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Atomic data and stellar chemical peculiarities for the elements Z=6 to 20

ABSTRACT

Current studies of main-sequence stars showing chemical anomalies, are briefly presented from the point of view of their connection with atomic spectroscopy. Analysis of their observed spectra and theoretical interpretation of their chemical peculiarities are shown to be strongly dependent on the amount of available atomic data and, to a lesser extent, on the accuracy of these data. We review the recent compilations available for laboratory wavelengths and transition probabilities of the elements Z=6 to 20. It is pointed out that some incompleteness may occur even for these light elements. A few examples concerning Si II are detailed to stress the astrophysical importance of progress in the study of high-excitation transitions and autoionisation.

1. INTRODUCTION

Investigation of stellar atmospheres requires a lot of atomic data from laboratory physics and, conversely, the stellar plasmas allow to observe experimental conditions that can not be reached in experiments. We will review some aspects of current studies of chemical peculiarities in main-sequences stars.

The scope of this paper is limited to the elements Z=6 to 20, from carbon to calcium. This avoids questions which are specific to the lighter elements and the severe problems raised by the heavier elements. The intermediate elements have generally well-established spectroscopic properties and they are favourable cases for constructing refined astrophysical models about stellar atmospheres, such as non-LTE transfer, abundance inhomogeneity, macroscopic movements and radiative diffusion. We will consider main-sequence stars of spectral types A and B (effective temperatures from about 7000 to 20000 K), with emphasis on those (about 20%) which show chemical anomalies by reference to a "normal" composition, close to the solar one. The proceedings of Cowley et al. (1986) review recent progress in understanding these peculiar stars. A great variety of chemical anomalies are found, often varying with time according to the stellar rotational phases. Therefore they offer the opportunity of differential studies, and, thanks to the continuous improvement of the observational performances, they may even appear as natural spectroscopic experiments.

Section 2 presents some astrophysical problems which are closely connected to atomic data. We give some details concerning the identification of the numerous observed lines in the UV spectra of hot stars. Then we briefly review the determination of elemental abundances and the theoretical computation of radiative forces acting on atoms and ions. These two steps are important to develop models of radiative diffusion to explain the chemical separation of elements. Section 3 recalls the available updated compilations of basic spectrocopic data and discuss some recent progress. Section 4 reports a few examples from our studies about Si II in stellar spectra, in order to illustrate their connexion with atomic physics.

2. ASTROPHYSICAL QUESTIONS ABOUT CHEMICALLY PECULIAR STARS

Identification of ultra-violet lines in stellar spectra

The ultra-violet spectra of A and B stars contains numerous absorption lines of atoms and ions, their density being much larger than in the visible range at similar wavelength dispersion. High-resolution spectral observations in the ultra-violet have already been obtained by the Copernicus satellite and by the International Ultraviolet Explorer (IUE), much more is expected soon from the Hubble Space Telescope (see the contribution of Leckrone et al, in these proceedings). Since its launch in 1978, the IUE satellite has recorded thousands of stellar spectra covering the range 115-320 nm, with a resolution of 10^4. Therefore it has already contributed greatly to extend the observational basis for many detailed investigations of physical processes in stellar atmospheres (see Kondo et al., 1987).

To interpret the new ultra-violet stellar spectra, one must correctly identify the species which account for the observed lines or features. This task is often difficult because of the large number of observed lines and the frequent occurrence of blends. For example there is a controversy about the appearance of the C IV and Si IV resonance lines in the UV spectra of some B stars: if present they may reveal superionization processes in the stellar atmospheres, but Hubeny et al (1985) have pointed out the risk of erroneous identifications due to blending lines, underlining the importance of careful identification work. In Ap stars the enhancement of rare elements may be detected by observing ultra-violet resonance lines of their ions, but these are generally weak and often blended: a correct identification is crucial and generally requires that all the lines of abundant elements have previously been recognized in the studied range.

A detailed line identification is also an important preliminary step when studying low dispersion spectra, especially to determine the origin of observed absorption features. An illustration is given in Fig. 1 which shows the rotational variation observed in a low-dispersion ultra-violet spectrum of a peculiar star (Artru and Freire, 1988): several absorption features appear to vary differently from

one phase to the other. This reveals inhomogenous surface abundances of the corresponding absorbers. At low resolution, single resonance lines (C II, Si II, Ga II) are readily recognized, but other features are not easily identified when they correspond to a local accumulation of medium lines from a complex spectrum. For instance, a large variation occurs at 142 nm (Fig.1) which can be attributed to titanium, since four Ti III lines has previously been identified at this wavelength by inspecting high-resolution spectra. These lines appears on the spectra of two stars with similar effective temperature (see Fig.2).

Much work has already been done to provide extensive lists of identified ultra-violet lines in various types of stellar spectra. Several published atlases of A and B stars are based on observations from the Copernicus satellite (one of Sirius by Rogerson, 1987, others are referenced therein). The IUE spectra displayed in Fig.2 are taken from our recent atlas of two normal B stars (Artru et al, 1989). It gives an identification for about 80% of 1460 lines measured in the short spectral range (125-198 nm). Most of the listed transitions (about 75%) belong to elements heavier than Z=20 (Fe II and Fe III being preponderant) and this proportion is expected to be even larger in the long wavelength range of IUE.

Systematic procedures of line identification must be based on a suitable list of laboratory wavelengths, including the most complete up-to-date data, but restricted to the atomic transitions which have a reasonable chance to give an observable stellar line. Because of the high probability of fortuitous wavelength coincidences in the ultra-violet, it is necessary to use other criteria of identification, usually based on predicted line intensities. This would require the knowledge of all oscillator strengths in the line list, which is generally far from being the case.

Methods of wavelength coincidence statistics (see Cowley and Merritt, 1987 and references therein) overcome the difficult identification of each individual line of complex spectra. They allow an objective and quick detection of rare elements from the crowded ultra-violet stellar spectra. However they also require complete atomic line lists, at least for the studied species, and even oscillator strengths in their most sophisticated versions.

Abundance determination

The quantitative abundance studies have always provided the basic observational constraints on the theoretical interpretation of chemical anomalies in stars. They must be further developped to fully benefit from numerous recent progress: modern detectors, ultra-violet observations, refined atmosphere models and accurate atomic data.

A review of abundances in A stars, including the Am and Ap peculiar stars, was given by Wolf (1983). Also Cowley and Adelman (1983) have discussed the different techniques to increase the accuracy of stellar abundance

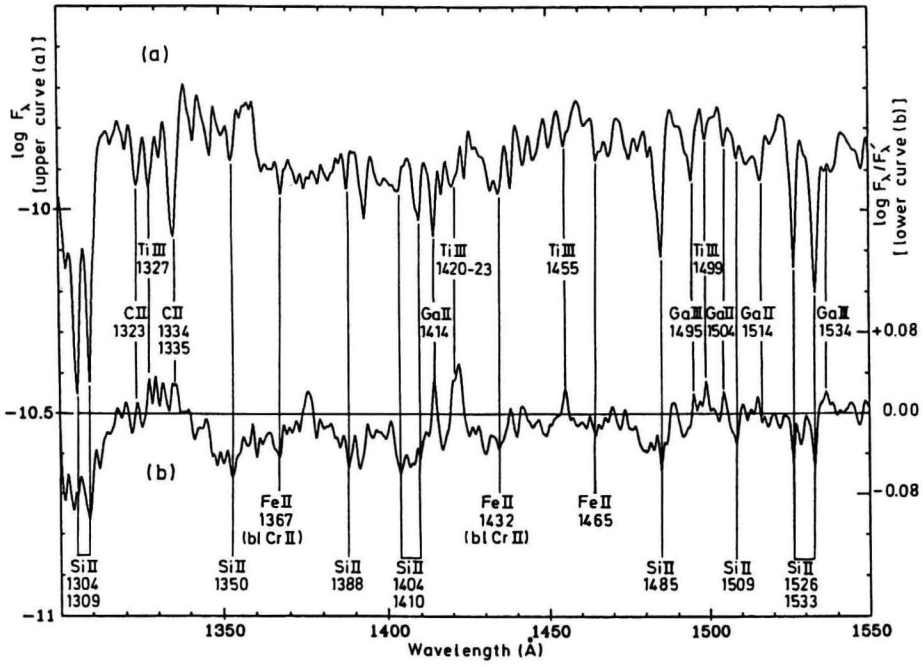

Fig. 1. Low-resolution spectrum of the star HD25823 (upper curve a) and ratio of two spectra recorded at different phases (lower curve b). From Artru and Freire-Ferrero (1988)

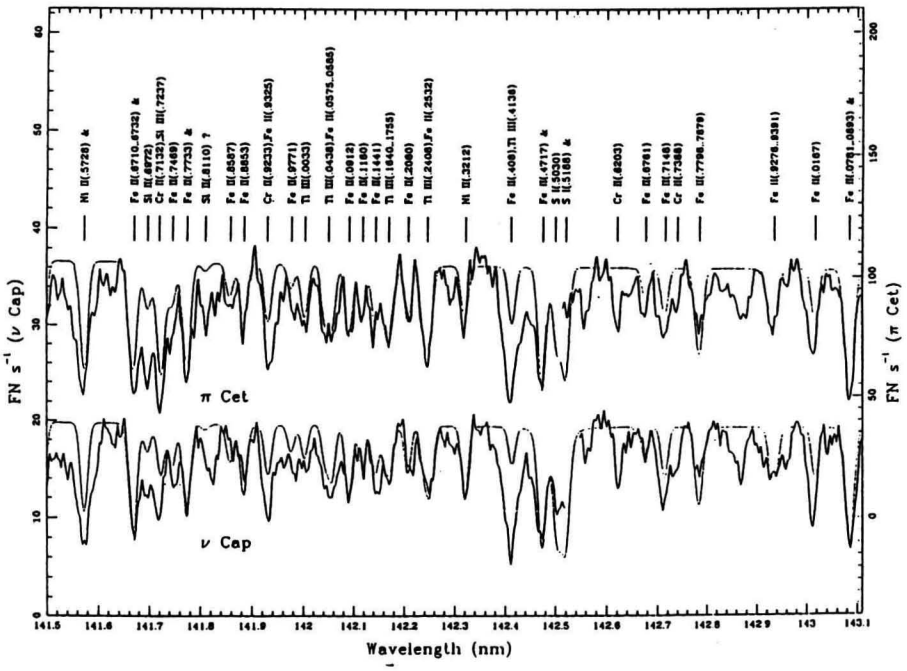

Fig .2. High-resolution spectra of two B stars: IUE observation (solid line) and LTE synthetic calculation (dotted lines). From Artru et al (1989)

determinations. Recent results are summarized in the proceedings of Cowley et al (1986) by Sadakane for hot stars (p.369), by Dworetsky for Hg-Mn stars (p.397), and by Boyarchuk and Savanov for Am stars (p.433). There is still a need for collecting reliable abundances for many elements in extended samples of peculiar and comparison stars. Such a study was done for Hg-Mn stars by Guthrie (1984). Series of consistent data are available from systematic abundance determinations in A and B stars by Adelman (1988) and Kocer et al (1987), earlier references being given therein. A recent workshop (Adelman and Lanz, 1988) achieved a decisive step towards clarifying the difficulties of this task, by means of a thorough comparison between independent elemental analyses of the same observational data (co-added visible spectra of two peculiar stars, o Peg and ϕ Her). Abundance of the elements C, Mg, Al, Si, S and Ca were determined with basically the same set of atomic data and the largest discrepancies obtained were typically about 0.2-0.3 dex.

The interpretation of ultra-violet spectra by synthetic computation requires preliminary reliable abundances. For instance Sadakane and Ueta (1989) have carefully redetermined abundances of 14 elements in Sirius from photographic spectra. Conversely, some ultra-violet lines, especially the strong resonance ones, can be used to determine abundances. This has been done for aluminum by Sadakane et al (1983) who confirm the general underabundance of this element in Ap star. Because of the heavy line blending in the ultra-violet, abundances must be derived by means of synthetic computations, often done in the LTE approximation. Then one or several abundances are adjusted as parameters to fit the observed spectrum. Such an exhaustive study of IUE spectra was done by Castelli et al (1985) for the He-weak star HR6000.

A number of abundances have been derived by Lanz (1987) in a sample of silicon stars,both from visible and ultra-violet spectra. The study of silicon in the ultra-violet is detailed by Artru and Lanz (1987). The silicon overabundances were found significantly smaller (2 to 5 times) than those deduced from the visible lines. These discrepancies are only partly explained by underestimates of the line damping in the visible (Lanz et al, 1988) and a strong departure from the LTE populations is expected.

The abundant elements, carbon, nitrogen and oxygen suffer from a severe lack of reliable abundance data although their study is of special importance in the context of the diffusion theory (Michaud, 1976, 1987). In the optical range they have been observed mainly by red or infra-red high-excitation transitions of the neutral atoms (Lambert et al, 1982; Faraggiana et al, 1988; Roby, 1987), while their stronger blue or UV lines may be affected by non-LTE effects (Lennon 1983, Lanz 1987). These elements are also essential in many stellar investigations related to the chemical history of the galactic material. For instance, Adelman et al (1986) have studied them in horizontal-branch stars.

Computation of radiative forces

The theory of radiative diffusion of elements gives a convincing explanation of chemical peculiarities observed in main-sequence stars: as a result of the competition between stellar gravity and radiative acceleration, a given element may be pushed up and accumulate on the stellar surface. Michaud (1976) gives the basic equations which allow to evaluate radiative accelerations. Further developments of the diffusion theory have been reviewed in Cowley et al (1986): in particular Alecian (p.381) discuss the role of magnetic fields and Michaud (p.459) the effects of stellar hydrodynamics, such as mass loss.

The first step of any diffusion model is the calculation of radiative accelerations: it involves the probabilities of all photoabsorption processes (lines and photoionisation) for every populated states of every ion, at each depth of the stellar atmosphere. Moreover the radiative acceleration due to a saturated line depends strongly on the broadening effects and on possible blends with other strong lines. Therefore, as recently pointed out by Michaud (1987), there are important needs for atomic data (up to high ionization stages) to calculate the radiative accelerations with sufficient accuracy (typically 30%).

Although the light elements are favourable cases, detailed calculations of their radiative acceleration in stellar atmospheres are still scarce. Complete non-LTE computations have been performed by Borsenberger et al (1981, 1984) for some of the alkaline-earths. The radiative diffusion of silicon has been calculated by Alecian and Vauclair (1981) who found that its accumulation is sensitive to the magnetic field.

3. SOURCES OF BASIC ATOMIC DATA

A great number of atomic lines should be introduced in any refined calculation concerning the stellar atmospheres of normal and peculiar stars. Therefore all exhaustive up-to-date compilations of basic atomic data are invaluable tools to insure the completeness and the quality of the astrophysical interpretations. Compared with heavier elements, those we consider here (Z= 6 to 20) are favourable cases, since their spectra have relatively simple

Compilations of energy-levels and multiplet tables

C I to VI	Moore, 1970 (sect.3)
N I to III	Moore, 1975 (sect.5)
N IV to VII	Moore, 1970 (sect.4)
O I	Moore, 1976 (sect.7)
O III	Moore, 1985 (sect.11)
O IV	Moore, 1983 (sect.10)
O V	Moore, 1980 (sect.9)
O VI to VIII	Moore, 1979 (sect.8)
Na I to XI	* Martin and Zalubas, 1981
Mg I to XII	* Martin and Zalubas, 1980
Al I to XIII	* Martin and Zalubas, 1979
Si I	Moore, 1967 (sect.2)
Si II to IV	Moore, 1965 (sect.1)
Si I to XIV	* Martin and Zalubas, 1983
P I to XV	* Martin et al, 1985
K I to XIX	* Corliss and Sugar, 1979
Ca I to XI	* Sugar and Corliss, 1979

* compilations of energy-levels only

structures and most of them have already been thoroughly studied.

The original NBS tables of atomic energy levels and multiplets still provide a basic source of spectroscopic data, thanks to the exceptionally good quality of these early data. They have been up-dated for a number of light elements as summarized in the following table. A finding list has been prepared by Adelman et al (1985).

Fairly complete data in the ultra-violet range are now available thanks to the new publications of Kelly (1979, 1987) who provides invaluable lists of classified lines (with convenient access to the original references, updated to 1977 and 1981) and their finding lists including all spectra of elements up to Z=36. Therefore at the moment the main need for updated finding lists is actually in the optical region. The NBS report from Reader and Corliss (1980) has the advantage of covering the whole spectral range and of including all heavy elements, but it gives a limited list of lines, selected on the basis of their intensity in emission spectra, and it does not provide any classification or excitation energy of the transitions.

Compiling transition probabilities is quite a difficult task because there is a wide variety of methods of determination and the true accuracy of published results is often hard to estimate. The NBS compilations of Wiese et al (1966,1969) are still widely used. A new list of critically evaluated transition probabilities has been published by Wiese and Martin (1980) for selected atomic and ionic transitions. Other compilations exist for the Li-like spectra (Martin and Wiese, 1976) and for Si II (Lanz and Artru, 1985). One is in preparation for the Be-like ions of carbon, nitrogen and oxygen (Allard et al, 1989). For example, to compile the gf-values of C III published since 1966, 45 new references were found with theoretical results, and 13 with lifetime measurements, allowing us to list oscillator strengths for one hundred new multiplets.

The NIST (NBS) bibliographical data base is a major help in extracting the best updated results from the literature. Commission 14 of the IAU gives regular lists of references, selected for their usefulness in astrophysics: the last one (Swings, 1988) contains hundreds of new publications from 1984 to 1987; a large part of them is still devoted to extended spectral analyses or new oscillators strengths, even for light elements.

Extensive computations of theoretical atomic data are very promising for many stellar applications. Their importance has been proved by the continuing use of the early data of Kurucz and Peytremann (1975) by astrophysicists. The international collaboration on the OPACITY project of Seaton (1987) is producing a lot of very accurate data (see his contribution to this colloquium).

4. EXAMPLES CONCERNING Si II IN THE SPECTRA OF Ap STARS

The Si II spectrum is an important contributor to the opacity in the photosphere of A and B stars and all its features are enhanced in the case of peculiar silicon stars. From our studies related to this spectrum, we will borrow some illustrative examples showing the close interaction between stellar and atomic spectroscopy.

The Si II lines appear so strongly in the IUE ultra-violet

spectra of A and B stars, even with normal abundance, that we can identify additional transitions which were not previously listed, neither in the laboratory lists (Kelly, 1987), nor in the list due to Kurucz and Peytreman (1975). For instance the stellar spectra shows a new doublet ($3s3p^2\ ^2D$--$3s^210f\ ^2F^o$) for which wavelengths can be predicted from known levels. A few such identifications have been made in our stellar atlas (Artru et al, 1989) for Si II and Ca II; others may still be missing for very abundant species. A new Si II identification in IUE spectra of Ap stars was given by Artru (1986, Fig.1): in this case the upper levels $3s3p(^1P)3d\ ^2D^o$ were previously unknown and we have established the identification simultaneously on laboratory and stellar spectra.

Our second Si II example concerns the autoionising transition $3s^23d^2D$ -$3s3p(^1P)\ ^2F^o$ which explains the wide depression, observed at 140 nm in silicon stars (Artru, 1986). This transition comes from a known excited level ($3s^23d\ ^2D$ at 9.84 eV) to an upper level which is theoretically predicted as strongly autoionising. Figure 3 shows its effect on the calculated spectrum of a silicon star. This identification was confirmed by synthetic calculations applied to several peculiar stars and compared to the IUE observations (Artru and Lanz, 1987). It is also consistent with the new theoretical energies of the $3s3p(^1P)3d$ states, computed by Le Dourneuf et al (1989). Nevertheless there exists no laboratory measurement of this photoionisation resonance which has actually been located at 140 nm by means of stellar observations.

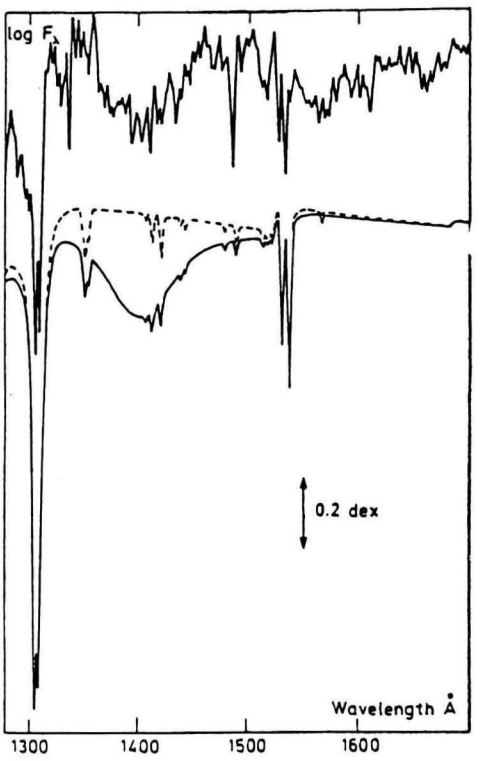

Fig. 3. Synthesis of the Si II autoionizing line (lower spectrum, solid line) and observed IUE spectrum of the silicon star HD34452 (upper spectrum). From Artru (1986)

In Fig.3 the strong observed Si II blend at 148.5 nm is badly reproduced by the calculation. This has been corrected later, as detailed in Artru and Lanz (1987), by revising the autoionisation width of the high-excitation transition to $3s3p(^3P)3d\ ^2F^o$. In a cooler star this blend is dominated by the other Si II transition of lower excitation (3d-7f) and, taking this into account, we have obtained a satisfactory interpretation by correctly re-evaluating the Stark broadening. This underlines the importance of correctly introducing line broadening in the synthesis of strong stellar lines.

AKNOWLEDGMENTS

I thank J. Hansen for improvement of this contribution.

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