New Molecular Collisional-Radiative Model in ADAS

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Outline

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Motivation

- Molecules desorbed from the wall contribute to the neutral density and influence the divertor physics.
- ADAS 900 series main objective is to extend ADAS Database to molecular data

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- We want to provide molecular data tools to use in plasma edge and divertor calculations and experiments.

Steps to follow for a Molecular CR model

1. Compile a database. Structure it and provide readings tool for it. Do maxwellian integration of cross sections to obtain rates(Boring part).
2. There are gaps!. Fill the gaps with estimation of molecular processes. Automatic process is needed due to the big number of states.
3. Solve CR model for all molecules and all dissociation products.

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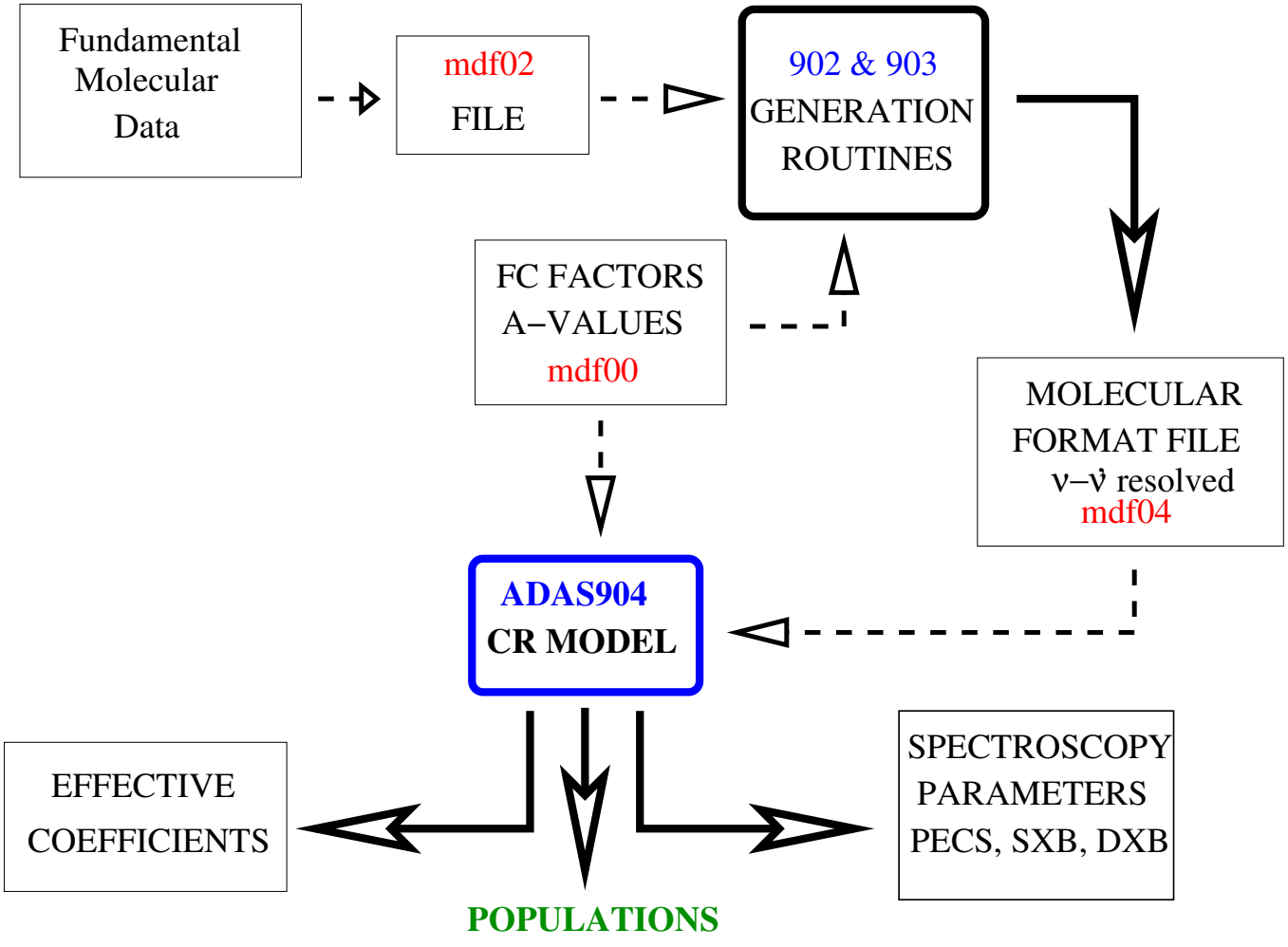
ADAS 900


Fundamental Molecular Data
mdf02 FILE
902 & 903 GENERATION ROUTINES
FC FACTORS A–VALUES mdf00
MOLECULAR FORMAT FILE v–v̇ resolved mdf04
ADAS904 CR MODEL
EFFECTIVE COEFFICIENTS
SPECTROSCOPY PARAMETERS PECS, SXB, DXB
POPULATIONS

Formats

mdf00 General information. Vibrational energies. FC factors. A-values.

mdf02 Cross sections and rates obtained from external sources or calculations.

mdf33/34 ADAS902 product. Rates (upsilons and $cm^3 s^{-1}$) obtained from maxwellian integratrion of *mdf02*.

mdf04/14 ADAS903 product. Maxwellian rates completed with EIQIP and EICIP to be used in population models.

mdf11 ADAS904 product. Molecular effective coefficients.

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- **Excitation data:** There is avalaible data[1] that have been checked to be in good agreement with the fitting formulas from Janev.
- **Ionization data** Only ionization from ground state available.
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- Calculation are performed over vibronic levels and summed in case of electronic resolution.
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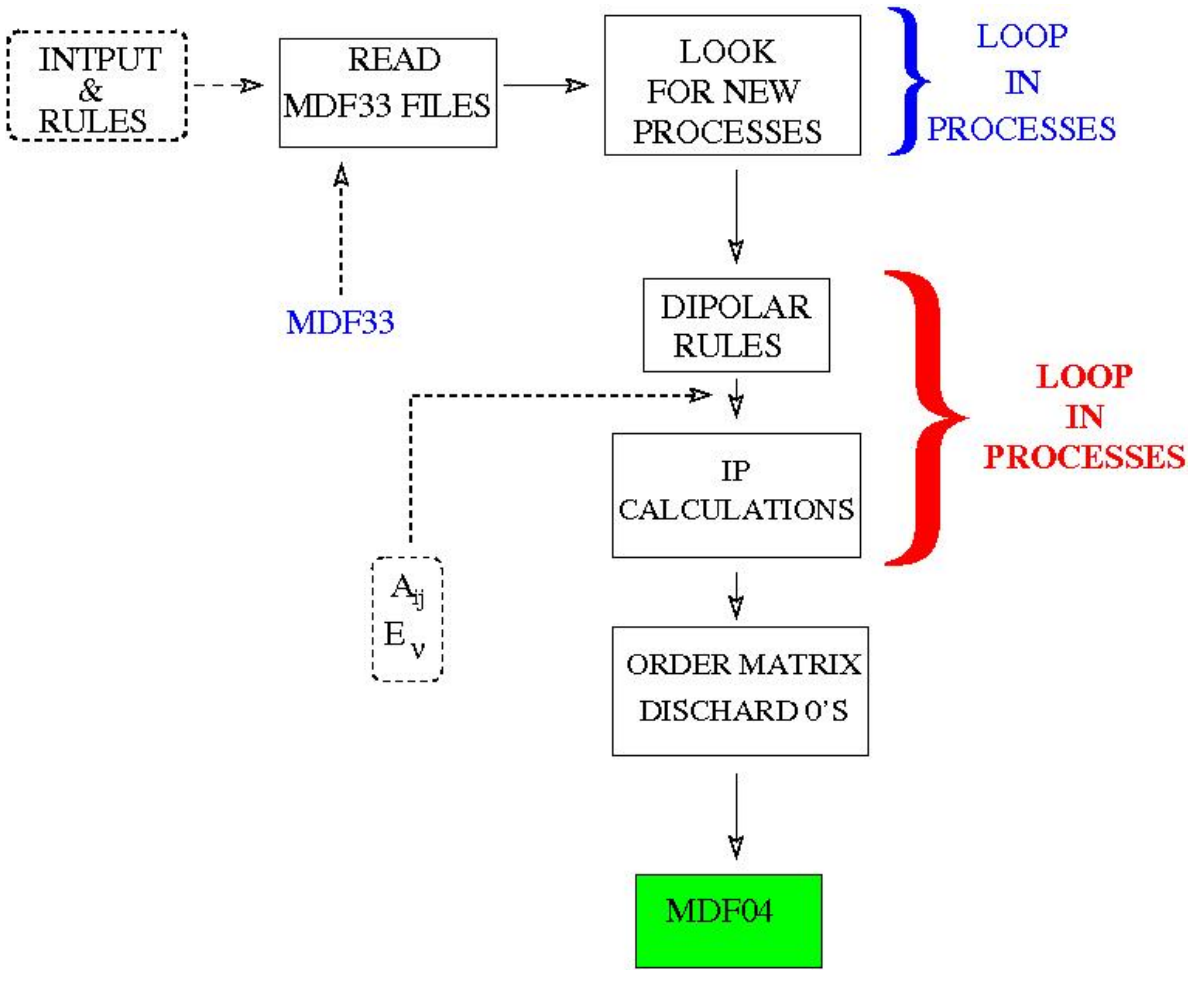
ADAS903: filling the matrix

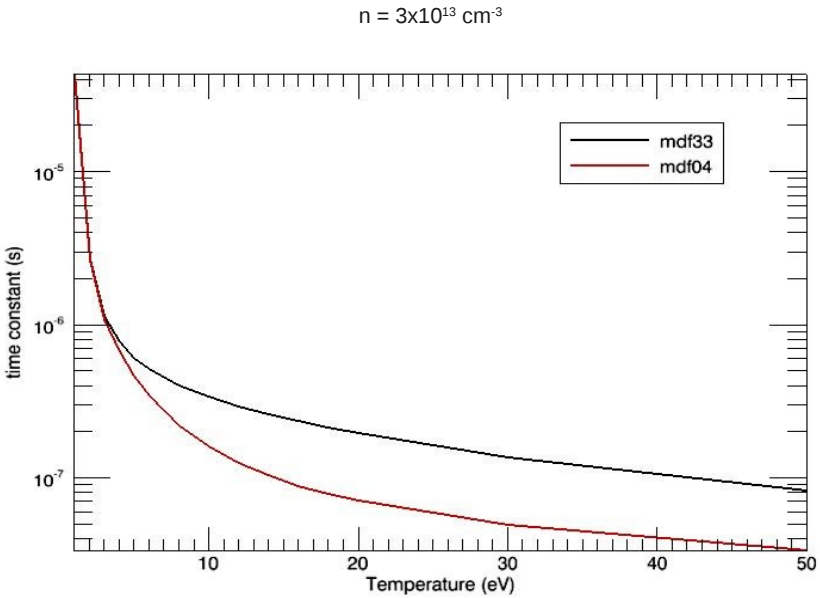


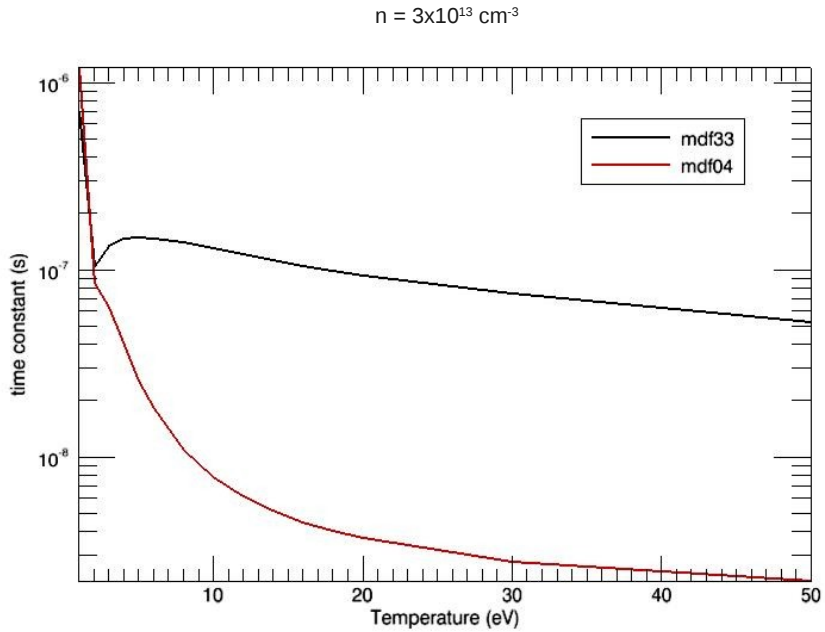
Why filling the matrix?

Maxwellian time constant: $\tau = \frac{1}{n_e \langle \sigma v \rangle}$

$$H_2(X, \nu = 0) \rightarrow H + H$$

$$H_2(X, \sum_\nu \nu) \rightarrow H + H$$





Processes from excited vibrational levels are needed.

ADAS904: Solving CR

- Dissociative processes are all that go to dissociation (diss. excitiation, ionisation, CX, recombination . . .).
- Metastables are allways vibrationally resolved
  $\longrightarrow$ 150 $\times$ 150 maximum dimension of metastable matrix.
- Autoionisation and predissociation are included at this stage from *mdf38* format data.
- Atomic dissociation products equilibrium ionisation balance is included in the CR model.

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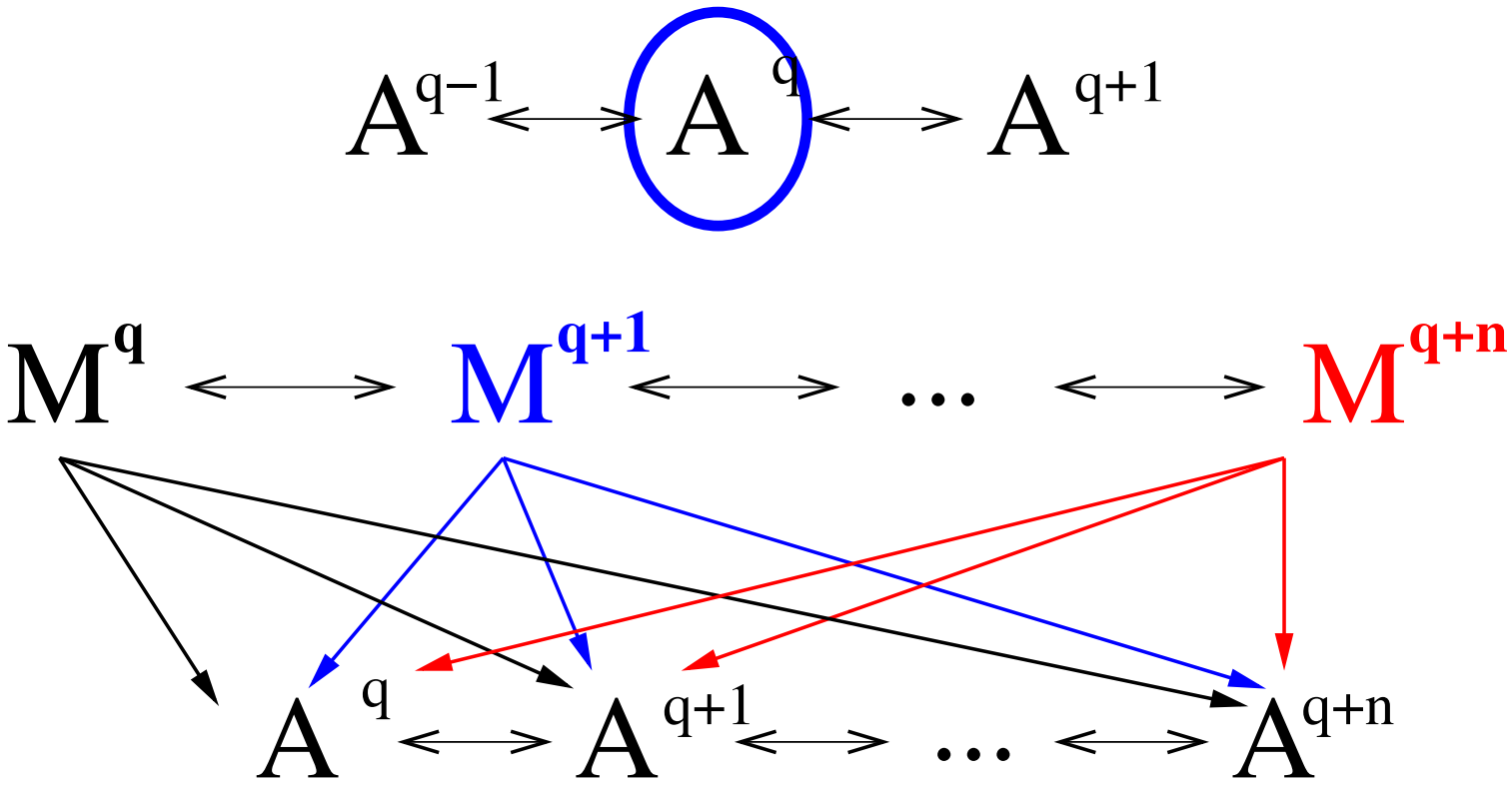
Molecules CR model



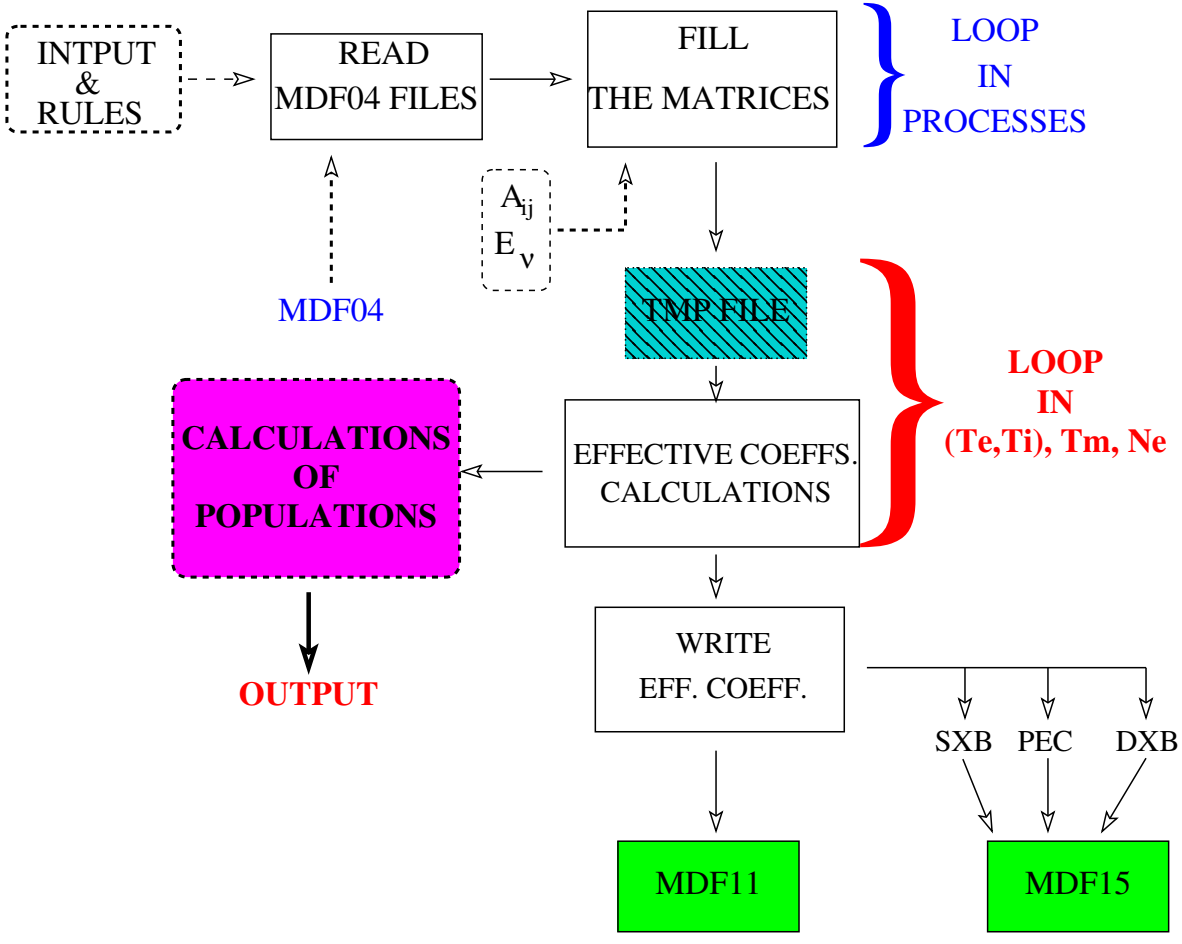
ADAS904: The population model

CR Equation

$$\begin{pmatrix} \frac{dN_X}{dt} \end{pmatrix} = \underbrace{\left(\begin{array}{c|c|c} H_2 & \sim 0 & 0 \\ \hline \neq 0 & H_2^+ & 0 \\ \hline \neq 0 & \neq 0 & H(n), H^+ \end{array}\right)}_{\begin{pmatrix} \cdots \\ \text{states} \\ \cdots \end{pmatrix}} \times \begin{pmatrix} N_X \end{pmatrix} - \begin{pmatrix} \Gamma_{in} \end{pmatrix}$$

Γ_{in} can correspond to the collisional terms from constant populations.

ADAS904: CR model



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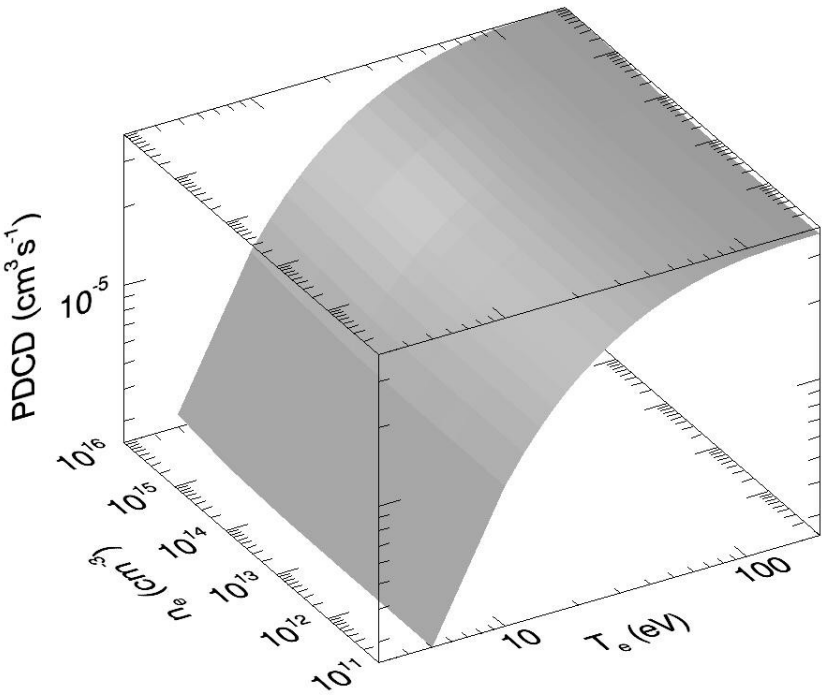
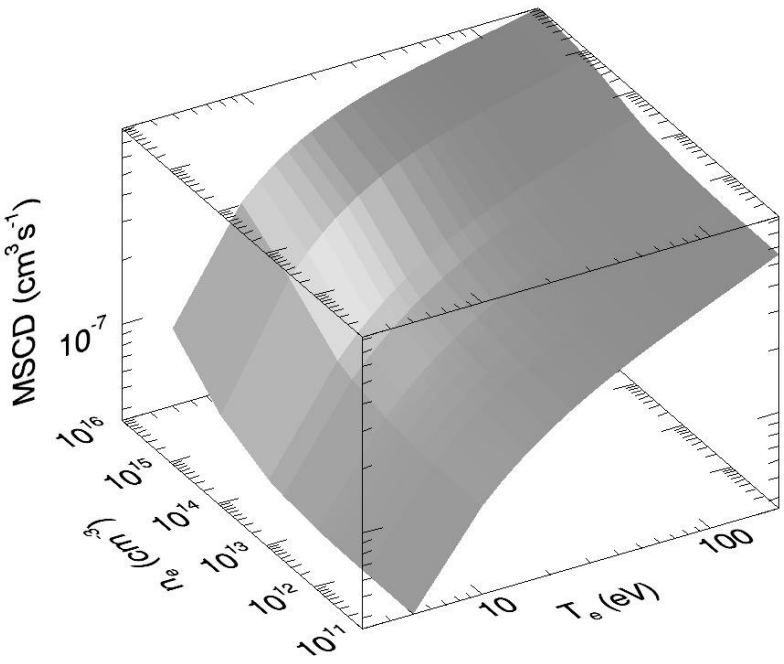
Effective coefficients

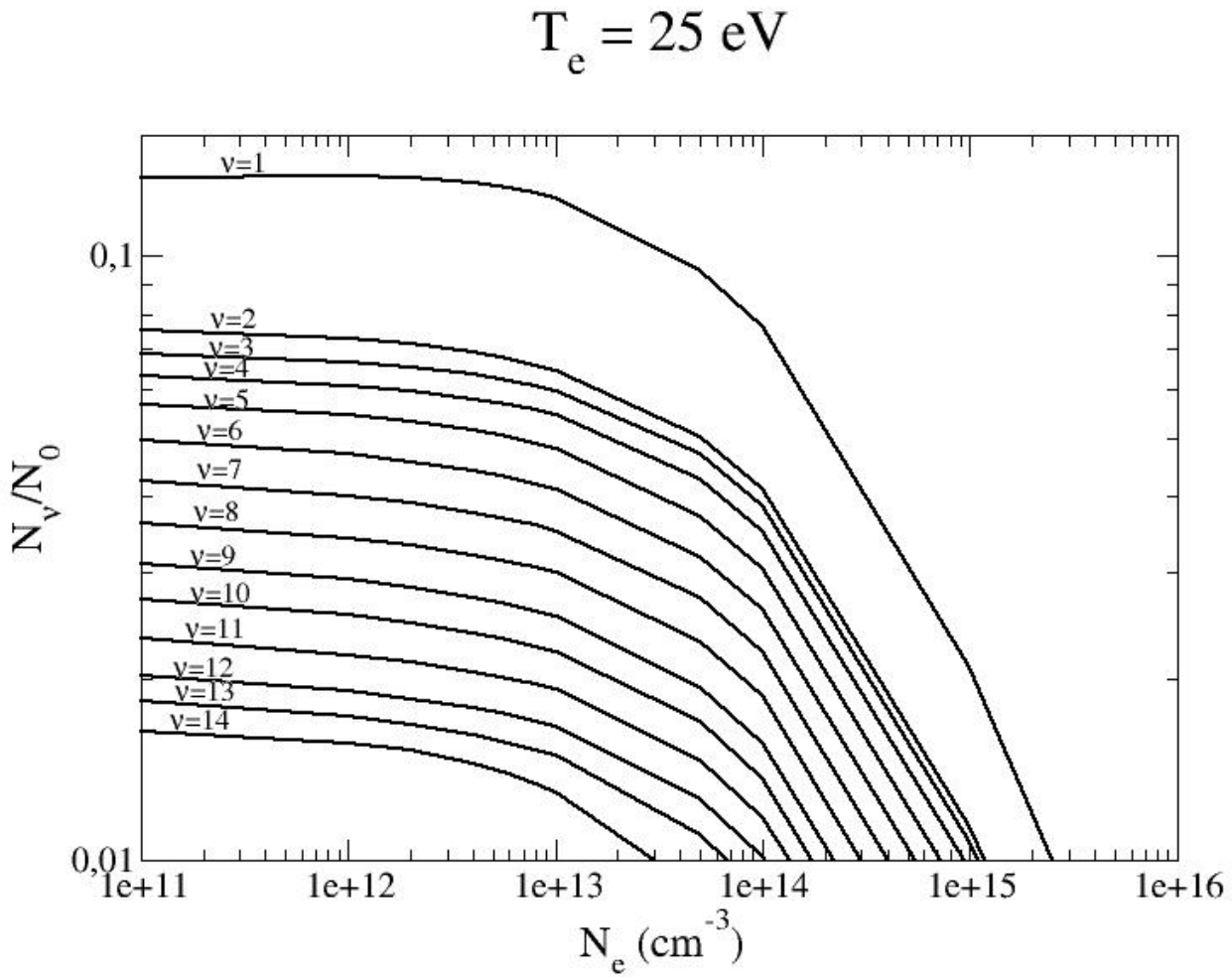
CR dissociation from ground state



CR ionization from ground state to ground state



Population


$T_e = 25$ eV
v=1
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v=3
v=4
v=5
v=6
v=7
v=8
v=9
v=10
v=11
v=12
v=13
v=14
0,1
0,01
N_v/N_0
1e+11
1e+12
1e+13
1e+14
1e+15
1e+16
N_e (cm^{-3})

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Summary

- New molecular collisional-radiative tools have been developped and will be soon available.
- The tools can be extended to other diatomic molecules other than H_2.
- Molecular data are the main problem in building such a model.
- Checking and developing of method of calculations under way.
- Easy implementation of results in models (ADAS structure).