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ON A NEW CATALOGUE OF ATOMIC DATA FOR ASTROPHYSICAL INVESTIGATIONS

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Astrophysics is one of the main fields where atomic data are extensively used. A lot of the data, often used in astrophysical investigations, will be compiled in a new atomic data catalogue, which we are preparing. This catalogue is a revised and extended version of the "Catalogue of Atomic Data for the Rarefied Astrophysical Plasma" (Golovatyj *et al.*, 1991). The structure, outline of the contents and the main compilation principles of the catalogue are described.

KEY WORDS Atomic data, catalogue of atomic data, atomic processes, gaseous nebulae

1 INTRODUCTION

Atomic data are important in many fields of astrophysics. It is important to note an essential difference between the data used by astrophysicists and spectroscopists. Astrophysicists prefer to use not directly the cross sections of atomic processes, but rather their rates (for the most of astrophysical objects, particle velocities are distributed in accordance with the Maxwell law). If, however, the cross sections themselves are sometimes used (mainly for photoionization from the ground level but sometimes also from the excited atom and ion levels) then only the angle-averaged cross sections are required. On the contrary, spectroscopists just investigate how these cross sections depend on the angles between directions of the incident and the scattered particles, on the energies of the colliding particles, etc. This is why we include in the catalogue mainly the rates of the processes considered. To reduce the volume of the tables, in most cases we present not the cross sections and the rates of the processes themselves, but the numerical values of the coefficients for their analytical approximations. The following data are included in the catalogue: the atomic energy levels and the wavelengths of transitions, the oscillator strengths

and the transition probabilities, the lifetimes of the atomic states, the photoionization cross sections, the radiative and dielectronic recombination rates, the thermal averaged collision strengths and the rates of the charge transfer processes. The catalogue contains both the atomic data obtained by us and those published in the literature. Application of numerous atomic data to the studies of the spectra of gaseous nebulae are also described. Due to the recent discovery of heavy-element lines in the spectra of planetary nebulae (Péquignot and Balateau 1994) we add the data for these elements and for some other heavy elements, including the data for the rare-earth elements.

2 THE STRUCTURE OF THE CATALOGUE

The catalogue consists of the following main parts: A short introduction to atomic spectroscopy (Chapter 1) serves as an explanation of the notation used. The units most often used for measuring energy and cross section are tabulated. We also describe briefly the standard LS-coupling scheme for the level classification. Relations between radiative transition probabilities, line strengths and oscillator strengths, as well as the classification of the radiative transition types, adopted in the astrophysical literature, are also given in this chapter.

The reader can find the most often needed astrophysical data in numerous tables. A description of the tables and a short guide for users are given in Chapters 1–3. If even more information than presented in the tables is needed, the Appendices may be helpful. In Appendix A one can find numerous references concerning a wide variety of data. Extensive data can be also found in the databases and catalogues of atomic data which are described in Appendix B, with a special attention drawn to the atomic database TOPbase (Canto *et al.*, 1993). If the data required cannot be found in the tables and the Appendices A and B, the reader may turn to Appendix C, where the most often employed programmes for atomic data calculations are listed. Some useful mathematical formulae are given in Appendix D.

3 RADIATIVE TRANSITIONS AND PHOTOPROCESSES

In the Chapter 3 we discuss the processes which are accompanied by emission or absorption of photons. The following topics are considered:

- (1) transition probabilities, oscillator strengths and lifetimes;
- (2) photoionization;
- (3) photoionization from K and L shells;
- (4) photorecombination;
- (5) photoheating and recombination cooling.

We give an extensive list of transition probabilities and oscillator strengths for H-like ions and HeI atoms. Due to a restricted volume of the catalogue we do not incorporate the transition probabilities of other elements. A detailed list of transition probabilities between low-excited levels of atoms and ions from C to Pb (mainly for forbidden and intercombination transitions) is presented in Table 16. A large number of the transition probabilities for the lines observed in the spectra of gaseous nebulae are given in Table 23. To find data not presented in the catalogue, the reader can turn to Appendix A, where extensive bibliography on transition probabilities is given.

4 COLLISION PROCESSES

In Chapter 4 we consider collisions of atoms and ions with electrons and other particles which are most important under physical conditions typical of astrophysical objects. The following topics are included:

- (1) electron impact ionization;
- (2) Electron impact excitation;
- (3) excitation by collisions with heavy particles;
- (4) autoionization;
- (5) dielectronic recombination;
- (6) charge transfer reactions.

The most important particle impact process which determines the distribution of atoms and ions on the excited states is the excitation of the atoms and ions by electron impact. Instead of excitation cross sections, the collision strengths are often used (see, for example, Mendoza, 1983). They are determined from

$$\sigma_{ik}(u) = [\pi a_0^2] \left(\frac{E_{ik}}{Ry} \right) \frac{\Omega_{ik}}{g_i(u+1)}, \quad (1)$$

where $\sigma_{ik}(u)$ and Ω_{ik} are the excitation cross section and the collision strength for the transition $i \rightarrow k$, respectively, a_0 is the Bohr radius, E_{ik} is the energy of the transition and g_i is the statistical weight of the lower level i of the transition. We use the standard notation Ry for rydberg. The incident electron energy E is expressed in the threshold-value units $u = E/E_{ik} - 1$.

The electron impact excitation rates are usually expressed in terms of the effective collision strengths:

$$q_{ik} = \frac{8.6287 \times 10^{-6}}{g_i T_e^{1/2}} \gamma_{ik} \exp \left[\frac{-E_{ik}}{kT_e} \right], \quad (2)$$

Table 1. Coefficients of a polynomial fit to the effective collision strengths of electron impact excitation for atomic hydrogen (Giovanardy *et al.*, (1987). The low temperature ($500 \text{ K} \leq T_e \leq 72000 \text{ K}$) coefficients are listed in the first line, and the high temperature coefficients ($55000 \text{ K} \leq T_e \leq 500000 \text{ K}$) in the second one

Transition	a	b	c	d
1s-2s	2.297-01	5.318-06	-1.180-10	8.636-16
	2.694-01	7.883-07	-1.394-12	1.451-18
1s-2p	3.435-01	1.297-05	2.178-12	7.928-17
	3.162-01	1.472-05	-8.275-12	-8.794-19
1s-3s	6.250-02	-1.299-06	2.666-11	-1.596-16
	3.337-02	2.223-07	-2.794-13	1.516-19
1s-3p	9.941-02	-3.714-07	6.134-11	-3.973-16
	6.985-02	2.538-06	-8.729-13	-1.291-18
1s-3d	5.030-02	7.514-07	-2.826-13	-1.098-17
	5.051-02	7.876-07	-2.072-12	1.902-18
1s-4s	1.909-04	1.983-07	-8.325-13	1.128-18
	2.867-03	1.222-07	-2.323-13	1.865-19
1s-4p	1.527-03	1.001-06	-2.192-12	9.348-18
	1.958-03	9.525-07	-9.668-13	4.807-19
	1.007-02	3.508-07	-8.024-13	6.764-19
1s-4f	3.266-03	3.908-07	-8.778-12	6.171-17
	9.103-03	-6.105-09	-6.191-15	1.268-20

where the effective collision strength of the transition γ_{ik} is determined by integrating the collision strength Ω_{ik} over the Maxwellian electron velocity distribution:

$$\gamma_{ik} = \int_0^{\infty} \Omega_{ik} \exp(-\beta_{ik} u) d(\beta_{ik} u), \quad (3)$$

where $\beta_{ik} = E_{ik}/kT_e$.

The effective collision strengths are slowly varying functions of temperature and they are often approximated by expressions of the type

$$\gamma_{ik} = a + bT_e + cT_e^2 + dT_e^3, \quad (4)$$

where the parameters a , b , c and d are the polynomial best-fit values to the calculated values of γ_{ij} . We shall present extended tables of these parameters for various atoms and ions. As an illustration we show in Table 1 a part of the table obtained for HI transitions.

5 SPECTRA OF GASEOUS NEBULAE

We consider both the calculated emission spectra of the nebulae and the observed line intensities in the gaseous nebulae spectra for diagnostics of the nebular gas

(including the determination of the electron density and the ion and element abundances). So, we briefly discuss the following problems:

- (1) recombination spectra;
- (2) collision-excited lines;
- (3) selective mechanisms of the line excitation;
- (4) plasma diagnostics of n_e and T_e ;
- (5) element abundance determination;
- (6) continuous spectra.

Most of the gaseous nebulae possess both density and thermal inhomogeneities (see, e. g., Kholtygin and Feklistova, 1992). We consider the impact of these inhomogeneities on both the line intensities in the spectra of nebulae and the nebular parameters obtained from the observed line intensities.

6 THE TABLES

Below we list a preliminary log of the tables. The final version of the catalogue is planned to be somewhat more complete.

Table 1. Transition probabilities for HI transitions.

Table 2. Transition probabilities for HeI transitions.

Table 3. Photoionization cross-sections from the ground and excited states for atoms and ions from H to Fe.

Table 4. Parameters of the photoionization cross-sections from the K-shell.

Table 5. Coefficients of analytical approximations for the collisional ionization, radiative and dielectronic recombination rates.

Table 6. Radiative recombination rates on the HeI ion levels.

Table 7. Photoheating rates for HI.

Table 8. HI recombination cooling rates.

Table 9. Parameters of analytical approximations for the electron impact ionization rates.

Table 10. Parameters for the determination of the collisional ionization rates for $(nl)^2$ shells.

Table 11. Parameters for the determination of the collisional ionization rates for low atomic states.

Table 12. Coefficients of a polynomial fit to the effective electron impact ionization strengths for atomic hydrogen.

Table 13. Electron impact excitation rates for atomic hydrogen.

Table 14. Approximation parameters for the electron impact excitation rates for some ions.

Table 15. Energies and designations for the ground and metastable levels of selected atoms and ions.

Table 16. Transition probabilities and effective collision strengths γ_{ik} of selected atoms and ions.

Table 17. Coefficients of analytical approximations for the total rates of dielectronic recombination on ground and metastable states.

Table 18. Parameters for approximating the total rates of dielectronic recombination for highly stripped ions.

Table 19. Charge transfer rates for atom and ion collisions with H and He.

Table 20. Coefficients of analytical approximations for recombination and ionization charge transfer rates.

Table 21. Parameters for approximating the rates of charge transfer with H^0 and He^+ .

Table 22. Recombination charge transfer rates between atoms and ions of heavy elements.

Table 23. List of the lines observed in the spectra of gaseous nebulae.

Table 24. Relative intensities of HI recombination lines.

Table 25. Relative intensities of HeI recombination lines.

Table 26. Relative intensities of HeII recombination lines.

Table 27. Relative intensities of C, N and O ions recombination lines.

Table 28. Parameters of analytical approximations of the effective dielectronic recombination coefficients for the lines of the ions of C, N, O, Ne, Mg, Al and Si.

Table 29. The values of total and partial effective recombination coefficients for C, N and O ion lines.

Table 30. The values of the fitting parameters to the function $X(T_e)$ connecting the recombination line intensities and the ion abundances.

Table 31. Parameters approximating the functions connecting the collisionexcited line intensities with the relative abundance of ions.

Table 32. Continuum emission coefficients.

7 BIBLIOGRAPHY

The atomic data bibliography during the last 15 years is reviewed. We present an extended and updated reference list which contains the following topics:

- (a) energy levels and wavelengths;
- (b) transition probabilities;
- (c) photoionization;
- (d) recombination;
- (e) collisional ionization;
- (f) collisional excitation;

- (g) charge transfer;
- (l) line broadening;
- (i) opacities.

This reference list is an extended continuation of the atomic data bibliography of Butler (1993). We added both new references up to date and those for the atoms and ions of heavy elements.

8 DELIVERY OF THE CATALOGUE AND ADDITIONAL INFORMATION

We plan to submit the catalogue to *Baltic Astronomy* or *Astron. Astroph. Transactions* (the other possibilities are also not excluded) before the end of 1995. Moreover, an electronic copy of the catalogue will be available by *anonymous ftp* via the ftp-server IP **193.125.206.230** in the directory `/usr/nome/afk` under the name `CatAda.tex`. The data included into the Catalogue will be updated at least twice a year. Any user is invited to contact A. F. Kholtygin to get additional information or solve any problems via e-mail at `afk@aispbu.spb.su`. We will greatly appreciate comments and information about any recent review papers, catalogues or atomic databases not referred to in the catalogue.

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