# ATOMIC DATA IN ASTROPHYSICS

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## Abstract

A short review of the atomic and molecular data which are necessary for astrophysics researches is presented. A list of atomic data is described which was chosen by first Soviet colloquium on atomic data in astrophysics.

## Introduction

Almost all information is gotten by astrophysicists form observed electromagnetic radiation. More part of observed objects is plasma formations which are strongly different in their characteristics. Radiation reaching observers is usually emitted by relatively low-density outer layers of cosmical bodies. Physical conditions in the places of emission are usually far from thermodynamical equilibrium. Therefore for quantitative analysis of spectra of cosmical objects it is necessary very often to use analysis based upon detailed balance of atomic and molecular processes in plasma. Thus, atomic data are the foundation without which astrophysical researches are practially impossible.

Modern astrophysics covers all wavelengths. There are observations of radiations with differences of wavelength by the factor $10^{20}$, from many kilometric radio waves to gamma-photons with energy $10^{12}$–$10^{14}$ eV. On continuum spectrum there are spectral lines. The longest wavelength line has $\lambda \approx 18$m and is transition on the level with number 732 in atomic hydrogen or carbon (Konovalenko and Sodin, 1981). The shortest wavelength lines are located in gamma-range and are radiated by excited atomic nuclei.

The principal structure unit of the Universe is stars. They radiate most of the energy in near IR, optical and UV ranges. These ranges are the most informative. Most observations are in these ranges. It is possible to get information about matter with low temperature ($T \approx 5$–$300$ K mainly in far IR and radio radiation, and about the most hot objects ($T > 10^6$K) by use of X-rays. Cold parts of matter are practically neutral and consist mainly of molecules, dust grains and atoms. Hot parts contain ions with charges until approximately 30 (see, e.g., Gibson, 1973).

Thus in modern astrophysical researches it is necessary to have data on elementary processes with atoms, molecules, atomic and molecular ions and sometime with solid bodies (dust grains).

## Atoms and Atomic Ions

Atoms and ions of different elements play different roles in astrophysics which are connected with the different abundances of elements in space. Chemical composition of atmospheres of most stars and other astrophysical objects is almost universal (Aller, 1961). The most abundant are atoms of H and He (90% and 10% in quantity of atoms). Among others the most abundant are atoms from C to Fe with even-even nuclei (abundance on 3-5 decades less than H). Together with atoms H and He they form physical conditions in cosmical plasma. Therefore it is necessary to have the most full and various data on them. Other isotopes and atoms are present in small quantities ($10^{-6}$–$10^{-14}$ relatively H). Nevertheless they give very interesting information on nuclear evolution of matter and therefore they are intensively studied.

In several groups of objects strong deviations from "standard cosmical" chemical and isotop abundance are observed, up to 3-5 orders of magnitude in both directions (higher or lower abundance). Peculiar Ap-stars show, e.g., overabundance of rare earth elements on factor $10^{3-5}$ (Pikel'ner, Kokhlova, 1972). In the interstellar medium strong depletion of elements was found (Spitzer and Jenkins, 1975). Therefore quantitative chemical and isotope analysis continues to be an important astrophysical problem.

Stars. In spite of faint brightness of stars it is possible now to get very detailed spectra: in the range of hundreds or thousands angstrom spectrum resolution can reach ~0.3–0.03Å. In such spectra there are thousands of spectral lines. For some of the lines it is possible to get forms of contours. Stars with different temperature and chemical composition of atmospheres have different lines.

In stellar spectra, lines of all elements were found, including radioactive elements such as techecium. For the determination of abundances typically several dozen lines of each ion of each element (mainly I-VI ionizations) are necessary. Therefore for quantitative analysis of the spectrums it is necessary to have a lot of spectrosopic data: energy levels, wavelengths and oscialltor strengths for hundereds, thousands or millions of lines. Kurucz (1971, 1981) calculates, e.g., the catalog of oscillator strengths for several million lines. But this catalog needs to be revised because in a number of cases strong lines are missed.

For detailed analysis it is necessary to know data on collision broadening lines (particulary for rare earths), and data on collisonal and radiative processes, which determine populations of levels and ionization in condition of stellar atmospheres (mainly $T=(2-50)10^3$K, $N=10^{11}-10^{16}$cm$^{-3}$, I-V ionizations; for white dwarfs N is higher and sometimes T can be higher).

Chomospheres, transition regions and coronae of sun and stars show higher temperature until $10^8$K and full collection of ions until $z \approx 30$. They radiate mainly in UV and X regions.

Parameters of ~$10^5$ spectrum lines including highly-ionized elements are necessary for calculations of opacity of stellar matter in inner parts of stars (Cox, 1965).

Stellar objects show often strong magnetic fields. The sun and other "ordinary" stars have magnetic fields from ~1 Gs to 5000 Gs, Ap-stars until $10^5$Gs, white dwarfs up to $10^8$Gs, and on neutron stars fields of $10^{11}-10^{13}$Gs. Therefore, it is necessary to have, also, data on magnetic field influence on atoms and ions.

Important mechanisms of opacities of stellar atmospheres are bf and ff processes with negative ions ($H^-$, $He^-$, sometimes $C^-$ and several molecular negative ions, see, e.g., Gray, 1976). Data on formation and destruction in collision and radiative processes and on radiation of them are needed.

Diffuse mediums. In stellar atmospheres conditions are usually not far from local thermodynamic equilibrium (LTE). In more diffuse media, such as gas nebula, interplanetary, interstellar, intergalactical media, nuclei of galaxies and quasars, in circumstellar envelopes etc. conditions are usually far from LTE. Analysis of radiation of such objects demands calculations of level populations and ionization, taking into account a large variety of atomic processes. Physical conditions in such objects cover a wide range: T from 4-6 K to many billion K in shock waves, N from $< 10^{-6}$ cm$^{-3}$ to $\gtrsim 10^{12}$cm$^{-3}$. These media are pierced by cosmical and X-rays, which produce strongly non-equilibrium ionization with coexistence in one place I-VI ions and, probably, sometimes I-XII ions (Bochkarev, 1979).

At the first Soviet meeting on systematization of atomic data, which are necessary for astrophysical researches (Bochkarev, 1983) was suggested the next list of principal data, which are necessary for research on the physics of rarified media in astrophysical objects.

The most important are data on the most abundant elements: H, He, C, N, O, Ne, Mg, Si, S, Fe, including all stages of ionization for them. Data about other observable I-VI ions of Na, Al, Ar, Ca, Ni are also necessary. For all these ions it is necessary to have data on radiative and dielectronic recombinations in a wide interval of temperatures (e.g. formation of neutral atoms for $T< 10-100$ K). Full rates of recombinations are needed, as for several ions with observed recombination spectra (H, He, CII, NII, OIII etc.) also data on recombination populations of individual levels. As a result of low density of cosmical plasmas there are important dielectronic recombinations not only through permitted levels but also through forbidden ones. In the last case, dependence of recombination coefficients on density is required.

There are important data on ionization of atoms and ions: photoionization of outer and inner electronic envelopes (photon energy $h\nu< 10-30$ KeV) and a number of cases of metastable levels; collisional ionization by thermal electrons of ground and the most important metastable levels; ionization of nonrelativistic particles of cosmic rays. Actual problem is collecting data on charge-transfer reactions II-XII ions of C-Fe with HI for $kT< 2$eV, with HeI for $kT<3-5$TeV and with HeII for $kT<10-15$TeV.

It is necessary to have information on excitation of thin structure of main terms of atoms and several ions (e.g. CII, OIII, SiII, SII, FeII) by collisions of electrons, protons, atoms and molecules of hydrogen ($T=10-10^4$ K), data on collisional excitations of low terms of atoms and ions without variations of main quantum number n and for a number of ions for collisional excitation with variation of n for several low levels, which are not hydrogen like. Developing of observational technics in millimeter range demands more accurate data on energetic splintering of ground levels of atoms and above mentioned ions.

For collision processes it is necessary to have dependencies of cross-sections on energy and rates of the processes as functions of temperature.

Finally, it is necessary to have Einstein coefficients of one-electron transitions between above metnioned levels and terms, including forbidden, (intercombinational etc.) transitions, and also probabilities of non-radiative filling of vacancies in inner envelopes of atoms and ions (Auger effect), including cascades of transitions in inner envelopes.

Total data bank, discussed in this section, must consist of several thousand numbers and functions of energy and temperature. Above mentioned meeting states that it would be very likely to complete such bank of date.

## Moleculars and dust grains

At present about 100 different molecules and molecular ions have been found in spectra of astrophysical objects. They are found in atmospheres of planets and cold stars ($T<6000$ K), in comets, interstellar medium and circumstellar envelopes. For stellar spectra there are oxides and hydrides of metals. The main problem is identification of faint molecular bands in optical and UV ranges. In comets there are visible optical fluorescence of CH, $CH^+$, NH, OH, $OH^+$, CN, $C_2$, $CO^+$, $N_2{}^+$, $NH_2$, $H_2O^+$, $C_3$, $CO_2{}^+$ in solar radiation. Here it is important to know constants of fluorescence and photodestruction (ionization, dissociation) of the molecules. In planetary atmospheres there are visible numerous IR bands of CO, $N_2$, $O_2$, HF, HCl, $H_2O$, DOH, CO, $SO_2$, HCN, $NH_3$, $PH_3$, $CH_4$, $C_2H_2$, $C_2H_6$, which are formed in a medium where T is hundreds of Kelvins and pressure from $10^{-3}$ atm. and higher.

The greatest quantity and variety of molecules are observed in the interstellar medium and circumstellar envelopes, especially in the most cold

(T=5-30K) and dense ($N=10^3-10^7 cm^{-3}$) parts of them. To the end of 1982 approximately 60 molecules and molecular ions in ~100 isotopic variant were found (Rudnitsky, 1983): 15 two atomic, 15 three-atomic molecules and multi-atomic, consisting until 13 atoms ($HC_{11}N$). All molecules, excluding NaOH, consist of H, C, N, O, Si, S; about 2/3 of them have carbon, among them $H_2CO$, HCOOH, methil and ethyl-alcohol, dimetilether. Cyclical molecules are not found. A real problem is to search 6-10 atomic molecules, mainly organical (simplest amino acids of glycin type etc.).

Most molecules were found from radio spectra of radiation, mainly in millimeter range. It is rotational transitions with J< 20-40, and also thin effects (K- and Λ-splitting, inversional transitions etc.). For reliable identification of lines it is necessary to have an accuracy of frequencies no worse than 0.5-1 MHz mainly in ranges 22-23 GHz, 35-37 GHz, 88-90 GHz, 110-116 GHz for which receivers exist.

In the next 10 years the submillimeter range will become more familiar.

The most important collision processes are exitation mainly of rotational and vibrational levels by thermal electrons, H, $H_2$ and He for $T=10-10^3K$ for molecules with observed maser effect (OH, $H_2O$, SiO, $CH_3OH$, $H_2CO$) and also for $H_2$,$H_2^+$, CO, CS, $NH_3$, etc.

It is necessary also to have data on rates of chemical reactions in low density and cold ($T=10-10^3K$) media, both on gas-phase reactions (mainly ion-molecular, including reactions of isotopic fractions) and on surfaces of dust grains (probability of absorption and desorption, interaction between molecules on the surface, desorption as the result of chemical reaction etc.). Knowledge of properties of dust grains, which is poor now, must be improved (Huffman, 1977; Martin 1978).

It is necessary to know optical and spectral properties of dust grains of different sizes from 0.005 to 5-10 μm in UV, optical and IR ranges, for grains with a large quantity defects of structure, admixtures and for heteogeneous grains (see Huffman 1977, Martin 1978).

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