# Atomic and Molecular Data for Stellar Physics

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ABSTRACT. This paper discusses a number of problems in the field of stellar astronomy which are caused by inadequate kinowledge of atomic and molecular data.

## 1. INTRODUCTION

When I was asked to give this talk just a few days ago, I decided to increase the size of the topic. The reason for which I did this was that I felt it was necessary to talk about the atomic and molecular data for stellar interiors.

There are three fundamental points to be made.

(1) In stellar interiors, we need some checking of the existing calculations.
(2) In stellar atmospheres, we need a certain amount of data, obtained using very high precision.
(3) Again in stellar atmospheres, we need a lot of data, but we can accept a rather lower degree of accuracy.

## 2. STELLAR INTERIORS

In the field of stellar interiors, there is a rather disconcerting disagreement between some work carried out at Livermore and the standard Los Alamos results. Fortunately, the previous disagreement between Carson and the Los Alamos group appears to have been resolved. However, Iglesias, Rogers and Wilson (1987) have compared their results for a number of species with the Los Alamos Astrophysical Opacity Library and find that, at T=20ev, they calculate an iron opacity which is six times larger. If such an increase occurs at higher temperatures (it does not occur at T=10ev) than at least some evolutionary tracks, such as those for low mass stars, will be affected. This will mean that globular cluster isochrones will be altered thereby altering the ages found for globular clusters. Simon (1982) has also suggested that stellar interior opacities are underestimated, using as his data the various results for the period ratios of Cepheids.

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## 3. STELLAR ATMOSPHERES

In stellar atmospheres, whether you need a small amount of very good data or a lot of less good data depends on the problem that you want to study.

The most accurate work on the determination of oscillator strength that I am aware of is that of Blackwell and his collaborators at Oxford, (e.g. Blackwell, et al. 1979, Andrews et al. 1979, Blackwell, Petford and Shallis, 1979, Blackwell and Shallis, 1979a) who claim an accuracy of 0.5 per cent. They have used this result to produce the very precise solar curve of growth shown by Blackwell and Shallis 1979b. This curve of growth is very well defined indeed. However, while very well defined, this curve is not ideal for determining the solar iron abundance--it simply does not extend to weak enough iron lines. The weakest line seen in it has log $W/\lambda = -5.4$ or in addition, in a star like Arcturus, these lines would be much stronger and therefore less suitable for abundance work.

However, there is a problem once one starts to analyze very weak lines. It is necessary to check very carefully that the identifications are secure and that the features are not blended. I recall a personal story here. One of my students had analyzed the spectrum of CH and, as an extension, had computed the wavelengths of $C^{13}H$. He wanted to search for these lines and found one whose strength was greater than expected. After a while he discovered that the reason for this was because of blending with a line of, I think, ruthenium. This line had been included in our line data list, but we might have been a little cavalier in the value we used for the abundance of ruthenium in the sun. So, while we do need the weak line data for the analysis of stellar spectra, we also need to know a lot of data about all other possible blending contributors.

One further point about this weak line problem is that, as far as I know, every line which has been seen in the laboratory spectrum of neutral iron has been seen in the solar spectrum. This means that when you start looking at sufficiently weak lines in the solar spectrum, or other stellar spectra, you really cannot be sure of your identifications.

Two other problems where we need lots of data are (a) the actual calculation of stellar spectra and (b) the calculation of models of stellar atmospheres.

Why should anyone want to compute an accurate spectrum of a star? One basic reason is that we want to understand stellar photometry, while another is the understanding of spectra. We want to be able to convert stellar colors into $T_{eff}$, log g and metal abundance. And we even want to understand the influence of different metals on stellar colors--if you have observed a spectral region which contains a lot of CH lines for example, than your magnitudes are affected by the abundance of CH and, consequently, C. Now some colors we seem to calculate quite well e.g. B-V for F dwarfs, but we need help elsewhere. For example, our model spectra are too bright in the region 3,000-4,000 A. This is very unfortunate, because it makes our interpretation of the colors much less certain. In order to do this job in this critical wavelength region, we need to have more atomic data--more, not just more accurate values for existing data.

What do we need for stellar model calculations? The point here is that we have to take account of the absorption lines when we are deriving the temperature structure of a model atmosphere. The problem is made tractable by the use of "opacity distribution functions" or ODFs. The idea here is that, instead of computing the opacity in great detail at every depth in a model i.e. using millions of wavelength points, we argue that it doesn't really matter where in a suitable wavelength interval each line is. We determine a histogram for each 100 angstrom interval, say, giving the fractions of that interval where the absorption coefficient exceeds the series of values. It is really essential to use these ODFs instead of simply calculating mean opacities.

What data is lacking? It depends upon the type of star. In the F stars like Procyon, it must be the weak atomic lines. This is also true in the G stars and, probably, the K stars. However, as we go to cooler stars, more and more of the flux comes out at longer wavelengths. In the M stars, we need the data for water vapor. This is still not available in a suitable form for the calculation of ODFs.

While Bengt Gustafsson was unable to give this talk, he did describe to me some of the problems which he and his colleagues had worked on and gave a very interesting example of the importance of this work. This concerns work on carbon stars. As you can imagine, in the hotter carbon stars the line opacity is mainly due to CO and CN and extensive data is available for these molecules. This data is adequate for the hotter carbon stars. However, in the cooler ones, the molecular equilibria change with the polyatomic molecules increasing in abundance at the expense of the diatomics. With only CO and CN opacities, the atmospheres become quite transparent and relatively thin. These atmospheres have caused problems in the analysis of observations. They have relatively high pressures. These high pressures lead to a lot of the hydrogen being in the present in the form of $H_2$. However, since the $H_2$ lines around 2 microns are observed to be relatively weak in the spectral carbon stars, the early models (Johnson 1982) led to the belief that cool carbon stars were relatively deficient in hydrogen.

Numerical experiments with a fudge factor i.e. a veil of weak metal lines, show that even the inclusion of relatively weak lines would have an important effect, reducing the pressures in the models and thereby reducing the $H_2$ abundance and the predicted strength of the $H_2$ molecular lines. Eriksson et al. (1984) were the first to consider the opacity of HCN and $C_2H_2$ and found that their model atmospheres expanded significantly, with a pressure reduction of two orders of magnitude compared to models calculated without the HCN and $C_2H_2$ opacity. Eriksson et al used semiclassical estimates for the absorption--later Jorgensen et al (1985, 1988) performed ab initio CASSCF calculations for HCN and $C_3$ and verified and strengthened these results.

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