     (R*8)  XCD(,,)   = MATRIX ACD COEFFICIENTS FOR THE DIFFERENT
C                          ATOMIC SPECIES
C     (L)    NODATA(,) = .FALSE. MATRIX FILLED FOR THIS ATOMIC SPECIE
```

```
C                        .TRUE. NO LEVELS TO FILL -> NO FILE ->
C                         -> NO ORDINARY LEVELS
C
C     INTERNAL
C
C     (I*4)  C#        = COUNTERS
C     (I*4)  IUNIT     = PARAMETER = UNIT TO WHICH INPUT FILE IS
C                         ALLOCATED
C     (I*4)  ISDIMD    = PARAMETER = MAXIMUM NUMBER OF (CHARGE, PARENT,
C                         GROUND) BLOCKS IN ISONUCLEAR MASTER FILES
C     (I*4)  IZDIMD    = PARAMETER = MAXIMUM NUMBER OF CHARGE STATES
C                         IN ISONUCLEAR MASTER FILES
C     (I*4)  ITDIMD    = PARAMETER = MAXIMUM NUMBER OF TEMP OR DENS
C                         VALUES IN ISOELECTRONIC MASTER FILES
C     (I*4)  NDPTNL    = PARAMETER = MAXIMUN LEVEL OF PARTITIONS
C     (I*4)  NDPTN     = PARAMETER = MAXIMUN NO. OF PARTITIONS IN ONE
C                         LEVEL
C     (I*4)  NDPTNC    = PARAMETER = MAXIMUN NO. OF COMPONENTS IN A
C                         PARTITION
C     (I*4)  NDCNCT    = PARAMETER = MAXIMUN NUMBER OF ELEMENTS IN
C                         CONNECTION VECTOR
C     (I*4)  NDMET     = PARAMETER = MAX. NUMBER OF METASTABLES ALLOWED
C                         FOR THE PARENT INDEX
C
C     (I*4)  ICLASS    = CLASS OF DATA (1 - 12 )
C     (I*4)  IS1MIN    = MINIMUM ION CHARGE + 1 (OUTPUT OF XXDATA_11)
C     (I*4)  IS1MAX    = MAXIMUM ION CHARGE + 1 (OUTPUT OF XXDATA_11)
C                             (NOTE EXCLUDES THE BARE NUCLEUS)
C     (I*4)  NPTNL     = NUMBER OF PARTITION LEVELS IN BLOCK
C                         (OUTPUT OF XXDATA_11)
C     (I*4)  NPTN()    = NUMBER OF PARTITIONS IN PARTITION LEVEL
C                         (OUTPUT OF XXDATA_11)
C                          1st DIM: PARTITION LEVEL
C     (I*4)  NPTNC(,)  = NUMBER OF COMPONENTS IN PARTITION
C                         (OUTPUT OF XXDATA_11)
C                          1st DIM: PARTITION LEVEL
C                          2nd DIM: MEMBER PARTITION IN PARTITION LEVEL
C     (I*4)  IPTNLA()  = PARTITION LEVEL LABEL (0=RESOLVED ROOT,1=
C                         UNRESOLVED ROOT) (OUTPUT OF XXDATA_11)
C                          1st DIM: PARTITION LEVEL INDEX
C     (I*4)  IPTNA(,)  = PARTITION MEMBER LABEL (LABELLING STARTS AT 0)
C                         (OUTPUT OF XXDATA_11)
C                          1st DIM  PARTITION LEVEL INDEX
C                          2nd DIM: MEMBER PARTITION INDEX IN PARTITION
C                          LEVEL
C     (I*4)  IPTNCA(,,)= COMPONENT LABEL (LABELLING STARTS AT 0)
C                         (OUTPUT OF XXDATA_11)
C                          1st DIM: PARTITION LEVEL INDEX
C                          2nd DIM: MEMBER PARTITION INDEX IN PARTITION
C                          LEVEL
C                          3rd DIM: COMPONENT INDEX IN MEMBER PARTITION
C     (I*4)  NCNCT     = NUMBER OF ELEMENTS IN CONNECTION VECTOR
C     (I*4)  ICNCTV()  = CONNECTION VECTOR OF NUMBER OF PARTITIONS OF
C                         EACH SUPERSTAGE IN RESOLVED CASE INCLUDING
C                         THE BARE NUCLEUS (OUTPUT OF XXDATA_11)
C                          1st DIM: CONNECTION VECTOR INDEX
C     (I*4)  IBLMX     = NUMBER OF (SSTAGE, PARENT, BASE) BLOCKS IN
```

```
C                           ISONUCLEAR MASTER FILE
C     (I*4)  ISMAX     = NUMBER OF CHARGE STATES IN ISONUCLEAR MASTER
C                           FILE (OUTPUT OF XXDATA_11)
C     (C*12) DNR_ELE   = CX DONOR ELEMENT NAME FOR ICLASS = 3 or 5
C                           (BLANK IF UNSET) (OUTPUT OF XXDATA_11)
C     (R*8)  DNR_AMS   = CX DONOR ELEMENT MASS FOR ICLASS = 3 or 5
C                           (0.0d0 IF UNSET) (OUTPUT OF XXDATA_11)
C     (I*4)  ISPPR()   = 1st (PARENT) INDEX FOR EACH PARTITION BLOCK
C                           (OUTPUT OF XXDATA_11)
C                           1st dim: INDEX OF (SSTATGE PARENTS BASE)
C                           BLOCK IN ISONUCLEAR MASTER FILE
C     (I*4)  ISPBR()   = 2nd (BASE) INDEX FOR EACH PARTITION BLOCK
C                           (OUTPUT OF XXDATA_11)
C                           1st DIM: INDEX OF (SSTAGE, PARENT, BASE)
C                            BLOCK IN ISONUCLEAR MASTER FILE
C     (I*4)  ISSTGR()  = S1 FOR EACH RESOLVED DATA BLOCK
C                           (OUTPUT OF XXDATA_11)
C                           1st DIM: INDEX OF (SSTAGE, PARENT, BASE)
C                            BLOCK IN ISONUCLEAR MASTER FILE
C     (I*4)  IDMAX     = NUMBER OF DENS VALUES IN ISONUCLEAR MASTER
C                           FILES (OUTPUT OF XXDATA_11)
C     (I*4)  ITMAX     = NUMBER OF TEMP VALUES IN ISONUCLEAR MASTER
C                           FILES (OUTPUT OF XXDATA_11)
C     (R*8)  DDENS()   = LOG10(ELECTRON DENSITY(cm-3)) FROM adf11
C                           (OUTPUT OF XXDATA_11)
C     (R*8)  DTEV()    = LOG10(ELECTRON TEMPERATERE (eV) FROM adf11
C                           (OUTPUT OF XXDATA_11)
C     (R*8)  DRCOF(,,) = IF(ICLASS <=9):
C                           LOG10(COLL.-RAD. COEFFT.) FROM ISONUCLEAR
C                            MASTER FILE
C                         IF(ICLASS >=10):
C                           COLL.-RAD. COEFFT. FROM ISONUCLEAR MASTER
C                           FILE (OUTPUT OF XXDATA_11)
C                            1st DIM: INDEX OF (SSTAGE, PARENT, BASE)
C                             BLOCK IN ISONUCLEAR MASTER FILE
C                            2nd DIM: ELECTRON TEMPERATURE INDEX
C                            3rd DIM: ELECTRON DENSITY INDEX
C
C     (L)    LRES      = .TRUE.  => PARTIAL FILE
C                      = .FALSE. => NOT PARTIAL FILE
C     (L)    LSTAN     = .TRUE.  => STANDARD FILE
C                      = .FALSE. => NOT STANDARD FILE
C     (L)    LPTN      = .TRUE.  => PARTITION BLOCK PRESENT
C                      = .FALSE. => PARTITION BLOCK NOT PRESENT
C     (I*4)  NA        = NUMBER OF ATOMIC SPECIES IN FILE
C     (I*4)  IASP()    = MADAS SPECIE NUMBER FOR EACH SPECIE IN FILE
C     (C*80) ATFLS()   = ADF04 PATH FOR EACH ATOMIC SPECIE
C                           (FROM ADAS DIRECTORY)
C     (I*4)  ATST()    = NUMBER OF ATOMIC STATES TO BE READ PER SPECIE
C     (R*8)  IZST()    = ION CHARGE OF EACH SPECIE
C     (I*4)  IMADAS(,) = NUMBER OF STATE IN THE MDF FILES
C     (C*2)  CMADAS(,) = CONFIGURATION FROM SEP. AT. CONF.
C     (I*4)  IADF04(,) = NUMBER OF STATE IN ADF04 FILE
C     (C*18) CADF04(,) = CONFIGURATION STRING IN ADF04 FILE
C     (C*80) ADFFILE   = ATFLS(I) FILE WITHOUT BLANKS
C     (C*100)IFILE     = FILE NAME FOR MDF25 WITH BLANKS
C     (C*100)FFILE     = FILE NAME FOR MDF25 WITHOUT BLANKS
```

```
C     (I*4)  LENGTH    = STRING LENGTH
C     (C*80) TFILE()   = PATH FOR ADF11 FILES
C     (I*4)  IOPT      = SPLINE END POINT CURVATURE/GRADIENT OPTION
C                             1 => DDY1 = 0, DDYN = 0
C                             4 => DY1 = 0 , DDYN = 0
C                        OTHER OPTION AVAILABLE WITH NEGATIVE
C                        DERIVATIVE AND NO CURVATURE. NOW IOPT WILL
C                        BE SET TO IOPT=1
C     (R*8)  XIN()     = INTERNAL SPLINE INDEPENDENT VARIABLE
C     (R*8)  YIN()     = INTERNAL SPLINE DEPENDENT VARIABLE
C     (R*8)  XIND()    = INTERNAL 2ND SPLINE INDEPENDENT VARIABLE
C     (R*8)  YIND()    = INTERNAL 2ND SPLINE DEPENDENT VARIABLE
C     (R*8)  XOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)  YOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)  DY()      = DERIVATIVES AT SPLINE KNOTS
C     (L)    LSETX     = VARIABLE TO SET THE KNOTS OF SPLINE
C                       .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                       .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                       ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                        RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                        TO USE IT AGAIN FOR THE SAME KNOTS)
C     (L)    LINTRP()  = INTERPOLATION INDEX
C                       .TRUE.  => POINT INTERPOLATED
C                       .FALSE. => POINT EXTRAPOLATED
C     (R*8)  RATINT    = INTERPOLATED RATE (CM3/S)
C     (I*4)  IZ0       = NUCLEAR CHARGE
C
C
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          XXDATM_25  MADAS     TO FETCH DATA FROM MAPPING FILES MDF25
C          XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C          XXDATA_11  ADAS      TO READ A COMPLETE ADF11 FILE
C          XXSPLE     ADAS      INTERPOLATES USING CUBIC SPLINES
C          R8FUN1     ADAS      EXTERNAL FUNCTION FOR NEEDED FOR
C          LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN STRING
C
C
C
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 02/03/2012
C                 FIRST VERSION
C
C-----------------------------------------------------------------------
```

C.4.7 wrt_mdf11

```
      SUBROUTINE WRT_MDF11( OUNIT , OPATH, TITE , MCLASS,
     &                      NMOLSP, NSP  , SYMBS, MSYMB ,
     &                      NMST  , NATM ,
     &                      NNES  , NMTE , NMTM ,
     &                      NE    , TE   , TI   , TM    ,
     &                      TMPCFF, SNMST, VNMST,
     &                      SNATM , VNATM, MOL  , IZ
     &                     )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: WRITE_MDF11 *******************
C
C     PURPOSE: CREATE THE MDF11 FORMAT FILES FOR THE DIFFERENT MOLECULAR
C              EFFECTIVE COEFICIENTS
C
C     MCLASS                      EFF COEF.
C
C       1                          MQCD
C       2                          MACD
C       3                          MSCD
C       4                          MCXIACD
C       5                          MCXCD
C       6                          PDCD
C       7                          MXCD
C       8                          PXDCD
C       9                          DXCD
C      10                          PXSDCD
C
C
C     INPUT:
C     (I*4)   OUNIT()    = UNITS WHERE THE OUTPUTS WILL BE WRITTEN
C     (C*80)  OPATH      = OUTPUT PATH
C     (L)     TITE       = .TRUE. TI=TE
C     (I*4)   MCLASS     = MOLECULAR COEFFICIENT CLASS (SEE BEFORE)
C     (I*4)   NMOLSP     = NUMBER OF MOLECULAR SPECIES
C     (I*4)   NSP        = NUMBER OF SPECIES
C     (C*10)  SYMBS()    = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (I*4)   NMST()     = ARRAY WITH THE NUMBER OF METASTABLES PER
C                          SPECIE
C     (I*4)   NATM       = NUMBER OF ATOMIC METASTABLES
C     (C*10)  MSYMB      = MOLECULAR SYSTEM SYMBOL
C     (I*4)   NNES       = NUMBER OF DENSITIES (MAX MNT)
C     (I*4)   NMTE       = NUMBER OF ELECTRON TEMPERATURES
C     (I*4)   NMTM       = NUMBER OF MOLECULAR TEMPERATURES
C     (R*8)   NE()       = ARRAY OF ELECTRON DENSITIES
C     (R*8)   TE()       = ARRAY OF TEMPERATURES FOR COLLISIONING
C                          ELECTRON (eV)
C     (R*8)   TI()       = ARRAY OF TEMPERATURES FOR COLLISIONING
C                          IONS/ATOMS (eV)
C     (R*8)   TM()       = ARRAY OF TEMPERATURES FOR TARGET
C                          PARTICLES(MOLECULES) (eV)
```

```
C     (I*4)   TMPCFF     = TEMP FILE UNIT WITH THE COEFS
C     (I*4)   SNMST()    = ELECTRONIC STATE INDEX FOR MOLECULAR
C                          METASTABLE
C     (I*4)   VNMST()    = VIB STATE INDEX FOR MOLECULAR METASTABLE
C     (I*4)   SNATM()    = ELECTRONIC STATE INDEX FOR ATOMIC METASTABLE
C     (I*4)   VNATM()    = VIB STATE INDEX FOR ATOMIC METASTABLE
C     (I*4)   MOL()      = ARRY OVER SPECIES INDEX: 1 MOLECULE, 0 ATOM
C     (R*8)   IZ()       = ION/MOLECULE CHARGE
C
C
C     INTERNAL:
C
C     (I*4)   NMMST      = PARAMETER = MAX NUMBER OF METASTABLE STATES
C     (I*4)   NCF        = PARAMETER = NUMBER OF COEFFICIENTS
C     (I*4)   MNSP       = PARAMETER = MAX. NUMBER OF SPECIES
C     (I*4)   MNT        = PARAMETER = MAX NUMBER OF DESIRED TEMPERATURES
C     (I*4)   NMAMST     = PARAMETER = MAX NUMBER OF ATOMIC METASTABLES
C
C     (I*4)   C#         = COUNTERS
C     (C*100) OFILE()    = NAMES OF THE OUTPUT FILES
C     (I*4)   NSPT       = NUMBER OF SPECIES FROM TEMPORAL FILE
C     (I*4)   LENGTH     = STRING LENGTH
C     (C*100) IFILE      = CHARACTER FOR FILE NAME
C     (I*4)   NBLCK()    = NUMBER OF BLOCKS OF THE FILE
C     (I*4)   TIEQTE     = 1 TI = TE, 0 OTHERWISE
C     (C*7)   RCLASS     = COEFFICIENTS' NAME
C     (I*4)   FSTAR      = FIRST MOLECULAR SPECIE TO WRITE FILE FOR
C     (I*4)   FFIN       = LAST MOLECULAR SPECIE TO WRITE FILE FOR
C     (I*4)   SSP        = FIRST MOLECULAR SPECIE TO READ FILE FOR
C     (I*4)   FSP        = LAST MOLECULAR SPECIE TO READ FILE FOR
C     (I*4)   NLMST      = LOWER INDEX STATE FOR WRITING
C     (I*4)   NUMST      = UPPER INDEX STATE FOR WRITING
C     (L*4)   ATFLG      = ATOMIC PRODUCTS FLAG
C     (I*4)   N          = BLOCK INDEX
C     (L*4)   EQSTFLG    = EQUAL STATES FLAG (APPLIES ONLY IN MQCD)
C     (I*4)   NNES       = NUMBER OF DENSITIES READ FROM TEMPORAL
C     (I*4)   NMTE       = NUMBER OF ELECTRON TEMPERATURES READ
C     (I*4)   NMTM       = NUMBER OF MOLECULAR TEMPERATURES READ
C     (R*8)   NET()      = ARRAY OF READ ELECTRON DENSITIES
C     (R*8)   TET()      = ARRAY OF READ TEMPERATURES FOR COLLISIONING
C                          ELECTRON (eV)
C     (R*8)   TMT()      = ARRAY OF READ TEMPERATURES FOR TARGET
C                          PARTICLES(MOLECULES) (eV)
C     (I*4)   NATM       = NUMBER OF READ ATOMIC METASTABLES
C     (I*4)   IC         = READING COEFFICIENTS INDEX
C     (I*4)   ISP        = SPECIE READ FROM FILE
C     (I*4)   NL         = LOWER STATE INDEX READ FROM FILE
C     (I*4)   NU         = UPPER STATE INDEX READ FROM FILE
C     (C*7)   CCLASS     = COEFFICIENT NAME READ FROM FILE
C     (R*8)   MCD(,)     = COEFFICENT STATES MATRIX
C     (R*8)   CF(,,)     = COEFFICIENT MATRIX IN NE,TE AND TM
C     (I*4)   NMOLSPT    = READ NUMBER OF MOLECULAR SPECIES
C     (I*4)   NMST()     = ARRAY WITH THE READ NUMBER OF METASTABLES PER
C                          SPECIE
C     (L*4)  ISPFLG      = .TRUE. THE SPECIES IS FOUND
C     (L*4)  GOFLG       = .TRUE. CONTINUE FOR THIS SPECIE AND THIS COEFF.
C     (I*4)  LSP, USP    = WRITING SPECIE INDEX
```

```
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN STRING
C
C     AUTHOR: F. GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 09/03/2012
C             FIRST VERSION
C
C  VERSION  : 1.1
C  DATE     : 30/04/2012
C  MODIFIED : F.GUZMAN
C             - dimension on te and ne is an argument and not readed from
C                tmpcff as before
C
C-----------------------------------------------------------------------
```

C.5 MDFLIBS

C.5.1 create_fmt_mdf02.for

```
      SUBROUTINE CREATE_FMT_MDF02( IUNIT   ,  OUNIT   ,  OFILE   ,
     &                             FUNIT   ,  STFILE
     &                           )
C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 PROGRAM: CREATE_FMT_02 *******************
C
C  PURPOSE: CREATE A PROPER PRE-FORMAT FILE FROM AN INPUT FILE WITH PART
C  OF THE DATA
C  SUBROUTINE:
C
C     INPUT  : (I*2)   IUNIT     = UNIT TO WHICH INPUT FILE IS ALLOCATED
C     INPUT  : (I*2)   OUNIT     = UNIT WHERE THE OUTPUT WILL BE WRITTEN
C     INPUT  : (C*100) OFILE     = NAME OF THE OUTPUT FILE
C     INPUT  : (I*2)   FUNIT     = UNIT WHERE THE FILE WITH THE STATES
C                                  INFORMATION WILL BE ALLOCATED
C     INPUT  : (C*100) STFILE    = NAME OF THE FILE WITH THE STATES
C                                  INFORMATION
C
C     READ   : (C*10)  MSYMB     = MOLECULAR SYMBOL
C                                  (FOR HETERONUCLEAR MOLECULES IT HAS
C                                  TO BE AN ARRAY)
C     READ   : (C*3)   TDATA     = TYPE OF DATA IN OMG'S OR CROSS SECTIONS
C     READ   : (I*4)   NBLOCKS   = NUMBER OF BLOCKS OF DATA
C     READ   : (I* )   RPARAM(,) = PARAMETERS OF THE REACTION
C     READ   : (L)     DISS      = REACTION DISSIOCIATIVE OR NOT
C     READ   : (C*8)   CH_DIS    = DISSOCIATION CHANNEL
C     READ   : (R*8)   W         = STATISTICAL WEIGTH
C     READ   : (R*8)   TPARAM    = ELECTRONIC TEMPERATURE (ENERGY) DATA
C     READ   : (R*8)   SPARAM    = CROSS SECTIONS (OR OMG'S) DATA
C     READ   : (R*8)   PARVAL(,) = PARAMETERS FOR THE FITTING FORMULA
C     READ   : (C*2)   PIMPCT()  = TYPE OF PROCESS:
C                                  CX = CHARGE EXCHANGE
C                                  EX = EXCITATION
C                                  IO = IONIZATION
C                                  DISSOSIATION PROCESSES ARE INCLUDED
C                                  BEFORE AS THEIR PRIMARY PROCESS IS
C                                  ALWAYS ONE OF THESE.
C
C
C
C     AUTHOR: F. GUZMAN  5/07/2010
C
C     MODIFIED: 9/11/2010
C     - added write of PIMPCT[RPARAM(,15)]: type of process.
C
```

C.5.2 rt2upsln.for

```
      FUNCTION RT2UPSLN (TEI,TM,WT,MMOL,MI,TRAT,OUT)
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 FUNCTION: XXDATM_00 *******************
C
C  PURPOSE:
C
C     CONVERTS FROM CM3/2 TO UPSILON OR VICEVERSA
C
C  ORIGINAL NAME: RT2UPSLN
C
C     INPUT:
C
C     (C*1)  OUT      = DESIRED OUTPUT: 'R' RATES, 'Y' UPSILONS
C     (R*8)  TEI      = TEMPERATURES FOR COLLISIONING
C                         PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)  TM       = TEMPERATURES FOR TARGET
C                         PARTICLES(MOLECULES) (eV)
C     (R*8)  WT       = STATISTICAL WEIGHT
C     (R*8)  MMOL     = TOTAL MOLECULAR MASS
C     (R*8)  MI       = PROJECTILE MASS (IF ION IMPACT, 0 OTHERWISE)
C     (R*8)  TRAT     = INPUT VALUE
C
C     INTERNAL:
C
C     (R*8)  TAU      = REDUCED TEMPERATURE
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          R8CONST    ADAS      RETURNS THE FUNDAMENTAL CONSTANT
C
C     AUTHOR F. GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 11/2011
C  MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C
C-----------------------------------------------------------------------
```

C.5.3 wrt_mdf02.for

```
      SUBROUTINE WRT_MDF02(  OUNIT,   MSYMB,    NBLOCKS,    RPARAM,
     &                        EPARAM,    DISS,     CH_DIS,     TDATA,
     &                             W,   NDATA,     TPARAM,    SPARAM,
     &                        PARVAL,  PIMPCT,
     &                         OFILE,      FUNIT,    STFILE
     &                      )

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: WRITE_MDF02 *******************
C
C  PURPOSE: CREATE A PROPER MDF02 FORMAT FILE
C  SUBROUTINE:
C
C     INPUT  : (I*2)   OUNIT     = UNIT WHERE THE OUTPUT WILL BE WRITTEN
C     INPUT  : (C*100) OFILE     = NAME OF THE OUTPUT FILE
C     INPUT  : (I*2)   FUNIT     = UNIT WHERE THE FILE WITH THE STATES
C                                  INFORMATION WILL BE ALLOCATED
C     INPUT  : (C*100) STFILE    = NAME OF THE FILE WITH THE STATES
C                                  INFORMATION
C
C     INPUT  : (C*10)  MSYMB     = MOLECULAR SYMBOL
C                                  (FOR HETERONUCLEAR MOLECULES IT HAS
C                                  TO BE AN ARRAY)
C     INPUT  : (C*3)   TDATA     = TYPE OF DATA IN OMG'S OR CROSS SECTIONS
C     INPUT  : (I*4)   NBLOCKS   = NUMBER OF BLOCKS OF DATA
C     INPUT  : (I* )   RPARAM(,) = PARAMETERS OF THE REACTION
C     INPUT  : (L)     DISS      = REACTION DISSIOCIATIVE OR NOT
C     INPUT  : (C*8)   CH_DIS    = DISSOCIATION CHANNEL
C     INPUT  : (R*8)   W         = STATISTICAL WEIGTH
C     INPUT  : (R*8)   TPARAM    = ELECTRONIC TEMPERATURE (ENERGY) DATA
C     INPUT  : (R*8)   SPARAM    = CROSS SECTIONS (OR OMG'S) DATA
C     INPUT  : (R*8)   PARVAL(,) = PARAMETERS FOR THE FITTING FORMULA
C     INPUT  : (C*2)   PIMPCT()  = TYPE OF PROCESS:
C                                  CX = CHARGE EXCHANGE
C                                  EX = EXCITATION
C                                  IO = IONIZATION
C                                  DISSOSIATION PROCESSES ARE INCLUDED
C                                  BEFORE AS THEIR PRIMARY PROCESS IS
C                                  ALWAYS ONE OF THESE.
C
C
C     AUTHOR: F. GUZMAN 5/07/2010
C
C     MODIFIED: 9/11/2010
C     - added write of PIMPCT[RPARAM(,15)]: type of process.
```

C.5.4 xxdatm_00.for

```
      SUBROUTINE XXDATM_00( S1 , S2   , E1   , E2   ,
     &                      FC , MAXV1, MAXV2, DFILE,
     &                      DST, ERROR
```

```
     &                     )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 FUNCTION: XXDATM_00 ********************
C
C  PURPOSE:
C
C     THIS FUNCTION READS THE FC FACTORS FILES IN DIRECTORIES OF MDF00
C     AND RETURNS THE ONE FOR THE INPUT VALUES
C
C  ORIGINAL NAME: FC_FACTOR
C
C  VERSION:  1.0
C
C
C
C INPUT:
C
C     (I*4) S1      = INITIAL STATE SPECIE INDEX
C     (I*4) E1      = INITIAL STATE ELECTRONIC INDEX
C     (I*4) S2      = FINAL STATE SPECIE INDEX
C     (I*4) E2      = FINAL STATE ELECTRONIC INDEX
C     (C*80)DFILE   = FCF DIRECTORY
C     (C*4) DST     = 'FC' or 'aval'
C
C OUTPUT
C
C     (R*8) FC(,)   = ARRAY WITH THE FC FACTORS FOR THE INPUT STATES
C     (I*4) MAXV1   = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                     STATE E1
C     (I*4) MAXV2   = HIGHEST QUANTUM NUMBER OF BOUND VIB LEVELS FOR
C                     STATE E2
C     (I*4) ERROR   = ERROR STATUS
C
C
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          XXRMWS      ADAS     REMOVES ALL BLANKS IN INPUT STRING
C          LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN STRING
C
C   AUTHOR: F. GUZMN
C
C   VERSION  : 1.0
C   DATE     : 24-03-2011
C   MODIFIED : F. GUZMAN
C              FIRST VERSION
C
C   VERSION  : 1.1
C   DATE     : 26/05/2011
C   MODIFIED : F. GUZMAN
```

```
C              - To include directory files so  isotopes can be count
C
C   VERSION  : 2.0
C   DATE     : 30/08/2011
C   MODIFIED : F. GUZMAN
C              NEW NAME XXDATM_00
C              Now is an mdflibs subroutine and can be used to read
C              mdf00 format as FCF and A-values. It has an official
C              name of the mdf format reading subroutines
C
C   VERSION  : 2.1
C   DATE     : 05/10/2011
C   MODIFIED : F. GUZMAN
C              Added an error status for output.
C
C
C-----------------------------------------------------------------------
```

C.5.5 xxdatm_02.for

```
      SUBROUTINE xxdatm_02( IUNIT  ,
     &                       MSYMB  , ATNUM  , ATSYMB  ,
     &                       IND_S  , SYMBS  , CH_ION , BWNO_I ,
     &                       CH_DIS , BWNO_D , NDIS   , WNO    ,
     &                       WNOD   , IND_P  , PATH_P , DESC_P ,
     &                       IND_E  , ECONUA , ECONSA , COUPSTA,
     &                       WT     , RPARAM , IND_R  , IN_E   ,
     &                       TPARAM , SPARAM , PARVAL , EPARAM ,
     &                       CMMT
     &                       )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: xxdatm_02 *******************
C
C  PURPOSE:  TO FETCH DATA FROM INPUT DATA SET OF TYPE MDF PREFORMAT.
C
C  CALLING PROGRAM: adas_901
C
C  DATA:
C
C           THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C
C           COLLISION ENERGIES  : KEV/AMU
C           TOTAL XSECTS.       : CM2
C           N-SHELL XSECTS.     : CM2
C           NL-SHELL DATA       : CM2
C
C
C  SUBROUTINE:
C  PARAM.: (I*4)  MXMMOLNT  = PARAMETER = MAXIMAL NUMBER OF CHARACTER
C                                         PER MOLECULE(NOW 4: At_N)
C  PARAM : (R*8)  ZEROST    = PARAMETER = LOWEST VALUE FOR CROSS SECTIONS
C  PARAM : (I*4)  MNE       = PARAMETER = MAX NUMBER OF ELECTRONIC STATES
C  PARAM : (I*4)  NCEST     = PARAMETER = MAX TOTAL NUMBER OF PROCESSES
C  PARAM : (I*4)  MNME      = PARAMETER = MAX NUMBER OF DESIRED TEMPERATURES
C  PARAM : (I*4)  MNS       = PARAMETER = MAX NUMBER OF SPECIES IN DIFFERENT
C                                          MDF02 FILES
C  PARAM : (I*4)  MDP       = PARAMETER = MAX NUMBER OF FORMULA PARAMETERS IN
C                              INPUT DATA IN MDF02 FILES
C  PARAM : (I*4)  MNC       = PARAMETER = MAX NUMBER OF DISSOCIATION CHANELS
C                                          BY SPECIE
C
C  INPUT : (I*4)  IUNIT     = UNIT TO WHICH INPUT FILE IS ALLOCATED
C
C  INT.  : (I*4)  IERR     = ERROR RETURN CODE.
C
C  OUTPUT :(C*2)  MSYMB     = MOLECULAR SYMBOL
C                             (FOR HETERONUCLEAR MOLECULES IT HAS TO BE
C                             AN ARRAY)
C  OUTPUT :(I*4)  ATNUM     = NUMBER OF ATOMS IN THE MOLECULE
```

```
C                             (FOR HETERONUCLEAR MOLECULES IT HAS TO BE
C                             AN ARRAY)
C  OUTPUT :(C*2)  ATSYMB    = ATOMIC SYMBOLS IN THE MOLECULE
C                             (FOR HETERONUCLEAR MOLECULES IT HAS TO BE
C                             AN ARRAY)
C  OUTPUT :(I*4)  IND_S     = MAX. INDEX OF SPECIES THAT IS DIFFERENT MOLECULES
C                             ATOMS AND THEIR IONS
C  OUTPUT :(I*4)  IN_E(,)   = INDEX OF ELECTRONIC STATE FOR EACH IND_S
C                              1ST DIM. SPECIES INDEX, 2ND DIM. EL. INDEX
C  OUTPUT :(I*4)  IND_P     = MAX, INDEX OF ELECTRON IMPACT PROCESSES BETWEEN
C                             DIFFERENT SPECIES
C                             ATOMS AND THEIR IONS
C  OUTPUT :(C*60) PATH_P()  = PATH OF THE DIFFERENTS PROCESS IN IND_P
C  OUTPUT :(C*40) DESC_P()  = DESCRIPTION OF THE DIFFERENT PROCESS IN IND_P
C  OUTPUT :(I*4)  IND_E()   = MAX. INDEX OF ELECTRONIC STATE FOR EACH IND_S
C  OUTPUT :(C*8)  ECONUA()  = ELECTRONIC CONFIGURATION IN THE UNITED ATOMS
C                             LIMIT
C                              1ST DIM. SPECIE, 2ND DIM. EL. STATE
C  OUTPUT :(C*4)  ECONSA()  = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                             ATOMS LIMIT
C                              1ST DIM. SPECIE, 2ND DIM. EL. STATE
C  OUTPUT :(C*10) COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC CONFIGURATION
C                              1ST DIM. SPECIE, 2ND DIM. EL. STATE
C  OUTPUT :(R*8)  WT(,)     = STATISTICAL WEIGHT
C                              1ST DIM. SPECIE, 2ND DIM. EL. STATE
C  OUTPUT :(C*6)  CH_ION()  = IONISATION CHANNELS
C  OUTPUT :(R*8)  BWNO_I()  = IONISATION ENERGY
C                             (MEASURED FROM LOWEST ELECTRONIC STATE
C                              MINIMUM) (cm^-1)
C  OUTPUT :(C*6)  CH_DIS(,) = DISSOCIATION CHANNELS
C                              1ST DIM. NUMBER OF SPECIES,
C                              2ND DIM. NUMBER OF DISS. CHANNEL
C, OUTPUT :(R*8)  BWNO_D()  = DISSOCIATION ENERGY
C                             (MEASURED FROM LOWEST ELECTRONIC STATE
C                              MINIMUM) (cm^-1)
C                              1ST DIM. NUMBER OF SPECIES,
C                              2ND DIM. NUMBER OF DISS. CHANNEL
C  OUTPUT :(I*4)  IND_R     = MAX. NUMBER OF REACTIONS
C  OUTPUT :(C*15) RPARAM(,) = PARAMETERS FOR EACH REACTION VALUES,
C                             ARRAY(IND_R,16)
C  OUTPUT :(R*8)  TPARAM(,) = TEMPERATURES ARRAY FOR DATA
C                              1ST DIM. PROCESS INDEX,
C                              2ND DIM. NUMBER OF ENERGIES
C  OUTPUT :(R*8)  SPARAM(,) = CROSS SECTION DATA ARRAY
C                              1ST DIM. PROCESS INDEX,
C                              2ND DIM. NUMBER OF ENERGIES
C  OUTPUT :(R*8)  PARVAL(,) = PARAMETERS ARRAY FOR FITTING FORMULA
C                              1ST DIM. PROCESS INDEX,
C                              2ND DIM. NUMBER OF PARAMETERS
C  OUTPUT :(R*8)  EPARAM(,) = TRANSITION ENERGY PARAMETER
C  OUTPUT :(I*4)  NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C  OUTPUT :(C*145)CMMT()    = COMMENTS ON THE INPUT FILE (100 LINES)
C  OUTPUT :(C*10) SYMBS()   = ARRAY OF THE SYMBOLS FOR EACH IND_S
C  OUTPUT :(C*10) WNO(,)    = BOUND ENERGY OF STATES
C                             (MEASURED FROM LOWEST ELECTRONIC STATE
C                              MINIMUM) (cm^-1)
C                              1ST DIM. SPECIE, 2ND DIM. EL. STATE
```

```
C  OUTPUT :(C*10) WNOD(,)   = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                              (MEASURED FROM LOWEST ELECTRONIC STATE
C                               MINIMUM) (cm^-1)
C                               1ST DIM. SPECIE, 2ND DIM. EL. STATE
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          -------------------------------------------------------------
C          LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN
C                               STRING (IGNORING TRAILING BLANKS)
C          XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C          I4FCTN     ADAS      RETURNS CHARACTER STRING AS AN INTEGER.
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C AUTHOR: FRANCISCO GUZMAN
C
C VERSION  : 1.0
C DATE     : 11/06/10
C MODIFIED : F.GUZMAN
C          FIRST VERSION
C        - based in the structure of program xxdata_01
C
C
C VERSION  : 1.1
C DATE     : 9/11/2010
C MODIFIED : F. GUZMN
C     included a new parameter RPARAM(,15) that
C     specifies the type of process (capture, ionization...).
C     Needed for extrapolation
C
C VERSION  : 1.2
C DATE     : 25/03/2011
C MODIFIED : F. GUZMN
C     included the new matrix WNO(,) that accounts for the
C     electronic bound energy
C     included rmws adas routine to avoid confusion in
C     multiple files case
C
C VERSION  : 1.2.1
C DATE     : 22/09/2011
C MODIFIED : F. GUZMN
C     included the new matrix WNOD(,) that accounts for the
C     electronic asymptotic energy needed after
C
C VERSION  : 2.0
C DATE     : 21/04/2012
C MODIFIED : F. GUZMN
C     included the new matrix IN_E to account for electronic
C     index independently
C
C VERSION  : 2.1
C DATE     : 12/08/2012
C MODIFIED : F. GUZMN
C     rationalized dimension in SPARAM,TPARAM and PARVAL.
C     creates MNME, MNS and MDP, MNC parameters
C
C-----------------------------------------------------------------------
```

C.5.6 xxdatm_04

```
      SUBROUTINE XXDATM_04( IUNIT  , TMPUNIT , NOTMP ,
     &                      IRDMD  , ITEI    , ITM   ,
     &                      SRCH   , TRS     , DEF_T ,
     &                      ISL    , IVL     , ISU   ,
     &                      IVU    , IPRCS   ,
     &                      ELIM   ,
     &                      NST    , MNV     ,
     &                      SYMBS  , MMOL    , MSYMB ,
     &                      CH_ION , CH_DIS  ,
     &                      BWNO_I , BWNO_D  ,
     &                      NSP    , STI     ,
     &                      INDS   , INDE    ,
     &                      COUPSTA, WT      , ECONSA,
     &                      WNO    , WNOD    ,
     &                      NMTE   , NMTM    ,
     &                      TEI    , TM      ,
     &                      TEO    , TMO     ,
     &                      INDR   ,
     &                      CATEGF , TCODE   ,
     &                      SU     , SL      ,
     &                      V1     , V2      ,
     &                      PRCS   , DCH     ,
     &                      TRAT   , RAT_ONET,
     &                      LINTRP
     &                     )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: xxdatm_04 *******************
C
C  PURPOSE:  TO FETCH DATA FROM INPUT DATA SET OF TYPE MDF33 FORMAT.
C
C     NOTE:  DUE TO THE NECESSITY TO DEAL WITH THE DIFFICULTIES OF
C            MANAGING BIG MATRICES IN ADAS904 ROUTINES THERE ARE
C            THREE MODES TO READ MDF04 FILES:
C                  1) READ ALL AT ONCE FOR SMALL MATRICES (LESS
C                          THAN 8500 ELEMENTS)
C                  2) READ THE MATRIX FOR ONLY ONE TEMPERATURE
C                  3) READ ALL TEMPERATURES FOR ONE PROCESS
C              IN THE SECOND CASE ALL THE PARAMETERS OF THE PROCESSES
C              WILL BE WRITEN IN A TEMPORAL FILE (IT MUST BE OPEN
C              BEFORE CALLING THIS ROUTINE)
C
C
C  CALLING PROGRAM: adas_903 adas_904
C
C  DATA:
C
C           THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C
C           COLLISION ENERGIES  : EV/AMU
```

```
C           RATES                   CM3/S
C
C
C-----------------------------------------------------------------------
C
C     INPUT
C
C     (I*4)   IUNIT     = UNIT TO WHICH INPUT FILE IS ALLOCATED
C     (I*4)   TMPUNIT   = UNIT FOR TEMPORAL FILE IN CASE IRDMD=2
C     (L)     NOTMP     = .TRUE. TMPFILE ALREADY WRITEN (DO NOT WRITE IT)
C     (I*1)   IRDMD     = SWITCH THE MODE OF READING MDF04
C                          1: READ ALL AT ONCE FOR SMALL MATRICES (LESS
C                             THAN 8500 ELEMENTS)
C                          2: READ THE MATRIX FOR ONLY ONE TEMPERATURE
C                          3: READ ALL TEMPERATURES FOR ONE PROCESS
C     (I*2)  ITEI,ITM   = INDEX OF THE ELECTRON/ION/MOLECULE DESIRED
C                          TEMPERATURES
C     (R*8)  TEO, TMO   =  ELECTRON/ION/MOLECULE DESIRED
C                          TEMPERATURES
C     (C*2)  SRCH       = 'TR' SEARCH FOR TRANSITION NUMBER
C                         'ST' SEARCH FOR STATES NUMBERS PLUS PROCESS NUMBER
C     (I*6)  TRS        = TRANSITION NUMBER (IRDMD=3)
C     (L)    DEF_T      = .TRUE. -> DEFAULT TEMPERATURES
C     (I*4)  ISL        = BOTTOM STATE OF TRANSITION (IRDMD=3)
C     (I*4)  ISU        = TOP STATE OF TRANSITION(IRDMD=3)
C     (I*4)  IVL        = BOTTOM VIBRATIONAL STATE OF TRANSITION (IRDMD=3)
C     (I*4)  IVU        = TOP VIBRATIONAL STATE OF TRANSITION(IRDMD=3)
C     (I*4)  IPRCS      = PROCESS NUMBER FOR TRANSITION
C     (I*4)  ELIM       = LIMIT OF THE NUMBER OF TRANSITIONS TO
C                          READ AT THE SAME TIME
C     (I*4)  NST        = MAX NUMBER OF ELECTRONIC STATES (DIM FOR RAT_ONET)
C     (I*4)  MNV        = MAX NUMBER OF VIB STATES (DIM FOR RAT_ONET)
C
C
C
C     OUTPUT
C
C     (C*10)  MSYMB     = MOLECULAR SYMBOL
C     (R*8)   MMOL      = TOTAL MOLECULAR MASS
C     (C*10)  SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (C*6)   CH_ION()  = IONISATION CHANNELS
C     (R*8)   BWNO_I()  = IONISATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (C*6)   CH_DIS(,) = DISSOCIATION CHANNELS
C     (R*8)   BWNO_D(,) = DISSOCIATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*4)   STI       = STATE INDEX AND NUMBER OF STATES
C     (I*4)   NSP       = NUMBER OF SPECIES
C     (I*4)   INDS()    = INDEX OF SPECIES
C     (I*4)   INDE()    = INDEX OF ELECTRONIC STATE
C     (C*10)  COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C     (C*4)  ECONSA()   = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C     (R*8)   WT()      = STATISTICAL WEIGHT
```

```
C     (C*10)  WNO()     = BOUND ENERGY OF STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)   WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C     (I*3)   NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C     (I*3)   NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C     (R*8)   TEI()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                         PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)   TM()      = ARRAY OF TEMPERATURES FOR TARGET
C                         PARTICLES(MOLECULES) (eV)
C     (I*6)   INDR      = NUMBER OF TRANSITIONS
C     (I*2)   CATEGF()  = CATEGORY OF COLLISIONAL TRANSITIONS
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER N0N MAXWELLIAN
C     (I*4)   TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
C                                 1 = DIPOLE
C                                 2 = NON-DIPOLE, NON SPIN CHANGE
C                                 3 = SPIN CHANGE
C                                 4 = OTHER (AMBIGUOUS)
C     (I*4)   SU()      = UPPER STATE INDEX OF A TRANSITION
C     (I*4)   SL()      = LOWER STATE INDEX OF A TRANSITION
C     (I*4)   V1()      = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)   V2()      = FINAL STATE VIBRATIONAL INDEX
C     (I*4)   PRCS()    = PROCESS NUMBER
C     (C*6)   DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (R*8)   TRAT(,,)  = ARRAY OF DEFAULT MAXWELLIAN RATES OUTPUT
C                          FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                          THIRD INDEX RUNS OVER TRANSITIONS
C                         IN CASE THATNM TE=0 ONLY FIRST AND THIRD INDEX
C                         FILLED.
C                         IN CASE IRDMD =2 OR 3 THIRD INDEX IS 1
C     (L)     LINTRP()  = INTERPOLATION INDEX
C                         .TRUE.  => POINT INTERPOLATED
C                         .FALSE. => POINT EXTRAPOLATED
C
C
C  INTERNAL
C
C     (C*110) CLINE     = LINE TEXT
C     (I*4)   C#        = COUNTERS
C     (I*4)   CNTL#     = COUNTER OF LINES
C     (R*8)   WM12 ()   = (WT-1)/2
C     (I*4)   ELIM      = LIMIT OF THE NUMBER OF TRANSITION TO
C                          READ AT THE SAME TIME
C     (I*1)   SPRTR     = SEPARATRIX (=-1)
C     (L)     LSETX     = VARIABLE TO SET THE KNOTS OF SPLINE
C                         .TRUE. => SPLINE PRESET FOR THESE KNOTS
C                         .FALSE. => SPLINE NOT SET FOR THESE KNOTS
C                         ( 'LSETX' IS ALWAYS RETURN AS '.FALSE.'  ON
C                          RETURN FROM THE SUBROUTINE SO IT IS POSSIBLE
C                          TO USE IT AGAIN FOR THE SAME KNOTS)
C     (I*4)   IOPT      = SPLINE END POINT CURVATURE/GRADIENT OPTION
C                             1 => DDY1 = 0, DDYN = 0
C                             4 => DY1 = 0 , DDYN = 0
C                         OTHER OPTION AVAILABLE WITH NEGATIVE
```

```
C                        DERIVATIVE AND NO CURVATURE. NOW IOPT WILL
C                        BE SET TO IOPT=1
C     (R*8)   XIN()     = INTERNAL SPLINE INDEPENDENT VARIABLE
C     (R*8)   YIN()     = INTERNAL SPLINE DEPENDENT VARIABLE
C     (R*8)   XOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   YOUT()    = INTERNAL OUTPUT SPLINE VARIABLE
C     (R*8)   DY()      = DERIVATIVES AT SPLINE KNOTS
C     (I3)    IENRP     = NUMBER OF ENERGIES TO INTERPOLATE
C     (R*8)   RTFI()    = ARRAY WITH INTERPOLATED VALUES FOR TI
C     (R*8)   RAT_ONET(,,,)= ARRAY WITH THE PROCESSES FOR ONLY ONE T
C     (I*4)   A,B       = VIB NUMBERS FOR RAT_ONE (100 => V =-3)
C
C
C
C ROUTINES:
C         ROUTINE    SOURCE    BRIEF DESCRIPTION
C         ------------------------------------------------------------
C         I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C         XXSPLE     ADAS      INTERPOLATES USING CUBIC SPLINES
C         R8FUN1     ADAS      EXTERNAL FUNCTION FOR NEEDED FOR
C                              XXSPLE THAT ONLY RETURNS ARGUMENT
C
C
C
C     AUTHOR F. GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 25/11/2011
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C  VERSION  : 1.1
C  DATE     : 22/12/2011
C  MODIFIED : F. GUZMAN
C             added ELIM to input
C
C  VERSION  : 2.0
C  DATE     : 22/12/2011
C  MODIFIED : F. GUZMAN
C             added interpolation in temperatures in case irmd=2
C
C  VERSION  : 2.1
C  DATE     : 22/12/2011
C  MODIFIED : F. GUZMAN
C             corrected negative index number for rat_one with a/b
C             indexes
C
C  VERSION  : 2.2
C  DATE     : 12/03/2012
C  MODIFIED : F. GUZMAN
C             added dimensions to the rat_one mat. to save memory in case
C              of different irdmd values
C
C
C
C-----------------------------------------------------------------------
```

C.5.7 xxdatm_11

```
       SUBROUTINE XXDATM_11( FUNIT , INBLCK,
     &                       SYMBS , MSYMB ,
     &                       NNES  , NMTE  , NMTM ,
     &                       TIEQTE, NBLCK , IZ   ,
     &                       TE    , TI    , TM   , NE    ,
     &                       SLMST , VLMST , SUMST, VUMST ,
     &                       CFO
     &                     )

       IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: xxdatm_11 *******************
C
C  PURPOSE:  TO FETCH DATA FROM INPUT DATA SET OF TYPE MDF11 FORMAT.
C
C  DATA:
C
C           THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C
C           COLLISION ENERGIES  : EV/AMU
C           RATES                 CM3/S
C
C
C-----------------------------------------------------------------------
C
C     INPUT
C
C     (C*100) FUNIT     = NAME OF THE INTPUT FILE
C     (I*4)   INBLOCK   = BLOCK NUMBER TO RETRIEVE
C
C     OUTPUT
C
C     (C*10)  SYMBS      = SPECIE SYMBOL
C     (C*10)  MSYMB      = MOLECULAR SYSTEM SYMBOL
C     (I*4)   NNES       = NUMBER OF DENSITIES
C     (I*4)   NMTE       = NUMBER OF ELECTRON TEMPERATURES
C     (I*4)   NMTM       = NUMBER OF MOLECULAR TEMPERATURES
C     (I*4)   TIEQTE     = 1 TI = TE, 0 OTHERWISE
C     (I*4)   NBLCK      = NUMBER OF BLOCKS OF THE FILE
C     (R*8)   TE()       = ARRAY OF TEMPERATURES FOR COLLISIONING
C                          ELECTRON (eV)
C     (R*8)   TI()       = ARRAY OF TEMPERATURES FOR COLLISIONING
C                          IONS/ATOMS (eV)
C     (R*8)   TM()       = ARRAY OF TEMPERATURES FOR TARGET
C                          PARTICLES(MOLECULES) (eV)
C     (R*8)   NE()       = ARRAY OF ELECTRON DENSITIES
C     (I*4)   SLMST      = ELECTRONIC STATE LOWER INDEX FOR METASTABLE
C     (I*4)   VLMST      = VIB STATE LOWER INDEX FOR METASTABLE
C     (I*4)   SUMST      = ELECTRONIC STATE UPPER INDEX FOR METASTABLE
C     (I*4)   VUMST      = VIB STATE UPPER INDEX FOR METASTABLE
C     (R*8)   IZ         = ION/MOLECULE CHARGE
```

```
C     (R*8)   CFO(,,)    = COEFFICIENT MATRIX IN NE,TE AND TM
C
C
C     INTERNAL
C
C     (I*4)   IUNIT     = PARAMETER = UNIT TO WHICH INPUT FILE IS ALLOCATED
C     (I*4)   MNT       = PARAMETER = MAX NUMBER OF DESIRED TEMPERATURES
C
C     (I*4)   C#        = COUNTERS
C     (I*4)   N         = BLOCK NUMBER READ
C     (R*8)   CF(,,)    = READ COEFFICIENT MATRIX IN NE,TE AND TM
C
C
C     AUTHOR F. GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 11/04/2012
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C-----------------------------------------------------------------------
```

C.5.8 xxdatm_25

```
      SUBROUTINE XXDATM_25(DMADAS,  MSYMB ,
     &                     NA    , IASP   , ATFLS  , TFILE ,
     &                     ATST  , IZST   ,
     &                     IMADAS, CMADAS , IADF04 , CADF04
     &                     )
      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: xxdatm_25 *******************
C
C  PURPOSE:  TO FETCH DATA FROM MAPPING FILES MDF25
C
C     NOTE: CONFIGURATION STRINGS FROM ADF04 ARE CONSIDERED TO BE 18
C           CHARACTERS LONG. BUT THAT COULD CHANGE. IN THIS CASE CADF04
C           STRING AND FORMAT 1002 LINE SHOULD CHANGE TO ADAPT
C
C
C     INPUT:
C
C     (C*80)  DMADAS    = MADAS/MADAS/ PATH
C     (C*10)  MSYMB     = MOLECULAR SYMBOL
C
C     OUTPUT:
C
C     (I*4)   NA        = NUMBER OF ATOMIC SPECIES IN FILE
C     (I*4)   IASP()    = MADAS SPECIE NUMBER FOR EACH SPECIE IN FILE
C     (C*80)  ATFLS(,)  = ADF04 AND ADF11 PATH FOR EACH ATOMIC SPECIE
C                         (FROM ADAS DIRECTORY)
C     (C*80)  TFILE()   = PATH FOR ADF11 FILES
C     (I*4)   ATST()    = NUMBER OF ATOMIC STATES TO BE READ PER SPECIE
C     (R*8)   IZST()    = ION CHARGE OF EACH SPECIE
C     (I*4)   IMADAS(,) = NUMBER OF STATE IN THE MDF FILES
C     (C*2)   CMADAS(,) = CONFIGURATION FROM SEP. AT. CONF.
C     (I*4)   IADF04(,) = NUMBER OF STATE IN ADF04 FILE
C     (C*18)  CADF04(,) = CONFIGURATION STRING IN ADF04 FILE
C
C
C     INTERNAL:
C
C     (I*4)   C#        = COUNTERS
C     (C*2)   ATSYMB    = ATOMIC SYMBOLS IN THE MOLECULE
C     (I*4)   LENGTH    = STRING LENGTH
C     (I*4)   AUNIT     = FILE UNIT FOR MDF25
C     (C*100) IFILE     = FILE NAME FOR MDF25 WITH BLANKS
C     (C*100) FFILE     = FILE NAME FOR MDF25 WITHOUT BLANKS
C     (C*5)   TYP       = TYPE OF FILE FOR READ
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          -------------------------------------------------------------
C          LENSTR     ADAS      RETURNS THE EFFECTIVE LENGTH OF A GIVEN
```

```
C                               STRING (IGNORING TRAILING BLANKS)
C          XXRMWS     ADAS      REMOVES ALL BLANKS IN INPUT STRING
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C
C     AUTHOR: F. GUZMN
C
C     VERSION   : 1.0
C     DATE      : 14/02/2012
C                 FIRST VERSION
C
C     VERSION   : 1.1
C     DATE      : 01/03/2012
C     MODIFIED  : F. GUZMAN
C     - added mapping for adf11 files and parameter needed to read them
C
C
C-----------------------------------------------------------------------
```

C.5.9 xxdatm_33

```
      SUBROUTINE XXDATM_33( IUNIT  ,
     &                      CATEG  , MI     ,
     &                      MSYMB  , MMOL   , NSP    ,
     &                      NDIS   , SYMBS  ,
     &                      CH_ION , CH_DIS,
     &                      BWNO_I , BWNO_D, STI    ,
     &                      INDS   , INDE   ,
     &                      COUPSTA, WT     , ECONSA,
     &                      WNO    , WNOD   ,
     &                      NMTE   , NMTM   ,
     &                      TEI    , TM     , INDR   ,
     &                      TCODE  , PRCS   ,
     &                      SU     , SL     ,
     &                      V1     , V2     ,
     &                      DE     , DCH    , CATEGF,
     &                      TRAT
     &                     )

      IMPLICIT NONE

C-----------------------------------------------------------------------
C
C
C  ***************** FORTRAN77 SUBROUTINE: xxdatm_33 *******************
C
C  PURPOSE:  TO FETCH DATA FROM INPUT DATA SET OF TYPE MDF33 FORMAT.
C
C
C  CALLING PROGRAM: adas_903
C
C  DATA:
C
C           THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C
C           COLLISION ENERGIES  : KEV/AMU
C           RATES                 CM3/S
C
C
C-----------------------------------------------------------------------
C
C  INPUT
C
C
C     (I*4)   IUNIT     = UNIT TO WHICH INPUT FILE IS ALLOCATED
C     (I*2)   CATEG     = CATEGORY OF OUTPUT COLLISIONAL TRANSITIONS
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER NON MAXWELLIAN
C     (R*8)   MI        = PROJECTILE MASS (IF ION IMPACT, 0 OTHERWISE)
C
C
C  OUTPUT
C
C
```

```
C     (C*10)  MSYMB     = MOLECULAR SYMBOL
C     (R*8)   MMOL      = TOTAL MOLECULAR MASS
C     (I*4)   NSP       = NUMBER OF SPECIES
C     (I*4)   STI       = STATE INDEX AND NUMBER OF STATES
C     (I*4)   NDIS()    = NUMBER OF DISSOTIATION CHANNELS PER SPECIE
C     (C*10)  SYMBS()   = FINAL ARRAY OF THE SYMBOLS FOR EACH INDS
C     (C*6)   CH_ION()  = IONISATION CHANNELS
C     (C*6)   CH_DIS(,) = DISSOCIATION CHANNELS
C     (R*8)   BWNO_I()  = IONISATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)   BWNO_D(,) = DISSOCIATION ENERGY
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*4)   INDS()    = INDEX OF SPECIES
C     (I*4)   INDE()    = INDEX OF ELECTRONIC STATE
C     (C*10)  COUPSTA() = COUPLED MOLECULAR STATE ELECTRONIC
C                         CONFIGURATION
C     (R*8)   WT()      = STATISTICAL WEIGHT
C     (C*10)  WNO()     = BOUND ENERGY OF STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (R*8)   WNOD()    = ASYMPTOTIC ENERGY OF ELECTRONIC STATES
C                         (MEASURED FROM LOWEST ELECTRONIC STATE
C                          MINIMUM) (cm^-1)
C     (I*3)   NMTM      = NUMBER OF MOLECULAR TEMPERATURES
C     (I*3)   NMTE      = NUMBER OF ELECTRON/ION TEMPERATURES
C     (R*8)   TEI()     = ARRAY OF TEMPERATURES FOR COLLISIONING
C                         PARTICLES(ELECTRON/IONS) (eV)
C     (R*8)   TM()      = ARRAY OF TEMPERATURES FOR TARGET
C                         PARTICLES(MOLECULES) (eV)
C     (I*4)   INDR      = NUMBER OF TRANSITIONS
C     (I*2)   CATEGF()  = CATEGORY OF COLLISIONAL TRANSITIONS
C                           1 -> UPSILON
C                           2 -> RATES (CM3/S)
C                           3 -> OTHER NON MAXWELLIAN
C     (I*4)   TCODE()   = ELECTRONIC TRANSITION SUBCATHEGORY
C                                 1 = DIPOLE
C                                 2 = NON-DIPOLE, NON SPIN CHANGE
C                                 3 = SPIN CHANGE
C                                 4 = OTHER (AMBIGUOUS)
C     (I*4)   PRCS()    = PROCESS NUMBER
C     (I*4)   SU()      = UPPER STATE INDEX OF A TRANSITION
C     (I*4)   SL()      = LOWER STATE INDEX OF A TRANSITION
C     (I*4)   V1()      = INITIAL STATE VIBRATIONAL INDEX
C     (I*4)   V2()      = FINAL STATE VIBRATIONAL INDEX
C     (R*8)   DE()      = TRANSITION/THRESHOLD ENERGY FOR A PROCESS
C     (C*6)   DCH()     = DISSOCIATION CHANNEL STRING FOR EACH PROCESS
C     (R*8)   TRAT(,,)  = ARRAY OF MAXWELLIAN RATES OUTPUT FROM THERMRAT
C                          FIRST INDEX RUNS OVER ION/ELECTRON TEMPERATURES
C                          SECOND INDEX OVER MOLECULAR TEMPERATURES
C                          THIRD INDEX RUNS OVER TRANSITIONS
C                         IN CASE THAT NMTE=0 ONLY FIRST AND THIRD INDEX
C                         FILLED
C     (C*4)  ECONSA()   = ELECTRONIC CONFIGURATION IN THE SEPARATED
C                          ATOMS LIMIT
C
```

```
C
C  INTERNAL
C
C     (R*8)   ME        = PARAMETER = ELECTRON MASS (g)
C     (R*8)   ELCH      = PARAMETER = ELECTRONIC CHARGE (C)
C     (R*8)   FERG      = PARAMETER = 1.D7 ERG/N
C     (R*8)   IH        = PARAMETER = RYDBERG ENERGY (eV)
C     (R*8)   A0        = PARAMETER = BOHR RADIUS (cm)
C     (R*8)   A02       = PARAMETER = A0**2
C
C     (C*110) CLINE     = LINE TEXT
C     (I*4)   C#        = COUNTERS
C     (I*4)   CNTL#     = COUNTER OF LINES
C     (R*8)   WM12 ()   = (WT-1)/2
C     (R*8)   CHECK     = FOR CHECKING THAT RATES HAVE BEEN READ
C     (R*8)   TAU       = REDUCED TEMPERATURE
C     (I*1)   SPRTR     = PARAMETER = SEPARATRIX (=-1)
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT     ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          R8CONST    ADAS      RETURNS THE FUNDAMENTAL CONSTANT
C                               CORRESPONDING TO 'KEY'.C
C
C
C     AUTHOR F. GUZMAN
C
C  VERSION  : 1.0
C  DATE     : 19/05/2011)
C  MODIFIED : F. GUZMAN
C             FIRST VERSION
C
C  VERSION  : 1.1
C  DATE     : 26/09/2011
C  MODIFIED : F. GUZMN
C     included the new matrix WNOD() that accounts for the
C     electronic asymptotic energy needed after and written to mdf33
C
C  VERSION  : 1.3
C  DATE     : 10/10/2011
C  MODIFIED : F. GUZMN
C     included separate atom configuration to account to dissociation
C     products.
C
C  VERSION  : 1.4
C  DATE     : 11/11/2011
C  MODIFIED : F. GUZMN
C     added NSP and STI to output
C
C
C
C-----------------------------------------------------------------------
```

C.5.10 xxrdpop.for

```
      PROGRAM XXRDPOP

      IMPLICIT NONE

      INTEGER IUNIT, IUNIT10, OUNIT
      PARAMETER (IUNIT = 15 , IUNIT10 = 10, OUNIT = 20 )
      CHARACTER POPF*80
      CHARACTER TENETM*2
      REAL*8    VAL(2)   , NE(20)      , TE(20)  , TI(20),TM(20)
      REAL*8    VALF(20) , FPOP(150,20), POP(150)
      INTEGER   C1       , C2          , C3      , C4
      INTEGER   NMMPOP   , NNES        , NTE     , NTM
      INTEGER   NVAL
      INTEGER   SPOP(150), VPOP(150)
```

Appendix D

Shell scripts

Appendix E

Fitting Formulas

Fitting formulas are numbered as:

- From 1 to 99: electron impact on H_2 formulae.
- From 101 to 199: proton impact on H_2 formulae.
- From 201 to 299: rate coefficients formulae.
- From 301 to 399: formulae for ${H_2}^+$.

E.1 Electron impact on H_2

Here E is the electron impact energy in eV and ΔE is the energy difference between upper and lower state in eV unless otherwise is stated.

- Formula number form=1

  Formula for cross sesctions on vibrational excitation by electron impact via electron attachment cross sections (not valid for diagonal $v = v'$ transitions).

  $$\sigma_{v,v'} = \frac{5.78A}{(\Delta E)^4 x^2}\left(1 - \frac{1}{x}\right)^{6.11/(\Delta E)^{1/2}} \left(\times 10^{-16}\text{cm}^2\right)$$

  with $x = E/\Delta E$ and A a parameter to be determined for each collision. Fitting formula from [11].

- Formula number form=2

  Formula for cross sections on vibrationally unresolved symetry forbiden transitions from $H_2(X, v = 0)$ to states EF, H$\bar{\text{H}}$, GK and I singlet states of H_2.

  $$\sigma_{\text{exc}}(X^1\Sigma_g^+(v = 0) \rightarrow N^1\Lambda_g) = \frac{5.984A_1}{\Delta E x}\left(1 - \frac{1}{x}\right)^{A_2} \left(\times 10^{-16}\text{cm}^2\right)$$

  with $x = E/\Delta E$ and A_x parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=3

  Formula for cross sections on dipole allowed transitions from $H_2(X, v = 0)$ to states B, B′, B″$\bar{\text{B}}$, C, D, and D′ states of H_2.

$$\begin{aligned}\sigma_{\mathrm{exc}}(X^1\Sigma_g^+(v=0)\rightarrow N^1\Lambda_u) &= \frac{5.984}{\Delta E x}\left(1-\frac{1}{x}\right)^{A_1} \\ &\times \left(A_1+\frac{A_2}{x}+\frac{A_3}{x^2}+A_4\ln(x)\right)\left(\times 10^{-16}\mathrm{cm}^2\right)\end{aligned}$$

with $x = E/\Delta E$ and A_x parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=4

  Formula for cross sections on vibrationally unresolved excitation from H_2(X,$v = 0$) to triplet electronic states a, b, c, d and e of H_2.

  $$\sigma_{\mathrm{exc}}(X^1\Sigma_g^+(v=0)\rightarrow N^3\Lambda_\sigma) = \frac{A_1}{x^3}\left(1-\frac{1}{x^{A_2}}\right)^{A_3}\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x = E/\Delta E$ and A_x parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=5

  Formula for cross section on dipole allowed excitation from vibrationally excited levels of ground state to B and C states of H_2.

  $$\sigma_{\mathrm{exc}}^{\mathrm{tot}}(X^1\Sigma_g^+(v)\rightarrow \Lambda(=B,C)) = \sigma_0(x)\left[\frac{Ry}{\Delta E_{X\Lambda}(R_{t,v})}\right]^3$$

  with $x = E/\Delta E_{X\Lambda}(R_{t,v})$ and $\Delta E_{X\Lambda}(R_{t,v}) = \Delta E$ is the vertical difference of energy at the outermost turning point for every v. Here:

  $$\sigma_0(x) = \frac{A_1}{x}\left(1-\frac{1}{x}\right)^{A_2}\left[A_3+\frac{A_4}{x}+\ln(x)\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  A_x are parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=6

  Formula for cross sections on dipole allowed transitions from vibrationally excited levels $v = 0, 1$ of ground state to B′, B″B̄, D and D′ of H_2.

  $$\sigma_{exc}^{tot}(X^1\Sigma_g(v=1)\rightarrow N^1\Lambda_u) = \frac{A_1}{x}\left(1-\frac{1}{x}\right)^{A_2}\left[A_3+\frac{A_4}{x}+\ln(x)\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x = E/\Delta E_{X\Lambda}(R_{t,v})$ and $\Delta E_{X\Lambda}(R_{t,v}) = \Delta E$ is the vertical difference of energy at the outermost turning point for every v. A_x are parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=7

  Formula for cross sections on excitation from vibrationally excited levels of ground state $v \geq 1$ to dissociative triplet state b of H_2.

  $$\begin{aligned}\sigma_{exc}^{diss}(X^1\Sigma_g^+; v\rightarrow b^3\Sigma_u^+) = \quad & \frac{5.824\times 10^3}{E^3}\left(\frac{\Delta E_1^{th}}{\Delta E_v^{th}}\right)^{0.08} \quad \times \\ & \exp\left(-\frac{A_2}{(x_v-1)^{A_5}+A_3(x_v-1)^{A_6}+A_4(x_v-1)^{A_7}}\right)\quad\left(\times 10^{-16}\mathrm{cm}^2\right)\end{aligned}$$

  with $x_v = E/\Delta E_v^{th}$, E is the electron impact energy and $\Delta E_v^{th} = \Delta E$ is the vertical difference from vibrational ground state v, A_x are parameters to be determined for each collision being $A_1 = \Delta E_1^{th}$. Fitting formula from [11].

- Formula number form=8

  Formula for cross sections on vibrationally unresolved ionization from ground electronic state and ground electronic level $v = 0$ of H_2 to ground state of $H_2{}^+$.

  $$\sigma_{ion}^{non\ diss}(X^1\Sigma_g^+; 0 \to X^2\Sigma_g^+) = \frac{1.628}{x_0}\left(1 - \frac{1}{x_0^{0.92}}\right)^{2.19} \ln\left(C_0 \Delta E_0 x_0\right)\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x_0 = E/\Delta E_0$ and $C_0 = 2.05$. ΔE_0 is the ionization energy from vibrational ground state $v = 0$. Fitting formula from [11].

- Formula number form=9

  Formula for cross section dissociative ionization from ground electronic state and ground electronic level $v = 0$ of H_2 to the vibrational continuum of ground state of $H_2{}^+$.

  $$\sigma_{ion}^{diss}(X^1\Sigma_g^+; 0 \to X^2\Sigma_g^+) = \frac{0.02905}{x_0^{1.25}}\left(1 - \frac{1}{x_0^{2.78}}\right)^{1.886}\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x_0 = E/\Delta E_0$. ΔE_0 is the energy difference from vibrational ground state $v = 0$ to the asymptotic part of gorund state of $H_2{}^+$. Fitting formula from [11].

- Formula number form=10

  Formula for cross section on ionization from ground electronic state and ground electronic level $v = 0$ of $H_2$to dissociative state B of $H_2{}^+$.

  $$\sigma_{ion}^{diss}(X^1\Sigma_g^+; 0 \to B^2\Sigma_u^+) = \frac{0.5627}{x_0^{1.20}}\left(1 - \frac{1}{x_0^{1.22}}\right)^{3.375}\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x_0 = E/\Delta E_0$. ΔE_0 is the vertical difference from vibrational ground state $v = 0$ to the dissociative state B. Fitting formula from [11].

- Formula number form=11

  Formula for cross sections on dissociative attachment from vibrationally excitedlevel v of ground state fo H_2 and H^- production via $H_2{}^-(X\,{}^2\Sigma_u^+)$.

  $$\sigma_{DA}(X^1\Sigma_g^+; v \to X^2\Sigma_u^+) = A_1 \exp\left(-\frac{E - \left|E_{th,v}\right|}{E_0}\right)\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $E_{th,v} = |\Delta E|$ the threshold energy, $E_0 = 0.45\mathrm{eV}$ and $A_1 = \sigma_v^{(0)}$ is the peak cross section (in 10^{-16} cm^2) for the initial vibrational state v at the threshold. Fitting formula from [11].

- Formula number form=12

  Formula for cross section on excitation from triplet $c({}^3\Pi_u; v = 0)$ to $a({}^3\Sigma_u^+; v' = 0)$ of H_2.

  $$\sigma_{exc}(c^3\Pi_u; v = 0 \to a^3\Sigma_g^+; v' = 0) = \frac{2.08}{x^{1.20}}\left(1 - \frac{1}{x}\right)^{3.80}\left(\times 10^{-11}\mathrm{cm}^2\right)$$

  with $x_v = E/\Delta E_{00}$. ΔE_{00} is the vertical energy difference between both states. Fitting formula from [11].

- Formula number form=13

  Formula for cross section on dipole allowed excitation from vibrationally excited levels of ground state to dissociative continuum of B and C states of H_2. This formula is essencially the same formula that form=5. The parameter A_1 must be multiplied by the fraction of the total cross section that the dissociative part constitutes.

  $$\sigma_{\mathrm{exc}}^{\mathrm{tot}}(X^1\Sigma_g^+(v) \to \Lambda(= B, C)) = \sigma_0(x)\left[\frac{Ry}{\Delta E_{X\Lambda}(R_{t,v})}\right]^3$$

with $x = E/A_5$ and $A_5 = \Delta E_{X\Lambda}(R_{t,\nu})$ is the vertical difference of energy at the outermost turning point for every ν which is now passed as a parameter as it is not anymore the real energy difference ΔE. Here:

$$\sigma_0(x) = \frac{A_1}{x}\left(1 - \frac{1}{x}\right)^{A_2}\left[A_3 + \frac{A_4}{x} + \ln(x)\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

A_x are parameters to be determined for each collision. Fitting formula from [11].

- Formula number form=14

  Formula for cross sections on dipole allowed transitions from vibrationally excited levels $\nu = 0, 1$ of ground state to the dissociative continuum of B′, B″$\bar{\mathrm{B}}$, D and D′ of H_2. The parameter A_1 must be multiplied by the fraction of the total cross section that the dissociative part constitutes.

$$\sigma^{tot}_{exc}(X^1\Sigma_g(\nu = 1) \to N^1\Lambda_u) = \frac{A_1}{x}\left(1 - \frac{1}{x}\right)^{A_2}\left[A_3 + \frac{A_4}{x} + \ln(x)\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  with $x = E/A_5$ and $A_5 = \Delta E_{X\Lambda}(R_{t,\nu}) = \Delta E$ is the vertical difference of energy at the outermost turning point for every ν which is now passed as a parameter as it is not anymore the real energy difference ΔE. A_x are parameters to be determined for each collision. Fitting formula from [11].

E.2 Proton impact on H_2

Here E is the proton impact energy in eV and ΔE is the laboratory energy difference between upper and lower state in eV unless otherwise is stated. For H_2 system $E_{\mathrm{lab}} = 1.5E_{\mathrm{rel}} = 1.5E_{\mathrm{CM}}$. The stored data are scaled after to center of mass (eV/amu) reference frame.

- Formula number form=101

  Formula for cross section on vibrational excitation of ground state of H_2.

$$\sigma_{exc}(0 \to \nu') = [\sigma^{<}(0 \to \nu') + \sigma^{>}(0 \to \nu')]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

$$\begin{aligned}\sigma^{<}(0 \to \nu') &= \frac{A_1 e^{-\frac{A_2}{E^{A_3}}}\theta(E - \Delta E^{th,Lab}_{0\nu'})}{E^{A_4}}\\ \sigma^{>}(0 \to \nu') &= \frac{A_5 e^{-\frac{A_6}{E^{A_7}}}}{E^{A_8}\left(1 + A_9 E^{A_{10}}\right)}\end{aligned}$$

  where E is the proton impact laboratory energy ($E_{CM}(eV/amu) = 2/3E$), $\Delta E^{th,Lab}_{0\nu'}$ is the threshold energy in the laboratory reference system for stationary H_2 and $\theta(E - \Delta E^{th,Lab}_{0\nu'})$ is:

$$\theta(E - \Delta E) = \begin{cases} 1 & \text{if} \quad E \geq \Delta E \\ 0 & \text{if} \quad E < \Delta E \end{cases}$$

  Fitting formula from [11].

- Formula number form=102

  Formula for cross sections on charge transfer from vibrational levels $\nu \leq 8$ of ground state of H_2.

$$\sigma^{CX}_{\nu\leq 8}(E^p) = [\sigma^{<}_{\nu}(E^p) + \sigma^{>}_{\nu}(E^p)]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

$$\begin{aligned}\sigma_v^{<}(E) &= A_1 E^{A_2}\left[1-\left(\frac{\Delta E_v^{th,Lab}}{E}\right)^{A_3}\right]^{A_4} e^{-A_5 E^{A_6}}\\ \sigma_v^{>}(E) &= \frac{A_7 e^{-A_8/E^{A_9}}}{A_{10}E^{A_{11}}+A_{12}E^{A_{13}}+A_{14}E^{A15}+A_{16}E^{A_{17}}}\end{aligned}$$

where E^p is the proton impact laboratory energy ($E_{CM}(eV/amu) = 2/3E^p$), $\Delta E_{0v'}^{th,Lab}$ is the threshold energy in the laboratory reference system for stationary H_2 and $\{A_i\}$ are fitting parameters. Fitting formula from [11].

- Formula number form=103

  Formula for cross sections on charge transfer from vibrational levels $v \geq 9$ of ground state of H_2.

$$\sigma_{v\geq 9}^{CX}(E) = \frac{27.0 f(v)}{E^{0.033} + 9.85\times 10^{-10}E^{2.16} + 1.66 f(v)\times 10^{-25}E^{5.25}}\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  where E is the proton impact laboratory energy ($E_{CM}(eV/amu) = 2/3E$) and:

$$f(v) = \begin{cases} 1 & \text{if} \quad v = 9 \\ \frac{1.97}{(v-8)^{1.23}} & \text{if} \quad v \geq 10 \end{cases}$$

  Here $v = A_1$ is the only fitting parameter. The data are scaled after to center of mass (eV/amu) reference frame. Fitting formula from [11].

- Formula number form=104

  Formula for cross sections on dissociation from vibrational levels v of ground state of H_2 to H(1s) + H(1s).

$$\sigma_v^{diss}(E) = \frac{A_1}{E^{A_2}}\left[1-\left(\frac{E_{0v}}{E}\right)^{A_3}\right]^{A_4}\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  where E is the proton impact laboratory energy ($E_{CM}(eV/amu) = 2/3E$), E_{0v} is the dissociation threshold energy from an initial v in the laboratory reference system for stationary H_2 and $\{A_i\}$ are fitting parameters. Fitting formula from [11].

- Formula number form=105

  Formula for cross section on total ionization of vibrational level $v = 0$ of ground state of H_2.

$$\sigma_v^{non-diss}(E) = \frac{56.34 ln(e + 1.115E)}{E(1+21.2E^{-2.41})}\exp\left[-\frac{9.136}{1+8.37\times 10^{-2}E^{1.2733}}\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  where E is the collision energy in keV/amu. Fitting formula from [11].

- Formula number form=106

  Formula for cross section on total dissociative ionization of vibrational level $v = 0$ of ground state of H_2.

$$\sigma_v^{non-diss}(E) = \frac{10.75}{E^{0.96}(1+2.35\times 10^{4}E^{-5.52})}\exp\left[-\frac{2.6882}{1+2.890\times 10^{-4}E^{3.25}}\right]\left(\times 10^{-16}\mathrm{cm}^2\right)$$

  where E is the collision energy in keV/amu. Fitting formula from [11].

E.3 Rate coefficients

- Formula number form=201

  Formula for rate coefficients on electron impact vibrational excitation of vibrational level $v = 0$ by electron attachment of ground state of H_2 and rate coefficients for dissociative electron attachment of vibrational levels v of ground state of H_2.

  $$ln\left[K_v^{exc/diss}(0 \rightarrow v'; v \rightarrow \text{diss})\right] = \frac{A_1}{(T')^{A_2}} + \frac{A_3}{(T')^{A_4}} + \frac{A_5}{(T')^{A_6}} \text{cm}^3/\text{s}$$

  where $T' = T/10^3$ and T is the electron temperature in K. A_x are the fitting parameters. Fitting formula from [11]

E.4 Formulae for ${H_2}^+$

Here E is the electron impact energy in eV and ΔE is the energy difference between upper and lower state in eV unless otherwise is stated.

- Formula number form=301

  Formula for cross sections on vibrational exitation of vibrational levels v to level $v + 1$ of ground state of ${H_2}^+$.

  $$\sigma_v^{\text{exc}}(v \rightarrow v') = \frac{0.14\,(A_1 + 1)}{\Delta E_{v,v+1}} \frac{1}{E^{0.928}} \left(\times 10^{-16}\text{cm}^2\right)$$

  where $A_1 = v$ is taken as a parameter and $\Delta E_{v,nu+1}$ is the energy difference between the vibrational levels. Formula from [11].

- Formula number form=302

  Bethe-Born formula for cross sections on dissociative excitation from vibracional levels v of ground state of ${H_2}^+$.

  $$\sigma_{v \rightarrow DE}^{\text{BB}}(E) = \frac{0.88Ry}{E}\left[0.5A_1 \ln(E/Ry) + A_2\right]\left(\times 10^{-16}\text{cm}^2\right)$$

  where Ry is the Rydberg constant in eV and A_x are parameters. Formula from [11].

- Formula number form=303

  Formula for cross sections on dissociative ionization from the vibrational levels v of the ground state of ${H_2}^+$ to two protons.

  $$\sigma_v^{\text{DI}}(E) = \frac{A_1}{\Delta E_v}\frac{7.39}{E}\ln(0.18E)\left\{1 - \exp\left[-0.105\left(\frac{E}{15.2} - 1\right)^{1.55}\right]\right\}\left(\times 10^{-16}\text{cm}^2\right)$$

  where $A_1 = \left(\sum_v \frac{1}{\Delta E_v}\right)^{-1}$ is the parameter which asures the proper normalization for an approximate expresion from total dissociative ionization and ΔE_v is the vertical energy in eV from the outermost turning point of the v level to the curve of the repulsive $H^+ + H^+$ state. Formula from [11].

- Formula number form=304

  Formula for cross sections on dissociative recombination from the vibrational levels v of the ground state of ${H_2}^+$ to two atoms.

  $$\sigma_v^{\text{DR}}(E) = A_1\left\{\frac{1}{E^{0.665}\left(1 + 1.1E^{0.512} + A_2E^{A_3}\right)} + A_4e^{-A_5(E-A_6)^2}\right\}\left(\times 10^{-16}\text{cm}^2\right)$$

  where E is expressed in eV units and the other parametres are given for each v. Formula from [11].