Dominating Molecules in the Photospheres of Cool Stars

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1 Introduction

Molecular data bases (including very different numbers of molecular lines, and based on computations spanning a wide range in quality) have been used in the construction of models of the stellar atmospheric structure, and effects of various molecules on the stellar structure and evolution have been described in the literature. A systematic study showing which molecules are of importance in which types of stars is, nevertheless, still lacking, and the line lists used in various model computations necessarily reflect what was at hand at the time of computation rather than a systematic effort to solve the molecular opacity problem. A pioneering investigation was presented in two extensive papers by Tsuji (1964, 1973) where the foundation of the reaction scheme used in most models today was laid down. Later Tsuji (1986) has given a review of the existing work on molecules known in stars, and Johnson (1986) and Gustafsson (1989) have touched upon the same subject in reviews covering a broader range of stellar aspects. Jørgensen (1992) has recently summarized the existing molecular data (and discussed the methods used) available for model atmosphere construction.

In the present review I attempt to present a systematic analysis of the effect of the most abundant molecules in cool stars, and to touch upon what can be the most important missing molecular data for further progress in the field. For this purpose, I have computed about 150 new model atmospheres where various molecules have been included in, or excluded from, the adopted opacity in a systematic way. The models are based on a recent version (Jørgensen et al. 1992) of the Marcs code (Gustafsson et al. 1975) with molecular opacities (described further in section 4) from CO, CN, C2, TiO, HCN, C2H2, C3, and H2O considered in the computations. The code, with the input data used, is particularly tuned for computations of giant stars (stars with low gravity), and the emphasis in the present review will therefore be on red giants, but dwarf models will be computed for comparison purposes and for evaluation of trends. Whereas most of the results for the giant stars presented in this review are as reliably as is possible today, the results for the dwarfs (log(g) = +4.5) are to be considered as more qualitative in nature. A thorough description of the dwarf
stars and opacity problems particular to these are described elsewhere in this book by Borysow, Liebert, Scholz & Wehrse, and by Tsuji.

A stellar atmosphere is the outer, observable layer of a star — as opposed to the invisible stellar interior. The photosphere is the (lower) layer of the atmosphere where most of the visible (and infrared) part of the stellar spectrum is produced, and where the temperature decreases outward from the star. Often the atmosphere is used synonymously with the photosphere because only very few models exist for the layers above the photosphere. The effective temperature, $T_{\text{eff}}$, is an “average” temperature of the photosphere, but there are both (deeper) layers in the photosphere with temperatures much higher than $T_{\text{eff}}$ and (higher) layers in the photosphere with temperatures somewhat below $T_{\text{eff}}$. Also the surface gravity ($g$, here referred to in cgs units), the metallicity $Z$ (the mass fraction of the elements heavier than helium) and the C/O ratio are of vital importance for the atmospheric structure. The basic stellar parameters in the models computed here consist of various combinations of $T_{\text{eff}} = 4500, 3500, 3100, 2800, 2500 \text{K}$; $\log(g) = -0.5, +0.5, +1.5, +4.5$; $C/O = 0.43, 0.86, 0.92, 0.95, 0.98, 1.0, 1.01, 1.02, 1.05, 1.35, 2.0$, and $Z = Z_\odot$ (i.e., the solar abundance except for carbon).

2 Stellar Evolution into the “Molecular Regime”

The majority of stars end their life in the red giant phase where the outer parts expand and cool, while the interior slowly transforms into a hot, compact object (a white dwarf) of material that will slowly cool and undergo no further nuclear processing. While the stars are red giants they will, for the first time in their life, mix nuclear processed material from the interior to the surface (see e.g., Iben & Renzini 1983 and Lambert this volume). The cooler and more luminous they get the more of this material will be blown into space (e.g., de Jager et al. 1988), and in this way the gas and dust clouds, that new stars and planets are created from, will slowly be more and more enriched with nuclear processed material from cool red giants. Today it is even possible to trace some of the material that our own solar system was created from back to various types of red giants (e.g., Anders & Zinner 1993).

The Sun will become a red giant in about 7 billion years from now, and during about 200 million years the Sun will develop from a phase where it is 3500 K (and has 1000 times its present luminosity) to a final stage another 5 times more luminous and with $T_{\text{eff}} \approx 2500 \text{K}$ (Jørgensen 1991). It is in this interval of effective temperature that molecules dominate the structure of the stellar atmosphere, and I will here call it the “molecular regime” of stellar evolution. In stars warmer than 3500 K, the atomic lines become of increasing importance relative to the molecular lines, although a proper study has never been performed of where exactly the transition between the “atomic regime” and the “molecular regime” is (see Seaton this volume). There are also stars assumed to be cooler than 2500 K, but we have no reliable models of them yet. Dust may be an important opacity source in such stars (see Alexander & Ferguson and Sedlmayr,