The Flower & Pineau des Forêts shock code

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An introduction

The shock model by Flower & Pineau des Forêts aims at describing the propagation of a supersonic shock wave in a layer of interstellar medium (ISM). Its fields of application include the modelling of shocked regions that accompany the powerful ejection episodes associated to star formation (in the form of bipolar jets and outflows), or those related to the late stages of supernova remnants (SNRs). A new class of extra-Galactic applications has also been developed recently. This document presents the code, and provides all the necessary information to run its online version. The first section contains a selected bibliography. The second section introduces the formalism of the shock, followed by a description of the corresponding modules in the third section. The fourth and fifth respectively describe its input and output files. Complementary detailed material can finally be found in the appendixes.

1 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.

1.1 Shock theory

This first section lists the historical articles that deal with the theoretical modelling of the propagation of a shock wave in the ISM, through its most prominent aspects. Note that this list is far from being exhaustive, as it only covers the publications that were the subject of a referreeing process:

- (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
- (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
- (5) *Draine, B. T., 1980, ApJ, 241, 1021*
  Interstellar shock waves with magnetic precursors
- (6) *Draine, B. T., 1981, ApJ, 245, 880*
  Infrared emission from dust in shocked gas
- (7) *Draine, B. T., Roberge, W. G., & Dalgarno, A., 1983, ApJ, 264, 485*
  Magnetohydrodynamic shock waves 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
- (10) *Neufeld, D. A., & Kaufman, M. J., 1993, ApJ, 418, 263*
  Radiative cooling of warm molecular gas
- (11) *Kaufman, M. J., & Neufeld, D. A., 1996, ApJ, 456, 611*
  Far-infrared water emission from magnetohydrodynamic shock waves

1.2 The first series of papers

This section contains the full list of papers in which the two main contributors to the shock code describe the physical and chemical processes that were taken into account from the beginning of the code developement:

- (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

1.3 The updates

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, H_2, and non-stationary shock models. 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) + O_2 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 Forts, 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

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

The molecular hydrogen.

- (39) *Verstraete, L., Falgarone, E., Pineau des Forêts, G., Flower, D. R., & Puget, J.-L., 1999, ESASP, 427, 779*
  Hot chemistry in the diffuse medium: spectral signature in the H_2 rotational lines
- (40) *Le Bourlot, J., Pineau des Forêts, G., & Flower, D. R., 1999, MNRAS, 305, 802*
  The cooling of astrophysical media by H_2
- (41) *Flower, D. R. & Pineau des Forêts, G., 1999, MNRAS, 308, 271*
  H_2 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-H_2 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
- (44) *Wilgenbus, D., Cabrit, S., Pineau des Forêts, G., & Flower, D. R., 2001, ASPC, 243, 347*
  Characteristics of shocks in bipolar outflows observed in pure rotational lines of H_2 with ISOCAM
- (45) *Pineau des Forêts, G., & Flower, D. R., 2001, MNRAS, 323, 7*
  Collisional excitation of H_2 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*
  The contributions of J-type shocks to the H_2 emission from molecular outflow sources
- (48) *Cabrit, S., Flower, D. R., Pineau des Forêts, G., Le Bourlot, J., & Ceccarelli, C., 2004, ApSS, 292, 501*
  H_2 diagnostics of magnetic molecular shocks in bipolar outflows
- (49) *Wrathmall, S. A., Gusdorf, A., & Flower, D. R., 2007, MNRAS, 382, 133*
  The excitation of molecular hydrogen by atomic hydrogen in astrophysical media

Non-stationary shocks.

- (50) *Chièze, J.-P., Pineau des Forêts, G., & Flower, D. R., 1998, MNRAS, 295, 672*
  Temporal evolution of MHD shocks in the interstellar medium
- (51) *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
- (52) *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

1.4 The spinoffs

Pseudo-multidimensional modelling.

- (53) *Kristensen, L. E., Ravkilde, T. L., Pineau des Forêts, G., et al., 2008, A&A, 477, 203*
  Observational 2D model of H2 emission from a bow shock in the Orion Molecular Cloud
- (54) *Gustafsson, M., Ravkilde, T., Kristensen, L. E., et al., 2010, A&A, 513, 5*
  3D model of bow shocks

Molecular emission.

- (55) *Flower, D. R., & Gusdorf, A., 2009, MNRAS, 395, 234*
  Emission and cooling by CO in interstellar shock waves
- (56) *Flower, D. R., & Pineau des Forêts, G., 2010, MNRAS, 406, 1745*
  Excitation and emission of H_2, CO and H_2O molecules in interstellar shock waves
- (57) *Flower, D. R., Pineau des Forêts, G., & Rabli, D., 2010, MNRAS, 409, 29*
  Methanol line formation in outflow sources
- (58) *Flower, D. R., & Pineau des Forêts, G., 2012, MNRAS, 421, 2786*
  Time-dependent modelling of the molecular line emission from shock waves in outflow sources

Dust processing.

- (59) *Guillet, V., Pineau des Forêts, G., & Jones, A. P., 2007, A&A, 476, 263*
  Shocks in dense clouds
  I - Dust dynamics
- (60) *Guillet, V., Jones, A. P., & Pineau des Forêts, G., 2009, A&A, 497, 145*
  Shocks in dense clouds
  II - Dust destruction and SiO formation in J shocks
- (61) *Guillet, V., Pineau des Forêts, & G., Jones, A. P., 2011, A&A, 527, 123*
  Shocks in dense clouds
  III - Dust processing and feedback effects in C-type shocks

Irradiated shocks.

1.5 A selection of publications based on the Flower & Pineau des Forêts shock code

Galactic.

- (62) *McCoey, C., Giannini, T., Flower, D. R., & Caratti o Garatti, A., 2004, MNRAS, 353, 813*
  On the excitation of the infrared knot in the HH99 outflow
- (63) *Giannini, T., McCoey, C., Caratti o Garatti, A., Net al., 2004, A&A, 419, 999*
  On the excitation of the infrared knots along protostellar jets
- (64) *Giannini, T., McCoey, C., Nisini, B., et al., 2006, A&A, 459, 821*
  Molecular line emission in HH54: a coherent view from near to far infrared
- (65) *Cabrit, S., Codella, C., Gueth, F., et al., A&A, 2007, 468, 29*
  PdBI sub-arcsecond study of the SiO microjet in HH212. Origin and collimation of class 0 jets
- (66) *Dionatos, O., Nisini, B., Cabrit, S., Kristensen, L. E., & Pineau des Forts, G., 2010, A&A, 521, 7*
  Spitzer spectral line mapping of the HH211 outflow
- (67) *Gusdorf, A., Giannini, T., Flower, D. R., et al., 2011, A&A, 523, 53*
  Revisiting the shocks in BHR71: new observational constraints and predictions for *Herschel*
- (68) *Panoglou, D., Cabrit, S., Pineau des Forts, G., et al., 2012, A&A, 538, 2*
  Molecule survival in magnetized protostellar disk winds. I. Chemical model and first results
- (69) *Gusdorf, A., Anderl, S., Güsten, R., et al., 2012, A&A, 542, 19*
  Probing magnetohydrodynamic shocks with high-J CO observations: W28F

Extra-Galactic.

- (70) *Guillard, P., Boulanger, F., Pineau des Forêts, G., & Appleton, P. N., 2009, A&A, 502, 515*
  H_2 formation and excitation in the Stephan's Quintet galaxy-wide collision
- (71) *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
- (72) *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
- (73) *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
- (74) *Meijerink, R., Kristensen, L. E., Weiss, A., et al., 2013, ApJ, 762, 16*
  Evidence for CO Shock Excitation in NGC 6240 from Herschel SPIRE Spectroscopy

2 The formalism of the code

2.1 The situation

2.2 The variables

2.3 The equations

As the magnetic field interacts directly only with the charged particles, it is necessary to consider at least a two-fluid model of the shock region. Substantial differences may develop between the flow velocities and kinetic temperatures of the ionised and neutrals fluids.

Whilst the preservation of charge neutrality requires that the flow velocity of the positive ions, $v_{\rm i}$, and the electrons, $v_{\rm e}$, 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 consider a three-fluid model of the medium. The suffixes *n*, *i*, and *e* will refer to the neutral fluid, the ionised fluid, and the electrons respectively.

Let us denote by *z* the independent variable, which is the distance from some arbitrary reference point along the positive flow direction. The magnetic induction, which is taken to be perpendicular to the flow, will be denoted by *B*. We consider a plane-parallel shock in a stationary state, in which the magnetic field is 'frozen' into the ionised gas. All the following equations are given in (12).

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

$$\frac{d}{dz}\left(\frac{\rho_{\rm n} v_{\rm n}}{\mu_{\rm n}}\right) = \mathcal{N}_{\rm n} \tag{1}$$

where $\rho_{\rm n}$ is the mass density of the neutral particle and $\mu_{\rm n}$ the mean molecular weight ; $\mathcal{N}_{\rm n}$ is the number of neutral particles created per unit volume and time. The corresponding equation for the positive ions is

$$\frac{d}{dz}\left(\frac{\rho_{\rm i} v_{\rm i}}{\mu_i}\right) = \mathcal{N}_{\rm i} \tag{2}$$

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

$$\frac{d}{dz}(n_\alpha v_\alpha) = C_\alpha \tag{3}$$

where n_α is the particle number per unit volume, v_α is the velocity of the considered particle, and $\mathcal{N}_\alpha$ is a source term for the species α.

Mass conservation. The equation expressing the conservation of the mass of the neutral particles and of the ionised particles may be written

$$\frac{d}{dz}(\rho_{\rm n} v_{\rm n}) = \mathcal{S}_{\rm n} \quad \text{and} \quad \frac{d}{dz}(\rho_{\rm i} v_{\rm i}) = \mathcal{S}_{\rm i} = -\mathcal{S}_{\rm n} \tag{4}$$

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

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

$$\frac{d}{dz}\left(\rho_{\rm n} v_{\rm n}^2 + \frac{\rho_{\rm n} k_{\rm B} T_{\rm n}}{\mu_{\rm n}}\right) = \mathcal{A}_{\rm n} \tag{5}$$

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

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

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 6 then becomes

$$\frac{d}{dz}\left[\rho_i v_i^2 + \frac{\rho_i k(T_i + T_e)}{\mu_i} + \frac{B_0^2}{8\pi}\left(\frac{v_s}{v_i}\right)^2\right] = -\mathcal{A}_n \tag{7}$$

Once again, the inertia of electrons has been neglected.

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

$$\frac{d}{dz}\left[\rho_n v_n^3 + \frac{5}{2}\frac{\rho_n v_n k T_n}{\mu_n} + \frac{\rho_n v_n U_n}{\mu_n}\right] = \mathcal{B}_n \tag{8}$$

where U_n is the mean internal energy per neutral particle, and $\mathcal{B}_n$ is the corresponding source term, the change in 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

$$\frac{d}{dz}\left[\rho_i v_i^3 + \frac{5}{2}\frac{\rho_i v_i k(T_i + T_e)}{\mu_i} + \frac{B_0^2}{4\pi}\frac{v_s^2}{v_i}\right] = \mathcal{B}_i + \mathcal{B}_e \tag{9}$$

For all these equations of conservation (number, mass, momentum, energy), source terms have to be estimated. These source terms can be the results of different kind of processes arising in the shock context. The most general chemical and physical processes are discussed in Appendix A, and Appendix B deals with the effects of molecular cooling.

3 The code source

4 The input files

4.1 The input parameters in input_mhd.in

Presentation. The input_mhd.in file contains all necessary parameters to run the shock code, regrouped in different categories: shock parameters, environmental parameters, numerical parameters, and output specifications. Each of those is described in the following pargraphs. The input_mhd.in file is located in the ~/mhd_gr/input directory, and an example is given in Figure 1.

Shock parameters. The first block of usable parameters contains the shock-related ones:

- the shock type
- the number of fluids $N_{\rm fluids}$
- the magnetic field parameter b
- the shock velocity v_s
- the initial drift velocity between the ion and neutral fluids
- the initial value for the ortho-to-para ratio of H_2 op_H_2
- the initial gas temperature
- the pre-shock density n_H
- the initial grain temperature $T_{\rm grains}$

- a choice for the cooling functions *Cool_KN*

Environment. The second block of usable parameters contains the environmental ones:
- the cosmic ray ionization rate *Zeta*
- the flux radiation *Rad*
- the initial extinction A_v

Numerical parameters. The third block of usable parameters contains the numerical ones:
-
-
-
-
-
-

Output specifications.

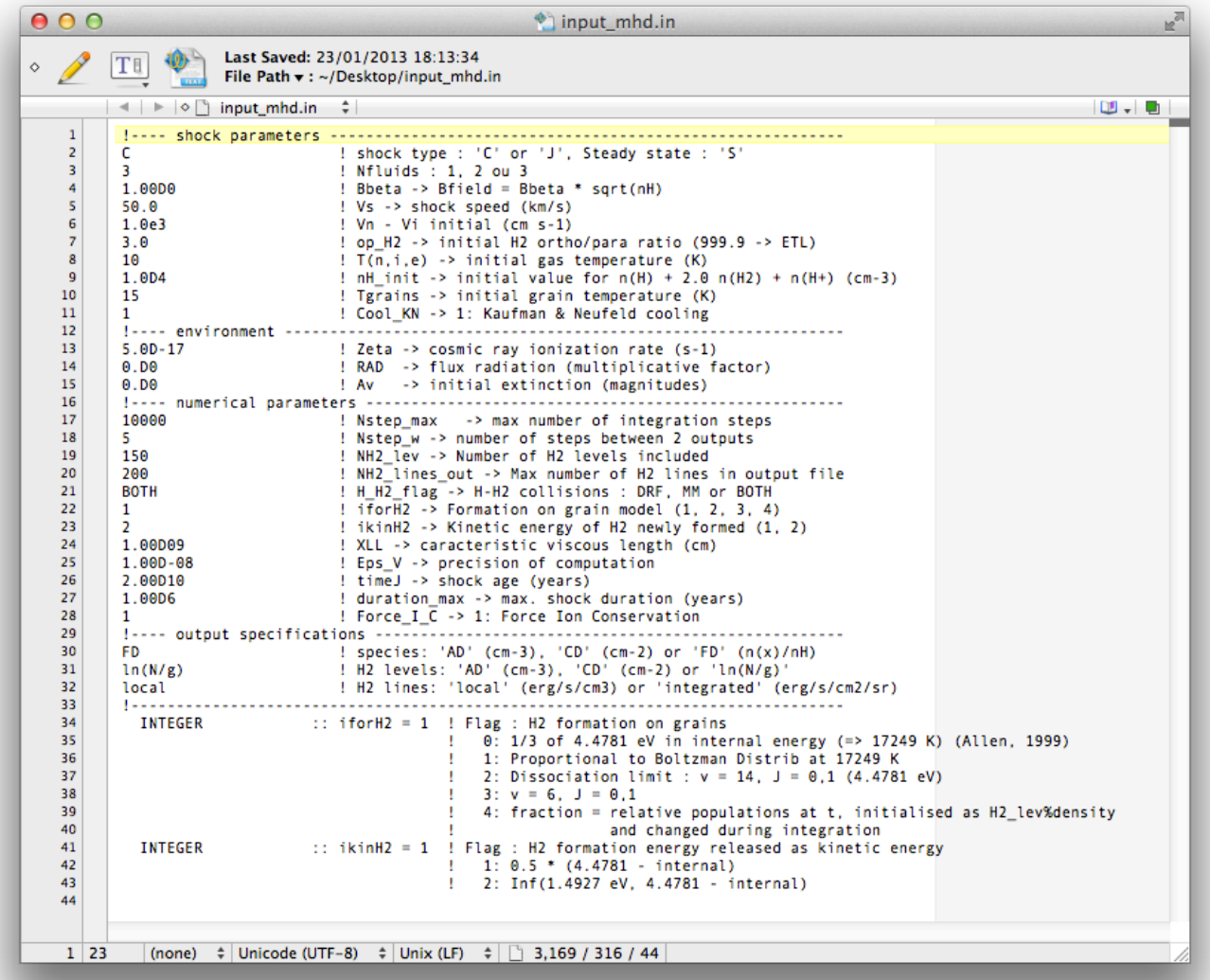

Figure 1: The input_mhd.in file, located in ~/mhd_gr/input directory.

element	fractional abundance	gas	mantles	cores
C	3.55×10^{-4}	8.27×10^{-5}	5.53×10^{-5}	2.17×10^{-4}
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}
Fe	3.23×10^{-5}	1.50×10^{-5}		3.23×10^{-5}

Table 1: Initial repartition of refractory elements in the gas-phase and in the grain mantles and cores, from (32). The atomic carbon from the PAHs has been incorporated in the carbonaceous grain cores. The total mass of the cores is 0.60% of that of the gas, divided up between silicate grains (70% of the mass, or 57% of the number of grains), and carbonaceous ones (30% in mass, 43% in number of grains).

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

Table 2: Initial repartition of chemical species in the grain mantles, relatively to hydrogen (first line), and to water ice (second line). The total mass of the mantles is 0.3% of that of the gas. From (32).

4.2 The considered chemical species in species.in

4.3 The considered chemical network in chemistry.in

4.4 The atomic and molecular data files

The H_2 molecule: coeff_GR_H2.in, coeff_H2_H2.in, coeff_H_H2_DRF.in.
Other species: coeff_X_oH2.in, coeff_X_pH2.in, coeff_X_H.in, coeff_X_He.in.

5 The output files

5.1 The physical and chemical structure of the shock

The physical parameters in mhd_phys.out .
The chemical abundances in mhd_speci.out .

5.2 The H_2-related files

The H_2 level populations H2_lev.out .
The H_2 line intensities H2_line.out .
The H_2 line integrated intensities excit.out .

5.3 Emissivities and cooling

The most important level populations populations.out .
The most important lines emissivities intensity.out .
The cooling functions cooling.out .

References

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A Source terms : chemistry

For further details concerning these equations, the interested reader can refer to (12), (13), and (14).

A.1 Number and mass of created particles

We note 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

$$\mathcal{N}_\alpha = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} C_\alpha \quad \text{and} \quad \mathcal{N}_\mathrm{i} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} C_\alpha \tag{10}$$

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

$$\mathcal{S}_\alpha = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} C_\alpha m_\alpha \quad \text{and} \quad \mathcal{S}_\mathrm{i} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} C_\alpha m_\alpha \tag{11}$$

The condition $\mathcal{S}_\mathrm{i} = -\mathcal{S}_\mathrm{n}$ provides a check-up of the consistency of the program.

A.2 Momentum

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

$$C_\alpha = \sum_\beta C_{\alpha\beta} \tag{12}$$

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

$$\mathcal{A}_\mathrm{n}^{(i)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_\beta C_{\alpha\beta} m_\alpha v_\beta \tag{13}$$

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, $v_\beta = v_\mathrm{n}$, whereas if there are all ions, $v_\beta = v_\mathrm{i}$. For a reaction between a neutral and an ion, $v_\beta = (m_\mathrm{i} v_\mathrm{i} + m_\mathrm{n} v_\mathrm{n})/(m_\mathrm{i} + m_\mathrm{n})$. Again, the condition

$$\sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_\beta C_{\alpha\beta} m_\alpha v_\beta = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_\beta C_{\alpha\beta} m_\alpha v_\beta \tag{14}$$

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

$$\sigma_\mathrm{in} = 2.41\pi \left(\frac{e^2 \alpha_\mathrm{n}}{\mu_\mathrm{in} v_\mathrm{in}^2} \right)^{1/2} \tag{15}$$

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

$$< \sigma v >_\mathrm{in} = 2.41\pi \left(\frac{e^2 \alpha_\mathrm{n}}{\mu_\mathrm{in}} \right)^{1/2} \tag{16}$$

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

$$\mathcal{A}_\mathrm{n}^{(ii)} = \frac{\rho_\mathrm{n}\rho_\mathrm{i}}{\mu_\mathrm{n} + \mu_\mathrm{i}} < \sigma v >_\mathrm{in} (v_\mathrm{i} - v_\mathrm{n}) \tag{17}$$

The electron-neutral scattering is negligible with respect to the ion-neutral scattering.

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

$$\mathcal{A}_{\rm n}^{(iii)} = \pi a^2 |v_{\rm i} - v_{\rm n}|(v_{\rm i} - v_{\rm n})\mu_{\rm in} \tag{18}$$

where a is the radius of the grain, and $\mu_{\rm in} = \mu_{\rm i}\mu_{\rm n}/(\mu_{\rm i} + \mu_{\rm n})$ is the reduced mass of the grain-neutral system.

A.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. One consequence of the photophysical activity of the interstellar medium (vii) is also mentioned.

(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

$$\mathcal{B}_{\rm n}^{(i)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_{\beta} C_{\alpha\beta} \frac{1}{2} m_\alpha v_\beta^2 \ \text{and} \mathcal{B}_{\rm i}^{(i)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\beta} C_{\alpha\beta} \frac{1}{2} m_\alpha v_\beta^2 \tag{19}$$

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 ($C_{\alpha\beta} > 0$) and destruction ($C_{\alpha\beta} < 0$) 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 $T_{\rm i}$ et $T_{\rm e}$, and are destructed through ionisation at temperature $T_{\rm n}$. Consequently, the rate at which enthalpy is added to the neutral fluid can be written

$$\mathcal{B}_{\rm n}^{(ii)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \left[\sum_{\substack{\beta, \\ C_{\alpha\beta}>0}} C_{\alpha\beta} \frac{3}{2} k \frac{T_{\rm i} + T_{\rm e}}{2} + \sum_{\substack{\beta, \\ C_{\alpha\beta}<0}} C_{\alpha\beta} \frac{3}{2} k T_{\rm n} \right] \tag{20}$$

Similarly, for ions

$$\mathcal{B}_{\rm i}^{(ii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \left[\sum_{\substack{\beta, \\ C_{\alpha\beta}>0}} C_{\alpha\beta} \frac{3}{2} k T_{\rm n} + \sum_{\substack{\beta, \\ C_{\alpha\beta}<0}} C_{\alpha\beta} \frac{3}{2} k T_{\rm i} \right] \tag{21}$$

And eventually, for electrons

$$\mathcal{B}_{\rm e}^{(ii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\substack{\beta, \\ C_{\alpha\beta}<0}} C_{\alpha\beta} \frac{3}{2} k T_{\rm e} \tag{22}$$

(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

$$\mathcal{B}_{\rm n}^{(iii)} = \sum_{\substack{\alpha, \\ \text{neutral} \\ \text{species}}} \sum_{\substack{\beta, \\ C_{\alpha\beta}>0}} C_{\alpha\beta} \frac{M_\beta - m_\alpha}{M_\beta} \Delta E_\alpha \tag{23}$$

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

$$\mathcal{B}_{\rm i}^{(iii)} = \sum_{\substack{\alpha, \\ \text{ionised} \\ \text{species}}} \sum_{\substack{\beta, \\ C_{\alpha\beta}>0}} C_{\alpha\beta} \frac{M_\beta - m_\alpha}{M_\beta} \Delta E_\alpha \tag{24}$$

(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

$$\mathcal{B}_{\rm n}^{(iv)} = \frac{\rho_{\rm n}\rho_{\rm i}}{\mu_{\rm n}\mu_{\rm i}} < \sigma v >_{\rm in} \frac{2\mu_{\rm n}\mu_{\rm i}}{(\mu_{\rm n}+\mu_{\rm i})^2}\left[\frac{3}{2}k(T_{\rm i}-T_{\rm n}) + \frac{1}{2}(v_{\rm i}-v_{\rm n})(\mu_i v_i + \mu_n v_{\rm n})\right] \tag{25}$$

(v) Elastic collisions between electronic and neutrals. A similar expression is still valid for electron-neutral scattering, and simplifies thanks to the fact that $m_{\rm e} \ll \mu_{\rm n}$

$$\mathcal{B}_{\rm n}^{(v)} = \frac{\rho_{\rm n}\rho_{\rm i}}{\mu_{\rm n}\mu_{\rm i}} < \sigma v >_{\rm en} \frac{2m_{\rm e}}{\mu_{\rm n}}\left[\frac{4}{2}k(T_{\rm e}-T_{\rm n}) + \frac{1}{2}(v_{\rm i}-v_{\rm n})\mu_{\rm n}v_{\rm n}\right] \tag{26}$$

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

$$< \sigma v >_{\rm en} = 10^{-19}\left(\frac{8kT_{\rm e}}{\pi m_{\rm e}}\right)^{1/2} \ {\rm m}^3\ {\rm s}^{-1} \tag{27}$$

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

$$\mathcal{B}_{\rm e}^{(vi)} = \frac{4e^4}{\mu_{\rm i}kT_{\rm e}}\left(\frac{2\pi m_{\rm e}}{kT_{\rm e}}\right)^{1/2} \ln\Lambda\left(\frac{\rho_{\rm i}}{\mu_{\rm i}}\right)^2 k(T_{\rm i}-T_{\rm e}) \tag{28}$$

with $\mathcal{B}_{\rm i}^{(vi)} = -\mathcal{B}_{\rm e}^{(vi)}$, and where

$$\Lambda = \frac{3}{2e^3}\left(\frac{k^3T_{\rm e}^3\mu_{\rm i}}{\pi\rho_{\rm i}}\right)^{1/2} \tag{29}$$

(vii) Other source terms for electrons. Non thermal electrons are also injected through ionisation of the atoms and molecules of the gas by cosmic rays, and significantly thermalised (heating via photoelectric effect on grains can also be significant, but is subjected to considerable uncertainties on the physical properties of the grains). The injection rate of energy (in the grains fluid) through this process is $\delta E\zeta\rho_{\rm n}/\mu_{\rm n}$, where δE is the average energy transferred to the electron gas via ionisation by cosmic rays, and ζ is the ionisation rate by cosmic rays. Ideally, the heating rate through photoionisation should be given by

$$\mathcal{B}_{\rm e}^{(vii)} = \sum_\alpha n_\alpha \int_{\nu_\alpha}^{\nu_{\rm H}} \frac{4\pi J_\nu}{h\nu} a_\nu(\alpha)(h\nu - h\nu_\alpha)d\nu \tag{30}$$

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 $h\nu_{\rm H} = 13.598$ eV). In practice, one often has to consider an estimate of the value of the integrate of the equation 30, because of the uncertainties on the mean radiation intensity and on the frequency dependance of the photoionisation cross section. We use the formula

$$\delta E({\rm eV}) \ = \ \max\left\{5.7, \left[32 - 7\log\left(\frac{\rho_{\rm n}}{\rho_{\rm i}}\frac{\mu_{\rm i}}{\mu_{\rm n}}\right)\right]\right\} \tag{31}$$

The corresponding photoionisation rate for the electrons fluid then writes

$$\mathcal{B}_{\rm e}^{(vii)} = \sum_\alpha \delta E_\alpha \gamma_\alpha n_\alpha \tag{32}$$

where δE_γ stands for the average energy of the photoelectron produced by the photoionisation of the α species, with a density n_α, and which photoionisation rate is γ_α.

B Source terms : molecular cooling

B.1 Molecular vibrations and rotations

The atoms of a molecule are never in a steady state, whatever value the temperature could be reaching. In fact, even in a solid which temperature approaches the absolute zero, atoms constantly oscillate around their equilibrium position. Two kinds of movements can be characterised in this oscillation : vibration and rotation.

Rotational movements of a molecule can be described by means of a model of rigid rotator. The resolution of the Schrodinger equation for a molecule in free three-dimensional rotation shows that the rotational energy of a diatomic rigid rotator is quantized. In other terms, the energy of two atoms bound by a rigid bond can only have well defined values. However, the description of molecule with a rigid rotator model is only an approximation, because the nuclei also vibrate. In addition to this, centrifugal forces due to the rotation of the molecule generate a slight distorsion which itself provokes a modification of its inertia momentum. Taking the effects into account, the rotational energy levels (in joules) are given by

$$E_{\mathrm{r}} = hcBJ(J+1) - hcDJ^2(J+1)^2 \tag{33}$$

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

$$B = h/8\pi^2 cI \tag{34}$$

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

$$D = 4B^3/\omega^2 \tag{35}$$

J is the rotational quantum number of the molecule ($J = 0, 1, 2, ...$), 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 Schrdinger 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

$$E_{\mathrm{v}} = (v+\frac{1}{2})hc\omega_{\mathrm{e}} - (v+\frac{1}{2})^2 hcx_{\mathrm{e}}\omega_{\mathrm{e}} + (v+\frac{1}{2})^3 hcy_{\mathrm{e}}\omega_{\mathrm{e}} + \ldots \tag{36}$$

where v is the vibrational quantum number ($v = 0, 1, 2, ...$), 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, distorsion 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, NH_3, ou H_2O are also taken into account in the model.

B.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 ambiant 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- H_2. In the ortho-H_2, nuclear spins are aligned, thus $I = 1$, whereas for para-H_2, 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-H_2) then corresponds to odd values of J, and the state $J = 0$ (para-H_2) 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.

B.3 Molecular hydrogen cooling

The method of evaluation of the contribution to the cooling by molecular hydrogen is presented in (13). We call $n_{\rm J}$ the population density of the rotational level J of molecular hydrogen. The total density of molecular hydrogen is thus

$$n(\mathrm{H_2}) = \sum_{\rm J} \mathrm{n_J} \tag{37}$$

and the total density of hydrogen nuclei is

$$n(H) = n(H^0) + 2n(\mathrm{H_2}) \tag{38}$$

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

$$C(J \rightarrow J-2) = n_J \left[n(H^0) + n(\mathrm{H_2}) \right] < \sigma v >_{J \rightarrow J-2} \tag{39}$$

where $< \sigma v >_{\rm J \longrightarrow J-2}$ is the coefficient rate of collisional de-excitation, which we assume identical for molecular or atomic hydrogen. The collisional excitation rate is related to 39 through the 'detailed balance'

$$(2J-3)C(J-2 \rightarrow J) = (2J+1)C(J \rightarrow J-2)\exp(-x) \tag{40}$$

with

$$x = 2(2J-1)B/kT_{\rm n} \tag{41}$$

In equation 41, 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

$$\begin{aligned} < \sigma v >_{\rm J \rightarrow J-2} &= 4.6 \times 10^{-12}(2J-3)T_{\rm n}^{1/2}(1+x)^{1/2} \\ &\times \exp\left[\frac{-5.01x}{1 + BJ(J+1)/kT_{\rm n}} - 0.1187(4J-2) \right] \end{aligned} \tag{42}$$

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

$$\begin{aligned} \frac{d}{dz}(v_{\rm n} n_{\rm J}) &= \left[C(J+2 \rightarrow J) + A(J+2 \rightarrow J) \right] n_{\rm J+2} \\ &- \left[C(J \rightarrow J+2) + C(J \rightarrow J-2) + A(J \rightarrow J-2) \right] n_{\rm J} \\ &+ C(J-2 \rightarrow J) n_{\rm J-2} \end{aligned} \tag{43}$$

where $v_{\rm n}$ is the neutral fluid velocity in the z direction. At the static limit, $v_{\rm n} = 0$, and left's part of the equation 43 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 43 can be generalized

$$\begin{aligned}\frac{d}{dz}(v_{\rm n} n_{\rm J}) &= [C(J+2 \rightarrow J) + A(J+2 \rightarrow J)]\, n_{\rm J+2} \\ &- [C(J \rightarrow J+2) + C(J \rightarrow J-2) + A(J \rightarrow J-2)]\, n_{\rm J} \\ &+ C(J-2 \rightarrow J) n_{\rm J-2} \\ &+ \frac{n_{\rm J}}{n({\rm H_2})} \frac{d}{dz}\left[u_{\rm n} n({\rm H_2})\right] \end{aligned} \tag{44}$$

where $u_{\rm n} n({\rm H_2})$ is the molecular flux of molecular hydrogen.

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

$$[\mathcal{B}_{\rm n}({\rm H_2})]_{radiative} = -\sum_{J \geq 2} n_{\rm J} A(J \rightarrow J-2) 2(2J-1) B \tag{45}$$

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

$$\frac{\rho_{\rm n}}{\mu_{\rm n}} U_{\rm n} = \sum_{v,{\rm J}} n(v,J) E(v,J) \tag{46}$$

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

$$\frac{\rho_{\rm n}}{\mu_{\rm n}} U_n = \sum_{v,J} n_J B J(J+1) \tag{47}$$

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

$$\frac{d}{dz}\left(\frac{\rho_{\rm n} v_{\rm n} U_{\rm n}}{\mu_{\rm n}}\right) = \sum_{J} B J(J+1) \frac{d}{dz}(u_{\rm n} n_{\rm J}) \tag{48}$$

where $d(u_{\rm n} n_{\rm J})/dz$ is provided by equation 44.

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 The species.in file

```
!————————— list of chemical species — Steady state at T = 19.67 K —————————
!———— WARNING : order = neutrals, species on mantles, 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          00000000010000  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         00000000001000  1.126D-15  106.700     A&G : 3.55e-5
38 SiH        01000000001000  7.402D-20  089.690
39 SiH2       02000000001000  7.267D-22  069.140 *
40 SiH3       03000000001000  4.825D-24  048.540 *
41 SiH4       04000000001000  3.171D-22  011.000
42 SiO        00000100001000  3.242D-16  -24.300
43 SiO2       00000200001000  2.114D-17  -73.000
44 Mg         00000000100000  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*      04000000001001  1.000D-16
42 SiO*       00000100001001  1.000D-16
43 SiO2*      00000200001001  1.000D-16
59 O**        00000100000002  1.399D-04              Noyaux = 4*3.50(-5)
60 Si**       00000000001002  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)
```

D The chemistry.in file

```
!-------------------------------------------------------------------------------
!
! 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 =C+ ELECTR
!                last reaction : 56 88 CO +CRP =C O
!                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 : Ahrrenius 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	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	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	ELECTR		3.30D-09	0.00	005500.0
	C54H18-	+C	=C54H18	C	ELECTR		9.60D-10	0.00	005500.0
	C54H18-	+CH	=C54H18	CH	ELECTR		9.60D-10	0.00	005500.0
	C54H18-	+O	=C54H18	O	ELECTR		8.30D-10	0.00	005500.0
	C54H18-	+OH	=C54H18	OH	ELECTR		8.30D-10	0.00	005500.0
56 88	C54H18	+SECPHO	=C54H18+	ELECTR			2.00D+04	0.00	140000.0
56 88	C54H18-	+SECPHO	=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	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		4.61D-07	0.50	000000.0
	G	+H3+	=G+	H	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
22Z90	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
22Z90	CH+	+ELECTR	=C	H			1.50D-07	-.42	000000.0
22Z90	CH2+	+ELECTR	=C	H2			1.25D-07	-.50	000000.0
22Z90	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	H2			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	H	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	=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
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+	+C3H2	=C3H+	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	He	5.10D-10	0.00	000000.0
P& H	He+	+C2H	=CH+	C	He	5.10D-10	0.00	000000.0
P& H	He+	+C2H	=C2+	H	He	5.10D-10	0.00	000000.0
3R75	He+	+C2H2	=CH+	CH	He	7.70D-10	0.00	000000.0
3R75	He+	+C2H2	=C2+	H2	He	1.61D-09	0.00	000000.0
3R75	He+	+C2H2	=C2H+	H	He	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	He	2.00D-09	0.00	000000.0
4 84	He+	+C3H2	=C3H+	H	He	1.00D-09	0.00	000000.0
4 84	He+	+C3H2	=C3+	H2	He	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+	H2	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
GUESS	HNC	H	HCN	H		1.00D-10	0.50	000200.0
GUESS	HNC	O	CO	NH		2.00D-10	0.50	000200.0
GUESS	HNC	OH	H2O	CN		2.00D-10	0.50	000200.0
GUESS	HNC	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
GUESS	CH5+	HNC	C2H3+	NH3		1.00D-09	0.00	000000.0
GUESS	CH5+	HCN	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+	HCN	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
22Z90	NH3+	ELECTR	NH2	H		3.00D-07	-0.50	000000.0
22Z90	NH4+	ELECTR	NH2	H2		7.60D-07	-0.50	000000.0
22Z90	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
22Z90	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	000000.0
7Z88	H2CN+	ELECTR	HNC	H			1.75D-07	-0.50	000000.0
7Z88	H2NC+	ELECTR	HNC	H			1.75D-07	-0.50	000000.0
7Z88	H2NC+	ELECTR	NH2	C			1.75D-07	-0.50	000000.0
22Z90	NO+	ELECTR	N	O			4.30D-07	-0.37	000000.0
P& H	HNO+	ELECTR	NO	H			3.00D-07	-0.50	000000.0
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+	0H			6.10D-10	0.00	011385.0
GUESS	H+	+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+	0	He		8.30D-10	0.00	000000.0
P& H	He+	+OCS	=CS+	0	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+	0			2.60D-10	0.00	000000.0
P& H	C+	+SO	=SO+	C			2.60D-10	0.00	000000.0
P& H	C+	+SO	=CO+	S			2.60D-10	0.00	000000.0
P& H	C+	+OCS	=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	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
21Z91	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	-0.53	000017.0
ROW01	Si	OH	SiO	H		1.72D-10	-0.53	000017.0
HRBST	SiO	OH	SiO2	H		1.00D-12	-0.70	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
	H3+	Si	SiH2+	H		1.70E-09	0.00	000000.0
648	H3+	SiH2	SiH3+	H2		2.00E-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.

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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
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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