

# PLOUTOS MANUAL

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## I. Introduction

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PLOUTOS is a visualization and manipulation toolkit for EIRENE A&M databases AMJUEL, HYDHEL and H2VIBR (see [Documentation](#)). It is distributed under [EIRENE license](#) and it is available [here](#) (to get access click *Ploutos* on the left column - restricted to registered users).

## II. Select reaction data

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Reactions data in AMJUEL, HYDHEL and H2VIBR databases refers to those processes with a background projectile (electron or bulk ion) impacting on a target (atom, molecule, test or bulk ion). EIRENE needs reaction rates and in some cases also cross sections (charge-exchange collisions) and interaction potentials (elastic collisions).

PLOUTOS initial page contains the following 4 tables of reaction data

- collisions with **e**, where e stands for electrons,
- collisions with **p**, where p stands for protons,
- collisions with **H**, meaning collisions with hydrogenic A&M species,
- collisions with **He**, meaning collisions with helium species.

Each table is organized such that the reaction data for the same physical process are grouped together and shown as consecutive rows. The following column features are present:

- **number**: a label for the physical process in the form of three integer digits split by dots, for instance 2.1.5 for hydrogen ionization by electron impact (Janev notation),
- **reaction**: the formula of the reaction, which uniquely identifies the group of reactions corresponding to the same physical process and different data in the same group may refer to different models and/or different particle internal states (electronic, vibrational and/or rotational ones).
- **range**: the limits of validity of the data in energy for cross sections (section H.1), in temperature for those rates in sections H.2 and H.8, in temperature and energy for those rates in sections H.3 and H.9, in temperature and density for those rates in sections H.4 and H.10.
- **reference**: the main reference from which data are taken,
- **data type**: the type of data, whether they are experimental or calculated from a theory,
- **peculiar properties**: a general comment about the data, as for instance the theoretical model used for computation, some specific properties or features,
- **generation**: a label to keep track of the insertion of new data: 0 for all reaction at present, it will increase in next developments,
- **data origin**: a specification of how the data have been obtained, for instance whether it is the original fit present in the reference, or it is an improved fit or for experimental data whether it is the fit of the original data,
- **File/chapter**: the corresponding chapter (see next table for the quantity in each chapter) and database (AMJUEL, HYDHEL or H2VIBR).

Chapter	Quantity	Variables	Comments
H.0	interaction potentials	energy	for elastic processes
H.1	cross section	energy	laboratory frame (comoving with the target species)
H.2	reaction rate	temperature	vanishing target energy and non-drifting background Maxwellian distribution
H.3	reaction rate	temperature, energy	non-vanishing target energy and/or drifting background Maxwellian distribution
H.4	reaction rate	temperature, density	from CRM accounting for ladder-like processes

Chapter	Quantity	Variables	Comments
H.8	cooling rate	temperature, density	$\langle \sigma v E_p \rangle$ with $\langle \sigma v \rangle$ from H.2
H.9	cooling rate	temperature, density	$\langle \sigma v E_p \rangle$ with $\langle \sigma v \rangle$ from H.3
H.10	cooling rate	temperature, density	$\langle \sigma v E_p \rangle$ with $\langle \sigma v \rangle$ from H.4
H.11, H.12	other parameters	temperature	mainly population coefficients

These columns except **number** are retractable and the user can freely choose the features to be shown through the **Visibility column** list at the top of the page: by clicking *on/off* a hidden/visible column is made visible/hidden.

Visibility columns:  
 reaction: switch to off  
 range: switch to off  
 reference: switch to off  
 data type: switch to off  
 Peculiar properties: switch to on  
 generation: switch to on  
 data origin: switch to on  
 File/chapter: switch to off

There are three additional columns that do not refer to data features but they contain some buttons to select the list of reaction data to be sent to the plotter or to the solver:

- **not included in solver:** one button for each group to remove any group element from the list of reaction to be sent to the solver,
- **selected data:** one button for each data to select one element of each group (radio button for group elements) to include in the list of reaction data to be sent to the solver - the header contains the clickable string *unselect all* to clear the list,
- **plot:** one or more buttons for each reaction data to be sent to the plotter - the header contains the clickable string *unselect all* to clear the list.

These buttons allows to send to the solver at most one element for each group of reaction data, while no restriction is made on the reaction data for the plotter.

On top of the first main table one can also find the alternative clickable strings *show only selected reactions (rows)/show all reactions (rows)* to show only those selected records for solver/all records. Similarly, the clickable strings *show only selected reactions (Groups)/show all reactions (Groups)* provides the same utility for all the elements of those groups containing the

selected reactions.

### III. PLOTTER

The reaction data selected through the third column (**plot**) are sent to the **plotter** that provides the plots with cross-sections/reaction rates on y-axis and energy/temperature on the x-axis. If the selected reaction data are cross sections **PLOUTOS** computes internally the reaction rate and plots it. Similarly, from interaction potentials both the corresponding cross-sections and reaction rates are computed and plotted.

At the bottom of **PLOUTOS** initial page one can find to the right the table to set the plotter options.

It contains two columns: one for cross-section and one for reaction rate plots. The first two rows define the minimum and maximum values in eV for energy and temperature. The third row fixes the number of points, while the fourth one contains radio buttons to set the scale for the x-axis, whether logarithmic (log) or linear (lin). The last three rows are for reaction rates only and they can be used to fix additional parameters:

	Parameter for cross section: aus up1	Parameter for Maxwellian rate coefficients:
inxmin	<input type="text" value="1"/>	<input type="text" value="1"/>
inxmax	<input type="text" value="1000"/>	<input type="text" value="1000"/>
eanz	<input type="text" value="50"/>	<input type="text" value="50"/>
xloglin	<input checked="" type="radio"/> log <input type="radio"/> lin	<input checked="" type="radio"/> log <input type="radio"/> lin
E		<input type="text" value="1.00e-01"/> <input type="button" value="add one more energy of beam particle"/>
ne		<input type="text" value="1.00e+14"/> <input type="button" value="add one more density option"/>
P		<input type="text" value="1.00e+00"/> <input type="button" value="add one more parameter"/>

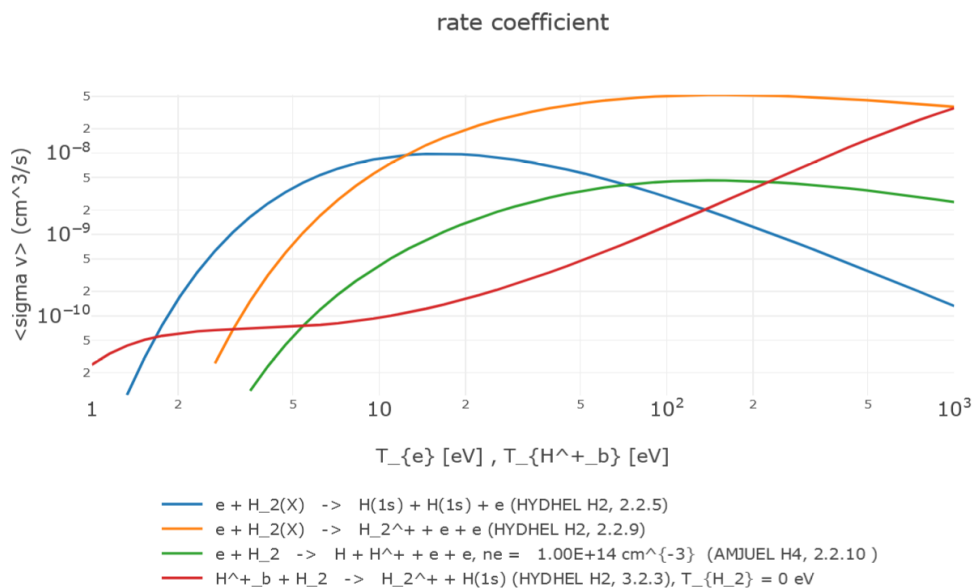
- energy for data in chapters H.3 and H.9,
- density for data in H.4 and H.10,
- other additional parameters.

For each additional parameter more values can be assigned by clicking on the buttons below the entries.

Below the table one can find the button **plot** to access the **plotter**.

The *\*plotter page* shows the graphs for the selected cross sections (for H.0 or H.1 data) as a function of center-of-mass energy and for the reaction rates as a function of beam temperature (see the figure below). At the top of the page one can download input and output data in various formats (db, fhg and json). The plots can be customized by showing/hiding the legend,

by setting logarithmic scales on X and/or Y axis and by changing X and/or Y ranges, clicking the button *re-draw* button to apply the changes. Other graphical options (such as zoom, download as png, reset axis) are available by moving the cursor on the plot at the top right.



## IV. SOLVER

The **solver** allows the user to solve a 1-dimensional linear collisional-radiative model (**CRM**) defined by the list of selected reaction data through the column **selected data** in the main tables of the initial page. Data for cooling rate (corresponding to chapters H.8, H.9, H.10) and for elastic reactions cannot be selected since they are irrelevant: the former are for energy distribution and the latter refer to processes that do not change particle concentration.

It is possible to save such a list in json format through the button *save configuration* at the bottom of the page and to load a previously saved list by loading the corresponding json file through the button *Start with own configuration* at the top of the page.

The 1-dimensiona characted of the CRM can be interpreted as time evolution or as space distribution. This features allow to model a finite velocity for each species and to perform a spectral analysis outlining the relevant time/spatial scales.

Some solver options can be fixed through the table at the bottom of **PLOUTOS** initial page to the left. It contains two rows to identify (*yes*) or treat as different (*no*) atomic (H) or molecular (H<sub>2</sub>) species with respect to their electronic ground state H(1s) and H<sub>2</sub>(X), respectively (this is a reasonable assumption in most cases). The next four rows fix some options

H = H(1s)	<input type="radio"/> yes <input checked="" type="radio"/> no
H <sub>2</sub> = H <sub>2</sub> (X)	<input type="radio"/> yes <input checked="" type="radio"/> no
tmin_json	<input type="text" value="1e-2"/>
tmax_json	<input type="text" value="1e+4"/>

for the time variable: the minimum and maximum time, the number of points and the scale, whether logarithmic (*log*) or linear (*lin*) one.

By clicking the solver button, one enters the *species selection* page in which different options for the reactants and the products of the selected reaction data can be chosen.

n_T_json	51
loglin_json	<input checked="" type="radio"/> log <input type="radio"/> lin
solver	

The first table in the *species selection* page contains all the reactants and products as records whose feature columns are:

- *select*: to select the species to include into the solver, with the buttons to select/unselect all the listed species in header,
- *species*: with species name, derived from the databases,
- *initial condition/incident flux*: to fix the initial condition, *i.e.* the concentration at initial time  $t=0$  (time evolution) or the incident flux at  $x=0$  (spatial distribution),
- *influx*: to fix the external source influx,
- *velocity*,
- *loss time*,
- *P, Q*: to select whether the corresponding species is P, *i.e.* it is tracked normally, or it is a short-living Q species (according to Greenland classification ref.),
- *sensitivity*,
- *most probable paths*,
- *plot/print*: to select the species to be shown in output (plot or file), with the buttons to select/unselect all the listed species in header,
- *reservoir*: to select additional reservoirs having fixed temperature and density, default reservoirs being electrons, photons and bulk ions only.

	Species	init. condition (t=0) or incident flux (x=0) in #/unit volume or #/s/unit area, resp.	influx (#/s/unit volume)	velocity (cm/s)	losstime (s)	P, Q	sensitivity	most probable paths	plot/print ?	reservoir ?
<input type="button" value="select all"/> <input type="button" value="unselect all"/>					<input type="text" value="1e+300"/> <input type="button" value="all losstime"/>	<input type="button" value="set all P"/> <input type="button" value="set all Q"/>	<input type="checkbox"/> enable continuation run WARNING: large systems may lead to long execution times	eps: <input type="text" value="1.e-7"/> n output: <input type="text" value="10"/> n calc: <input type="text" value="10"/>	<input type="button" value="select all"/> <input type="button" value="unselect all"/>	
default	e	fixed reservoir								
default	h <sub>v</sub>	fixed reservoir								
default	H <sup>+</sup> <sub>b</sub>	fixed reservoir								
<input type="checkbox"/>	1 - H <sup>+</sup>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="1e+300"/>	<input checked="" type="radio"/> P <input type="radio"/> Q	<input type="text" value="0"/>	<input type="radio"/>	<input type="checkbox"/>	<input type="button" value="reservoir"/>
<input type="checkbox"/>	2 - H(1s)	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="1e+300"/>	<input checked="" type="radio"/> P <input type="radio"/> Q	<input type="text" value="0"/>	<input type="radio"/>	<input type="checkbox"/>	<input type="button" value="reservoir"/>
<input type="checkbox"/>	3 - H <sub>2</sub> (X)	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="1e+300"/>	<input checked="" type="radio"/> P <input type="radio"/> Q	<input type="text" value="0"/>	<input type="radio"/>	<input type="checkbox"/>	<input type="button" value="reservoir"/>
<input type="checkbox"/>	4 - H <sub>2</sub> <sup>+</sup>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="1e+300"/>	<input checked="" type="radio"/> P <input type="radio"/> Q	<input type="text" value="0"/>	<input type="radio"/>	<input type="checkbox"/>	<input type="button" value="reservoir"/>

Additional tables allow the user to select the temperature and density of the reservoirs (in red), the maximal time, the threshold value below which the rate is assumed to vanish (for ill-conditioned CRMs), the output (linear or logarithmic) scale for x (time/space coordinates) and y (concentration) axis.

time-step/spatial step 1			
E	<input type="text" value="1"/>		
$T_{nv_b}$ (eV)	<input type="text" value="1.00e+01"/>	$n_{nv_b}$ (#/cm <sup>3</sup> )	<input type="text" value="1.00e+13"/>
$T_{H^+_b}$ (eV)	<input type="text" value="1.00e+01"/>	$n_{H^+_b}$ (#/cm <sup>3</sup> )	<input type="text" value="1.00e+13"/>
$T_e$ (eV)	<input type="text" value="1.00e+01"/>	$n_e$ (#/cm <sup>3</sup> )	<input type="text" value="1.00e+13"/>
$t_{max}$ (s)	<input type="text" value="1e-4"/>		

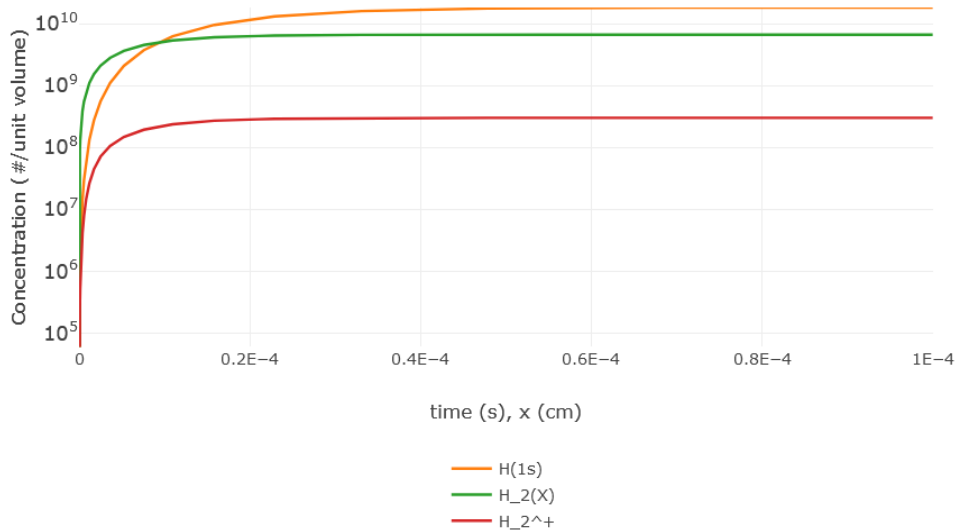
epsrate	<input type="text" value="1.e-30"/>		
xloglin	<input checked="" type="radio"/> log <input type="radio"/> lin	yloglin	<input checked="" type="radio"/> log <input type="radio"/> lin
	<input type="button" value="submit"/>		

After setting the options the user can send the corresponding CRM to the solver and inspect the output through the *submit* button at the bottom of the *species selection* page .

The *solver output page* provides several tables and plots outlining the results of the CRM. A first table presents a resume of the selections done in previous page (species, influx, ..), while the output files can be downloaded by clicking the printout list (see the image to the right). Then, one can find the plot of the species concentrations vs time/spatial coordinate (see the figure below), that is customizable as in the *plotter page*, and a technical summary of the solver run is presented.

#### Printout in tabular form

[matrix elements](#)  
[Table reactions - species](#)  
[EIRENE-json](#)  
[all rates in tabular form](#)  
[Output for EIRENE](#)  
[printout of solution in tabular form](#)  
[Download plot data \(Concentration\) as json](#)



Next, the user can find the results of **spectral analysis** (see the figure below). The threshold eigenvalue absolute value  $|\lambda|$  and the maximal number of non-vanishing eigenvalues can be changed with respect to the shown values and the analysis can be redone clicking the *re-submit* button. The last lines contains the clickable links for downloading the results. Finally one finds the plot of the minimal non-vanishing eigenvalue absolute value with respect to the eigenvalue number up to the maximal one.

### Spectral analysis of reaction kinetics

non-zero eigenvalues: 3,  $|\lambda|_{\min} = 8.716062e+04$ ,  $|\lambda|_{\max} = 1.388490e+06$   
total number of species: 4  
stiffness parameter,  $\lambda_{\max} / \lambda_{\min}$ : 1.593024e+01  
fastest timescale in system:  $\tau_{\text{fastest}} \sim 1. / |\lambda|_{\max} = 7.202070e-07$  s  
slowest timescale in system:  $\tau_{\text{slowest}} \sim 1. / |\lambda|_{\min} = 1.147307e-05$  s  
number of non-zero eigenmodes with  $|\lambda| < 1000 * 8.716062e+04$ : 3  
used non-zero eigenvalues with smallest modulus: 3  
re-evaluate solution with  non-zero slowest eigenmodes.

- [Eigenvalues](#)
- [Eigenvalues, Eigenvectors](#)
- [Download plot data \(eigenvalues\) as json](#)

The bottom part of the *solver output page* allows the user to change some of the background parameters and perform a new run on top of the old one (i.e. the final concentrations are taken as initial conditions) by clicking the *re-submit* button.



### Continue this run with new background parameters ?

- new run, with new initial condition, runs from  $t_{\min} = 0$  to new  $t_{\max}$
- use final concentrations of previous run as initial condition
- keep same influx as in previous run

E

$T_e$  (eV)   $n_e$  (#/cm<sup>3</sup>)

$T_{hv\ b}$  (eV)   $n_{hv\ b}$  (#/cm<sup>3</sup>)

$T_{H^+\ b}$  (eV)   $n_{H^+\ b}$  (#/cm<sup>3</sup>)

$t_{\max}$  (s)

xloglin  log  lin yloglin  log  lin

## V. Default cases

H2-F.Cianfrani,2022-2023: Default cases for molecular hydrogen decay can be selected through the buttons placed at the top of the initial page. They correspond to the vibrationally unresolved case and to the two vibrationally resolved cases, with 7 and 14 internal states, whose reaction data are shown in the table below (in the last column *vibr.res.* specify the source for the vibrationally-resolved cases if different from that in the unresolved one).

Start with default-Cases:

Unresolved
Vibrationally resolved 7
Vibrationally resolved 14

Formula	Type of reaction	Source (database,chapter,number)
$H_2 + e \rightarrow H_2^+ + e + e$	molecular ionization	HYDHEL H.2 2.2.9, H2VIBR H.2 2.[ $\nu$ ]v14 <i>vibr.res.</i>
$H_2 + e \rightarrow H_2(b_{triplet}) \rightarrow H + H + e$	neutral dissociation	HYDHEL H.2 2.2.5, H2VIBR H.2 2.[ $\nu$ ]v11 <i>vibr.res.</i>

Formula	Type of reaction	Source (database,chapter,number)
$H_2 + e \rightarrow H + H^+ + e + e$	dissociative ionization	AMJUEL H.4 2.2.10
$H_2 + H^+ \rightarrow H_2^+ + H$	charge exchange	HYDHEL H.2 3.2.3, H2VIBR H.2 2.[ $\nu$ ]v 2 <i>vibr.res.</i>
$H_2(\nu) + e \rightarrow H_2(\nu \pm 1) + e$	ladder-like vibrational transitions	H2VIBR H.2 2.[ $\nu$ ]v[ $\nu \pm 1$ ] <i>vibr.res.</i>
$H + e \rightarrow H^+ + e + e$	ionization	AMJUEL H.4 2.1.5
$H_2^+ + e \rightarrow H + H^+ + e$	neutral dissociation (MAD)	AMJUEL H.4 2.2.12
$H_2^+ + e \rightarrow H^+ + H^+ + e + e$	dissociative ionization (MAI)	AMJUEL H.4 2.2.11
$H_2^+ + e \rightarrow H + H$	dissociative recombination (MAR)	AMJUEL H.4 2.2.14

In the unresolved case one needs to identify  $H_2$  with  $H_2(X)$  and the resulting CRM is non-trivial only if a non-vanishing  $H_2$  influx is chosen in the *species selection* page. In the two vibrationally resolved cases the user can freely split the full molecular source over different states  $H_2(\nu)$ .