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Most of the material in this section has been taken from chapter I of the book
Elementary Processes in Hydrogen-Helium Plasmas
R.K.Janev et al., Springer Series on Atoms and Plasmas, Springer 1987, [1], with additions/clarifications by Detlev Reiter mainly in 8.

1 Preface

Atomic and molecular processes play an important role in laboratory and astrophysical plasmas for a wide range of conditions, and determine, in part, their electrical, transport, thermal, and radiation properties. The study of these and other plasma properties requires a knowledge of the cross section, reaction rate coefficients, and inelastic energy transfers for a variety of collisional reactions. In this review, we provide quantitative information about the most important collision processes occurring in hydrogen, helium, and hydrogen-helium plasmas in the temperature range from 0.1 eV to 20 keV. The material presented here is based on published atomic and molecular collision data, theoretical calculations, and appropriate extrapolation and interpolation procedures. This review gives the properties of each reaction, graphs of the cross section and reaction rate coefficients, and the coefficients of analytical fits for these quantities. We present this information in a form that will enable researchers who are not experts in atomic physics to use the data easily.
The authors thank their colleagues at the Princeton Plasma Physics Laboratory and in the atomic physics community who have made many useful suggestions for the section and presentation of the material. We gratefully acknowledge the excellent technical assistance of Elizabeth Carey for the typing, and Bernie Giehl for the drafting.
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2 Scope of the Present Survey

The goal of this survey is to provide as complete as possible collection of atomic and molecular collision data for hydrogen and helium plasmas with temperatures between 0.1 eV and 20 keV, and electron and ion densities less than $\sim 5 \cdot 10^{14}$ cm^{-3}. We present descriptions of the reactions, and graphs of the cross sections and reaction rate coefficients for all types of inelastic processes between the charged and neutral constituents of hydrogen-helium plasmas: $\mathrm{e}, \mathrm{H}^+, \mathrm{H}, \mathrm{H}_2^+, \mathrm{H}_2, \mathrm{H}_3^+, \mathrm{He}^{2+}, \mathrm{He}^+$ and He. We also include processes involving excited species such as $\mathrm{H}^*, \mathrm{He}^*, \mathrm{H}_2^*$ (electronically, vibrationally and rotationally), and H^-, and processes involving important electron and proton rearrangement reactions. The survey also contains a brief description of the energetics of the reaction (energy loss or gain in the reaction, energy distribution of reaction products, etc.). Finally, we provide analytic fits to the cross sections and reaction rate coefficients. Their coefficients are tabulated in Chap. 8.

3 Organization of Information

We have arranged the material according to the charge and structural complexity of colliding particles. The units used for the more common quantities are
E: impact energy (in the laboratory reference system) in eV, unless otherwise stated;
σ: cross section in cm^2;
$\langle\sigma v\rangle$: reaction rate coefficient in cm^3/s, the average being taken over a Maxwellian distribution with temperature T in eV.
For each individual reaction we give the following information in order of presentation:
– its symbolic notation, – the energy loss or gain, – the method (experimental, theoretical, or semi-empirical), by which the cross section has been obtained in various energy regions with the reference to the corresponding data source, – the energetics on the reaction products (when applicable), – comments on the reaction and/or the procedures applied to determine the cross sections, – a graphic representation of the cross section σ as a function of energy E (represented by a dashed curve with the scale on the right-hand side) and the corresponding reaction rate coefficient $\langle\sigma v\rangle$ as a function of temperature T (given by a solid line with the scale on the left side), – in the case of reactions between heavy particles the target particle's energy (velocity) can be important, and the figures show the reaction rate coefficients as a function of plasma temperature for several energies of the target particle, – in the case of reactions between plasma electrons and heavier particles, the heavy particle's energy is taken to be zero and only the temperature dependence is plotted.
Nearly all the figures use the same scales for σ and $\langle\sigma v\rangle$ so that these quantities can easily be compared. For groups of similar reactions, where energetics and cross sections are given by analytic formulas, the figures contain only a few representative examples. The Appendix gives information, such as energy levels, oscillator strengths, potential energy curves for H_2, H_2^+, and H_2^-, etc., common to several classes of reactions.

4 Sources and Criteria for Selection and Evaluation of Data

The main sources of information for the cross sections were previous compilations, such as those mentioned above, and the current journal literature. In selecting the data for a particular reaction, we gave priority to information with a stated accuracy. In cases where the original cross section data did not cover the entire energy range considered here, we have extended the range by employing appropriate interpolation or extrapolation procedures based either on reliable theoretical models or on a reasonable extension or scaling of the experimental data. In most cases, the extrapolations, which are necessary to calculate reaction rate coefficients, occur where the cross section is small. We calculated cross sections using existing theoretical methods (cf. Mott and Massey 1965; Smirnov 1973) for reactions for which no measurements could be found in the literature. We used simple two-state models (such as Landau-Zener and Rozen-Zener-Demkov models or the first Born approximation) to extend and generate new cross-section data. These theoretical methods provide results generally accurate to within a factor of two, or so. For the processes involving excited states (excitation, ionization, and charge transfer), we give generalized formulas for calculation of the cross sections. These formulas are, in most cases, based on a

semiclassical or purely classical model of the processes in question, and in some cases are supplemented by appropriate semi-empirical corrections. Their accuracy usually increases with the principal quantum number of the corresponding state. For processes involving heavy-particle collisions (excluding those induced by protons) for which no systematic experimental or theoretical data exist, we give appropriate scaling rules for cross sections and/or reaction rate coefficients based on the known data for the corresponding proton-induced processes. Our survey does not explicitly include collision processes that are related by the detailed balance principle to a corresponding "direct" process (for example, collisional de-excitation or collisional three-body electron-ion recombination). We include the radiative transition rates for hydrogen and helium atoms in the Appendix to complement the direct collisional processes.

5 Accuracy

In general, the accuracy for the cross section data for processes involving ground state species is $\pm 50\%$ or better, since, with few exceptions, we based the data presented here on experimental or evaluated theoretical results. For the processes involving excited species, the cross sections probably have an accuracy of a factor of two when they are based only on theoretical calculations or generalized formulas. A similar accuracy should apply to those molecular processes for which we determined the cross sections by averaging over vibrationally excited states (corresponding to a distribution of states typical for low-temperature plasmas), unless the cross section is known experimentally.

6 References

We used the following compilations as basic sources for the data whenever possible, after checking their consistency with more recent data: Freeman and Jones (1974), Jones (1977), Barnett et al. (1977), Takayanagi and Suzuki (1978), Fujimoto (1978), and Sataka et al. (1981). If no modifications were necessary, the reference we give is to these data sources (where the original references for the data can be found). In cases where other cross-section data are available for a given process, we have performed either a least-squares average of all the data or present the best results. In these latter cases, in order to avoid an excessive reference list, we include only the references used to construct the cross section in the figures.

7 Digitization of the Cross Sections

Most of the data available in either the original published sources or in the data surveys are presented in the form of a graph. We transformed these data to numbers using a Tektronix Graphics Tablet and combined digitized data from several sources in order to cover the required energy range (0.1 eV to 20 keV). For reactions with a nonzero threshold,a data point has been added at threshold.

8 Calculation of Reaction Rate Coefficients

The Maxwellian-averaged reaction rate coefficients for a particle of mass m and fixed energy $E = mV^2/2$ incident on a (stationary) Maxwellian distribution of particles of mass M and temperature $T = Mu^2/2$, i.e. thermal velocity $u = \sqrt{2T/M}$, for the heavy-particle reactions is

$$\langle \sigma v \rangle (T, V) = \frac{1}{\pi^{1/2} u V} \int_{v_{th}}^{\infty} v_r^2 dv_r \sigma(E_r) \{ \exp[-(v_r - V)^2/u^2] - \exp[-(v_r + V)^2/u^2] \}, \quad (1)$$

where $v_r = |\vec{V} - \vec{v}_{Maxw}|$ is the relative (collision) velocity related to E_r by $E_r = m_r v_r^2/2$, $m_r = mM/(m + M)$ being the reduced mass of colliding particles, $\vec{v}_{Maxw}$ is a velocity from the Maxwellian distribution at temperature and mass T, M, respectively, and v_{th} is the value of v_r at threshold, $E_r = E_{th}$.
For the electron reactions one can typically assume $u \gg V$, $M \ll m$. Hence, setting $M = m_r, T = T_e$ and stationary particles with mass m: $\lim E, V \to 0$

$$\langle \sigma v \rangle (T) = \frac{4}{\pi^{1/2} u^3} \int_{v_{th}}^{\infty} v_r^3 dv_r \sigma(E_r) \exp(-v_r^2/u^2), \quad (2)$$

or

$$\langle \sigma v \rangle (T) = \frac{2^{3/2}}{\pi^{1/2} M^{1/2}} \frac{1}{T^{3/2}} \int_{E_{th}}^{\infty} dE_r E_r \sigma(E_r) \exp(-E_r/T), \quad (3)$$

We used a number of mathematical techniques to assure the reaction rate integrals were computed accurately for the nearly five orders of magnitude variation in E and T.
For the calculation of reaction rate coefficients, it is necessary to know the cross section from threshold to very large values of the energy. However, the digitized data necessarily represent the cross section for a finite energy range and for a finite number of points (less than 100). Our solution to this problem is: (1) to calculate values of σ within the digitized range by linear interpolation of $\ln \sigma$ in $\ln E$; and (2) to extrapolate σ outside the digitized range by a method depending on the type of reaction as discussed below.

Type 1 Reactions with a nonzero threshold and a zero cross section at threshold. No low-energy extrapolation is necessary. We calculate the high-energy extrapolation from the formula $\sigma = ax^{-n} \ln x$, where $x = E/E_{th}$, and obtain the quantities a and n by matching the function at the last data point and with the average slope for the last few data points.

Type 2 Reactions fit well by $\ln \sigma = a + b \ \ln E$.

(N.B. these are cross sections of the form $\sigma(v) = \alpha v^{\beta}$ and zero threshold)

We obtain both low- and high-energy extrapolations with the coefficients, a and b.

Type 3 Reactions with a zero threshold.

The form $\ln \sigma = a + b \ \ln E$ fits both the high- and low-energy extrapolations. The coefficients are obtained by matching the function at the first (last) point and the average slope at the first (last) few points, respectively.

Type 4 Reactions with a nonzero threshold and a nonzero cross section at threshold.

No low-energy extrapolation is necessary since there is a point at threshold, and σ is taken to be zero below threshold. The high-energy extrapolation is of the form $\ln \sigma = a + b \ln E$, with the coefficients calculated to match the function at the last point and the average slope at the last few points.

We calculated the cross sections used in the plots, in the numerical tables, and in the integrals for the reaction rate coefficients by the above procedures. There are sufficient data points for the interpolated values to be at least as accurate as the data. In most cases the extrapolations occur where the cross section is negligibly small. Where this is not the case, there is no better alternative to the above procedure.

9 Numerical Fits to σ and $\langle \sigma v \rangle$

We derived numerical fits for σ and $\langle \sigma v \rangle$ so that these processes can be evaluated easily in numerical codes and in other instances that demand simple and/or repeated evaluations. Since σ and $\langle \sigma v \rangle$ vary over many orders of magnitude, we made polynomial fits for $\ln \sigma$ in terms of $\ln E$ and for $\ln \langle \sigma v \rangle$ in terms of $\ln T$:

$$\ln \sigma = \sum_{n=0}^{N} a_n (\ln E)^n,$$

$$\ln \langle \sigma v \rangle = \sum_{n=0}^{N} b_n (\ln T)^n,$$

For the electron reactions, $\langle \sigma v \rangle$ is essentially independent of E within the range of energies considered here. A more useful fit for the heavy-particle reactions is a double polynomial fit in both E and T:

$$\ln \langle \sigma v \rangle = \sum_{n=0}^{N} \sum_{m=0}^{M} \alpha_{mn} (\ln E)^n (\ln T)^m.$$

Such a fit requires a large number of coefficients in order to be accurate, but can be used for arbitrary E and T. We tabulate the coefficients for a 9 x 9 double fit of this form in Sect. 8.3 of [1].

N.B. Neither of these fits guarantees correct asymptotic behaviour, at the low and high end of the parameters E or T. Parameters for proper extension of the fits, or to enforce zero cross sections at threshold, have to be found on a case by case basis. (The same would apply, of course, if tabulated rather than fitted data would have been given). Asymptotically better forms for cross sections or rate coefficients are given in the literature.

An error is given for each fit as an indication of the quality of the fit. The error is defined as

$\frac{1}{N}\sum_{i=1}^{N}(\ln x_i - \ln x_{fit,i})^2$,
where N is the number of points fit, and x is σ or $\langle\sigma v\rangle$. An error of 10^{-4} is a good fit; that is, the fit is very close to the actual values, most likely well within the error in the data. Sections 8.1, 8.2 and 8.3 of [1] contain examples of fits with several values of errors for each type of fit. It was hard to obtain the double fits with an error of 10^{-4} or better and Sect. 8.3 of [1] contains a more extensive discussion of their errors.

10 Example of Use of Fits

As an example of the use of the tables of fits for cross sections and reaction rate coefficients consider the calculation of $\langle\sigma v\rangle$ for reaction 2.1.5, $e + H(ls) \rightarrow e + H^+ + e$. Below we evaluate

$$\ln\langle\sigma v\rangle = \sum_{n=0}^{8} b_n (\ln T)^n$$

for T = 10 eV (i.e. $\ln(10) = 2.30259\ldots$) using the coefficients for reaction 2.1.5 in Sect. 8.2 of [1]. In the calculation below, only six digits need to be kept for these to be nearly perfect fits (see Sect. 8.2 of [1]) and the coefficients have been truncated at six digits.

$$\begin{aligned}
\ln\langle\sigma v\rangle &= -3.27139e+01 + 1.35365e+01\ (2.30259) \\
&\quad -5.73932e+00\ (2.30259)^2 + 1.56315e+00\ (2.30259)^3 \\
&\quad -2.87705e-01\ (2.30259)^4 + 3.48255e-02\ (2.30259)^5 \\
&\quad -2.63197e-03\ (2.30259)^6 + 1.11954e-04\ (2.30259)^7 \\
&\quad -2.03914e-06\ (2.30259)^8 \\
\\
\ln\langle\sigma v\rangle &= -19.07995.
\end{aligned}$$

Thus,

$$\langle\sigma v\rangle = 5.17228e-09\ cm^3/s.$$

(see p14 in [1]).

References

[1] R.K. Janev, B. Langer et al. Springer Series on Atoms+Plasmas, Vol 4, 1987