

DOCUMENTATION

Shock code

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Image of the bipolar jet HH212 in the ro-vibrational H₂ line $\nu = 1-0$ S(1) at 2.12 μ m tracing hydrogen molecules shock-heated to ≈ 2000 K, and revealing a series of remarkably symmetric bowshocks caused by periodic outbursts in the jet (Credit: J. Bally, U. of Colorado, USA).

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Overview

This document presents the main ingredients of the "Paris-Durham" Shock Code distributed on the ISM Platform of the Paris Observatory Data Center at <http://ism.obspm.fr>. It provides all the necessary information to run its last public version, and use its output files.

The last current version, **V1.1**, allows for an external far-ultraviolet (FUV) irradiation field and for the crossing of sonic point. It is described in Godard et al. 2019 [51].

The rest of this chapter presents the main physical and chemical ingredients of the model, and its limitations. Chapter 2 presents instructions for installing and running the code on your local computer. Chapters 3 and 4 describe in detail the input and output files, respectively. Chapter 5 contains suggested reading and a selected bibliography, that the interested user is strongly advised to consult. Appendices present complementary material (including the main equations solved by the code in the C-shock case, and examples of input chemical files).



The source code is distributed under an open licence GPL V3. Applications using any parts of the code must be distributed under the same license or higher.

Acknowledgement and citations

For statistical purposes, please acknowledge in your publications the use of this code and the ISM Platform Service as:

This work has made use of the Paris-Durham public shock code Vx [where x stands for the version that you used], distributed by the CNRS-INSU National Service "ISM Platform" at the Paris Observatory Data Center (<http://ism.obspm.fr>)

Please also refer to the following papers:

- Flower, D. R., Pineau des Forêts, G., & Hartquist, T. W. , 1985, MNRAS, 216, 775, **and**
- **for V0:** Flower, D. R., & Pineau des Forêts, G., 2003, MNRAS, 343, 390
- **for V1.1:** Godard, B., Pineau des Forêts, G., Lesaffre, P., et al. 2019, A&A 622, A100
- **if you used option Cool_KN=1:** Neufeld, D.A. & Kaufman, M.J. 1993, ApJ 418, 263

Contact:

For questions and suggestions of updates, please do not hesitate to contact the scientific team in charge of code development and documentation (B. Godard, S. Cabrit, A. Gusdorf, P. Lesaffre, G. Pineau des Forêts). The generic email address is shock.support@obspm.fr.

Credits:

The interactive software tools to run the on-line version and to analyse the `hdf5` output files are developed and maintained by David Languignon, Nicolas Moreau and Carlo-Maria Zwolf (LERMA, Observatoire de Paris).

1.1 The "Paris-Durham" shock code in a nutshell:

The code was originally created jointly by David Flower (Durham, UK) & Guillaume Pineau des Forets (IAS Orsay, France) to treat multi-fluid MHD shocks in the diffuse interstellar medium [12]. It was then continuously updated and developed to include an ever growing number of micro-processes and physical situations. A list of the main updates and of the papers that describe them is given in Chapter 5.

Its fields of application include galactic interstellar shocks driven by

- super-alfvénic turbulence and cloud collisions
- jets and outflows from forming stars
- slow AGB winds
- old supernova remnant shells.

Extra-galactic applications have also been developed recently.

Main assumptions and geometry: This shock code calculates the

- *steady-state* ($\partial/\partial t = 0$) dynamical, thermal, and chemical structure of a
- *plane-parallel shock wave* propagating in a
- *molecular and dusty homogeneous medium* permeated by
- *a uniform magnetic field transverse to the shock propagation*, and possibly irradiated by
- *an external FUV field from upstream* (see Figure 1.1).

Types of shocks:

The code can handle all the possible shock types for a transverse B-field:

- steady "jump" (J-type) shocks, where the gas is suddenly compressed across a viscous front.
- steady "continuous" (C-type) shocks, where ions and neutral decouple and the neutral fluid remains supersonic throughout.
- young C-shocks (where the C-type precursor is truncated and followed by a truncated J-front).
- steady C* and C-J shocks, where the neutral fluid goes through a sonic point [51].

Range of validity and limitations: The thermo-chemistry is validated up to $n_H \leq 10^8 \text{ cm}^{-3}$ and $G_0 \leq 10^5$. The code does not (yet) treat the transfer of Lyman photons, and only considers singly ionized species, hence J-shocks should be restricted to $V_s \leq 30 \text{ km s}^{-1}$. Grain-grain collisions are not (yet) included, hence the release of refractory and ice species in gas phase is underestimated (for detailed modeling see [60, 61, 62]).

The main strength of the Paris-Durham model is that it *solves in parallel* for the dynamics and non-equilibrium chemistry: Indeed, ionization regulates the decoupling between neutral and charged fluids ("magnetic precursor"), ion-neutral drag heating, and gas-grain sputtering, which in turn has a strong feedback on the shock dynamics. This ensures a self-consistent solution.

Observational predictions: The code also computes and outputs the *predicted surface brightness* ($\text{erg/s/cm}^2/\text{sr}$) in optically thin lines of H_2 and atomic lines (O, C, C^+ , N, N^+ , Si, Si^+ , S, S^+ , Fe^+) that can be directly compared with observations, eg. with JWST. Line profiles for optically thick molecules (eg. CO, H_2O , SiO, OH, CH_3OH , NH_3 etc..) can be computed a posteriori from local abundances, temperature, and density, e.g. in the Large-Velocity-Gradient (LVG) approximation.

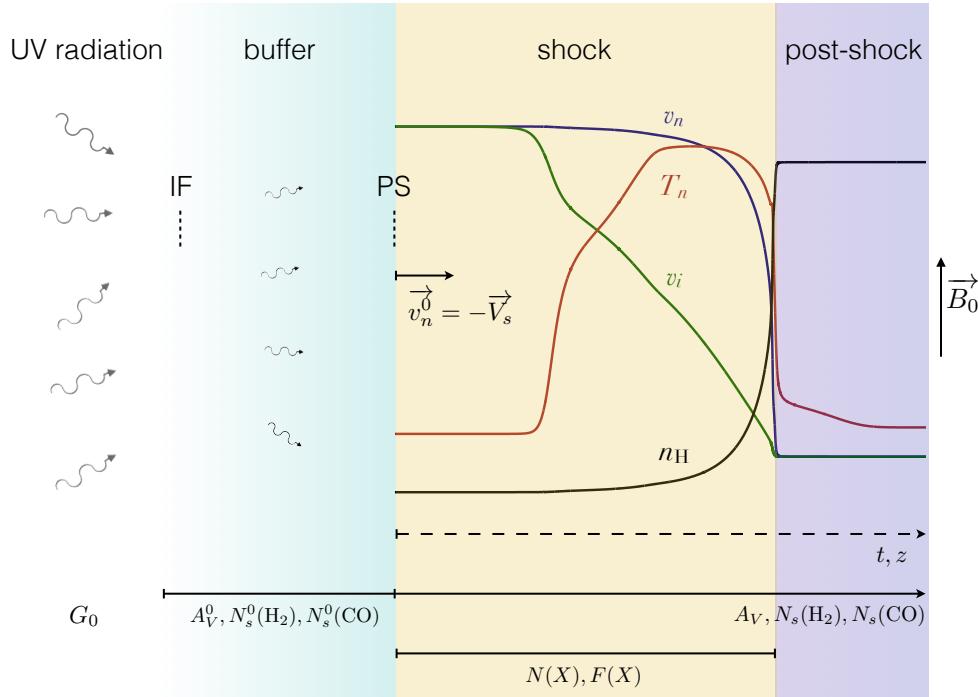


Figure 1.1: This figure represents the different zones in a planar C-type shock irradiated from upstream: the preshock radiative buffer in light blue, which must be computed separately (from the ionization front IF up to the desired attenuation A_V^0) to provide initial conditions for the shock; The C-shock layer per se in yellow; and its post-shock region in purple (defined as the region with no further compression) whose contribution to the line intensities is not included. Some key parameter notations are also indicated. From [51].

1.2 Main ingredients in the Paris-Durham code

1.2.1 Dynamics

The Paris-Durham shock code computes the coupled evolution of velocity, density, temperature and chemical abundances along the 1D flow assuming steady-state; this is made by integrating as a function of z (see Figure 1.1) a series of ordinary coupled differential equations describing the conservation of particle number, mass, momentum, energy, in each fluid (neutrals, ions, electrons), and the rate of change of each chemical species. These equations are presented in Appendix A in the case of C-type shocks, and the corresponding momentum and energy source terms, including chemical reactions, are detailed in Appendix B. The H_2 level populations are also integrated in parallel with the dynamics (as they can deviate from local equilibrium). The full set of coupled equations is solved with the DVODE integrator, able to handle stiff systems.

The type of steady shock wave allowed to propagate through the medium depends crucially on its magnetization and ionization properties.

If V_s is larger than the magneto sonic speed in the charged fluid $V_{A,c} = B / \sqrt{4\pi\rho_c}$ (where the density ρ_c of the charged fluid includes the inertia of charged grains coupled to the magnetic field), then no magnetic precursor can develop; only a viscous J-type shock front can form. (runs with the 'C' option in such a case will not give any sizable change in variables).

In contrast, if $V_s < V_{A,c}$, a C-type magnetic precursor can develop in the charged fluid, where ions are rapidly decelerated by the magnetic pressure gradient while the neutrals are decelerated much more progressively by collisions with the slower ions (see Figure 1.1). These ion-neutral collisions dissipate the incident kinetic energy flux over a much wider region (of order the mean free path of neutrals through the ions) than in J-type shock (where it is dissipated over the viscous length = mean free path of neutrals through neutrals). If the gas cools sufficiently well to remain supersonic, a steady C-shock results. If a sonic point is encountered, a C* shock or a steady C-J shock result. Such transitions occur as soon as $G_0 > 0.2\sqrt{n_H/\text{cm}^{-3}}$ [51] and are automatically handled by version V1.1 of the shock code.

1.2.2 Heating and cooling processes

The cooling mechanisms included in the code are

- H₂ line cooling following collisional excitation by H, H₂, He, H⁺, and electrons [?],
- Rotational and vibrational radiative cooling by CO, H₂O, and ¹³CO in the Large Velocity Gradient approximation [10]
- Pure rotational cooling by OH and NH₃ in the low-density optically thin limit [12],
- Atomic cooling by fine-structure and metastable lines of C, N, O, S, Si, C⁺, N⁺, O⁺, S⁺, Si⁺ [47] and Fe⁺ [?].
- Inelastic scattering of electrons on H and H₂ [?, ?, ?],
- Collisional dissociation and ionisation

The heating mechanisms included in the code are

- Viscous and compressive heating
- Ambipolar-diffusion heating = elastic scattering between the neutral fluid and charged ions and grains,
- Heating by cosmic-rays
- Photoelectric effect on small grains and PAHs
- Photoionization and photodissociation heating [12]
- Collisional de-excitation of H₂ levels, including FUV-pumped or formation-pumped H₂

Additional mechanisms are included that can either heat or cool :

- Energy heat / loss through gas-grain collisions [?]
- Enthalpy transfer between the neutral, ion, and electron fluids [12] (net balance = 0)
- Exo / endo-thermicity of chemical reactions [12]

The reader is referred to the corresponding references for a discussion of the physical context and hypotheses involved in modelling each of the above processes.

1.2.3 Chemical species and grains

Chemical species can be constructed from any of the elements H, D, He, C, N, O, Na, Mg, Si, S, Fe. They can be neutral, singly ionized, on grain icy mantles (name followed by *), or inside grain refractory cores (name followed by **). The list of species to be integrated by the code is read from an input file [species.in](#), with a specific format described in Chapter 3. It can be modified by the user to suit specific needs. Standard models involve 134-138 species (see eg. Appendix ??).

A representative polycyclic aromatic hydrocarbon (PAH) species can be included ($C_{54}H_{18}$), that can be singly charged and contribute to ion-neutral coupling [32].

Finally, a representative grain species (G) is also included to track the grain charge. The number of grains per H nucleus is determined self-consistently from the initial mass of refractory elements in grain cores, the initial grain size distribution, and the core bulk density (all user-specified, see Section 3).

The thickness of ice mantles is determined self-consistently from the total abundances of elements in mantles, the ice bulk density specified by the user (see Section 3), and the size distribution of grain cores at the current point.

1.2.4 Chemical network

The list of reactions used by the code can be freely specified by the user (see Section [?]). The standard network involves ≈ 1000 reactions linking about 130 species. But it can be expanded to include, eg., deuterated species.

The current version of the code allows for the following types of gas-phase chemical reactions (limited to a maximum of 4 products):

- neutral-neutral reactions
- ion-neutral reactions (enhanced by ion-neutral drift, following the effective temperature prescription of [?]). Reverse reactions are included up to an endothermicity of 2 eV.
- radiative and dissociative recombinations
- charge exchange
- Ionisation and dissociation by secondary energetic electrons from cosmic ray ionizations
- photodissociation by "secondary photons" close to 1000 Å from H_2 Lyman fluorescence excited by secondary electrons [?]
- Ionisation and dissociation by far-ultraviolet (FUV) photons, including an approximate treatment for self-shielding of H_2 and CO [50, 51]

Some chemical reactions involving H_2 are treated level by level for improved accuracy:

- H_2 reformation on grains (with sticking coefficient from [?])

- H₂ ortho to para conversion [42]
- H₂ collisional dissociation (following [?])

The code also models several processes that transfer species between grains and gas:

- sputtering of icy mantles by drifting heavy neutrals (with attendant reduction in mantle thickness)
- sputtering ("erosion") of refractory species from grain cores by drifting heavy neutrals (with attendant reduction in grain core size)
- charge balance of grains and PAHs (treated as in [32])
- adsorption of species on ice mantles, immediately followed by complete saturation
- FUV-induced and cosmic-ray induced desorption from ice mantles [51]
- thermal desorption of ice mantles [51]

Installation and run on local computers

Requirements

All versions of the Paris-Durham Shock code require a recent Fortran 90 compiler.

Python 2.7 and Python modules (numpy, h5py, PyQt4) are not mandatory, but they are also required if you wish to produce output files in HDF5 format. The same Python modules are also required to run the two interactive tools **Extractor** and **ChemistryAnalyzer** provided in the release package, that allow to browse these HDF5 files and analyze interactively the code results, in particular to check the dominant chemical reactions for producing a given species.

Installation of Python 2.7 and required modules with MacPorts on Mac:

```
sudo port install python27 py27-numpy py27-h5py py27-pyqt4
```

Installation of Python 2.7 and required modules on Ubuntu with apt-get:

```
sudo apt-get install gfortran libblas3gf libblas-doc  
libblas-dev liblapack3gf liblapack-doc liblapack-dev
```

The procedure to install the code is:

- 1- download the source code at <http://ism.obspm.fr> (go to the 'Shock' page, then to the 'Download' page, then click on the "download" link corresponding to the desired version)
- 2- unwrap the zip archive; it will create a "Shock" directory (Shock_1.1_godard2019) that you can rename to your taste.

The "Shock" directory should contain the following subdirectories:

- **src**: with all FORTRAN source codes
- **bin**: with Makefile and all compiled modules
- **input**: with all input parameter files, chemistry files, as well as atomic, molecular and grain data.
- **output**: will contain subdirectories (one per run) with output files
- **AnalysisTools**: contains the two Python tools **Extractor** and **ChemistryAnalyzer** to analyze HDF5 files, and their Documentation files [Doc_Extractor.pdf](#) and [Doc_ChemistryAnalyzer.pdf](#).
- **mtx**: numerical libraries

To finish the installation:

- 3- go to **bin/** and edit and configure the file **Makefile** to suit your local compiler
- 4- compile the code with **make**

This should create the executable **mhd_vode** in the "Shock" directory.

First test run

Go back to your main "Shock" directory and type `./mhd_vode`. This will run the code with the default input files present in `input/`. It is a standard C-shock with $V_s = 10 \text{ km s}^{-1}$, $n_H = 10^4 \text{ cm}^{-3}$, magnetic field scaling parameter $b = 1$, and no FUV field ($G_0 = 0$). The execution time on a laptop should be about 10 minutes.

All the output files will be written in the subdirectory `output/example_shock/`. The content of these output files is described in Chapter 4.

Now, edit the input file `input/input_mhd.in` and change the value of the parameter `modele` from "example_shock" to something else, such as "Cv10n4b1G0". Then, go back up to the "Shock" directory and re-run the code. It will write the output files in a different subdirectory `output/Cv10n4b1G0`, created with the new name that you gave. **This prevents the code from overwriting the output files of consecutive model runs !**

We recommend using short names for output directories, that recall the main shock parameters (e.g."Cv10n4b1G0").

The other input parameters, and how to modify them to suit one's need, are described in Chapter 3.

Basic instructions for a specific shock run

The basic steps to compute a new shock model, and the most important input parameters to set at each step are the following:

Step 1: Compute the relevant thermo-chemical pre-shock conditions:

Of course, this first step only needs to be done once for a given set of environmental conditions. The following input parameters must be carefully set in the input file `input_mhd.in`(described in more detail in Chapter 3) :

- Name of file with chemical network (with or without ice adsorption/desorption)
- Name of file with initial species abundances (generally only atoms + H₂ + grains for pre shock)
- Name of output directory for pre shock run
- Preshock density n_H
- Type of pre-shock : S1 = isodensity with constant FUV, S2 = isobaric with constant FUV, P1 = isodensity with FUV attenuation, P2 = isobaric with FUV attenuation
- Incident FUV field intensity G_0 at the ionization front (IF), in units of the local interstellar FUV field
- FUV attenuation A_V at $z=0$ ($\approx 10^{-9}$ for P1 and P2 types, any value for S1 and S2)
- Advection speed V_s from ionization front ($\leq 0.3 \text{ km/s}$ to reach steady-state conditions)
- Advection time $t_{\max} = \text{duration}_{\max}$

Step 2: Insert computed pre-shock conditions into shock model input file

The following parameters need to be updated in [input_mhd.in](#):

- File with initial species abundances = *path to species.out* of preshock model run
- File with initial H₂ levels = *path to H2_lev.out* of preshock model run
- Attenuation A_V_0 at shock entrance = Total A_V through preshock buffer
- self-shielding N_H2_0 at shock entrance = Total column density of H₂ through preshock buffer
- self-shielding N_CO_0 at shock entrance = Total column density of CO through preshock buffer

When there is no FUV irradiation ($G_0 = 0$), the last three parameters can remain set to zero. Otherwise, they must be read from the last line of the output file [mhd_coldens.out](#) written by the pre shock run. This can be done automatically with a shell or Python script.

Step 3: Define the chemistry-independent, "dynamical" shock parameters:

The following input parameters must be specified :

- Name of shock output directory
- Shock speed V_s
- Transverse magnetic field, parametrized as $b = B(\mu\text{G}) / \sqrt{n_H/\text{cm}^{-3}}$
- Initial shock type (C or J)
- Number of fluids (3 for C, 1 for J)
- Shock age = `timeJ`

Step 4: Run the shock model

A whole grid of shock models with same initial preshock conditions can be run simply by repeating Step 3 for different dynamical parameters.

Input files

The code reads several input files that must be located in the `input/` directory. The main ones to be modified or carefully checked by the user are

- `input_mhd.in`: specific model parameters (described in Section 3.1).
- "species.in" : list of chemical species with their initial abundances, including grains and PAHs (see Section 3.2)
- "chemistry.in" : list of chemical reactions and their rates, including gas-grain and photo reactions (see Section 3.3)

The other input files provided in the download package contain various atomic, molecular, and grain data (level energies, Einstein A_{ij} coefficients, collisional excitation rates, grain sputtering yields...); they are only meant to be updated whenever newer data become available and should not be modified without expert advice.

3.1 Summary of input parameters in `input_mhd.in`

The `input_mhd.in` file contains all necessary input parameters to run the shock code, grouped under several categories:

- file parameters
- shock parameters
- environmental parameters
- grain properties
- excitation and cooling
- numerical parameters
- output specifications
- developer options

The input parameters in each category are described in the following Table.

List of input parameters in the `input_mhd.in` file

<i>File parameters</i>	
<code>modele</code>	Model name. subdirectory <code>output/modele</code> will be created containing all output files; also added as prefix to the <code>.hdf5</code> binary output files.
<code>specfile</code>	Path of file with species list and their initial abundances. Example format given in <code>species.in</code> . Can be the output file <code>species.out</code> created by a previous "initialization" run (types S1, S2, P1 or P2, see below). .
<code>chemfile</code>	Path of file with chemical reactions list. Example format given in <code>chemistry.in</code> .
<code>h2exfile</code>	File with initial H₂ level populations. Standard value "none" initializes H ₂ levels at LTE at temperature = <code>Tn</code> with an ortho to para ratio = <code>op_H2_in</code> (see <i>Shock parameters</i> below). Can be the file <code>H2_lev.out</code> from preshock run.
<code>gridfile</code>	File with FUV radiation field at each point. Only used for self-irradiated shock models (under development). Standard value "none".

Shock parameters

shock_type	Type of model can take the following values <ul style="list-style-type: none"> • C = Continuous C-type shock (with ion-neutral decoupling) • J = Jump J-type shock (neutral viscosity term added to dynamical equations)
	preshock with Sideways irradiation: <ul style="list-style-type: none"> • S1 = isodensity advection at V_s with constant FUV flux • S2 = isobaric advection at V_s with constant FUV flux
	Preshock buffer with upstream irradiation: <ul style="list-style-type: none"> • P1 = isodensity advection at V_s with FUV attenuation along z • P2 = isobaric advection at V_s with FUV attenuation along z
Nfluids	Number of fluids can take the following values <ul style="list-style-type: none"> • 1 (standard for J-shocks) • 2 : neutrals and ions decoupled, but $T_e = T_i$ • 3 (standard for C-shocks) : neutrals and ions decoupled, and $T_e \neq T_i$
Bbeta	Magnetic field parameter $b = B(\mu\text{G}) / \sqrt{n_H(\text{cm}^{-3})}$, has a major impact on type of shock (see section [?]). Standard values = 1 for a C-shock and 0.1 for a J-shock.
Vs_km	Shock entrance speed (types C, J) or advection speed (types S1, S2, P1, P2) (km s^{-1})
DeltaVmin	Initial ion-neutral drift speed (cm s^{-1}). Standard = 1.00E03
nH_init	Initial proton density (cm^{-3}) related to gas volumic density through $\rho = 1.4 \times m_H n_H$ (for 10% of Helium by number). V1.1 is only validated up to $n_H \leq 10^8 \text{ cm}^{-3}$.
Tn	Initial temperature of neutrals (in K). Standard value = 15 K.
op_H2_in	Initial ortho to para ratio of H₂ . Standard value = 3 (ratio of spin degeneracies).

Environment parameters

Zeta	Cosmic ray ionization rate per H₂ molecules(s⁻¹) . For a gas with 10% of Helium, it is related to the usual cosmic ray ionisation rate per H nucleus, ζ_{CR} , through $\text{Zeta} = \zeta_{CR}/0.54$. Standard value: 5.00E-17. Can be increased to mimic ionization by hard X-rays $\gg 100 \text{ eV}$.
F_ISRF	Shape of the incident FUV field . This flag can take two values: <ul style="list-style-type: none"> • 1 (Standard): Mathis prescription • 2: Draine prescription Photorates in the chemistry.in file provided with V1.1 are for a Mathis field. Photorates for a Draine field can be found in Heays et al. (2017).
RAD	Mean intensity G_0 of the FUV field over the interval 910-2066 Å, in Habing units
Av0	Visual extinction at $z=0$ (in magnitudes); Typical value is 1.00E-01
F_COUP_RAD	FUV radiative transfer flag to compute photodissociation and desorption rates 0 : No FUV transfer. Photo rates computed from chemfile (in the form $\gamma \exp -\beta A_\nu$) 1 : Calculation of FUV field attenuation along z and local photo rates.
F_AV	A_ν integration flag . 0 = A_ν constant (sideways irradiation); 1 = A_ν integrated along z from upstream.
F_inAv	A_ν to N_H conversion flag : 0 = computed from grain distribution; 1 = grain abundance scaled to match inv_Av_fac
inv_Av_fac	A_ν to N_H ratio (cm^2) (only if $F_{inAv} = 1$). Standard value (galactic ISM) = 5.34D-22
N_H2_0	Column density of H₂ buffer (cm^{-2}) providing H ₂ self-shielding.
N_CO_0	Column density of CO buffer (cm^{-2}) providing CO self-shielding.
vturb	Turbulent velocity (km s^{-1}) used for H ₂ self-shielding calculations in the FGK formalism. Typical value: 1-3 km s^{-1} .

Grain properties

F_TGR	Grain temperature flag . 0 = constant (Standard), 1 = computed at each position.
-------	---

Tgrains	Initial grain temperature (in K). Standard value = 15 K
amin_mrn	Grain minimum radius (in cm), excluding PAHs. Typical value: 1.00E-06 (0.01 μm).
amax_mrn	Grain maximum radius (in cm). Typical value: 3.00E-05 (0.3 μm).
alpha_mrn	Index α of power-law grain size distribution , $dn(a)/da \propto a^{-\alpha}$. Standard value = 3.5 according to Mathis, Rumpl and Nordsieck, 1977, ApJ, 217, 425.
rho_grc	grain core bulk density (in g cm^{-3}). The number of grains per unit volume of gas is inversely proportional to rho_grc. Standard value = 2 g cm^{-3} .
rho_grm	ice mantle bulk density (in g cm^{-3}). Determines the thickness of the ice layer, hence the total grain cross-section for collisions with gas. Standard value = 1 g cm^{-3} .

Excitation and cooling

ieqth	Gas temperature flag ; 1 (Standard) = solved self-consistently; 0 = fixed (only for 'S' and 'P' type models)
Cool_KN	CO and H₂O cooling flag ; 1 (standard) = interpolate in LVG cooling tables from Neufeld & Kaufman (1993); 0 = low-density and optically thin approximation (diffuse medium).
NH2_lev	Number of H₂ levels whose populations are solved in parallel along the flow. Must be 49 when H_H2_flag = DRF. Can be higher when H_H2_flag = MM or BOTH. <i>Make sure to include all H₂ levels with energies up to the maximum temperature in the shock, as they will contribute to H₂ collisional dissociation. Standard = 100</i>
NH2_lines_out	Maximum number of H₂ lines whose emissivities will be written in output files. Standard = 100.
H_H2_flag	H-H₂ collisional rates ; can take 3 values <ul style="list-style-type: none">• DRF : quantum rates from Flower et al. with prescription for reactive collisions adapted from Schofield• MM : semi-classical rates from Martin & Mandy• BOTH (Standard): DRF for the first 49 levels and MM above.
iforH2	H₂ excitation after formation : can take 6 values: <ul style="list-style-type: none">• -1: formation in the lowest levels v,J =0,0 and 0,1• 0 : 1/3 of the formation energy (4.4781 eV) is distributed among the NH2_lev levels according to a Boltzman distribution• 1 (Standard) : proportional to LTE distribution at Tex = 17249 K = 1/3 of 4.4781 eV• 2: all into level v=14, J=0,1 at the dissociation limit (4.4781 eV)• 3: all into v=6, J=0,1• 4: proportional to H₂ relative populations in the gas at current point NB: This parameter can strongly influence the H ₂ line intensities in dissociative or irradiated shocks: Verifications are strongly advised.
ikinh2	Kinetic energy carried by reformed H₂ can take 2 values: <ul style="list-style-type: none">• 1 : 0.5 \times (4.4781 eV - internal)• 2 (Standard): minimum between 1/3 \times 4.4781 eV and (4.4781 eV - internal)
pumpH2	H₂ FUV pumping 0 = not treated, 1 = calculated.
NCO_lev	Number of CO levels included in FGK calculations (obsolete: CO FUV lines are too broad for FGK)

Numerical parameters

Nstep_max	Maximum number of integration steps . Standard = 10000
timeJ	C-shock age (years). This parameter allows to model young C-shocks of ages smaller than the timescale to recouple the ion and neutral fluids (eg. in protostellar outflows). To approximate the structure of such a young C-shock, the code automatically truncates the steady C-type shock at a flow time = timeJ, and switches to a steady J-type viscous front. To compute a steady shock, make sure that timeJ > duration_max. Standard value = 9.999E99

duration_max	Maximum duration of the model (years) at which calculation stops (if Nstep_max not already reached). In a young C-shock, it should be set to $2 \times \text{timeJ}$. In a young J-shock, it should be set to the true shock age. In other instances, it should be sufficiently long to reach the equilibrium postshock temperature and chemistry. For initialization runs of type 'S' starting from atomic conditions, it takes typically $3 \times 10^6 \times (10^4/n_H)$ yrs. For initialization runs of type 'P' (irradiated buffer), the duration should be set to $N_H^0/(n_H V_s)$ where N_H^0 is the desired attenuating column of H nuclei through this buffer.
eps_V XLL	Precision parameter for DVODE numerical integrator. Standard = 1.00D-07 Viscous length for $n_H = 1 \text{ cm}^{-3}$ (cm). Divided by n_H in the code. Standard = 1.00E14.

Output specifications

F_W_HDF5_STD	Write hdf5 standard output file (1 = Yes, 0 = No). for Extractor tool.
F_W_HDF5_CHE	Write hdf5 chemical output file (1 = Yes, 0 = No). for Chemistry Analyser tool.
F_W_ASCII	Write ASCII output files (1 = Yes, 0 = No), for usual graphic tools.
Npthdf5	Maximum number of points in hdf5 files . Standard = 10000
Nstep_w	Number of steps between 2 outputs for ASCII and chemical hdf5 files
speci_out	Quantity written in ASCII file mhd_speci.out can take 3 values: <ul style="list-style-type: none"> AD : absolute number densities at current point $n(X)$ (in cm^{-3}) CD : column densities integrated up to current point $N(X) = \int_0^z n(X) dz$ (in cm^{-2}) FD : fractional abundances at current point $n(X)/n_H$ (dimensionless) Quantity written in ASCII file H2_lev.out can take 3 values: <ul style="list-style-type: none"> AD : local number density in each H₂ level, $n(v, J)(z)$ (in cm^{-3}) CD : column densities integrated up to current point, $N(v, J) = \int_0^z n(v, J) dz$ (in cm^{-2}) In(N/g) : list of $\ln(N(v, J))/g_{v,J}$ (dimensionless) where $g_{v,J} = 2J+1$ is the level statistical weight; allows to plot Boltzman excitation diagrams of H₂ at each z to monitor changes in excitation and ortho/para. Quantity written in ASCII file H2_line.out can take 2 values: <ul style="list-style-type: none"> 'local' : local emissivity in each H₂ line (in $\text{erg s}^{-1} \text{cm}^{-3}$) 'integrated' : flux integrated up to current point in each H₂ line (in $\text{erg s}^{-1} \text{cm}^{-2} \text{sr}^{-1}$) Chemical analysis (Y = Yes, N = No). Output list of dominant reactions at each z (obsolete).
H2_out	
line_out	
flag_analysis	

Developer options

F_SORT	Sort chemical reactions before computing derivatives (1 = Yes, 0 = No)
F_CONS	Enforce elemental and charge conservation (1 = Yes, 0 = No)
F_CH	compute CH velocity instead of adopting the neutral fluid velocity (1 = Yes, 0 = No)
F_S	compute S velocity instead of adopting the neutral fluid velocity (1 = Yes, 0 = No)
F_SH	compute SH velocity instead of adopting the neutral fluid velocity (1 = Yes, 0 = No)
z_0	flow divergence scale under development

3.2 The chemical species file "species.in"

The chemical evolution through any shock model will strongly depend on the chosen initial chemical composition. Hence this initialization is a major point to pay attention to.

The list of chemical species to be considered, and their initial abundances at $z = 0$, is read from a

specifically formatted "species file" located in directory `input/`. In V1.0 and V0, this file had to be named `species.in`. Starting from V1.1, the filename and its path can be freely specified by the user through the parameter `specfile` in `info_mhd.in`; However, to help recognize these files, it is strongly recommended to keep names of the type `species.in_X` where X describes the specifics.

An example of "species file" and its format is given in Appendix D.

It contains one line per species, which must contain:

- index (not used anymore by the code)
- species name with a maximum of 8 characters
- 14 digit number (not used anymore by the code)
- fractional abundance relative to the total number of **protons**, $n_H = n(H) + 2n(H_2) + n(H^+)$
- enthalpy of formation in kcal mol^{-1} (1/4.1 of the value in kJ mol^{-1})
- a comment (optional)

NB: Since the format is so critical, it is strongly advised to save the standard `species.in` given in the code package under a different name, e.g. `species.in.sav`, before any editing.

Three kind of species names are recognized:

- gas-phase species: denoted by their usual symbol and followed by + or - if charged (eg. HCO+)
- neutral species on ice mantles: symbol followed by a * (eg. SiO*)
- neutral atoms in grain cores: symbol followed by a ** (e.g. Mg**)

The species name is automatically interpreted by the code and assigned the corresponding mass. Currently, the code can handle species made of the following elements: H, D, He, C, N, O, Na, Mg, Si, S, Fe. Only single-ionization stages are supported.

An additional generic "grain species" G is also defined, that can be positively or negatively charged. It enters in the chemistry through reactions of charge transfer with gas species. The code verifies that the total number of grains, $n(G) + n(G+) + n(G-)$ in the "species.in" file is consistent with the total mass of ** species in grain cores, for the grain size distribution and the bulk grain density specified in `input_mhd.in`. Otherwise, a warning is issued on screen asking to run a pre shock model (types 'S' or 'P'), where the abundance of G will be properly initialised.

Several important points must be checked about the "species file" before running a model:

- The total elemental abundances summed over all species, and the gas/grain mass ratio: they are computed by the code at the start of the computation and written in the ascii output file `info_mhd.out`, where they can be consulted to make sure they agree with the desired values (eg. solar abundances).
- the distribution of elemental abundances among gas, PAHs, grain cores, and icy grain mantles: the depletion onto grains affects the shock predictions in that it determines the gas-phase abundance of the most important coolants (CO, H2O, O) and the total mass in grains (which controls the inertia of the charged fluid and the C-shock structure). Table 3.2 gives the standard distribution adopted in [32] for dark cloud conditions and a PAH abundance of 10^{-6} . However, these numbers should of course be adjusted depending on the specific environment considered.
- the assumed composition of ice mantles. This will determine the line intensity of shock tracers that are mainly sputtered off grain mantles rather than formed in the gas phase (eg. CH3OH,

element	elemental abundance	in gas phase	in PAHs ($C_{54}H_{18}$)	in ice mantles	in grain cores
H	1	1			
He	0.1	0.1			
C	3.55×10^{-4}	8.27×10^{-5}	5.4×10^{-5}	5.53×10^{-5}	1.63×10^{-4}
N	7.94×10^{-5}	6.39×10^{-5}		1.55×10^{-5}	
O	4.42×10^{-4}	1.24×10^{-4}		1.78×10^{-4}	1.40×10^{-4}
Mg	3.70×10^{-5}				3.70×10^{-5}
Si	3.37×10^{-5}				3.37×10^{-5}
S	1.86×10^{-5}	1.47×10^{-5}		3.93×10^{-6}	
Fe	3.23×10^{-5}	1.50×10^{-8}			3.23×10^{-5}

Table 3.2: Standard initial distribution of elemental fractional abundances among gas-phase species, PAHs, icy grain mantles, and grain cores, as adopted by [32]. The fractional abundance of PAH molecules ($C_{54}H_{18}$) is 10^{-6} per H nucleus. Silicates are assumed to be olivine ($SiO_4[Fe,Mg]_2$). The mass in grain cores is 0.6% of that of the gas, divided up between silicate grains (70% of the grain mass, 57% by number), and carbonaceous ones (30% of the grain mass, 43% by number).

CO^* 8.3×10^{-6} 8.3%	CO_2^* 1.3×10^{-5} 13%	CH_4^* 1.6×10^{-6} 1.6%	NH_3^* 1.6×10^{-5} 16%	H_2O^* 1.0×10^{-4} 100%
CH_3OH^* 1.9×10^{-5} 19%	H_2CO^* 6.2×10^{-6} 6.2%	$HCOOH^*$ 7.2×10^{-6} 7.2%	OCS^* 2.1×10^{-7} 0.21%	H_2S^* 3.7×10^{-6} 3.7%

Table 3.3: Example of initial species abundances in ice mantles relative to hydrogen nuclei in the gas (first line), and relative to water ice (second line, expressed in %), estimated by [32] from absorption observations in Gibb et al. (2000). The resulting total mass in ice mantles is 0.3% that of the gas. Detailed modeling of the L1157-B1 protostellar shock favors 6-10 times smaller abundances of CH_3OH^* and NH_3^* than given here[55].

NH_3 , OCS , H_2S ...). Table 3.3 gives the standard ice abundances adopted in [32] for dark cloud conditions, based on observations of W3OH by Gibb et al. (2000).

However, the ice composition in the cold ISM is still very uncertain. For example, modeling the full set of *Herschel* observations of the B1 shock in the L1157 protostellar outflow with the Paris-Durham shock code suggests that CH_3OH and NH_3 ices are 6-10 times less abundant in that region than assumed in Table 3.3.

Fortunately, most ice species (except for H_2O and CH_3OH) are not major shock coolants and are not strongly reactive; hence their assumed ice abundance does not impact the shock structure, and they can be scaled a posteriori to match observations.

3.3 The chemical network file "chemistry.in"

The chemical reaction rates are read from a specifically formatted file located in directory `input/`. The file name is user-specified through the parameter `chemfile` in `info_mhd.in`. The standard name is `chemistry.in`. The V1.1 download package provides two examples of chemistry files:

- `chemistry.in_standard`: with a standard network of 1300 reactions (adapted to the standard `species.in` file provided with the same package).

- `chemistry.in_noads`, which is the same network but without adsorption reactions onto grains.

The latter file should be used whenever one wishes to impose the initial abundances in ice mantles, for example to match those in Table 3.3.

Adsorption reactions should also be removed for computing the pre-shock composition ('S' or 'P' models) when photodesorption is so weak that most species would deplete on grain mantles and disappear from the gas phase before the end of the calculation. According to Equs. A.17 and A.18 in [51], photodesorption will no longer compete with adsorption when $G_0 \leq 0.01 \times (n_H/10^4 \text{cm}^{-3})$.

The chemical network file uses a specific tabular format, which looks as follows:

				gamma	alpha	beta			
16B83	O	H2	OH	H	1.55D-13	2.80	2980.0	0 !	
UMIST	CO	H	OH	C	1.10D-10	0.50	77700.0	0 !	
72	83	O2	H	OH	O	1.63D-09	-.90	8750.0	0 !

Each line corresponds to one reaction, where:

- the first 5 characters are a code (reference, database, family of reactions..)
- the next 2 columns are the reactant names, followed by the products (up to 4 columns).
- the following three floats, called respectively γ , α and β , parametrize the reaction rate.
- the integer after the 3 floats is a flag to identify the reaction type, and how γ , α and β are used by the code to compute chemical reaction rates
- the text after ! is a free comment

In the example above, the reaction type is 0, corresponding to gas phase reactions. in that case, γ , α and β are taken to be Arrhenius coefficients. and each reaction rate coefficient will be computed as:

$$k = \gamma \left(\frac{T}{300} \right)^\alpha e^{-\beta/T} \text{ cm}^3 \text{ s}^{-1}$$

Most of the gas-phase reaction rate coefficients in the current network can be computed using such an Arrhenius form; However, several important types of reactions need specific parametrizations; These special cases are generally signaled by reactants and/or products that do not correspond to existing species:

- CRP : ionization or dissociation by impact of secondary electrons resulting from cosmic rays
- SECPHO: dissociation or ionization by H₂ UV fluorescence resulting from cosmic rays (excitation of H₂ by secondary electron impacts).
- PHOTON (reactant) : dissociation or ionization by attenuated external FUV field
- GRAIN (reactant): adsorption onto grains
- GRAIN (product): sputtering of ices, erosion of grain cores, photodesorption
- VOISIN: thermal evaporation from ice mantle [51]
-

The exo / endothermicity ΔE of gas-phase reactions are computed from the enthalpy difference between the reactants and the products (the enthalpy of formation of each species is read from file `species.in`). Reverse reactions are added whenever their endothermicity is less than 2 eV. Their

rate is then taken equal to the forward rate but with an exponential term $\exp^{-\Delta E/kT}$.

Because of the complexity of such a network, and the necessity to check for internal consistency and "closure" reactions, it is not advised to modify the [chemistry.in](#) files without advice from an expert of the code.

Output files

Starting with V1.1, two (non mutually exclusive) options are offered for the output data format of the Shock Code: namely, a series of ASCII files in tabular format (see Section 4.1), or two single files in hdf5 binary format allowing the use of interactive analysis tools and VO-compliant interfaces (see Section 4.2).

4.1 ASCII output files

With `F_W_ASCII = 1` in `species.in` the code creates a series of ASCII files with computed quantities. Their content is arranged in tabulated data columns, that can be read by usual file editors and plotted by classical graphic softwares (eg. gnuplot, etc...). While the output subdirectory name changes according to the parameter `modele`, the ASCII filenames are always the same, allowing to use predefined graphic scripts. The list of output ASCII files and their content is summarized in the Table below.

List of main output ASCII files and their content

Information files

`info_mhd.out`

Summary of model (text file): List all input model parameters, initial abundances, and chemical reactions used for the run. Also provides the total elemental abundances summed over gas-phase, grain cores, and ice mantles (to check against solar abundances), and the gas / grain ratio.

`species.out`

Abundances at last computed point, $n(X)/n_H$. NB: After running initialization models of type 'S' or 'P', this file must be used as `species.in` for the subsequent shock run (type 'C' or 'J').

`excit.out`

predicted H₂ excitation diagram contains 3 columns: level number, level energy $E(v, J)$, and $\ln(N(v, J)/g_{v,J})$ where $N(v, J)$ is integrated from $z = 0$ to the last computed point.

Physical and chemical structure of the shock (one line per z)

`mhd_phys.out`

Physical variables as a function of z , such as density, temperature, velocity of each fluid, magnetic field, grain size and mass...

`mhd_speci.out`

Chemical abundances. Content depends on parameter `speci_out` in `input_mhd.in`:

- AD : absolute number densities at current point $n(X)$ (in cm⁻³)
- CD : column densities integrated up to current point $N(X) = \int_0^z n(X)dz$ (in cm⁻²)
- FD : fractional abundances at current point $n(X)/n_H$ (Standard)

`mhd_coldens.out`

Column densities of each species, integrated up to current point $N(X) = \int_0^z n(X)dz$ (in cm⁻²)

H₂ excitation and cooling (one line per z)

`H2_lev.out`

H₂ level populations. content depends on parameter `H2_out` in `input_mhd.in`:

- AD : local number density in each H₂ level, $n(v, J)(z)$ (in cm⁻³)
- CD : column densities integrated up to current point, $N(v, J) = \int_0^z n(v, J)dz$ (in cm⁻²)

- $\ln(N/g)$: list of $\ln(N(v, J)/g_{v,J})$ (dimensionless) where $g_{v,J} = 2J + 1$ is the level statistical weight (useful to plot excitation diagrams of H₂ at each z to monitor changes in excitation).

H2_line.out

H₂ line intensities. content depends on parameter line_out in [input_mhd.in](#):

- 'local' : local emissivity in each H₂ line (in erg s⁻¹ cm⁻³)
- 'integrated' : flux integrated up to current point in each H₂ line (in erg s⁻¹ cm⁻²)

Emissivities and cooling (one line per z)

intensity.out

Flux of main atomic / ionic lines integrated up to current point (erg/s/cm²/sr)

populations.out

Local level populations of main atoms / ions

fe_lines.out

Flux of Fe+ lines integrated up to current point (erg/s/cm²/sr)

fe_pops.out

Local level populations of Fe+

thermal_balance.out

Cooling and heating rates (erg/s/cm³) total and split by fluid, process, species.

4.2 hdf5 output files

The hdf5 files are much larger than the ASCII output files, as they include many more computed quantities. But they allow for interactive analysis tools with a user-friendly graphical interface, and exportation into VO-compliant databases (eg. IMSDB). They are also recommended for beginners who wish to browse through all available output variables, and check their definitions and units.

- The binary file modele_s.hdf5 (written when F_W_HDF5_STD =1 in [input_mhd.in](#)), contains all of the "standard" data computed at each position. The **Extractor tool** in [AnalysisTools/](#) allows to identify, select, and plot interactively any physical quantities, and export them to an ASCII file or a VO-Table. A script mode allows extraction from a large number of models. A detailed documentation is available in [Doc_Extractor.pdf](#) in [AnalysisTools/](#).
- The binary file modele_c.hdf5 (written when F_W_HDF5_CHE =1 in [input_mhd.in](#)), contains all of the "chemical" information (abundances, local reaction rates,...) at each position. This file is read by the **Chemistry_analyzer** tool, provided in [AnalysisTools/](#); an interactive graphical user interface presents the main formation and destruction mechanisms of any chosen species, and all information necessary to analyse the chemical state. Chemical rates can be exported to ASCII files or VO-Tables. A detailed documentation is available in [Doc_ChemistryAnalyzer.pdf](#) in [AnalysisTools/](#).

A non-exhaustive bibliography

This section provides the interested reader with a set of recommended-reading papers, whose variety spans from general knowledge about shock theory to publications specifically based on the use of the shock code described here.

5.1 Basic ISM shock theory

This first section lists the historical articles that deal with the theoretical modelling of the propagation of a shock wave in the dusty ISM, through its most prominent aspects. Note that this list is far from exhaustive, and only covers refereed publications :

Fast dissociative "jump" (J-type) molecular shocks

- [1] *Hollenbach, D., & McKee, C. F., 1980, ApJ, 241, L47*
Molecule formation and infrared emission in fast interstellar shocks
I - Physical processes
- [2] *McKee, C. F., & Hollenbach, D. J., 1980, ARA&A, 18, 219*
Interstellar shock waves
- [3] *Hollenbach, D., & McKee, C. F., 1980, ApJ, 241, 47*
Molecule formation and infrared emission in fast interstellar shocks
II - Dissociation speeds for interstellar shock waves
- [6] *Draine, B. T., 1981, ApJ, 245, 880*
Infrared emission from dust in shocked gas
- [4] *Hollenbach, D., & McKee, C. F., 1989, ApJ, 342, 306*
Molecule formation and infrared emission in fast interstellar shocks
III - Results for J shocks in molecular clouds
- [8] *Neufeld, D. A., & Dalgarno, A., 1989, ApJ, 340, 869*
Fast molecular shocks. I - Reformation of molecules behind a dissociative shock
- [9] *Neufeld, D. A., & Dalgarno, A., 1989, ApJ, 344, 251*
Fast molecular shocks. II - Emission from fast dissociative shocks

"Continuous" (C-type) shocks with magnetic precursor

- [5] *Draine, B. T., 1980, ApJ, 241, 1021*
Interstellar shock waves with magnetic precursors
- [7] *Draine, B. T., Roberge, W. G., & Dalgarno, A., 1983, ApJ, 264, 485*
Magnetohydrodynamic shock waves in molecular clouds
- [11] *Kaufman, M. J., & Neufeld, D. A., 1996, ApJ, 456, 611*
Far-infrared water emission from magnetohydrodynamic shock waves

Young C-shocks: Numerical MHD simulations with coupled chemistry

- [63] Chièze, J.-P., Pineau des Forêts, G., & Flower, D. R., 1998, *MNRAS*, 295, 672
Temporal evolution of MHD shocks in the interstellar medium
- [64] Lesaffre, P., Chièze, J.-P., Cabrit, S., & Pineau des Forêts, G., 2004, *A&A*, 427, 147
Temporal evolution of magnetic molecular shocks
I - Moving grid simulations
- [65] Lesaffre, P., Chièze, J.-P., Cabrit, S., & Pineau des Forêts, G., 2004, *A&A*, 427, 157
Temporal evolution of magnetic molecular shocks
II - Analytics of the steady state and semi-analytical construction of intermediate ages

5.2 First series of papers on the Paris-Durham shock code

This section contains the full list of early papers in which the two main contributors to the shock code describe the physical and chemical processes taken into account from the beginning of the code development. They are initially focussed on applications to the diffuse ISM, and then extended to denser clouds.

- [12] Flower, D. R., Pineau des Forêts, G., & Hartquist, T. W., 1985, *MNRAS*, 216, 775
Theoretical studies of interstellar molecular shocks
I - General formulation and effects of the ion-molecule chemistry
- [13] Flower, D. R., Pineau des Forêts, G., & Hartquist, T. W., 1986, *MNRAS*, 218, 729
Theoretical studies of interstellar molecular shocks
II - Molecular hydrogen cooling and rotational level populations
- [14] Pineau des Forêts, G., Flower, D. R., Hartquist, T. W., & Dalgarno, A., 1986, *MNRAS*, 220, 801
Theoretical studies of interstellar molecular shocks
III - The formation of CH+ in diffuse clouds
- [15] Pineau des Forêts, G., Roueff, E., & Flower, D.R., 1986, *MNRAS*, 223, 743
Theoretical studies of interstellar molecular shocks
IV - The sulphur chemistry in diffuse clouds
- [16] Flower, D. R., & Pineau des Forêts, G., 1987, *MNRAS*, 224, 403
Theoretical studies of interstellar molecular shocks
V - Solutions for J-type shocks as an initial value problem
- [17] Pineau des Forêts, G., Flower, D. R., Hartquist, T. W., & Millar, T. J., 1987, *MNRAS*, 227, 993
Theoretical studies of interstellar molecular shocks
VI - The formation of molecules containing two or three carbon atoms
- [18] Monteiro, T. S., Flower, D. R., Pineau des Forêts, G., & Roueff, E., 1988, *MNRAS*, 234, 863
Theoretical studies of interstellar molecular shocks
VII - The photodissociation of molecular hydrogen
- [19] Pineau des Forêts, G., Flower, D.R., & Dalgarno, A., 1988, *MNRAS*, 235, 621
Theoretical studies of interstellar molecular shocks
VIII - Polycyclic aromatic hydrocarbons in dark clouds
- [20] Flower, D. R., Heck, L., & Pineau des Forêts, G., 1989, *MNRAS*, 239, 741
Theoretical studies of interstellar molecular shocks
IX - The influence of PAH molecules on the ratio C/CO in dark clouds

- [21] Pineau des Forêts, G., Roueff, E., & Flower, D. R., 1989, *MNRAS*, 240, 167
Theoretical studies of interstellar molecular shocks
X - The chemical fractionation of deuterium in dark clouds
- [22] Heck, L., Flower, D. R., & Pineau des Forêts, 1990, *Computer Physics communications*, 58, 169
A computer program for calculating the structure of magnetohydrodynamical shocks in interstellar clouds

5.3 Updates of the Paris-Durham shock code

Through the years, the code was developed to account for different kinds of observations, mostly spreading from the infrared (IR) to the sub-millimeter/millimeter ranges. To this aim, several focused updates were implemented in the shock code, and were the subject of various publications, that are here divided up in the following themes: grains and SiO, chemistry, H₂, and FUV irradiation. Again, the list given is not supposed to be exhaustive.

Grains and SiO

- [23] Flower, D. R., Heck, L., Pineau des Forêts, G., & Millar, T. J., 1990, *MNRAS*, 242, 512
The erosion of PAH molecules within shocks in dark clouds
- [24] Flower, D. R., & Pineau des Forêts, G., 1994, *MNRAS*, 268, 724
Grain/Mantle erosion in Magnetohydrodynamic shocks
- [25] Flower, D. R., Pineau des Forêts, G., & Walmsley, C. M., 1995, *A&A*, 294, 815
Hot shocked ammonia towards Sgr B2
- [26] Flower, D. R., & Pineau des Forêts, 1995, *MNRAS*, 275, 1049
Non-thermal sputtering of interstellar grains in magnetohydrodynamic shocks
- [27] Flower, D. R., Pineau des Forêts, G., Field, D., & May, P. W., 1996, *MNRAS*, 280, 447
The structure of MHD shocks in molecular outflows: grain sputtering and SiO formation
- [28] Field, D., May, P. W., Pineau des Forêts, G., & Flower, D. R., 1997, *MNRAS*, 285, 839
Sputtering of the refractory cores of interstellar grains
- [29] Schilke, P., Walmsley, C. M., Pineau des Forêts, G., & Flower, D. R., 1997, *A&A*, 321, 293
SiO production in interstellar shocks
- [30] May, P. W., Pineau des Forêts, G., Flower, D. R., et al., 2000, *MNRAS*, 318, 809
Sputtering of grains in C-type shocks
- [31] Le Picard, S. D., Canosa, A., Pineau des Forêts, G., Rebrion-Rowe, C., & Rowe, B. R., 2001, *A&A*, 372, 1064
The Si(³P_J) + O₂ reaction: a fast source of SiO at very low temperature; CRESU measurements and interstellar consequences
- [32] Flower, D. R., & Pineau des Forêts, G., 2003, *MNRAS*, 343, 390
The influence of grains in the propagation and the structure of C-type shock waves in interstellar molecular clouds
- [33] Gusdorf, A., Cabrit, S., Flower, D. R., & Pineau des Forêts, G., 2008, *A&A*, 482, 809
SiO line emission from C-type shock waves: interstellar jets and outflows
- [34] Gusdorf, A., Pineau des Forêts, G., Cabrit, S., & Flower, D. R., 2008, *A&A*, 490, 695
SiO line emission from interstellar jets and outflows: silicon-containing mantles and non-stationary shock waves

Warm gas chemistry

- [35] Pineau des Forêts, G., Roueff, E., & Flower, D. R., 1990, *MNRAS*, 244, 668
The formation of nitrogen-bearing species in dark interstellar clouds
- [36] Pineau des Forêts, G., Roueff, E. L., Schilke, P., & Flower, D. R., 1993, *MNRAS*, 262, 915
Sulphur-bearing molecules as tracers of shocks in interstellar clouds
- [37] Roueff, E., Pineau des Forêts, G., & Flower, D. R., 1995, *ApJSS*, 233, 125
The importance of chemical data for the study of interstellar shocks
- [38] Flower, D. R., & Pineau des Forêts, G., 1998, *MNRAS*, 297, 1182
C-type shocks in the interstellar medium: profiles of CH⁺ and CH absorption lines

Molecular hydrogen

- [40] Le Bourlot, J., Pineau des Forêts, G., & Flower, D. R., 1999, *MNRAS*, 305, 802
The cooling of astrophysical media by H₂
- [41] Flower, D. R. & Pineau des Forêts, G., 1999, *MNRAS*, 308, 271
H₂ emission from shocks in molecular outflows: the significance of departures from a stationary state
- [42] Wilgenbus, D., Cabrit, S., Pineau des Forêts, G., & Flower, D. R., 2000, *A&A*, 356, 1010
The ortho:para-H₂ ratio in C- and J-type shocks
- [43] Flower, D. R., Le Bourlot, J., Pineau des Forêts, G., & Roueff, E., 2000, *MNRAS*, 314, 753
The cooling of astrophysical media by HD
- [45] Pineau des Forêts, G., & Flower, D. R., 2001, *MNRAS*, 323, 7
Collisional excitation of H₂ by grains in C-type shocks
- [46] Le Bourlot, J., Pineau des Forêts, G., Flower, D. R., & Cabrit, S., 2002, *MNRAS*, 332, 985
New determinations of the critical velocities of C-type shock waves in dense molecular clouds: applications to the outflow source in Orion
- [47] Flower, D. R., Le Bourlot, J., Pineau des Forêts, G., & Cabrit, S., 2003, *MNRAS*, 341, 70
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5.4 Spinoffs

This section lists further developments directly based upon the Paris-Durham shock model but not (yet) included in the current on-line versions.

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Excitation and emission of H₂, CO and H₂O molecules in interstellar shock waves
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Methanol line formation in outflow sources
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Time-dependent modelling of the molecular line emission from shock waves in outflow sources (with introduction of NH₃ chemistry and excitation)
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(with introduction of OH excitation)

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IV. Effects of grain-grain processing on molecular line emission

5.5 A selection of observational applications of the Paris-Durham shock code

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Characteristics of shocks in bipolar outflows observed in pure rotational lines of H₂ with ISO-CAM

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On the excitation of the infrared knots along protostellar jets

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- [72] Gusdorf, A., Giannini, T., Flower, D. R., et al., 2011, *A&A*, 523, 53

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- [74] Gusdorf, A., Anderl, S., Güsten, R., et al., 2012, *A&A*, 542, 19

Probing magnetohydrodynamic shocks with high-J CO observations: W28F

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- [76] Neufeld, D.A., DeWitt, C., Lesaffre, P., Cabrit, S., Gusdorf, A., Le Ngoc, T., Richter, M. 2019, *ApJ* 878, L18

SOFIA/EXES observations of warm H₂ at high spectral resolution: witnessing para-to-ortho conversion behind a molecular shock wave in HH7

Extra-Galactic

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H₂ formation and excitation in the Stephan's Quintet galaxy-wide collision

- [78] [Guillard, P., Ogle, P. M., Emonts, B. H. C., et al., 2012, ApJ, 747, 95](#)
Strong molecular hydrogen emission and kinematics of the multiphase gas in radio galaxies with fast jet-driven outflows
- [79] [Guillard, P., Boulanger, F., Pineau des Forêts, G., et al., 2012, ApJ, 749, 158](#)
Turbulent molecular gas and star formation in the shocked intergalactic medium of Stephan's quintet
- [80] [Hailey-Dunsheath, S., Sturm, E., Fischer, J., et al., 2012, ApJ, 755, 57](#)
Turbulent molecular gas and star formation in the shocked intergalactic medium of Stephan's quintet
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Model formalism

A.1 Setup of the problem and notations

We consider a plane-parallel shock in a stationary state, in which the magnetic field is ‘frozen’ into the ionised gas. The magnetic induction, which is taken to be perpendicular to the flow, will be denoted by B , with an initial value of B_0 . Let us denote by z the independent variable, which is the distance from some arbitrary reference point along the positive flow direction. We will solve for the steady-state equations of dynamics *in the reference frame of the shock wave*, where material is entering from $z = 0$ at velocity V_s and slows down to a final velocity $V_\infty = V_s/C$ where C is the maximum gas compression allowed by the magnetic field.

As the magnetic field interacts directly only with charged particles, the increase of magnetic pressure caused by shock compression will be felt by the neutral fluid only through ion-neutral collisions. If these collisions are rare (i.e. at low fractional ionization), substantial differences may develop between the velocities and kinetic temperatures of the ionised and neutrals fluids. Hence it is necessary to consider at least a two-fluid model of the shock region : charged fluid and neutral fluid.

However, whilst the preservation of charge neutrality requires that the flow velocity of the positive ions, V_i , and the electrons, V_e , should be the same, the kinetic temperatures of ions and electrons may differ if Coulomb scattering is insufficiently rapid to maintain a common thermal distribution. Accordingly, we will generally consider a three-fluid model of the medium, where $V_e = V_i$ but $T_e \neq T_i$. In the following, the suffixes n , i , and e will refer to the neutral fluid, the ionised fluid, and the electrons respectively.

A.2 Multi-fluid dynamical equations

All the following equations are taken from [12].

Particle number conservation. For the three fluids, conservation of particle number density requires that

$$\frac{d}{dz} \left(\frac{\rho_n V_n}{\mu_n} \right) = \mathcal{N}_n \quad (\text{A.1})$$

where ρ_n is the mass density of the neutral fluid and μ_n the mean molecular weight ; \mathcal{N}_n is the number of neutral particles created per unit volume and time. The corresponding equation for the positive ions is

$$\frac{d}{dz} \left(\frac{\rho_i V_i}{\mu_i} \right) = \mathcal{N}_i \quad (\text{A.2})$$

As we assume charge neutrality, the equation for electrons is identical to A.2. One can also write the conservation of particle number density for each individual species α

$$\frac{d}{dz} (n_\alpha V_\alpha) = \mathcal{C}_\alpha \quad (\text{A.3})$$

where n_α is the number of particles α per unit volume, V_α is the velocity of the considered particle, and \mathcal{N}_α is the source term for creation of the species α .

Mass conservation. The equations expressing the conservation of mass of the neutral and ionised fluids may be written

$$\frac{d}{dz}(\rho_n V_n) = \mathcal{S}_n \text{ and } \frac{d}{dz}(\rho_i V_i) = \mathcal{S}_i = -\mathcal{S}_n \quad (\text{A.4})$$

considering that neutral mass may be created only through the destruction of ionised mass. \mathcal{S}_n is the corresponding source term. The mass of electrons is negligible.

Momentum conservation. The equation of momentum conservation is, for the neutrals,

$$\frac{d}{dz} \left(\rho_n V_n^2 + \frac{\rho_n k_B T_n}{\mu_n} \right) = \mathcal{A}_n \quad (\text{A.5})$$

where T_n is the kinetic temperature of the neutral gas and k_B is Boltzmann's constant ; \mathcal{A}_n is the source term that denotes the change in momentum of the neutral fluid per unit volume and time (due to ion-neutral collisions and normal viscosity). In the case of the ion-electron fluid, account must also be taken of the compression of the magnetic field

$$\frac{d}{dz} \left[\rho_i V_i^2 + \frac{\rho_i k(T_i + T_e)}{\mu_i} + \frac{B^2}{8\pi} \right] = -\mathcal{A}_n \quad (\text{A.6})$$

Denoting the unperturbed value of the magnetic induction by B_0 , and the shock velocity by V_s , the fact that the field is frozen in the ionised fluid implies that $B \times V_i = B_0 \times V_s$, the flow velocity being expressed in the frame of reference of the shock. Equation A.6 then becomes

$$\frac{d}{dz} \left[\rho_i V_i^2 + \frac{\rho_i k(T_i + T_e)}{\mu_i} + \frac{B_0^2}{8\pi} \left(\frac{V_s}{V_i} \right)^2 \right] = -\mathcal{A}_n \quad (\text{A.7})$$

Once again, the inertia of electrons has been neglected.

Energy conservation. The conservation of energy of the neutral fluid may be expressed as

$$\frac{d}{dz} \left[\rho_n V_n^3 + \frac{5}{2} \frac{\rho_n V_n k T_n}{\mu_n} + \frac{\rho_n V_n U_n}{\mu_n} \right] = \mathcal{B}_n \quad (\text{A.8})$$

where U_n is the mean internal energy per neutral particle, and \mathcal{B}_n is the corresponding source term: the change in total energy of the neutral fluid per unit volume and time. For the ion-electron fluid, if we neglect the contribution of the internal energy of the ions, we have

$$\frac{d}{dz} \left[\rho_i V_i^3 + \frac{5}{2} \frac{\rho_i V_i k(T_i + T_e)}{\mu_i} + \frac{B_0^2}{4\pi} \frac{V_s^2}{V_i} \right] = \mathcal{B}_i + \mathcal{B}_e \quad (\text{A.9})$$

For all these equations of conservation (number, mass, momentum, energy), source terms have to be estimated. These source terms can be the results of many different processes arising in the

shock context. The most general chemical and physical processes are discussed in Appendix B. Appendix C deals with the calculation of molecular radiative cooling.

Source terms: chemistry and collisions

The following are the chemical and collisional source terms for a 3-fluid C-shock calculation. They do not include the viscous friction and associated heating which dominate in a J-shock. For further details concerning these equations, the interested reader is referred to [12], [13], and [14].

B.1 Number and mass of particles

We note \mathcal{C}_α the production rate of atomic and molecular species per unit of volume and time. The total number of neutral and ionised particles created through chemical processes per unit of volume and time can be written

$$\mathcal{N}_n = \sum_{\alpha, \text{neutral species}} \mathcal{C}_\alpha \quad \text{and} \quad \mathcal{N}_i = \sum_{\alpha, \text{ionised species}} \mathcal{C}_\alpha \quad (\text{B.1})$$

Similarly the equations of mass transfer from the ionised fluid to the neutral fluid, and from the neutral fluid to the ionised fluid read

$$\mathcal{S}_n = \sum_{\alpha, \text{neutral species}} \mathcal{C}_\alpha m_\alpha \quad \text{and} \quad \mathcal{S}_i = \sum_{\alpha, \text{ionised species}} \mathcal{C}_\alpha m_\alpha \quad (\text{B.2})$$

The condition $\mathcal{S}_i = -\mathcal{S}_n$ provides a check-up of the consistency of the program.

B.2 Momentum

We note $\mathcal{C}_{\alpha\beta}$ the creation ($\mathcal{C}_{\alpha\beta} \geq 0$) or destruction ($\mathcal{C}_{\alpha\beta} \leq 0$) rate of the α species through the β reaction. Thus

$$\mathcal{C}_\alpha = \sum_\beta \mathcal{C}_{\alpha\beta} \quad (\text{B.3})$$

The momentum transfer between neutral and ionised fluid can be the result of three different processes.

(i) Reactive (inelastic) collisions between ions and neutrals. The momentum transfer rate towards the neutral fluid per unit of volume and time is

$$\mathcal{A}_n^{(i)} = \sum_{\alpha, \text{neutral species}} \sum_\beta \mathcal{C}_{\alpha\beta} m_\alpha V_\beta \quad (\text{B.4})$$

where the α species is assumed to be created with the velocity of the centre of mass of the reaction β , V_β . If all the reactants are neutrals, $V_\beta = V_n$, whereas if there are all ions, $V_\beta = V_i$. For a reaction between a neutral and an ion, $V_\beta = (m_i V_i + m_n V_n) / (m_i + m_n)$. Again, the condition

$$\sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_{\beta} \mathcal{C}_{\alpha\beta} m_\alpha V_\beta = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\beta} \mathcal{C}_{\alpha\beta} m_\alpha V_\beta \quad (\text{B.5})$$

provides a check-up of the execution of the program.

(ii) Elastic collisions between ions and neutrals (ambipolar diffusion). The cross section of this process is approximated by

$$\sigma_{in} = 2.41\pi \left(\frac{e^2 \alpha_n}{\mu_{in} V_{in}^2} \right)^{1/2} \quad (\text{B.6})$$

where e is the charge of the electron, α_n the polarisability of neutrals, $\mu_{in} = \mu_i \mu_n / (\mu_i + \mu_n)$ the reduced mass of the ion-neutral system, and V_{in} their relative velocity. The corresponding rate coefficient is

$$<\sigma V>_{in} = 2.41\pi \left(\frac{e^2 \alpha_n}{\mu_{in}} \right)^{1/2} \quad (\text{B.7})$$

and the momentum is transferred from ions to neutrals at the rate of

$$\mathcal{A}_n^{(ii)} = \frac{\rho_n \rho_i}{\mu_n + \mu_i} <\sigma V>_{in} (V_i - V_n) \quad (\text{B.8})$$

(iii) Elastic collisions between grains and neutrals (ambipolar diffusion). Because they are coupled to the charged fluid, charged grains also have a drift velocity with respect to the neutrals and play a role in momentum transfer. A good approximate of the corresponding momentum transfer rate is

$$\mathcal{A}_n^{(iii)} = n_g \pi a^2 |V_i - V_n| (V_i - V_n) \rho_n \quad (\text{B.9})$$

where a is the rms radius of the grain size distribution at the local point, and n_g is the number of charged grains per unit volume.

B.3 Energy

Energy transfers also exist between neutral and charged fluids, through chemical, collisional, or radiative processes. In this section, chemical ((i) to (iii)) and collisional ((iv) to (vi)) processes are described, as well as some consequences of FUV irradiation (vii).

(i) Reactive collisions between ions and ions, neutrals and neutrals, ions and neutrals. Chemical reactions generate a transfer of kinetic energy because the product of the reaction has an actual velocity in the frame of the fluid. The corresponding rates for the neutral and ionised fluids are

$$\mathcal{B}_n^{(i)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_{\beta} \mathcal{C}_{\alpha\beta} \frac{1}{2} m_\alpha V_\beta^2 \quad \text{and} \quad \mathcal{B}_i^{(i)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\beta} \mathcal{C}_{\alpha\beta} \frac{1}{2} m_\alpha V_\beta^2 \quad (\text{B.10})$$

The corresponding term for electrons can be neglected.

(ii) Energy transfer between reactants (ions, electrons and neutrals). If the enthalpy transfer between ionised and charged fluids is taken into account, formation ($\mathcal{C}_{\alpha\beta} > 0$) and destruction ($\mathcal{C}_{\alpha\beta} < 0$) must be treated separately. If the reactions generating more than two products (like molecular dissociation, for example) are of no importance, as was assumed in the previous model, then neutrals are created via the recombination of an ion with an electron, with respective kinetic temperatures T_i et T_e , and are destructed through ionisation at temperature T_n . Consequently, the rate at which enthalpy is added to the neutral fluid can be written

$$\mathcal{B}_n^{(ii)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \left[\sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} > 0}} \mathcal{C}_{\alpha\beta} \frac{3}{2} k \frac{T_i + T_e}{2} + \sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} < 0}} \mathcal{C}_{\alpha\beta} \frac{3}{2} k T_n \right] \quad (\text{B.11})$$

Similarly, for ions

$$\mathcal{B}_i^{(ii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \left[\sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} > 0}} \mathcal{C}_{\alpha\beta} \frac{3}{2} k T_n + \sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} < 0}} \mathcal{C}_{\alpha\beta} \frac{3}{2} k T_i \right] \quad (\text{B.12})$$

And eventually, for electrons

$$\mathcal{B}_e^{(ii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} < 0}} \mathcal{C}_{\alpha\beta} \frac{3}{2} k T_e \quad (\text{B.13})$$

(iii) Endothermicity and exothermicity of chemical reactions. This contribution can take part in the heating or to the cooling of the medium. Consequently, ΔE , the energy default of chemical reactions can influence the thermal balance, with a heating (or cooling) rate of the neutral fluid per unit of volume and time equal to

$$\mathcal{B}_n^{(iii)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} > 0}} \mathcal{C}_{\alpha\beta} \frac{M_\beta - m_\alpha}{M_\beta} \Delta E_\alpha \quad (\text{B.14})$$

where M_β is the total mass of the products of the reaction β . Similarly we have for the ionised fluid

$$\mathcal{B}_i^{(iii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\substack{\beta, \\ \mathcal{C}_{\alpha\beta} > 0}} \mathcal{C}_{\alpha\beta} \frac{M_\beta - m_\alpha}{M_\beta} \Delta E_\alpha \quad (\text{B.15})$$

(iv) Elastic collisions between ions and neutrals. Heat is also exchanged between the different fluids through ion-neutral scattering. The heating rate of the neutrals generated by this process is given by

$$\mathcal{B}_n^{(iv)} = \frac{\rho_n \rho_i}{\mu_n \mu_i} \langle \sigma V \rangle_{in} \frac{2 \mu_n \mu_i}{(\mu_n + \mu_i)^2} \left[\frac{3}{2} k (T_i - T_n) + \frac{1}{2} (V_i - V_n) (\mu_i V_i + \mu_n V_n) \right] \quad (\text{B.16})$$

(v) Elastic collisions between electrons and neutrals. A similar expression is still valid for electron-neutral scattering, and simplifies thanks to the fact that $m_e \ll \mu_n$

$$\mathcal{B}_n^{(v)} = \frac{\rho_n \rho_i}{\mu_n \mu_i} <\sigma V>_{en} \frac{2m_e}{\mu_n} \left[\frac{4}{2} k(T_e - T_n) + \frac{1}{2} (V_i - V_n) \mu_n V_n \right] \quad (B.17)$$

where the scattering cross section is considered as independent on the energy, with

$$<\sigma V>_{en} = 10^{-19} \left(\frac{8kT_e}{\pi m_e} \right)^{1/2} m^3 s^{-1} \quad (B.18)$$

(vi) Elastic collisions between electrons and ions (Joule heating). The heating rate of the fluid of electrons through coulombian scattering on ions can be estimated with

$$\mathcal{B}_e^{(vi)} = \frac{4e^4}{\mu_i k T_e} \left(\frac{2\pi m_e}{k T_e} \right)^{1/2} \ln \Lambda \left(\frac{\rho_i}{\mu_i} \right)^2 k(T_i - T_e) \quad (B.19)$$

with $\mathcal{B}_i^{(vi)} = -\mathcal{B}_e^{(vi)}$, and where

$$\Lambda = \frac{3}{2e^3} \left(\frac{k^3 T_e^3 \mu_i}{\pi \rho_i} \right)^{1/2} \quad (B.20)$$

(vii) Photoionization Ideally, the heating rate of the electron fluid through photoionisation should be given by

$$\mathcal{B}_e^{(vii)} = \sum_{\alpha} n_{\alpha} \int_{\nu_{\alpha}}^{\nu_H} \frac{4\pi J_{\nu}}{h\nu} a_{\nu}(\alpha) (h\nu - h\nu_{\alpha}) d\nu \quad (B.21)$$

where J_{ν} is the mean intensity at frequency ν , $a_{\nu}(\alpha)$ is the photoionisation cross section for the species α (depending on the frequency), and ν_{α} is the threshold frequency of photoionisation. The integrate should be calculated until the Lyman limit of hydrogen (given by $h\nu_H = 13.598$ eV). In practice, one often has to consider an estimate of the value of the integrate of the equation B.21, because of the uncertainties on the mean radiation intensity and on the frequency dependance of the photoionisation cross section. We use the formula

$$\delta E(\text{eV}) = \max \left\{ 5.7, \left[32 - 7 \log \left(\frac{\rho_n}{\rho_i} \frac{\mu_i}{\mu_n} \right) \right] \right\} \quad (B.22)$$

The corresponding heating rate for the electrons fluid then writes

$$\mathcal{B}_e^{(vii)} = \sum_{\alpha} \delta E_{\alpha} \gamma_{\alpha} n_{\alpha} \quad (B.23)$$

where δE_{γ} stands for the average energy of the photoelectron produced by photoionisation of species α , with number density n_{α} and which photoionisation rate is γ_{α} .

Non-thermal electrons are also injected in the gas through two other processes:

- photoelectric effect on grains: is subject to considerable uncertainties depending on the physical properties of the grains and PAHs. An approximate prescription is implemented in V1.1 of the code, following [51].
- ionisation of atoms and molecules by cosmic rays: The injection rate of energy through this process may be written as $\Delta E \zeta n_H$, where ΔE is the average energy transferred to the electron gas per

cosmic-ray ionization and ζ is the cosmic ray ionisation rate per H nucleus. Monte-Carlo simulations show that in molecular gas, a large fraction of this energy is not used to heat the electron fluid, but to excite and dissociate H_2 . Hence the corresponding heating term is negligible compared to other source terms.

Source terms : molecular cooling

C.1 Basics of molecular rotational and vibrational excitation

The atoms of a molecule are never totally at rest. In fact, even in a solid which temperature approaches the absolute zero, atoms constantly oscillate around their equilibrium position. Three kinds of movements can occur in a molecule : global rotation, vibration (ie. periodic oscillation of the inter-atomic distance, as if the nuclei were connected by a spring), and bending modes (where angles between bonds oscillate about their equilibrium value).

Rotational movements of a molecule can be described to zero-th order by means of a model of rigid rotator. The resolution of the Schrödinger equation shows that the rotational energy is quantized and can only have well defined values. However, the description with a rigid rotator model is only an approximation, because centrifugal forces due to rotation tend to stretch the atomic bonds, which provokes a modification of the momentum of inertia. Taking the effects into account, the rotational energy levels (in joules) for a diatomic molecule are given by

$$E_r = hcBJ(J+1) - hcDJ^2(J+1)^2 \quad (\text{C.1})$$

where B is the rotational constant, expressed in cm^{-1} , related to the momentum of inertia I via

$$B = h/8\pi^2 c I \quad (\text{C.2})$$

and where D is the centrifugal distortion constant, related to the vibration frequency ω of the molecule through the equation

$$D = 4B^3/\omega^2 \quad (\text{C.3})$$

J is the rotational quantum number of the molecule ($J = 0, 1, 2, \dots$), which gives the value of the rotational kinetic moment (equal to $\sqrt{J(J+1)}h/2\pi$), c is the light velocity in the vacuum, and h is Planck's constant. The order of magnitude of the rotational energy is typically 1 J mol^{-1} .

The vibrational movements of a molecule can be described by means of the harmonic oscillator model. Once again, the resolution of the equation of Schrödinger for a unidimensional oscillator shows that the vibrational energy of a molecule is also quantized. Nevertheless, nuclei vibrations are never simple harmonic vibrations. The stretch of the oscillator is never perfectly elastic, and the vibrations are anharmonic. Taking this effect into account, the possible values of the vibrational energy of a diatomic molecule (in joules) are given by

$$E_v = (\nu + \frac{1}{2})hc\omega_e - (\nu + \frac{1}{2})^2hcx_e\omega_e + (\nu + \frac{1}{2})^3hcy_e\omega_e + \dots \quad (\text{C.4})$$

where ν is the vibrational quantum number ($\nu = 0, 1, 2, \dots$), ω_e is the hypothetical frequency of the small amplitude vibrations around the equilibrium position of the nuclei, and x_e and y_e are the anharmonic constants. The typical value of the vibrational energy is around 10^3 J mol^{-1} .

To these values of rotational and vibrational energy correspond several populated levels, between which quantum mechanics allows us to determine every permitted transition. Precisely, these transitions can be provoked by collisions likely to occur in interstellar shocks. These transitions accompany emission of photons, which can contribute to the cooling or heating of the interstellar gas. In the following calculations, distortion or anharmonicity is not taken into account (that is, all the terms following the '-' in the expressions of rotational and vibrational energies). Only the case of molecular hydrogen is shown here, keeping in mind that rotational and/or vibrational de-excitation of other molecules such as CO, OH, NH₃, ou H₂O are also taken into account in the model.

C.2 The case of molecular hydrogen

Molecular hydrogen is of particular interest because of its important fractional abundance in the interstellar medium. Indeed, even if coefficient rates of the reactions in which molecular hydrogen is involved are rather low, they occur so many times that they have to be taken into account as major processes.

Molecular hydrogen being an homonuclear molecule, its mass centre is the same as the electric charge's barycentre. Consequently, molecular hydrogen has no permanent electric dipolar moment, and radiative transitions associated to an electronic transition are of quadrupolar kind. Nevertheless, molecular hydrogen being by far the most abundant molecule of the interstellar medium, its contribution to the heating or cooling of the ambient gas is prevailing.

The lack of permanent electric dipolar moment has two important consequences for molecular hydrogen :

- molecular hydrogen exists in two forms, called ortho- or para- H₂. In the ortho-H₂, nuclear spins are aligned, thus $I = 1$, whereas for para-H₂, nuclear spins are anti-parallel, and consequently $I = 0$. Nuclei being made of identical fermions, the nuclear wave function that includes vibrational, rotational, and spin effects, must be antisymmetric with respect to the swap of photons. The wave function describing the fundamental state for vibration is invariant through this operation, whereas the rotational part of the wave function is multiplied by $(-1)^J$, where J is the rotational quantum number. The spin function of the triplet, $I = 1$, is symmetric with respect to proton swap, whereas the spin function of the singulet, $I = 0$, is antisymmetric. The state $I = 1$ (ortho-H₂) then corresponds to odd values of J , and the state $J = 0$ (para-H₂) is associated to even J values ;
- quadrupolar transitions don't allow the transition to one form from another.

Nevertheless, transitions remain possible between rovibrational levels of molecular hydrogen, which can play an important role in the energy transfers along the shock. This contribution must be taken into account in the source terms of the equations of conservation. Consequently, the populations of all the levels of molecular hydrogen must be computed.

C.2.1 Molecular hydrogen cooling

The method of evaluation of the contribution to the cooling by molecular hydrogen is presented in [13]. We call n_J the population density of the rotational level J of molecular hydrogen. The total

density of molecular hydrogen is thus

$$n(H_2) = \sum_J n_J \quad (C.5)$$

and the total density of hydrogen nuclei is

$$n(H) = n(H^0) + 2n(H_2) \quad (C.6)$$

$A(J \rightarrow J-2)$ is the rate of spontaneous radiative decay of the level $J \geq 2$ (in s^{-1}). The corresponding collisional de-excitation rate is

$$C(J \rightarrow J-2) = n_J [n(H^0) + n(H_2)] <\sigma v>_{J \rightarrow J-2} \quad (C.7)$$

where $<\sigma V>_{J \rightarrow J-2}$ is the coefficient rate of collisional de-excitation, which we assume identical for molecular or atomic hydrogen. The collisional excitation rate is related to C.7 through the ‘detailed balance’

$$(2J-3)C(J-2 \rightarrow J) = (2J+1)C(J \rightarrow J-2) \exp(-x) \quad (C.8)$$

with

$$x = 2(2J-1)B/kT_n \quad (C.9)$$

In equation C.9, B is the rotational constant of H_2 in his fundamental vibrational state, and k is Boltzmann’s constant. In our calculations, we use the expression

$$\begin{aligned} <\sigma V>_{J \rightarrow J-2} &= 4.6 \times 10^{-12} (2J-3) T_n^{1/2} (1+x)^{1/2} \\ &\times \exp \left[\frac{-5.01x}{1+B(J+1)/kT_n} - 0.1187(4J-2) \right] \end{aligned} \quad (C.10)$$

If we only consider radiative and collisional transitions between rotational levels, the gradient of the population flux of the state J in a stationary state writes

$$\begin{aligned} \frac{d}{dz}(V_n n_J) &= [C(J+2 \rightarrow J) + A(J+2 \rightarrow J)] n_{J+2} \\ &- [C(J \rightarrow J+2) + C(J \rightarrow J-2) + A(J \rightarrow J-2)] n_J \\ &+ C(J-2 \rightarrow J) n_{J-2} \end{aligned} \quad (C.11)$$

where v_n is the neutral fluid velocity in the z direction. At the static limit, $v_n = 0$, and left’s part of the equation C.11 vanishes.

In practice, the population flux of the J level can also evolve because of the chemical reactions that create or destroy molecular hydrogen. If we assume that chemical reactions populate (and de-populate) the levels proportionally to their local density, then the equation C.11 can be generalized

$$\begin{aligned} \frac{d}{dz}(V_n n_J) &= [C(J+2 \rightarrow J) + A(J+2 \rightarrow J)] n_{J+2} \\ &- [C(J \rightarrow J+2) + C(J \rightarrow J-2) + A(J \rightarrow J-2)] n_J \\ &+ C(J-2 \rightarrow J) n_{J-2} \\ &+ \frac{n_J}{n(H_2)} \frac{d}{dz} [u_n n(H_2)] \end{aligned} \quad (C.12)$$

where $u_n n(H_2)$ is the molecular flux of molecular hydrogen.

The radiative cooling rate of the gas via rotational transitions for molecular hydrogen can then write

$$[\mathcal{B}_n(H_2)]_{radiative} = - \sum_{J \geq 2} n_J A(J \rightarrow J-2) 2(2J-1) B \quad (C.13)$$

As the populations of the excited states of molecular hydrogen are likely to grow a lot along the shocks, their contribution to the internal energy of the fluid must also be taken into account. The internal energy of neutral gas per volume unit is

$$\frac{\rho_n}{\mu_n} U_n = \sum_{V,J} n(V,J) E(V,J) \quad (C.14)$$

where $n(V,J)$ is the density of molecular hydrogen in the rovibrational state (V,J) , and where $E(V,J)$ is the corresponding excitation energy. We don't take the excited vibrational states into account, and we then obtained

$$\frac{\rho_n}{\mu_n} U_n = \sum_{V,J} n_J B_J (J+1) \quad (C.15)$$

Among the necessary conditions to seal the neutral particles energy conservation, we thus have

$$\frac{d}{dz} \left(\frac{\rho_n v_n U_n}{\mu_n} \right) = \sum_J B_J (J+1) \frac{d}{dz} (u_n n_J) \quad (C.16)$$

where $d(u_n n_J)/dz$ is provided by equation C.12.

Previously, we have assumed that the de-excitation coefficients for atomic and molecular hydrogen were identical. The key point is that molecular hydrogen requires a special treatment because of its important abundance in the interstellar medium, and in spite of its symmetry that prevents the existence of a permanent electric dipolar moment.

C.3 Cooling by other molecules

In non-dissociative (or partly dissociative) molecular shocks, CO and H₂O are the main contributors to radiative shock cooling besides H₂. Methanol (CH₃OH) could also have a significant contribution if its abundance reaches a few 10⁻⁵ per H nuclei. However, modeling of Herschel observations of the B1 shock in the L1157 protostellar outflow indicate 5-10 times lower methanol abundances than this limit [54]. Current public versions of the code therefore neglect methanol cooling to compute the shock structure.

Rotational and vibrational cooling rates of CO and H₂O in warm interstellar gas were computed by Neufeld & Kaufman 1993 [10] in the Large Velocity Gradient (LVG) approximation for a wide range of parameters (densities, temperature, velocity gradients). These authors provided tables of results as well as a fortran routine to interpolate in them; it was implemented in the Paris-Durham Shock Code and is being called at each step when the parameter `cool_KN= 1`. The same routine is used for ¹³CO, scaling the CO abundance by a factor 80. The interested reader is referred to the original paper [10] for further details on the assumptions made and their range of validity.

Example of "species.in" file

This is a standard **species.in** file used in the public version V0 (run on-line).

```
!----- list of chemical species — Steady state at T = 19.67 K -----
!----- WARNING : order = neutrals, species on manfles, ions >0, ions <0 -----
!----- name, composition, initial density(cm-3), formation enthalpy (kCal/mol) -----
!
1 H 01000000000000 2.033D-04 051.634
2 H2 02000000000000 4.999D-01 000.000
3 He 00000010000000 1.000D-01 000.000
4 C 00010000000000 4.769D-07 169.980 -> C/H = 8.27e-5
5 CH 01010000000000 9.254D-09 141.600 A&G : 3.55e-4
6 CH2 02010000000000 3.342D-08 093.900
7 CH3 03010000000000 1.097D-09 034.800
8 CH4 04010000000000 3.644D-08 -15.970
9 O 00000100000000 1.732D-05 058.980 -> O/H = 1.24e-4
10 O2 00000200000000 1.181D-05 000.000 A&G : 7.41e-4
11 OH 01000100000000 1.230D-07 009.250
12 H2O 02000100000000 4.638D-07 -57.100
13 CO 00010100000000 8.166D-05 -27.200
14 CO2 00010200000000 8.027D-07 -93.965
15 C2 00020000000000 1.663D-09 198.200
16 C2H 01020000000000 7.773D-09 113.300
17 C2H2 02020000000000 8.667D-11 056.320
18 C3 00030000000000 6.924D-14 194.000
19 C3H 01030000000000 3.891D-13 177.000 ***
20 C3H2 02030000000000 2.850D-12 114.000 ***
39 CH3OH 04010100000000 1.000D-16 -99.999
42 H2CO 02010100000000 1.000D-16 -99.999
42 HCO2H 02010200000000 1.000D-16 -99.999
21 N 00001000000000 8.136D-06 112.530 -> N/H = 6.39e-5
22 NH 01001000000000 6.002D-08 090.000 A&G : 9.33e-5
23 NH2 02001000000000 1.004D-06 046.200
24 NH3 03001000000000 3.492D-07 -09.299
25 CN 00011000000000 5.552D-08 103.200
26 HCN 01011000000000 7.974D-08 032.390
27 HNC 01011000000000 8.993D-08 048.000
28 N2 00002000000000 2.704D-05 000.000
29 NO 00001100000000 3.072D-08 021.460
32 S 000000000010000 1.413D-05 065.600 A&G : 1.86e-5
33 SH 01000000010000 2.613D-08 032.600
34 H2S 02000000010000 2.996D-08 -04.230
35 CS 00010000010000 1.396D-07 063.000
36 SO 00000100010000 5.980D-08 001.200
37 SO2 00000200010000 2.475D-07 -70.300
38 OCS 00010100010000 2.036D-10 -34.000
37 Si 000000000010000 1.126D-15 106.700 A&G : 3.55e-5
38 SiH 01000000010000 7.402D-20 089.690
39 SiH2 02000000010000 7.267D-22 069.140 *
40 SiH3 03000000010000 4.825D-24 048.540 *
41 SiH4 04000000010000 3.171D-22 011.000
42 SiO 00000100001000 3.242D-16 -24.300
43 SiO2 00000200001000 2.114D-17 -73.000
44 Mg 00000000010000 1.000D-16 035.000
39 Fe 00000000000010 1.451D-08 098.700
38 C54H18 18540000000000 8.701D-07 -99.999 PAH/nH =1(-8)
63 G 00600000000000 4.027D-11 -99.999 Ngrain = 8.30(-11)
41 H2O* 02000100000001 1.029D-04 H2O*/nH =1.03(-4)
42 O2* 00000200000001 1.000D-16
42 CO* 00010100000001 8.271D-06 CO*/nH =8.27(-6)
43 CO2* 00010200000001 1.339D-05 CO2*/nH =1.34(-5)
39 CH4* 04010000000001 1.549D-06 CH4*/nH =1.55(-6)
44 NH3* 03001000000001 1.549D-05 NH3*/nH =1.55(-5)
44 N2* 00002000000001 1.000D-16
39 CH3OH* 04010100000001 1.859D-05 CH3OH*/nH =1.86(-6)
42 H2CO* 02010100000001 6.199D-06 H2CO*/nH =6.20(-6)
42 HCO2H* 02010200000001 7.240D-06 HCO2H*/nH =7.24(-6)
42 OCS* 00010100010001 2.069D-07 OCS*/nH =2.07(-7)
55 H2S* 02000000010001 3.720D-06 H2S*/nH =3.72(-6)
62 Fe* 00000000000011 3.245D-15
41 SiH4* 04000000000001 1.000D-16
42 SiO* 00000100000001 1.000D-16
43 SiO2* 00000200000001 1.000D-16
59 O** 00000100000002 1.399D-04 Noyaux = 4*3.50(-5)
60 Si** 00000000000002 3.370D-05 Noyaux = 3.370(-5)
61 Mg** 00000000100002 3.230D-05 Noyaux = 3.700(-5)
62 Fe** 00000000000012 3.230D-05 Noyaux = 3.230(-5)
63 C** 00010000000002 1.629D-04 Noyaux = 1.630(-4)
48 H+ 01000001000000 2.756D-09 365.200
49 H2+ 02000001000000 2.285D-12 355.700
50 H3+ 03000001000000 8.939D-09 265.000
51 He+ 00000011000000 8.213D-10 567.000
52 C+ 00010001000000 1.906D-09 429.700 A&G : 3.55e-4
53 CH+ 01010001000000 4.907D-14 387.000
```

54 CH2+	02010001000000	8.715D-14	331.000
55 CH3+	03010001000000	6.897D-10	262.000
56 CH4+	04010001000000	8.658D-15	272.000 **
57 CH5+	05010001000000	2.494D-11	216.000 *
58 O+	00000101000000	3.618D-14	373.000
59 O2+	00000201000000	1.577D-09	278.400
60 OH+	01000101000000	2.924D-13	309.310
61 H2O+	02000101000000	3.851D-13	233.700
62 H3O+	03000101000000	2.982D-09	143.000
63 CO+	00010101000000	2.717D-14	295.970
64 HCO+	01010101000000	3.936D-08	197.300
65 HCO2+	01010201000000	5.660D-11	141.000 *
66 C2+	00020001000000	3.510D-17	476.000
67 C2H+	01020001000000	7.229D-17	404.000
68 C2H2+	02020001000000	7.053D-12	317.500
69 C2H3+	03020001000000	4.930D-12	267.900
70 C3+	00030001000000	9.910D-18	479.000 *
71 C3H+	01030001000000	7.503D-16	381.000 *
72 C3H2+	02030001000000	3.081D-15	330.000 ***
73 C3H3+	03030001000000	1.388D-13	282.000 * **
74 N+	00001001000000	1.481D-10	447.690
75 NH+	01001001000000	9.212D-15	401.100
76 NH2+	02001001000000	4.136D-13	302.700
77 NH3+	03001001000000	1.240D-10	224.900
78 NH4+	04001001000000	2.439D-09	151.000 *
79 CN+	00011001000000	5.987D-16	429.300
80 C2N+	00021001000000	7.071D-11	410.000 *
81 HCN+	01011001000000	1.190D-14	346.000
83 H2CN+	02011001000000	2.813D-09	226.000 *
84 H2NC+	02011001000000	2.954D-11	265.000 *
85 N2+	00002001000000	1.777D-14	359.298
86 N2H+	01002001000000	2.603D-09	247.500
87 NO+	00001101000000	2.896D-10	235.330
88 HNO+	01001101000000	8.150D-12	256.800
92 S+	00000001010000	5.319D-08	304.000 -> S/H = 1.47e-5
93 SH+	01000001010000	9.585D-09	271.800 A&G : 1.86e-5
94 H2S+	02000001010000	5.897D-11	237.000
95 H3S+	03000001010000	1.970D-10	190.000 *
96 CS+	00010001010000	2.834D-14	324.000
97 HCS+	01010001010000	5.237D-10	243.000
98 SO+	00000101010000	7.732D-09	239.200
99 HSO+	01000101010000	2.774D-10	210.000
100HSO2+	01000201010000	2.872D-10	143.000
101HOCS+	01010101010000	2.565D-12	181.000
51 Si+	00000001001000	2.650D-17	295.000
109SiH+	01000001001000	2.769D-19	271.820
110SiH2+	02000001001000	6.140D-20	276.360 *
111SiH3+	03000001001000	4.275D-22	237.320 *
112SiH4+	04000001001000	2.794D-30	279.900
113SiH5+	05000001001000	1.596D-24	219.380 *
114SiO+	00000101001000	4.486D-23	239.520
115SiOH+	01000101001000	2.715D-18	-99.999
102Fe+	00000001000010	4.853D-10	280.240 LM: Fe/nH=1.5(-8)
103C54H18+	18540001000000	1.143D-09	-99.999
63 G+	00600001000000	2.420D-12	-99.999
104C54H18-	18540000000100	1.288D-07	-99.999 PAH/nH = 1(-8)
63 G-	00600000000100	3.599D-12	-99.999 Ngrain = 8.30(-11)

Example of "chemistry.in" file

This is a standard `chemistry.in` file used in the public version V0 (run on-line). Since this version does not allow for an external FUV field, the file does not include photo reactions other than those induced by "secondary photons" (H_2 fluorescence by cosmic ray electron impact).

```
|-----  
| update :  
|  
| 29/08/01: ajout de C** (meme taux d'erosion que Si**)   
| 12/01/01: ajout des reactions d'erosion pour les especes Si**, Mg**, Fe**, O**  
|   attention: les alpha,beta, gamma d'ont plus le meme sens  
|  
| 24/08/00 :  
|   * creation from the file Chemistry.dat  
|   * suppression of one reaction that appears twice :  
|     ADSOR C3 +GRAIN =CH4* CH4* CH4*  
|   * suppression of the column 'DE':  
|     the excess of energy is computed in the shock code.  
|   Remark : The old format is unchanged, if there is a value  
|             for DE, it is not read in the code.  
|   * change in one reaction (problem of conservation)  
|     SiOH+ +PHOTON =SiO+ O --->SiOH+ +PHOTON =SiO+ H  
|   * change 17 reactions : ->new specy=SECPHO (secondary photon)  
|     first reaction : 56 88 C +CRP => ELECTR  
|     last reaction : 56 88 CO +CRP => CO  
|     changes are (idem for the 17 reactions):  
|       CRP ->SECPHO in reactants  
|       beta = 140000.0 ->beta = 0.0  
| 31/08/00 :  
|   * change 23 reactions : same as last change of 24/08/00  
|   first reaction : 56 88 C54H18 +SECPHO =>C54H18+ ELECTR  
|   last reaction : 13 87 SiH4 +SECPHO =>SiH3 H  
|   changes are (idem for the 22 reactions):  
|     CRP ->SECPHO in reactants  
|     beta = 0.0 or 140000.0 ->beta = 0.0  
|  
| columns :  
|  
|   * reference or comment  
|   * R1, R2, P1, P2, P3, P4 : reactants and product of the reaction  
|     R1 + R2 ->P1 + P2 + P3 + P4  
|   * gamma(cm3.s-1), beta(K), alpha : Arrhenius coefficients  
|     in general :  
|       rate = gamma*EXP(-beta/T)*(T/300)**alpha  
|   special cases :  
|     * photo-reactions  
|       rate = gamma*EXP(-beta*Av)*RAD  
|     * CR induced desorption from grains  
|       rate = gamma*sigma(grain)*N(grains)/N(species on grains)  
|     * CR ionisation or dissociation  
|       rate = gamma*EXP(-beta/T)*(T/300)**alpha + other terms...  
|     * H2 and HD formation  
|       rate = gamma*(T/300)**alpha*nH/n(H)  
|     * three body reactions on grains surface  
|       rate = gamma*<sigma.v>(grain)*N(grains)/N(species on grains)  
|         /(Teff/beta+1)  
|     * sputtering of grain mantle  
|       complicated !  
|     * erosion of grain cores  
|       rate = gamma*EXP(-beta/T)*(T/300)**alpha * <sigma.v>(grain)  
|     * adsorption on grains  
|       rate = gamma*<sigma.v>(grain)
```

	R1	R2	P1	P2	P3	P4	gamma	alpha	beta
87 88	H	+H	=H2				8.14D-17	0.5	
IONIZ	H	+ELECTR	=H+	ELECTR	ELECTR		9.20D-10	0.5	157890.0
IONIZ	H2	+ELECTR	=H2+	ELECTR	ELECTR		1.40D-09	0.5	179160.0
IONIZ	H	+H+	=H+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+H3+	=H3+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+He+	=He+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+H3O+	=H3O+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+H3S+	=H3S+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+HCO+	=HCO+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+Fe+	=Fe+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+NH3+	=NH3+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+NH4+	=NH4+	H+	ELECTR		1.30D-13	0.5	157890.0
IONIZ	H	+S+	=S+	H+	ELECTR		1.30D-13	0.5	157890.0

IONIZ	H	+SiOH+	=SiOH+	H+	ELECTR	1.30D-13	0.5	157890.0
IONIZ	H	+O2+	=O2+	H+	ELECTR	1.30D-13	0.5	157890.0
IONIZ	H2	+H+	=H+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+H3+	=H3+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+He+	=He+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+H3O+	=H3O+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+H3S+	=H3S+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+HCO+	=HCO+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+Fe+	=Fe+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+NH3+	=NH3+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+NH4+	=NH4+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+S+	=S+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+SiOH+	=SiOH+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	H2	+O2+	=O2+	H2+	ELECTR	1.10D-13	0.5	179160.0
IONIZ	He	+H+	=H+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+H3+	=H3+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+He+	=He+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+H3O+	=H3O+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+H3S+	=H3S+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+HCO+	=HCO+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+Fe+	=Fe+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+NH3+	=NH3+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+NH4+	=NH4+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+S+	=S+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+SiOH+	=SiOH+	He+	ELECTR	1.10D-13	0.5	285328.0
IONIZ	He	+O2+	=O2+	He+	ELECTR	1.10D-13	0.5	285328.0
DISSO	H2	+ELECTR	=ELECTR	H	H	2.00D-09	0.5	116300.0
DISSO	H2	+H	=H	H	H	1.00D-10	0.0	052000.0
DISSO	H2	+He	=He	H	H	1.00D-11	0.0	052000.0
DISSO	H2	+H2	=H2	H	H	1.25D-11	0.0	052000.0
DISSO	H2	+H+	=H+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+H3+	=H3+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+He+	=He+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+H3O+	=H3O+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+H3S+	=H3S+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+HCO+	=HCO+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+Fe+	=Fe+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+NH3+	=NH3+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+NH4+	=NH4+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+S+	=S+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+SiOH+	=SiOH+	H	H	3.00D-11	0.5	052000.0
DISSO	H2	+O2+	=O2+	H	H	3.00D-11	0.5	052000.0
C54H18	+ELECTR	=C54H18-	PHOTON			1.00D-07	0.00	000000.0
C54H18+	+ELECTR	=C54H18	PHOTON			3.30D-06	-.50	000000.0
C54H18+ + C54H18-		=C54H18	C54H18			3.00D-09	-.50	000000.0
C54H18- + H+		=C54H18	H			7.50D-08	-.50	000000.0
C54H18- + H3+		=C54H18	H2	H		2.20D-08	-.50	000000.0
C54H18- + H3+		=C54H18	H	H		2.20D-08	-.50	000000.0
C54H18- + He+		=C54H18	He			3.80D-08	-.50	000000.0
C54H18- + C+		=C54H18	C			2.20D-08	-.50	000000.0
C54H18- + H3O+		=C54H18	H2O	H		1.70D-08	-.50	000000.0
C54H18- + H3S+		=C54H18	H2S	H		1.30D-08	-.50	000000.0
C54H18- + NH4+		=C54H18	NH3	H		1.80D-08	-.50	000000.0
C54H18- + HCO+		=C54H18	CO	H		1.40D-08	-.50	000000.0
C54H18- + HCS+		=C54H18	CS	H		1.10D-08	-.50	000000.0
C54H18- + Si+		=C54H18	Si			1.40D-08	-.50	000000.0
C54H18- + Fe+		=C54H18	Fe			1.00D-08	-.50	000000.0
C54H18- + S+		=C54H18	S			1.30D-08	-.50	000000.0
C54H18- + H+		=C54H18-	H			4.40D-09	0.00	000000.0
C54H18- + H3+		=C54H18-	H2	H		1.30D-09	0.00	000000.0
C54H18- + H3+		=C54H18-	H	H		1.30D-09	0.00	000000.0
C54H18- + He+		=C54H18-	He			2.20D-09	0.00	000000.0
C54H18- + C+		=C54H18-	C			1.30D-09	0.00	000000.0
C54H18- + H3O+		=C54H18-	H2O	H		1.00D-09	0.00	000000.0
C54H18- + H3S+		=C54H18-	H2S	H		7.40D-10	0.00	000000.0
C54H18- + NH4+		=C54H18-	NH3	H		1.00D-09	0.00	000000.0
C54H18- + HCO+		=C54H18-	CO	H		8.20D-10	0.00	000000.0
C54H18- + HCS+		=C54H18-	CS	H		6.50D-10	0.00	000000.0
C54H18- + Si+		=C54H18-	Si			8.30D-10	0.00	000000.0
C54H18- + Fe+		=C54H18-	Fe			5.90D-10	0.00	000000.0
C54H18- + S+		=C54H18-	S			7.80D-10	0.00	000000.0
C54H18- + H+		=C54H18-	H			3.30D-09	0.00	005500.0
C54H18- + C+		=C54H18-	C			9.60D-10	0.00	005500.0
C54H18- + CH		=C54H18-	CH			9.60D-10	0.00	005500.0
C54H18- + O		=C54H18-	O			8.30D-10	0.00	005500.0
C54H18- + OH		=C54H18-	OH			8.30D-10	0.00	005500.0
56 88	C54H18	+SECOPHO	=C54H18-	ELECTR		2.00D+04	0.00	140000.0
56 88	C54H18	+SECOPHO	=C54H18	ELECTR		2.00D+04	0.00	140000.0
G-	+ELECTR	=G-	PHOTON			6.90D-05	0.50	000000.0
G-	+H+	=G	H			1.60D-06	0.50	000000.0
G-	+H3+	=G	H2	H		4.61D-07	0.50	000000.0
G-	+H3+	=G	H	H		4.61D-07	0.50	000000.0
G-	+He+	=G	He			8.00D-07	0.50	000000.0
G-	+C+	=G	C			4.61D-07	0.50	000000.0
G-	+H3O+	=G	H2O	H		3.66D-07	0.50	000000.0
G-	+H3S+	=G	H2S	H		2.70D-07	0.50	000000.0
G-	+NH4+	=G	NH3	H		3.76D-07	0.50	000000.0
G-	+HCO+	=G	CO	H		2.96D-07	0.50	000000.0
G-	+HCS+	=G	CS	H		2.38D-07	0.50	000000.0
G-	+Si+	=G	Si			3.01D-07	0.50	000000.0
G-	+Fe+	=G	Fe			2.13D-07	0.50	000000.0
G-	+S+	=G	S			2.82D-07	0.50	000000.0

G	+H+	=G+	H			1.60D-06	0.50	000000.0
G	+H3+	=G+	H2	H	H	4.61D-07	0.50	000000.0
G	+H3+	=G+	H	H		4.61D-07	0.50	000000.0
G	+He+	=G+	He			8.00D-07	0.50	000000.0
G	+C+	=G+	C			4.61D-07	0.50	000000.0
G	+H3O+	=G+	H2O	H		3.66D-07	0.50	000000.0
G	+H3S+	=G+	H2S	H		2.70D-07	0.50	000000.0
G	+NH4+	=G+	NH3	H		3.76D-07	0.50	000000.0
G	+HCO+	=G+	CO	H		2.96D-07	0.50	000000.0
G	+HCS+	=G+	CS	H		2.38D-07	0.50	000000.0
G	+Si+	=G+	Si			3.01D-07	0.50	000000.0
G	+Fe+	=G+	Fe			2.13D-07	0.50	000000.0
G	+S+	=G+	S			2.82D-07	0.50	000000.0
G+	+ELECTR	=G	PHOTON			6.90D-05	0.50	000000.0
G	+SECPHO	=G+	ELECTR			0.63D+08	0.00	140000.0
G-	+SECPHO	=G	ELECTR			0.41D+09	0.00	140000.0
P & H	H	+CRP	=H+	ELECTR		4.60D-01	0.00	000000.0
P & H	He	+CRP	=He+	ELECTR		5.00D-01	0.00	000000.0
P & H	H2	+CRP	=H+	H	ELECTR	4.00D-02	0.00	000000.0
P & H	H2	+CRP	=H	H		1.50D+00	0.00	000000.0
P & H	H2	+CRP	=H2+	ELECTR		9.60D-01	0.00	000000.0
P & H	C	+CRP	=C+	ELECTR		1.80D+00	0.00	000000.0
P & H	O	+CRP	=O+	ELECTR		2.80D+00	0.00	000000.0
56 88	C	+SECPHO	=C+	ELECTR		1.02D+03	0.00	140000.0
2Z89	CH	+SECPHO	=C	H		1.46D+03	0.00	140000.0
13 87	CH4	+SECPHO	=CH3	H		4.68D+03	0.00	140000.0
2Z89	CH+	+SECPHO	=C	H+		3.52D+02	0.00	140000.0
2Z89	OH	+SECPHO	=O	H		1.02D+03	0.00	140000.0
2Z89	H2O	+SECPHO	=OH	H		1.94D+03	0.00	140000.0
2Z89	O2	+SECPHO	=O2+	ELECTR		2.34D+02	0.00	140000.0
2Z89	O2	+SECPHO	=O	O		1.50D+03	0.00	140000.0
2Z89	CO2	+SECPHO	=CO	O		3.42D+03	0.00	140000.0
2Z89	C2	+SECPHO	=C	C		4.74D+02	0.00	140000.0
77 87	C2H	+SECPHO	=C2	H		8.16D+03	0.00	140000.0
2Z89	C2H2	+SECPHO	=C2H	H		1.03D+04	0.00	140000.0
2Z89	C2H2	+SECPHO	=C2H2+	ELECTR		2.62D+03	0.00	140000.0
2Z88	C3	+SECPHO	=C2	C		2.24D+03	0.00	140000.0
13 87	C3H	+SECPHO	=C3	H		8.16D+03	0.00	140000.0
13 87	C3H2	+SECPHO	=C3H	H		8.16D+03	0.00	140000.0
56 88	CO	+SECPHO	=C	O		6.80D+02	1.20	140000.0
16B83	O	+H2	=OH	H		1.55D-13	2.80	002980.0
UMIST	CO	+H	=OH	C		1.10D-10	0.50	077700.0
72 83	O2	+H	=OH	O		1.63D-09	-.90	008750.0
16B83	OH	+H	=O	H2		7.00D-14	2.80	001950.0
16B83	OH	+H2	=H2O	H		9.54D-13	2.00	001490.0
16B83	H2O	+H	=OH	H2		5.24D-12	1.90	009265.0
17B73	C	+H2	=CH	H		1.16D-09	0.50	014100.0
P & H	C	+H	=CH	PHOTON		1.00D-17	0.00	000000.0
22 86	CH	+H2	=CH2	H		2.38D-10	0.00	001760.0
17B73	CH2	+H2	=CH3	H		5.18D-11	0.17	006400.0
23B83	CH3	+H2	=CH4	H		3.00D-10	0.00	005460.0
59 82	C2	+H2	=C2H	H		1.60D-10	0.00	001419.0
S88	C2H	+H2	=C2H2	H		1.14D-11	0.00	000950.0
17B73	CH	+H	=C	H2		1.16D-09	0.50	002200.0
22 86	CH2	+H	=CH	H2		4.70D-10	0.00	000370.0
17B73	CH3	+H	=CH2	H2		5.18D-11	0.17	005600.0
23B83	CH4	+H	=CH3	H2		3.00D-10	0.00	006560.0
P & H	O2	+C	=CO	O		3.30D-11	0.50	000000.0
93 88	OH	+CO	=CO2	H		4.40D-13	-1.15	000390.0
95 88	OH	+C	=CO	H		3.10D-11	-.36	000000.0
94 88	OH	+O	=O2	H		3.10D-11	-.36	000000.0
61 81	CH	+O	=HCO+	ELECTR		2.40D-14	0.50	000000.0
61 81	CH	+O	=CO	H		9.50D-11	0.50	000000.0
P & H	CH2	+O	=CO	H	H	2.00D-11	0.50	000000.0
X	CH3	+O	=CO	H2	H	1.80D-10	0.50	000000.0
P & H	C2	+O	=CO	C		5.00D-11	0.50	000000.0
P & H	C2H	+O	=CO	CH		1.00D-10	0.00	000250.0
X	C3	+O	=CO	C2		5.00D-11	0.50	000000.0
13 87	C3H	+O	=C2H	CO		5.00D-11	0.50	000000.0
13 87	C3H2	+O	=C2H2	CO		5.00D-11	0.50	000000.0
24Y83	C+	+H	=CH+	PHOTON		7.00D-17	0.00	000000.0
GRE92	C+	+H2	=CH2+	PHOTON		5.00D-16	0.00	000000.0
14 87	C+	+H2	=CH+	H		1.50D-10	0.00	004640.0
14 87	CH+	+H	=C+	H2		1.50D-10	0.00	000000.0
27B77	CH+	+H2	=CH2+	H		1.20D-09	0.00	000000.0
27B77	CH2+	+H	=CH+	H2		1.20D-09	0.00	002700.0
28B75	CH2+	+H2	=CH3+	H		7.00D-10	0.00	000000.0
28B75	CH3+	+H	=CH2+	H2		7.00D-10	0.00	010560.0
4Z89	CH3+	+H2	=CH5+	PHOTON		6.00D-15	0.00	000000.0
28B75	CH3+	+H2	=CH4+	H		2.00D-10	0.00	032500.0
28B75	CH4+	+H	=CH3+	H2		2.00D-10	0.00	000000.0
28B75	CH4+	+H2	=CH5+	H		4.00D-11	0.00	000000.0
28B75	CH5+	+H	=CH4+	H2		4.00D-11	0.00	002200.0
H+	+ELECTR	=H	PHOTON			2.90D-12	-.74	000000.0
22290	H2+	+ELECTR	=H	H		1.60D-08	-.43	000000.0
P & H	He+	+ELECTR	=He	PHOTON		4.50D-12	-.67	000000.0
McC03	H3+	ELECTR	H	H	H	5.10D-08	-.52	000000.0
McC03	H3+	ELECTR	H2	H		1.70d-08	-.52	000000.0
P & H	C+	+ELECTR	=C	PHOTON		4.40D-12	-.61	000000.0
22290	CH+	+ELECTR	=C	H		1.50D-07	-.42	000000.0
22290	CH2+	+ELECTR	=C	H2		1.25D-07	-.50	000000.0
22290	CH2+	+ELECTR	=CH	H		1.25D-07	-.50	000000.0

22Z90	CH3+	+ELECTR	=CH2	H		1.75D-07	.50	000000.0
22Z90	CH3+	+ELECTR	=CH	H		1.75D-07	.50	000000.0
P & H	CH4+	+ELECTR	=CH3	H		3.00D-07	.50	
P & H	CH4+	+ELECTR	=CH2	H	H	3.00D-07	.50	
22Z90	CH5+	+ELECTR	=CH	H2	H2	8.75D-08	.30	000000.0
22Z90	CH5+	+ELECTR	=CH2	H2	H	8.75D-08	.30	000000.0
22Z90	CH5+	+ELECTR	=CH3	H2		8.75D-08	.30	000000.0
22Z90	CH5+	+ELECTR	=CH4	H		8.75D-08	.30	000000.0
79 79	H+	+H2	=H2+	H		6.40D-10	0.00	021300.0
01R79	H2+	+H	=H+	H2		6.40D-10	0.00	000000.0
P & H	H2+	+H2	=H3+	H		2.10D-09	0.00	000000.0
P & H	H3+	+H	=H2+	H2		2.10D-09	0.00	020000.0
52R84	H+	+O	=O+	H		6.00D-10	0.00	000227.0
P & H	H+	+OH	=OH+	H		2.10D-09	0.00	000000.0
80R74	H+	+O2	=O2+	H		1.20D-09	0.00	000000.0
80R74	H+	+H2O	=H2O+	H		8.20D-09	0.00	000000.0
P & H	H+	+CH	=CH+	H		1.90D-09	0.00	000000.0
P & H	H+	+CH2	=CH+	H2		1.40D-09	0.00	000000.0
P & H	H+	+CH2	=CH2+	H		1.40D-09	0.00	000000.0
P & H	H+	+CH3	=CH3+	H		3.40D-09	0.00	000000.0
80R74	H+	+CH4	=CH3+	H2		2.28D-09	0.00	000000.0
80R74	H+	+CH4	=CH4+	H		1.52D-09	0.00	000000.0
18R80	H+	+CO2	=HCO+	O		4.20D-09	0.00	000000.0
P & H	H2+	+C	=CH+	H		2.40D-09	0.00	000000.0
P & H	H2+	+O	=OH+	H		1.50D-09	0.00	000000.0
38R75	H2+	+CO	=HCO+	H		2.16D-09	0.00	000000.0
38R75	H2+	+CO	=CO+	H2		6.44D-10	0.00	000000.0
P & H	H2+	+OH	=OH+	H2		7.60D-10	0.00	000000.0
38R75	H2+	+H2O	=H2O+	H2		3.90D-09	0.00	000000.0
38R75	H2+	+H2O	=H3O+	H		3.40D-09	0.00	000000.0
P & H	H2+	+CH	=CH+	H2		7.10D-10	0.00	000000.0
P & H	H2+	+CH	=CH2+	H		7.10D-10	0.00	000000.0
P & H	H2+	+CH2	=CH3+	H		1.00D-09	0.00	000000.0
P & H	H2+	+CH2	=CH2+	H2		1.00D-09	0.00	000000.0
P & H	H3+	+O	=OH+	H2		8.00D-10	0.00	000000.0
P & H	H3+	+OH	=H2O+	H2		1.30D-09	0.00	000000.0
5Z89	H3+	+CO	=HCO+	H2		1.70D-09	0.00	000000.0
39R82	H3+	+CO2	=HCO2+	H2		2.00D-09	0.00	000000.0
40R75	H3+	+H2O	=H3O+	H2		4.30D-09	0.00	000000.0
P & H	H3+	+C	=CH+	H2		2.00D-09	0.00	000000.0
P & H	H3+	+CH	=CH2+	H2		1.20D-09	0.00	000000.0
P & H	H3+	+CH2	=CH3+	H2		1.70D-09	0.00	000000.0
P & H	H3+	+CH3	=CH4+	H2		2.10D-09	0.00	000000.0
5Z89	H3+	+CH4	=CH5+	H2		1.90D-09	0.00	000000.0
85 86	He+	+H2	=H+	H	He	1.10D-13	-.24	000000.0
P & H	He+	+OH	=OH+	He		5.50D-10	0.00	000000.0
P & H	He+	+OH	=O+	H	He	5.50D-10	0.00	000000.0
74 85	He+	+H2O	=OH+	H	He	2.30D-10	-.94	000000.0
74 85	He+	+H2O	=H2O+	He		4.86D-11	-.94	000000.0
74 85	He+	+H2O	=H+	OH	He	1.64D-10	-.94	000000.0
42R85	He+	+CO	=C+	O	He	1.50D-09	0.00	000000.0
42R85	He+	+O2	=O+	O	He	1.00D-09	0.00	000000.0
81R77	He+	+CO2	=CO+	O	He	7.70D-10	0.00	000000.0
81R77	He+	+CO2	=O+	CO	He	1.80D-10	0.00	000000.0
81R77	He+	+CO2	=C+	O2	He	4.00D-11	0.00	000000.0
P & H	He+	+CH	=C+	H	He	1.10D-09	0.00	000000.0
P & H	He+	+CH2	=C+	H2	He	7.50D-10	0.00	000000.0
P & H	He+	+CH2	=CH+	H	He	7.50D-10	0.00	000000.0
P & H	He+	+CH3	=CH+	H2	He	9.00D-10	0.00	000000.0
P & H	He+	+CH3	=CH2+	H	He	9.00D-10	0.00	000000.0
43R76	He+	+CH4	=H+	CH3	He	4.00D-10	0.00	000000.0
43R76	He+	+CH4	=CH+	H2	He	2.56D-10	0.00	000000.0
43R76	He+	+CH4	=CH2+	H2	He	8.48D-10	0.00	000000.0
43R76	He+	+CH4	=CH3+	H	He	8.00D-11	0.00	000000.0
43R76	He+	+CH4	=CH4+	He		1.60D-11	0.00	000000.0
88 85	C+	+OH	=CO+	H		8.00D-10	0.00	000000.0
88 85	C+	+OH	=H+	CO		8.00D-10	0.00	000000.0
74 85	C+	+H2O	=HCO+	H		2.43D-09	-.63	000000.0
73R84	C+	+O2	=O+	CO		5.15D-10	0.00	000000.0
73R84	C+	+O2	=CO+	O		3.15D-10	0.00	000000.0
82R81	C+	+CO2	=CO+	CO		1.10D-09	0.00	000000.0
78 83	C+	+CH	=C2+	H		3.80D-10	0.00	000000.0
78 83	C+	+CH	=CH+	C		3.80D-10	0.00	000000.0
P & H	C+	+CH2	=CH2+	C		5.20D-10	0.00	000000.0
P & H	C+	+CH2	=C2H+	H		5.20D-10	0.00	000000.0
7R82	C+	+CH4	=C2H2+	H2		3.25D-10	0.00	000000.0
7R82	C+	+CH4	=C2H3+	H		9.75D-10	0.00	000000.0
52R84	O+	+H	=H+	O		6.00D-10	0.00	000000.0
52R84	O+	+H2	=OH+	H		1.20D-09	0.00	000000.0
P & H	O2+	+C	=CO+	O		5.20D-11	0.00	000000.0
P & H	O2+	+C	=C+	O2		5.20D-11	0.00	000000.0
44R81	OH+	+H2	=H2O+	H		1.01D-09	0.00	000000.0
44R81	H2O+	+H2	=H3O+	H		8.30D-10	0.00	000000.0
P & H	H3O+	+H	=H2O+	H2		6.10D-10	0.00	020500.0
P & H	H3O+	+C	=HCO+	H2		1.00D-11	0.00	000000.0
P & H	H3O+	+CH	=CH2+	H2O		6.80D-10	0.00	000000.0
P & H	H3O+	+CH2	=CH3+	H2O		9.40D-10	0.00	000000.0
P & H	O+	+ELECTR	=O	PHOTON		3.40D-12	-.64	000000.0
1Z83	O2+	+ELECTR	=O	O		1.95D-07	-.70	000000.0
22Z90	OH+	+ELECTR	=O	H		3.75D-08	-.50	000000.0
22Z90	H2O+	+ELECTR	=OH	H		3.15D-07	-.50	000000.0
90 88	H3O+	+ELECTR	=OH	H2		8.45D-07	-.50	000000.0

90 88	H3O+	+ELECTR	=H2O	H	4.55D-07	.50	000000.0
49R76	CH3+	+O	=HCO+	H2	3.10D-10	0.00	000000.0
49R76	CH3+	+O	=H3+	CO	1.30D-11	0.00	000000.0
8R80	CH5+	+O	=H3O+	CH2	2.16D-10	0.00	000000.0
51R80	CH5+	+CO	=HCO+	CH4	9.90D-10	0.00	000000.0
40R75	CH5+	+H2O	=H3O+	CH4	3.70D-09	0.00	000000.0
52R84	CO+	+H2	=HCO+	H	1.30D-09	0.00	000000.0
52R84	CO+	+H	=H+	CO	7.50D-10	0.00	000000.0
52R84	HCO+	+H	=CO+	H2	1.30D-09	0.00	024500.0
P& H	HCO+	+C	=CH+	CO	1.10D-09	0.00	000000.0
P& H	HCO+	+CH	=CH2+	CO	6.30D-10	0.00	000000.0
P& H	HCO+	+CH2	=CH3+	CO	8.60D-10	0.00	000000.0
27R77	HCO+	+CH3	=CH4+	CO	1.40D-09	0.00	009060.0
51R80	HCO+	+CH4	=CH5+	CO	9.90D-10	0.00	004920.0
65R78	HCO+	+H2O	=H3O+	CO	2.50D-09	0.00	000000.0
15	HCO+	+O2	=HCO2+	O	1.00D-09	0.00	001450.0
15	HCO2+	+O	=HCO+	O2	1.00D-09	0.00	000000.0
15	HCO+	+OH	=HCO2+	H	1.00D-09	0.00	000000.0
15	HCO2+	+H	=HCO+	OH	1.00D-09	0.00	007500.0
15	HCO2+	+CO	=HCO+	CO2	1.00D-09	0.00	000000.0
15	HCO+	+CO2	=HCO2+	CO	1.00D-09	0.00	005000.0
6R80	HCO2+	+CH4	=CH5+	CO2	7.80D-10	0.00	000000.0
22Z90	CO+	+ELECTR	=C	O	1.00D-07	-.46	000000.0
22Z90	HCO+	+ELECTR	=CO	H	2.40D-07	-.69	000000.0
6Z88	HCO2+	+ELECTR	=CO2	H	2.24D-07	-.50	000000.0
6Z88	HCO2+	+ELECTR	=CO	OH	1.16D-07	-.50	000000.0
27C77	C2+	+H2	=C2H+	H	1.40D-09	0.00	000000.0
45C77	C2+	+H2	=H+	C2H	1.50D-09	0.00	001260.0
45C77	C2H+	+H2	=C2H2+	H	1.70D-09	0.00	000000.0
46C84	C2H2+	+H2	=C2H3+	H	5.00D-10	0.00	000800.0
22Z90	C2+	+ELECTR	=C	C	3.00D-07	-.50	000000.0
22Z90	C2H+	+ELECTR	=C2	H	1.35D-07	-.50	000000.0
22Z90	C2H+	+ELECTR	=CH	C	1.35D-07	-.50	000000.0
75 88	C2H2+	+ELECTR	=C2H	H	1.50D-07	-.50	000000.0
75 88	C2H2+	+ELECTR	=CH	CH	1.50D-07	-.50	000000.0
75 88	C2H3+	+ELECTR	=C2H	H2	1.35D-07	-.50	000000.0
75 88	C2H3+	+ELECTR	=CH2	CH	1.35D-07	-.50	000000.0
75 88	C2H3+	+ELECTR	=C2H2	H	3.00D-08	-.50	000000.0
58 83	C3+	+H2	=C3H+	H	3.00D-10	0.00	000000.0
46C84	C3H+	+H2	=C3H2+	H	1.00D-09	0.00	000500.0
62 86	C3H+	+H2	=C3H3+	PHOTON	3.00D-13	-1.0	000000.0
46C84	C3H2+	+H2	=C3H3+	H	1.00D-10	0.00	002000.0
27C77	C2+	+H2	=C2H+	H	1.40D-09	0.00	000000.0
45C77	C2+	+H2	=H+	C2H	1.50D-09	0.00	001260.0
45C77	C2H+	+H2	=C2H2+	H	1.70D-09	0.00	000000.0
46C84	C2H2+	+H2	=C2H3+	H	5.00D-10	0.00	000800.0
22Z90	C2+	+ELECTR	=C	C	3.00D-07	-.50	000000.0
22Z90	C2H+	+ELECTR	=C2	H	1.35D-07	-.50	000000.0
22Z90	C2H+	+ELECTR	=CH	C	1.35D-07	-.50	000000.0
75 88	C2H2+	+ELECTR	=C2H	H	1.50D-07	-.50	000000.0
75 88	C2H2+	+ELECTR	=CH	CH	1.50D-07	-.50	000000.0
75 88	C2H3+	+ELECTR	=C2H	H2	1.35D-07	-.50	000000.0
75 88	C2H3+	+ELECTR	=C2H2	H	3.00D-08	-.50	000000.0
58 83	C3+	+H2	=C3H+	H	3.00D-10	0.00	000000.0
46C84	C3H+	+H2	=C3H2+	H	1.00D-09	0.00	000500.0
62 86	C3H+	+H2	=C3H3+	PHOTON	3.00D-13	-1.0	000000.0
46C84	C3H2+	+H2	=C3H3+	H	1.00D-10	0.00	002000.0
P& H	C3+	+ELECTR	=C2	C	3.00D-07	-.50	000000.0
P& H	C3H+	+ELECTR	=C2	CH	1.50D-07	-.50	000000.0
P& H	C3H+	+ELECTR	=C2H	C	1.50D-07	-.50	000000.0
75 88	C3H2+	+ELECTR	=C3H	H	1.50D-07	-.50	000000.0
75 88	C3H2+	+ELECTR	=C2H	CH	1.50D-07	-.50	000000.0
75 88	C3H3+	+ELECTR	=C3H2	H	1.50D-07	-.50	000000.0
75 88	C3H3+	+ELECTR	=C2H2	CH	1.50D-07	-.50	000000.0
P& H	H+	+C2	=C2+	H	3.10D-09	0.00	000000.0
P& H	H+	+C2H	=C2+	H2	1.50D-09	0.00	000000.0
P& H	H+	+C2H	=C2H+	H	1.50D-09	0.00	000000.0
78 83	H+	+C2H2	=C2H+	H2	2.00D-09	0.00	000000.0
78 83	H+	+C2H2	=C2H2+	H	2.00D-09	0.00	000000.0
4 84	H+	+C3H	=C3+	H2	2.00D-09	0.00	000000.0
4 84	H+	+C3H	=C3H+	H	2.00D-09	0.00	000000.0
4 84	H+	+C3H	=C3H2	H2	2.00D-09	0.00	000000.0
4 84	H+	+C3H2	=C3H2+	H	2.00D-09	0.00	000000.0
P& H	He+	+C2H	=C+	CH	5.10D-10	0.00	000000.0
P& H	He+	+C2H	=CH+	C	5.10D-10	0.00	000000.0
P& H	He+	+C2H	=C2+	H	5.10D-10	0.00	000000.0
3R75	He+	+C2H2	=CH+	CH	7.70D-10	0.00	000000.0
3R75	He+	+C2H2	=C2+	H2	1.61D-09	0.00	000000.0
3R75	He+	+C2H2	=C2H+	H	8.75D-10	0.00	000000.0
3R75	He+	+C2H2	=C2H2+	He	2.45D-10	0.00	000000.0
4 84	He+	+C3H	=C3+	H	2.00D-09	0.00	000000.0
4 84	He+	+C3H2	=C3H+	H	1.00D-09	0.00	000000.0
4 84	He+	+C3H2	=C3+	H2	1.00D-09	0.00	000000.0
P& H	H3+	+C2H	=C2H2+	H2	1.70D-09	0.00	000000.0
2R77	H3+	+C2H2	=C2H3+	H2	2.90D-09	0.00	000000.0
4 84	H3+	+C3H	=C3H2+	H2	2.00D-09	0.00	000000.0
4 84	H3+	+C3H2	=C3H3+	H2	2.00D-09	0.00	000000.0
P& H	C+	+C2H	=C3+	H	1.00D-09	0.00	000000.0
7R82	C+	+C2H2	=C3H+	H	2.20D-09	0.00	000000.0
P& H	HCO+	+C2H	=C2H2+	CO	7.80D-10	0.00	000000.0
54R77	HCO+	+C2H2	=C2H3+	CO	1.36D-09	0.00	000000.0

4 84	HCO+	+C3H	=C3H2+	CO		1.40D-09	0.00	000000.0
4 84	HCO+	+C3H2	=C3H3+	CO		1.40D-09	0.00	000000.0
10R86	H3O+	+C2H	=C2H2+	H2O		2.20D-10	0.00	004100.0
15	H3O+	+C2H2	=C2H3+	H2O		1.00D-09	0.00	007330.0
75 88	H3O+	+C3H	=C3H2+	H2O		2.00D-09	0.00	000000.0
75 88	H3O+	+C3H2	=C3H3+	H2O		3.00D-09	0.00	000000.0
10R86	C2H2+	+H2O	=H3O+	C2H		2.20D-10	0.00	000000.0
10R86	C2H3+	+H2O	=H3O+	C2H2		1.11D-09	0.00	000000.0
83R83	C3H+	+H2O	=HCO+	C2H2		2.48D-10	0.00	000000.0
83R83	C3H+	+H2O	=C2H3+	CO		2.02D-10	0.00	000000.0
P& H	H+	+Fe	=Fe+	H		7.40D-09	0.00	000000.0
P& H	H3+	+Fe	=Fe+	H		4.90D-09	0.00	000000.0
P& H	C+	+Fe	=Fe+	C		2.60D-09	0.00	000000.0
P& H	HCO+	+Fe	=Fe+	CO	H	1.90D-09	0.00	000000.0
P& H	H3O+	+Fe	=Fe+	H2O	H	3.10D-09	0.00	000000.0
P& H	O2+	+Fe	=Fe+	O2		1.10D-09	0.00	000000.0
P& H	Fe+	+ELECTR	=Fe	PHOTON		3.70D-12	-65	000000.0
P& H	N	CRP	N+	ELECTR		2.10E+00	0.00	000000.0
2Z89	CN	+SECPHO	=C	N		2.12D+04	0.00	140000.0
2Z89	HCN	+SECPHO	=CN	H		6.23D+03	0.00	140000.0
2Z89	HNC	+SECPHO	=CN	H		6.23D+03	0.00	140000.0
2Z89	NH2	+SECPHO	=NH	H		1.60D+02	0.00	140000.0
2Z89	NH2	+SECPHO	=NH2+	ELECTR		1.30D+03	0.00	140000.0
2Z89	NH3	+SECPHO	=NH2	H		2.63D+03	0.00	140000.0
2Z89	NH3	+SECPHO	=NH	H2		1.08D+03	0.00	140000.0
2Z89	NH3	+SECPHO	=NH3+	ELECTR		1.15D+03	0.00	140000.0
2Z89	NO	+SECPHO	=N	O		9.64D+02	0.00	140000.0
2Z89	NO	+SECPHO	=NO+	ELECTR		9.88D+02	0.00	140000.0
97 83	N	H2	NH	H		8.66D-10	0.50	014600.0
97 83	NH	H2	NH2	H		5.25D-12	0.79	006700.0
97 83	NH2	H2	NH3	H		6.22D-11	0.50	006300.0
14Z90	CN	H2	HCN	H		3.53D-13	3.31	000756.0
97 83	NH	H	N	H2		8.66D-10	0.50	002400.0
97 83	NH2	H	NH	H2		5.25D-12	0.79	002200.0
97 83	NH3	H	NH2	H2		6.22D-11	0.50	005700.0
P& H	NH	O	OH	N		2.90D-11	0.50	000000.0
P& H	NH2	O	NH	OH		3.50D-12	0.50	000000.0
97 83	NH3	O	NH2	OH		2.50D-12	0.00	003020.0
P& H	CN	O	CO	N		1.80D-11	0.50	000050.0
97 83	NH3	OH	NH2	H2O		2.30D-12	0.00	000800.0
P& H	NH	C	CN	H		1.10D-10	0.50	000000.0
94 88	CH	N	CN	H		2.10D-11	0.00	000000.0
97 83	CN	N	N2	C		7.30D-10	0.00	004500.0
P& H	NH	N	N2	H		5.00D-11	0.50	000000.0
94E88	OH	N	NO	H		5.30D-11	0.00	000050.0
97 83	O2	N	NO	O		3.30D-12	1.00	003150.0
P& H	NO	C	CN	O		1.10D-10	0.50	000000.0
94E88	NO	N	N2	O		3.40D-11	0.00	000050.0
97 83	NO	O	O2	N		7.50D-13	1.00	016000.0
GUESSHNC	H	HCN	H			1.00D-10	0.50	000200.0
GUESSHNC	O	CO	NH			2.00D-10	0.50	000200.0
GUESSHNC	OH	H2O	CN			2.00D-10	0.50	000200.0
GUESSHNC	O2	CO2	NH			2.00D-11	0.50	002000.0
3Z82	NH2	C	HNC	H		2.00D-11	0.50	000000.0
P& H	CH2	N	HCN	H		2.00D-11	0.50	000000.0
P& H	CH3	N	HCN	H2		2.00D-11	0.50	000000.0
GUESSCH5+	HNC	C2H3+	NH3			1.00D-09	0.00	000000.0
GUESSCH5+	HNC	C2H3+	NH3			1.00D-09	0.00	005120.0
13R85	N+	H2	NH+	H		8.40D-10	0.00	000168.5
10R80	NH+	H2	NH2+	H		1.27D-09	0.00	000000.0
10R80	NH+	H2	H3+	N		2.25D-10	0.00	000000.0
10R80	NH2+	H2	NH3+	H		2.70D-10	0.00	000000.0
07R83	NH3+	H2	NH4+	H		2.40D-12	0.00	000000.0
13R85	NH+	H	N+	H2		6.52D-10	0.00	000000.0
10R80	NH2+	H	NH+	H2		1.27D-09	0.00	024000.0
10R80	NH3+	H	NH2+	H2		2.25D-10	0.00	012800.0
15	NH4+	H	NH3+	H2		1.00D-09	0.00	011000.0
04R84	CN+	H2	HCN+	H		1.00D-09	0.00	000000.0
04R84	HCN+	H	CN+	H2		1.00D-09	0.00	015800.0
01R79	HCN+	H2	H2CN+	H		9.80D-10	0.00	000000.0
01R79	H2CN+	H	HCN+	H2		9.80D-10	0.00	034400.0
9Z89	N2+	H2	N2H+	H		2.00D-09	0.24	000000.0
10R80	N2H+	H	N2+	H2		2.10D-09	0.00	030300.0
08R82	N2H+	H2	H3+	N2		1.80D-09	0.00	008300.0
52	H+	HNC	H+	HCN		1.00D-09	0.00	000000.0
15	H+	HNC	H+	HNC		1.00D-09	0.00	007850.0
P& H	H+	NH	NH+	H		2.10D-09	0.00	000000.0
P& H	H+	NH2	NH2+	H		2.90D-09	0.00	000000.0
12R85	H+	NH3	NH3+	H		5.20D-09	0.00	000000.0
15	H+	CN	CN+	H		2.10D-09	0.00	006150.0
12R85	H+	HCN	HCN+	H		1.10D-08	0.00	000000.0
01R72	H+	NO	NO+	H		1.90D-09	0.00	000000.0
P& H	He+	NH	N+	H	He	1.10D-09	0.00	000000.0
P& H	He+	NH2	NH+	H	He	8.00D-10	0.00	000000.0
P& H	He+	NH2	N+	H2	He	8.00D-10	0.00	000000.0
02R75	He+	NH3	NH3+	He		2.64D-10	0.00	000000.0
02R75	He+	NH3	NH2+	H	He	1.76D-09	0.00	000000.0
02R75	He+	NH3	NH+	H2	He	1.76D-10	0.00	000000.0
P& H	He+	CN	C+	N	He	8.80D-10	0.00	000000.0
P& H	He+	CN	N+	C	He	8.80D-10	0.00	000000.0
01R77	He+	HCN	CN+	H	He	1.46D-09	0.00	000000.0
01R77	He+	HCN	CH+	N	He	6.20D-10	0.00	000000.0

01R77	He+	HCN	C+	NH	He	7.75D-10	0.00	000000.0
01R77	He+	HCN	N+	CH	He	2.48D-10	0.00	000000.0
01R77	He+	HNC	CN+	H	He	1.55D-09	0.00	000000.0
01R77	He+	HNC	C+	NH	He	1.55D-09	0.00	000000.0
02R77	He+	N2	N+	N	He	7.92D-10	0.00	000000.0
02R77	He+	N2	N2+	He		4.08D-10	0.00	000000.0
02R77	He+	NO	N+	O	He	1.38D-09	0.00	000000.0
02R77	He+	NO	O+	N	He	2.24D-10	0.00	000000.0
P& H	H3+	NH	NH2+	H2		1.30D-09	0.00	000000.0
P& H	H3+	NH2	NH3+	H2		1.80D-09	0.00	000000.0
5Z89	H3+	NH3	NH4+	H2		9.10D-09	0.00	000000.0
	H3+	N	NH2+	H		4.50D-20	0.00	000000.0
P& H	H3+	CN	HCN+	H2		1.00D-09	0.00	000000.0
P& H	H3+	CN	H2CN+	H		1.00D-09	0.00	000000.0
12R85	H3+	HCN	H2CN+	H2		9.50D-09	0.00	000000.0
12R85	H3+	HNC	H2CN+	H2		9.50D-09	0.00	000000.0
5Z89	H3+	N2	N2H+	H2		1.30D-09	0.00	000000.0
08R82	H3+	NO	HNO+	H2		1.10D-09	0.00	000000.0
19R80	H3O+	NH3	NH4+	H2O		2.20D-09	0.00	000000.0
	H3O+	CN	H2CN+	OH		4.50D-09	0.00	000000.0
19R78	H3O+	HCN	H2CN+	H2O		4.50D-09	0.00	000000.0
19R78	H2CN+	H2O	H3O+	HCN		4.50D-09	0.00	002460.0
19R78	H3O+	HNC	H2CN+	H2O		4.50D-09	0.00	000000.0
19R78	H2CN+	H2O	H3O+	HNC		4.50D-09	0.00	010300.0
P& H	HCO+	NH	NH2+	CO		6.40D-10	0.00	000000.0
P& H	NH2+	CO	HCO+	NH		6.40D-10	0.00	006100.0
P& H	HCO+	NH2	NH3+	CO		8.90D-10	0.00	000000.0
05R78	HCO+	NH3	NH4+	CO		1.90D-09	0.00	000000.0
12R85	HCO+	HCN	H2CN+	CO		3.70D-09	0.00	000000.0
12R85	HCO+	HNC	H2CN+	CO		3.70D-09	0.00	000000.0
04R71	HCO2+	NO	HNO+	CO2		1.00D-10	0.00	000000.0
P& H	C+	NH	CN+	H		7.80D-10	0.00	000000.0
P& H	C+	NH2	HCN+	H		1.10D-09	0.00	000000.0
05R79	C+	NH3	NH3+	C		5.29D-10	0.00	000000.0
05R79	C+	NH3	H2NC+	H		7.80D-10	0.00	000000.0
05R79	C+	NH3	H2CN+	H		7.80D-10	0.00	000000.0
05R79	C+	NH3	HCN+	H2		2.08D-10	0.00	000000.0
12R85	C+	HCN	C2N+	H		3.40D-09	0.00	000000.0
12R85	C+	HNC	C2N+	H		3.40D-09	0.00	000000.0
09R84	C+	NO	NO+	C		3.40D-09	0.00	000000.0
09R84	C+	NO	N+	CO		9.02D-10	0.00	000000.0
09R84	N+	CO	C+	NO		9.02D-10	0.00	015400.0
17R77	O2+	N	NO+	O		7.84D-11	0.00	000000.0
18R83	O2+	NH3	NH3+	O2		2.00D-09	0.00	000000.0
08R78	O2+	NO	NO+	O2		4.40D-10	0.00	000000.0
P& H	CH2+	N	HCN+	H		9.40D-10	0.00	000000.0
P& H	C2H+	N	C2N+	H		8.30D-10	0.00	000000.0
P& H	CH3+	N	HCN+	H2		6.70D-11	0.00	000000.0
M88	CH3+	N	H2CN+	H		6.70D-11	0.00	000000.0
M88	C2H2+	N	CH+	HCN		2.50D-11	0.00	000000.0
M88	C2H2+	N	CH+	HNC		2.50D-11	0.00	002600.0
M88	C2H2+	N	C2N+	H2		2.25D-10	0.00	000000.0
17R80	N+	O2	O2+	N		2.81D-10	0.00	000000.0
17R80	N+	O2	NO+	O		2.37D-10	0.00	000000.0
17R80	N+	O2	O+	NO		3.30D-11	0.00	000000.0
09R84	N+	CO	CO+	N		8.25D-10	0.00	000000.0
09R84	N+	CO	NO+	C		1.46D-10	0.00	000000.0
10R80	N+	NO	NO+	N		4.51D-10	0.00	000000.0
10R80	N+	NO	N2+	O		7.95D-11	0.00	000000.0
13R83	NH3+	H2O	NH4+	OH		2.50D-10	0.00	000000.0
13R83	NH4+	OH	NH3+	H2O		2.50D-10	0.00	003400.0
06R80	N2H+	O	OH+	N2		1.40D-10	0.00	003400.0
08R82	N2H+	H2O	H3O+	N2		2.60D-09	0.00	000000.0
06R80	N2H+	CO	HCO+	N2		8.80D-10	0.00	000000.0
06R80	HCO+	N2	N2H+	CO		8.80D-10	0.00	011200.0
08R82	N2H+	CO2	HCO2+	N2		1.40D-09	0.00	000000.0
08R82	HCO2+	N2	N2H+	CO2		1.40D-09	0.00	006400.0
15R74	N2H+	NH3	NH4+	N2		2.30D-09	0.00	000000.0
15R74	NH4+	N2	N2H+	NH3		2.30D-09	0.00	044000.0
08R82	N2H+	NO	HNO+	N2		3.40D-10	0.00	000000.0
01R83	C2N+	NH3	N2H+	C2H2		1.90D-10	0.00	000000.0
01R83	C2N+	NH3	H2CN+	HCN		1.70D-09	0.00	000000.0
P& H	HNO+	C	CH+	NO		1.00D-09	0.00	000000.0
04R71	HNO+	CO	HCO+	NO		1.00D-10	0.00	000000.0
04R71	HNO+	CO2	HCO2+	NO		1.00D-10	0.00	000000.0
P& H	HNO+	OH	H2O+	NO		6.20D-10	0.00	000000.0
08R82	HNO+	H2O	H3O+	NO		2.30D-09	0.00	000000.0
P& H	NO+	Fe	Fe+	NO		1.00D-09	0.00	000000.0
P& H	N+	ELECTR	N	PHOTON		3.80D-12	-0.62	000000.0
P& H	NH+	ELECTR	N	H		2.00D-07	-0.50	000000.0
P& H	NH2+	ELECTR	NH	H		1.50D-07	-0.50	000000.0
P& H	NH2+	ELECTR	N	H	H	1.50D-07	-0.50	000000.0
22290	NH3+	ELECTR	NH2	H		3.00D-07	-0.50	000000.0
22290	NH4+	ELECTR	NH2	H2		7.60D-07	-0.50	000000.0
22290	NH4+	ELECTR	NH3	H		7.60D-07	-0.50	000000.0
P& H	CN+	ELECTR	C	N		1.80D-07	-0.50	000000.0
75 88	C2N+	ELECTR	C2	N		1.00D-07	-0.50	000000.0
75 88	C2N+	ELECTR	CN	C		2.00D-07	-0.50	000000.0
75 88	HCN+	ELECTR	CN	H		1.50D-07	-0.50	000000.0
75 88	HCN+	ELECTR	CH	N		1.50D-07	-0.50	000000.0
22290	N2+	ELECTR	N	N		3.60D-08	-0.42	000000.0
6Z88	N2H+	ELECTR	N2	H		1.70D-07	-1.00	000000.0

7Z88	H2CN+	ELECTR	HCN	H		1.75D-07	-0.50	0000000.0
7Z88	H2CN+	ELECTR	HNC	H		1.75D-07	-0.50	0000000.0
7Z88	H2NC+	ELECTR	HNC	H		1.75D-07	-0.50	0000000.0
7Z88	H2NC+	ELECTR	NH2	C		1.75D-07	-0.50	0000000.0
22Z90	NO+	ELECTR	N	O		4.30D-07	-0.37	0000000.0
P & H	HNO+	ELECTR	NO	H		3.00D-07	-0.50	0000000.0
15	SO	+SECPHO	=S	O		9.64D+02	0.00	140000.0
15	CS	+SECPHO	=S	C		2.12D+04	0.00	140000.0
15	SH	+SECPHO	=S	H		1.46D+03	0.00	140000.0
2Z89	OCS	+SECPHO	=CO	S		1.07D+04	0.00	140000.0
2Z89	H2S	+SECPHO	=S	H2		1.03D+04	0.00	140000.0
2Z89	H2S	+SECPHO	=H2S+	ELECTR		3.39D+03	0.00	140000.0
2Z89	SO2	+SECPHO	=SO	O		1.77D+03	0.00	140000.0
16Z88	S	+H2	=SH	H		1.04D-10	.132	009620.0
16Z88	SH	+H2	=H2S	H		6.41D-12	.087	008050.0
16Z88	SH	+H	=S	H2		2.50D-11	0.00	000000.0
16Z88	H2S	+H	=SH	H2		1.29D-11	0.00	000860.0
16Z88	SO	+H	=OH	S		5.90D-10	-.31	011100.0
16Z88	SO2	+H	=SO	OH		9.25D-09	-.74	014700.0
16Z88	OCS	+H	=SH	CO		1.70D-11	0.00	002000.0
UMIST	SH	+O	=SO	H		1.60D-10	0.00	000100.0
17Z88	SH	+O	=OH	S		1.70D-11	0.67	000950.0
16Z88	H2S	+O	=SH	OH		1.40D-11	0.00	001920.0
16Z88	H2S	+OH	=SH	H2O		6.30D-12	0.00	000080.0
16Z88	CS	+O	=CO	S		2.70D-10	0.00	000760.0
16Z88	CS	+OH	=OCS	H		1.55D-13	1.12	000800.0
24Z87	S	+O2	=SO	O		5.19D-12	0.00	000265.0
16Z88	SO	+O	=S	O2		6.60D-13	0.00	002760.0
16Z88	SO	+O2	=SO2	O		1.40D-12	0.00	002820.0
23Z90	SO	+OH	=SO2	H		1.96D-10	-.17	000000.0
UMIST	SO	+N	=NO	S		1.73D-11	0.50	000750.0
16Z88	SO	+C	=CO	S		7.20D-11	0.00	000000.0
16Z88	SO	+C	=CS	O		1.70D-10	0.00	000000.0
16Z88	SO2	+O	=SO	O2		9.27D-11	-.46	009140.0
16Z88	OCS	+O	=SO	CO		2.60D-11	0.00	002250.0
16Z88	CH	+S	=CS	H		1.10D-12	0.00	000000.0
16Z88	CH	+S	=SH	C		1.73D-11	0.50	004000.0
16Z88	OH	+S	=SO	H		1.00D-10	0.00	000100.0
16Z88	SH	+C	=CS	H		2.00D-11	0.00	000000.0
16Z88	SH	+C	=CH	S		1.20D-11	0.58	005880.0
16Z88	SH	+CO	=OCS	H		5.95D-14	1.12	008330.0
18Z86	S+	+H2	=SH+	H		2.20D-10	0.00	009860.0
18Z86	SH+	+H2	=H2S+	H		1.90D-10	0.00	008500.0
P & H	SH+	+H2	=H3S+	PHOTON		1.00D-15	0.00	000000.0
18Z86	H2S+	+H2	=H3S+	H		1.40D-11	0.00	002300.0
1R84	CS+	+H2	=HCS+	H		4.80D-10	0.00	000000.0
18Z86	SH+	+H	=S+	H2		1.10D-10	0.00	000000.0
18Z86	H2S+	+H	=SH+	H2		2.00D-10	0.00	000000.0
18Z86	H3S+	+H	=H2S+	H2		6.00D-11	0.00	000000.0
P & H	SO+	+H	=S+	OH		6.10D-10	0.00	011385.0
GUESSH+	+S	=S+	H			1.00D-15	0.00	000000.0
P & H	H+	+SH	=SH+	H		1.60D-09	0.00	000000.0
P & H	H+	+SH	=S+	H2		1.60D-09	0.00	000000.0
P & H	H+	+H2S	=H2S+	H		7.60D-09	0.00	000000.0
P & H	H+	+CS	=CS+	H		4.90D-09	0.00	000000.0
P & H	H+	+SO	=SO+	H		3.20D-09	0.00	000000.0
P & H	H+	+OCS	=SH+	CO		5.90D-09	0.00	000000.0
P & H	H3+	+S	=SH+	H2		2.60D-09	0.00	000000.0
P & H	H3+	+SH	=H2S+	H2		1.90D-09	0.00	000000.0
P & H	H3+	+H2S	=H3S+	H2		3.70D-09	0.00	000000.0
P & H	H3+	+CS	=HCS+	H2		2.90D-09	0.00	000000.0
P & H	H3+	+SO	=HSO+	H2		1.90D-09	0.00	000000.0
8R82	H3+	+SO2	=HSO2+	H2		1.30D-09	0.00	000000.0
8R82	H3+	+OCS	=HOCS+	H2		1.90D-09	0.00	000000.0
P & H	He+	+SH	=S+	H	He	1.70D-09	0.00	000000.0
P & H	He+	+H2S	=S+	H2	He	3.60D-09	0.00	000000.0
P & H	He+	+H2S	=SH+	H	He	4.80D-10	0.00	000000.0
P & H	He+	+H2S	=H2S+	He		3.10D-10	0.00	000000.0
P & H	He+	+CS	=C+	S	He	1.30D-09	0.00	000000.0
P & H	He+	+CS	=S+	C	He	1.30D-09	0.00	000000.0
P & H	He+	+SO	=O+	S	He	8.30D-10	0.00	000000.0
P & H	He+	+SO	=S+	O	He	8.30D-10	0.00	000000.0
P & H	He+	+OCS	=CS+	O	He	7.60D-10	0.00	000000.0
P & H	He+	+OCS	=S+	CO	He	7.60D-10	0.00	000000.0
P & H	He+	+OCS	=CO+	S	He	7.60D-10	0.00	000000.0
P & H	He+	+OCS	=O+	CS	He	7.60D-11	0.00	000000.0
2R73	He+	+SO2	=S+	02	He	8.60D-10	0.00	000000.0
2R73	He+	+SO2	=SO+	0	He	3.44D-09	0.00	000000.0
P & H	C+	+S	=S+	C		1.50D-09	0.00	000000.0
P & H	C+	+SH	=CS+	H		1.10D-09	0.00	000000.0
3R78	C+	+H2S	=HCS+	H		1.28D-09	0.00	000000.0
3R78	C+	+H2S	=H2S+	C		4.25D-10	0.00	000000.0
P & H	C+	+CS	=CS+	C		1.60D-09	0.00	000700.0
P & H	C+	+SO	=S+	CO		2.60D-10	0.00	000000.0
P & H	C+	+SO	=CS+	O		2.60D-10	0.00	000000.0
P & H	C+	+SO	=SO+	C		2.60D-10	0.00	000000.0
P & H	C+	+OCS	=CO+	S		2.60D-10	0.00	000000.0
P & H	C+	+CS	=CS+	CO		1.60D-09	0.00	000000.0
P & H	C+	+SO2	=SO+	CO		2.30D-09	0.00	000000.0
P & H	CH+	+S	=S+	CH		4.70D-10	0.00	000000.0
P & H	CH+	+S	=SH+	C		4.70D-10	0.00	000000.0
P & H	CH+	+S	=CS+	H		4.70D-10	0.00	000000.0

19Z82	CH+	+SO	=OH+	CS		1.00D-09	0.00	000000.0
19Z82	CH+	+SO	=SH+	CO		1.00D-09	0.00	000000.0
P& H	CH3+	+S	=HCS+	H2		1.40D-09	0.00	000000.0
P& H	CH3+	+SO	=HOCS+	H2		9.50D-10	0.00	000000.0
P& H	CH5+	+S	=SH+	CH4		1.30D-09	0.00	000000.0
P& H	H3O+	+S	=SH+	H2O		3.20D-10	0.00	004930.0
4R79	H3O+	+H2S	=H3S+	H2O		1.90D-09	0.00	000000.0
P& H	HCO+	+S	=SH+	CO		3.30D-10	0.00	000000.0
P& H	HCO+	+SH	=H2S+	CO		8.20D-10	0.00	000000.0
P& H	HCO+	+CS	=HCS+	CO		1.20D-09	0.00	000000.0
P& H	HCO+	+SO	=HSO+	CO		7.50D-10	0.00	000000.0
7R75	HCO+	+H2S	=H3S+	CO		1.60D-09	0.00	000000.0
5R78	HCO+	+OCS	=HOCS+	CO		1.10D-09	0.00	000000.0
P& H	O2+	+S	=SO+	O		5.40D-10	0.00	000000.0
P& H	O2+	+S	=S+	O2		5.40D-10	0.00	000000.0
P& H	O2+	+H2S	=H2S+	O2		1.40D-09	0.00	000000.0
P& H	S+	+CH	=CS+	H		6.20D-10	0.00	000000.0
P& H	S+	+CH2	=HCS+	H		1.00D-11	0.00	000000.0
P& H	S+	+OH	=SO+	H		6.10D-10	0.00	000000.0
P& H	S+	+OH	=SH+	O		2.90D-10	0.00	008820.0
P& H	S+	+SH	=SH+	S		9.70D-10	0.00	000350.0
1R84	S+	+NO	=NO+	S		3.20D-10	0.00	000000.0
10R81	S+	+NH3	=NH3+	S		1.60D-09	0.00	000000.0
1R84	S+	+O2	=SO+	O		2.30D-11	0.00	000000.0
5R84	NH3+	+H2S	=NH4+	SH		6.00D-10	0.00	000000.0
P& H	HNO+	+S	=SH+	NO		1.10D-09	0.00	000000.0
P& H	N2H+	+S	=SH+	N2		1.10D-09	0.00	000000.0
P& H	SH+	+O	=SO+	H		2.90D-10	0.00	000000.0
P& H	SH+	+O	=S+	OH		2.90D-10	0.00	000000.0
P& H	SH+	+S	=S+	SH		9.70D-10	0.00	000000.0
P& H	SH+	+C	=CS+	H		9.90D-10	0.00	000000.0
P& H	SH+	+CH	=CH2+	S		5.80D-10	0.00	000000.0
P& H	SH+	+OH	=H2S+	O		3.10D-10	0.00	007500.0
P& H	SH+	+OH	=H2O+	S		4.30D-10	0.00	009200.0
10R81	SH+	+H2O	=H3O+	S		6.30D-10	0.00	000000.0
10R81	SH+	+H2S	=H2S+	SH		5.00D-10	0.00	001000.0
10R81	SH+	+H2S	=H3S+	S		5.00D-10	0.00	000000.0
1R84	SH+	+NO	=NO+	SH		3.30D-10	0.00	000000.0
10R81	SH+	+NH3	=NH3+	SH		5.25D-10	0.00	000000.0
10R81	SH+	+NH3	=NH4+	S		9.75D-10	0.00	000000.0
P& H	H2S+	+O	=SH+	OH		3.10D-10	0.00	000000.0
P& H	H2S-	+O	=SO+	H2		3.10D-10	0.00	000000.0
P& H	H2S+	+C	=HCS+	H		1.00D-09	0.00	000000.0
P& H	H2S+	+S	=S+	H2S		1.10D-09	0.00	000000.0
10R81	H2S+	+SH	=SH+	H2S		5.00D-10	0.00	000000.0
10R81	H2S+	+NO	=NO+	H2S		3.70D-10	0.00	000000.0
10R81	H2S+	+H2O	=H3O+	SH		8.10D-10	0.00	000000.0
10R81	H2S+	+NH3	=NH4+	SH		1.36D-09	0.00	000000.0
10R81	H2S+	+NH3	=NH3+	H2S		3.40D-10	0.00	000000.0
10R81	H3S+	+NH3	=NH4+	H2S		1.90D-09	0.00	000000.0
13R78	H3S+	+HCN	=H2CN+	H2S		1.90D-09	0.00	000000.0
19Z82	HCS+	+O	=HCO+	S		1.00D-09	0.00	000000.0
P& H	SO+	+NH3	=NH3+	SO		1.30D-09	0.00	000000.0
P& H	S+	+Fe	=Fe+	S		1.80D-10	0.00	000000.0
P& H	SH+	+Fe	=Fe+	SH		1.60D-09	0.00	000000.0
P& H	SO+	+Fe	=Fe+	SO		1.60D-09	0.00	000000.0
P& H	H2S+	+Fe	=Fe+	H2S		1.80D-09	0.00	000000.0
P& H	S+	+ELECTR	=S	PHOTON		3.90D-12	-.63	000000.0
P& H	SH+	+ELECTR	=S	H		2.00D-07	-.50	000000.0
P& H	H2S+	+ELECTR	=SH	H		1.50D-07	-.50	000000.0
P& H	H2S+	+ELECTR	=S	H		1.50D-07	-.50	000000.0
P& H	H2S+	+ELECTR	=H2S	PHOTON		1.10D-10	-.70	000000.0
P& H	H3S+	+ELECTR	=H2S	H		3.00D-07	-.50	000000.0
P& H	H3S+	+ELECTR	=SH	H2		1.00D-07	-.50	000000.0
P& H	CS+	+ELECTR	=C	S		2.00D-07	-.50	000000.0
P& H	CS+	+ELECTR	=C	S		2.00D-07	-.50	000000.0
21291	HCS+	+ELECTR	=CS	H		7.00D-07	-.50	000000.0
P& H	SO+	+ELECTR	=S	O		2.00D-07	-.50	000000.0
P& H	HSO+	+ELECTR	=SO	H		2.00D-07	-.50	000000.0
UMIST	HSO2+	ELECTR	SO	H	O	1.00E-07	-.50	000000.0
UMIST	HSO2+	ELECTR	SO	OH		1.00E-07	-.50	000000.0
P& H	HOCS+	+ELECTR	=OH	CS		2.00D-07	-.50	000000.0
P& H	HOCS+	+ELECTR	=OCS	H		2.00D-07	-.50	000000.0
L&G90	Si	+SECPHO	=Si+	ELECTR		3.00D+03	0.00	140000.0
L&G90	SiO	+SECPHO	=Si	O		3.00D+03	0.00	140000.0
L&G90	SiO2	+SECPHO	=SiO	O		3.00D+03	0.00	140000.0
2Z89	SiH	+SECPHO	=Si	H		1.46D+03	0.00	140000.0
13 87	SiH4	+SECPHO	=SiH3	H		4.68D+03	0.00	140000.0
McKay	SiH4	H	SiH3	H2		2.60D-11	0.00	001400.0
McKay	SiH3	H	SiH2	H2		2.00D-11	0.00	000000.0
McKay	SiH2	H	SiH	H2		2.00D-11	0.00	000000.0
McKay	SiH	H	Si	H2		2.00D-11	0.00	000000.0
McKay	SiH2	O2	SiO	H2O		7.50D-12	0.00	000000.0
McKay	SiH	O2	SiO	OH		1.70D-10	0.00	000000.0
UMIST	SiH2	O	SiO	H	H	5.00D-11	0.50	000000.0
UMIST	SiH	O	SiO	H		4.00D-11	0.50	000000.0
ROW01	Si	O2	SiO	O		1.72D-10	-.53	000017.0
ROW01	Si	OH	SiO	H		1.72D-10	-.53	000017.0
HRBST	SiO	OH	SiO2	H		1.00D-12	-.70	000000.0
2063	Si+	H2	SiH2+	PHOTON		3.00D-18	0.00	000000.0
2227	SiH+	H2	SiH3+	PHOTON		3.00D-17	-1.00	000000.0
2459	SiH3+	H2	SiH5+	PHOTON		1.00D-18	-0.50	000000.0

1724	Si+	H2	SiH+	H		1.50D-10	0.00	014310.0
27B77	SiH+	H2	SiH2+	H		1.20D-09	0.00	028250.0
28B75	SiH2+	H2	SiH3+	H		7.00D-10	0.00	006335.0
28B75	SiH3+	H2	SiH4+	H		2.00D-10	0.00	047390.0
2570	SiH4+	H2	SiH5+	H		1.00D-09	0.00	000000.0
2223	SiH+	H	Si+	H2		1.90D-09	0.00	000000.0
27B77	SiH2+	H	SiH+	H2		1.20D-09	0.00	000000.0
28B75	SiH3+	H	SiH2+	H2		7.00D-10	0.00	000000.0
28B75	SiH4+	H	SiH3+	H2		2.00D-10	0.00	000000.0
28B75	SiH5+	H	SiH4+	H2		4.00D-11	0.00	004470.0
2791	SiO+	H2	SiOH+	H		3.20D-10	0.00	000000.0
383	H+	Si	Si+	H		9.90E-10	0.00	000000.0
411	H+	SiH	SiH+	H		1.70E-09	0.00	000000.0
412	H+	SiH	Si+	H2		1.70E-09	0.00	000000.0
419	H+	SiH2	SiH2+	H		1.50E-09	0.00	000000.0
420	H+	SiH2	SiH+	H2		1.50E-09	0.00	000000.0
425	H+	SiH3	SiH3+	H		1.50E-09	0.00	000000.0
426	H+	SiH3	SiH2+	H2		1.50E-09	0.00	000000.0
429	H+	SiH4	SiH4+	H		1.50E-09	0.00	000000.0
430	H+	SiH4	SiH3+	H2		1.50E-09	0.00	000000.0
461	H+	SiO	SiO+	H		3.30E-09	0.00	000000.0
759	He+	Si	Si+	He		3.30E-09	0.00	000000.0
812	He+	SiH	Si+	H	He	1.80E-09	0.00	000000.0
821	He+	SiH2	SiH+	H	He	1.00E-09	0.00	000000.0
822	He+	SiH2	Si+	H2	He	1.00E-09	0.00	000000.0
829	He+	SiH3	SiH2+	H	He	1.00E-09	0.00	000000.0
830	He+	SiH3	SiH+	H2	He	1.00E-09	0.00	000000.0
834	He+	SiH4	SiH3+	H	He	1.00E-09	0.00	000000.0
835	He+	SiH4	SiH2+	H2	He	1.00E-09	0.00	000000.0
879	He+	SiO	Si+	O	He	8.60E-10	0.00	000000.0
880	He+	SiO	O+	Si	He	8.60E-10	0.00	000000.0
L&G90	He+	SiO2	SiO+	O	He	5.00E-10	0.00	000000.0
L&G90	He+	SiO2	Si+	O2	He	5.00E-10	0.00	000000.0
1033	C+	Si	Si+	C		2.10E-09	0.00	000000.0
1072	C+	SiH2	SiH2+	C		1.00E-09	0.00	000000.0
1078	C+	SiH3	SiH3+	C		1.00E-09	0.00	000000.0
1125	C+	SiO	Si+	CO		5.40E-10	0.00	000000.0
L&G90	C+	SiO2	SiO+	CO		1.00E-09	-0.60	000000.0
2471	S+	Si	Si+	S		1.60E-09	0.00	000000.0
2489	S+	SiH	SiH+	S		4.20E-10	0.00	000000.0
618	H3+	Si	SiH+	H2		2.00E-09	0.00	000000.0
644	H3+	SiH	SiH2+	H2		2.00E-09	0.00	000000.0
648	H3+	SiH2	SiH3+	H2		1.70E-09	0.00	000000.0
652	H3+	SiH3	SiH4+	H2		2.00E-09	0.00	000000.0
654	H3+	SiH4	SiH5+	H2		2.00E-09	0.00	000000.0
680	H3+	SiO	SiOH+	H2		2.00E-09	0.00	000000.0
1731	H3O+	Si	SiH+	H2O		1.80E-09	0.00	000000.0
1745	H3O+	SiH	SiH2+	H2O		9.70E-10	0.00	000000.0
1746	H3O+	SiH2	SiH3+	H2O		2.00E-09	0.00	000000.0
1764	H3O+	SiO	SiOH+	H2O		2.00E-09	0.00	000000.0
2258	HCO+	Si	SiH+	CO		1.60E-09	0.00	000000.0
2279	HCO+	SiH	SiH2+	CO		8.70E-10	0.00	000000.0
2283	HCO+	SiH2	SiH3+	CO		2.00E-09	0.00	000000.0
2286	HCO+	SiH4	SiH5+	CO		1.40E-09	0.00	000000.0
2305	HCO+	SiO	SiOH+	CO		7.90E-10	0.00	000000.0
2071	Si+	OH	SiO+	H		6.30E-10	0.00	000000.0
L&G90	Si+	H2O	SiOH+	H		2.30E-10	-0.60	000000.0
2082	Si+	O2	SiO+	O		1.00E-13	0.00	000000.0
2226	SiH+	O	SiO+	H		4.00E-10	0.00	000000.0
2229	SiH+	NH3	NH4+	Si		1.00E-09	0.00	000000.0
2230	SiH+	H2O	H3O+	Si		8.00E-10	0.00	000000.0
2391	SiH2+	O	SiOH+	H		6.30E-10	0.00	000000.0
2393	SiH2+	O2	SiOH+	OH		2.40E-11	0.00	000000.0
2458	SiH3+	O	SiOH+	H2		2.00E-10	0.00	000000.0
2571	SiH4+	H2O	H3O+	SiH3		2.00E-09	0.00	000000.0
2572	SiH4+	CO	HCO+	SiH3		1.00E-09	0.00	000000.0
2623	SiH5+	H2O	H3O+	SiH4		2.00E-09	0.00	000000.0
3116	Si+	ELECTR	Si	PHOTON		4.90E-12	-0.60	000000.0
3125	SiH+	ELECTR	Si	H		2.00E-07	-0.50	000000.0
3135	SiH2+	ELECTR	Si	H	H	2.00E-07	-0.50	000000.0
3136	SiH2+	ELECTR	SiH	H		1.50E-07	-0.50	000000.0
3137	SiH2+	ELECTR	Si	H2		1.50E-07	-0.50	000000.0
3146	SiH3+	ELECTR	SiH2	H		1.50E-07	-0.50	000000.0
3147	SiH3+	ELECTR	SiH	H2		1.50E-07	-0.50	000000.0
3156	SiH4+	ELECTR	SiH3	H		1.50E-07	-0.50	000000.0
3157	SiH4+	ELECTR	SiH2	H2		1.50E-07	-0.50	000000.0
3163	SiH5+	ELECTR	SiH4	H		1.50E-07	-0.50	000000.0
3164	SiH5+	ELECTR	SiH3	H2		1.50E-07	-0.50	000000.0
3227	SiO+	ELECTR	Si	O		2.00E-07	-0.50	000000.0
3247	SiOH+	ELECTR	SiO	H		1.50E-07	-0.50	000000.0
3248	SiOH+	ELECTR	Si	OH		1.50E-07	-0.50	000000.0
EROSI	Mg**	+He	=GRAIN	He	Mg	1.221D-2	73.0	0041.187
EROSI	Fe**	+He	=GRAIN	He	Fe	1.151D-2	73.0	0040.976
EROSI	Si**	+He	=GRAIN	He	Si	1.224D-2	73.0	0042.175
EROSI	C**	+He	=GRAIN	He	C	1.224D-2	73.0	0042.175
EROSI	O**	+He	=GRAIN	He	O	5.348D-2	73.0	0036.030
EROSI	Mg**	+C	=GRAIN	C	Mg	2.935D-2	48.0	0036.740
EROSI	Fe**	+C	=GRAIN	C	Fe	2.386D-2	47.0	0042.794
EROSI	Si**	+C	=GRAIN	C	Si	2.698D-2	48.0	0036.502
EROSI	C**	+C	=GRAIN	C	C	2.698D-2	48.0	0036.502
EROSI	O**	+C	=GRAIN	C	O	1.054D-1	48.0	0030.812

EROSI Mg**	+N	=GRAIN	N	Mg	2.935D-2	48.0	0036.740
EROSI Fe**	+N	=GRAIN	N	Fe	2.386D-2	47.0	0042.794
EROSI Si**	+N	=GRAIN	N	Si	2.698D-2	48.0	0036.502
EROSI C**	+N	=GRAIN	N	C	2.698D-2	48.0	0036.502
EROSI O**	+N	=GRAIN	N	O	1.054D-1	48.0	0030.812
EROSI Mg**	+O	=GRAIN	O	Mg	2.884D-2	48.0	0030.238
EROSI Fe**	+O	=GRAIN	O	Fe	4.116D-2	44.0	0059.438
EROSI Si**	+O	=GRAIN	O	Si	3.373D-2	47.0	0037.810
EROSI C**	+O	=GRAIN	O	C	3.373D-2	47.0	0037.810
EROSI O**	+O	=GRAIN	O	O	1.006D-1	47.0	0031.588
EROSI Mg**	+H2O	=GRAIN	H2O	Mg	2.884D-2	48.0	0030.238
EROSI Fe**	+H2O	=GRAIN	H2O	Fe	4.116D-2	44.0	0059.438
EROSI Si**	+H2O	=GRAIN	H2O	Si	3.373D-2	47.0	0037.810
EROSI C**	+H2O	=GRAIN	H2O	C	3.373D-2	47.0	0037.810
EROSI O**	+H2O	=GRAIN	H2O	O	1.006D-1	47.0	0031.588
EROSI Mg**	+N2	=GRAIN	N2	Mg	2.093D-2	48.0	0027.730
EROSI Fe**	+N2	=GRAIN	N2	Fe	4.324D-2	47.0	0042.335
EROSI Si**	+N2	=GRAIN	N2	Si	2.217D-2	47.0	0028.013
EROSI C**	+N2	=GRAIN	N2	C	2.217D-2	47.0	0028.013
EROSI O**	+N2	=GRAIN	N2	O	1.149D-1	46.0	0046.018
EROSI Mg**	+CO	=GRAIN	CO	Mg	2.093D-2	48.0	0027.730
EROSI Fe**	+CO	=GRAIN	CO	Fe	4.324D-2	47.0	0042.335
EROSI Si**	+CO	=GRAIN	CO	Si	2.217D-2	47.0	0028.013
EROSI C**	+CO	=GRAIN	CO	C	2.217D-2	47.0	0028.013
EROSI O**	+CO	=GRAIN	CO	O	1.149D-1	46.0	0046.018
EROSI Mg**	+O2	=GRAIN	O2	Mg	2.093D-2	48.0	0027.730
EROSI Fe**	+O2	=GRAIN	O2	Fe	4.324D-2	47.0	0042.335
EROSI Si**	+O2	=GRAIN	O2	Si	2.217D-2	47.0	0028.013
EROSI C**	+O2	=GRAIN	O2	C	2.217D-2	47.0	0028.013
EROSI O**	+O2	=GRAIN	O2	O	1.149D-1	46.0	0046.018
ADSORC	+GRAIN	=CH4*			1.00D+00		0000102.
ADSORCH	+GRAIN	=CH4*			1.00D+00		0000102.
ADSORCH2	+GRAIN	=CH4*			1.00D+00		0000102.
ADSORCH3	+GRAIN	=CH4*			1.00D+00		0000102.
ADSORCH4	+GRAIN	=CH4*			1.00D+00		0000102.
ADSORO	+GRAIN	=H2O*			1.00D+00		0000102.
ADSORO2	+GRAIN	=O2*			1.00D+00		0000102.
ADSOROH	+GRAIN	=H2O*			1.00D+00		0000102.
ADSORH2O	+GRAIN	=H2O*			1.00D+00		0000102.
ADSORCO	+GRAIN	=CO*			1.00D+00		0000102.
ADSORCO2	+GRAIN	=CO2*			1.00D+00		0000102.
ADSORC2	+GRAIN	=CH4*	CH4*		1.00D+00		0000102.
ADSORC2H	+GRAIN	=CH4*	CH4*		1.00D+00		0000102.
ADSORC2H2	+GRAIN	=CH4*	CH4*		1.00D+00		0000102.
ADSORC3	+GRAIN	=CH4*	CH4*	CH4*	1.00D+00		0000102.
ADSORC3H	+GRAIN	=CH4*	CH4*	CH4*	1.00D+00		0000102.
ADSORC3H2	+GRAIN	=CH4*	CH4*	CH4*	1.00D+00		0000102.
ADSORN	+GRAIN	=NH3*			1.00D+00		0000102.
ADSORNH	+GRAIN	=NH3*			1.00D+00		0000102.
ADSORNH2	+GRAIN	=NH3*			1.00D+00		0000102.
ADSORNH3	+GRAIN	=NH3*			1.00D+00		0000102.
ADSORCN	+GRAIN	=CH4*	NH3*		1.00D+00		0000102.
ADSORHCN	+GRAIN	=CH4*	NH3*		1.00D+00		0000102.
ADSORHNC	+GRAIN	=CH4*	NH3*		1.00D+00		0000102.
ADSORN2	+GRAIN	=N2*			1.00D+00		0000102.
ADSORNO	+GRAIN	=H2O*	NH3*		1.00D+00		0000102.
ADSORS	+GRAIN	=H2S*			1.00D+00		0000102.
ADSORSH	+GRAIN	=H2S*			1.00D+00		0000102.
ADSORH2S	+GRAIN	=H2S*			1.00D+00		0000102.
ADSORCS	+GRAIN	=CH4*	H2S*		1.00D+00		0000102.
ADSORSO	+GRAIN	=H2O*	H2S*		1.00D+00		0000102.
ADSORSO2	+GRAIN	=H2O*	H2O*	H2S*	1.00D+00		0000102.
ADSOROCS	+GRAIN	=OCS*			1.00D+00		0000102.
ADSORFe	+GRAIN	=Fe*			1.00D+00		0000102.
ADSORSi	+GRAIN	=SiH4*			1.00D+00		0000102.
ADSORSiH	+GRAIN	=SiH4*			1.00D+00		0000102.
ADSORSiH2	+GRAIN	=SiH4*			1.00D+00		0000102.
ADSORSiH3	+GRAIN	=SiH4*			1.00D+00		0000102.
ADSORSiH4	+GRAIN	=SiH4*			1.00D+00		0000102.
ADSORSiO	+GRAIN	=SiO*			1.00D+00		0000102.
ADSORSiO2	+GRAIN	=SiO2*			1.00D+00		0000102.
SPUTT CH4*	+H	=CH4	H	GRAIN	4.00D-05	0.00	002000.0
SPUTT CH4*	+H2	=CH4	H2	GRAIN	1.00D-04	0.00	002000.0
SPUTT CH4*	+He	=CH4	He	GRAIN	8.00D-04	0.00	002000.0
SPUTT H2O*	+H	=H2O	H	GRAIN	4.00D-05	0.00	006000.0
SPUTT H2O*	+H2	=H2O	H2	GRAIN	1.00D-04	0.00	006000.0
SPUTT H2O*	+He	=H2O	He	GRAIN	8.00D-04	0.00	006000.0
SPUTT CO*	+H	=CO	H	GRAIN	4.00D-05	0.00	001900.0
SPUTT CO*	+H2	=CO	H2	GRAIN	1.00D-04	0.00	001900.0
SPUTT CO*	+He	=CO	He	GRAIN	8.00D-04	0.00	001900.0
SPUTT CO2*	+H	=CO2	H	GRAIN	4.00D-05	0.00	003100.0
SPUTT CO2*	+H2	=CO2	H2	GRAIN	1.00D-04	0.00	003100.0
SPUTT CO2*	+He	=CO2	He	GRAIN	8.00D-04	0.00	003100.0
SPUTT NH3*	+H	=NH3	H	GRAIN	4.00D-05	0.00	003600.0
SPUTT NH3*	+H2	=NH3	H2	GRAIN	1.00D-04	0.00	003600.0
SPUTT NH3*	+He	=NH3	He	GRAIN	8.00D-04	0.00	003600.0
SPUTT CH3OH*	+H	=CH3OH	H	GRAIN	4.00D-05	0.00	006000.0
SPUTT CH3OH*	+H2	=CH3OH	H2	GRAIN	1.00D-04	0.00	006000.0
SPUTT CH3OH*	+He	=CH3OH	He	GRAIN	8.00D-04	0.00	006000.0
SPUTT H2CO*	+H	=H2CO	H	GRAIN	4.00D-05	0.00	006000.0
SPUTT H2CO*	+H2	=H2CO	H2	GRAIN	1.00D-04	0.00	006000.0
SPUTT H2CO*	+He	=H2CO	He	GRAIN	8.00D-04	0.00	006000.0

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SPUTT HCO2H* +H      =HCO2H  H      GRAIN      4.00D-05  0.00  006000.0
SPUTT HCO2H* +H2     =HCO2H  H2     GRAIN      1.00D-04  0.00  006000.0
SPUTT HCO2H* +He     =HCO2H  He    GRAIN      8.00D-04  0.00  006000.0
SPUTT OCS*   +H      =OCS   H      GRAIN      4.00D-05  0.00  006000.0
SPUTT OCS*   +H2     =OCS   H2     GRAIN      1.00D-04  0.00  006000.0
SPUTT OCS*   +He     =OCS   He    GRAIN      8.00D-04  0.00  006000.0
SPUTT H2S*   +H      =H2S   H      GRAIN      4.00D-05  0.00  006000.0
SPUTT H2S*   +H2     =H2S   H2     GRAIN      1.00D-04  0.00  006000.0
SPUTT H2S*   +He     =H2S   He    GRAIN      8.00D-04  0.00  006000.0
DESORCH4*  +CRP    =CH4    GRAIN    7.00D+01  0.00  000000.0
DESORH2O*   +CRP   =H2O    GRAIN    7.00D+01  0.00  000000.0
DESORCO*    +CRP   =CO     GRAIN    7.00D+01  0.00  000000.0
DESORCO2*   +CRP   =CO2    GRAIN    7.00D+01  0.00  000000.0
DESORNH3*   +CRP   =NH3    GRAIN    7.00D+01  0.00  000000.0
DESORCH3OH* +CRP   =CH3OH  GRAIN    7.00D+01  0.00  000000.0
DESORH2CO*  +CRP   =H2CO   GRAIN    7.00D+01  0.00  000000.0
DESORHCO2H* +CRP   =HCO2H  GRAIN    7.00D+01  0.00  000000.0
DESOROCS*   +CRP   =OCS   GRAIN    7.00D+01  0.00  000000.0
DESORH2S*   +CRP   =H2S    GRAIN    7.00D+01  0.00  000000.0
END

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