SF2A 2015
F. Martins, S. Boissier, V. Buat, L. Cambrésy and P. Petit (eds)

MOLECULES IN STELLAR ATMOSPHERES

T. Masseron[1]

Abstract. In order to analyse "warm" stars (G-type, K or M) spectra -mostly optical-, astronomers need specific and accurate molecular lists, which include, at least, their wavelengths and loggf. A non-negligible number of laboratory data and tools already exist in literature, but it is necessary to convert into format useful for stellar spectroscopists. After addressing the recent progress in the field and illustrating them with astronomical applications, I also mention the remaining needs.

Keywords: molecules, stars, spectroscopy

1 Introduction

Molecules appear in the stellar atmospheres of cool stars, namely all stars wiht effective temperature cooler than ∼6000K. In order to infer stellar parameters and surface abundances, stellar spectroscopists use radiative transfer programs to model the star's spectra. One of the fundamental input to those programs are linelists that allow to reproduce simlutaneously all the bound-bound transitions appearing in the spectra. In parallel, with the advance of modern astronomical facilities, the data quality allow now to resolve the stars spectra down to few $m\mathring{A}$, i.e. enough to observe any single transition of any atom or molecule. Therefore, it is important now to ensure that all the linelists used to model stellar spectra achieve at least similar precision.

2 Molecular linelists

Molecular linelists as used by stellar spectroscopists consists mainly in a listing of transition wavelengths, their excitation potential and their oscillator strength. Existing program for simulating molecular structures such as PGopher * allow to derive lines position from laboratory constants, while program such as LEVEL † can compute molecular levels wave function and couple them with a provided transition moments to obtain transition strength. Therefore, the combination of the two codes can provide molecular linelists. This what has been done recently to make an accurate new molecular linelist for CN (Sneden et al. 2014) and C_2 (Brooke et al. 2013). However, thermodynamical conditions in stellar atmosphere often allow to observe more transition than observed in laboratories. By combining the molecular structure codes with a stellar radiative transfer code, we were able to improve the molecular constants and thus the linelists for the CH molecule Masseron et al. (2014).

3 Applications

3.1 The first stars

One of the most exciting results coming from large spectroscopic survey such as SDSS, is the discovery of the most ancient stars in the Galaxy. To hunt such object, stellar spectroscopists are looking for the stars with the most pristine composition possible, in other words with the lowest metallic signature in their spectra. The current record older is SMSSJ03100.36 with only an upper limit on its metallicity such as $[Fe/H] < -7.5$ (Bessell

[1] Institute of Astronomy, Cambridge, UK

*PGOPHER, a Program for Simulating Rotational, Vibrational and Electronic Structure, C. M. Western, University of Bristol, `http://pgopher.chm.bris.ac.uk`

†R. J. Le Roy, Level 8.2: A Computer Program for Solving the Radial Schrodinger Equation for Bound and Quasibound Levels, University of Waterloo Chemical Physics Research Report CP-663 (2014); see `http://leroy.uwaterloo.ca/programs/.Leroy`

et al. 2015). Indeed, its chemical content is so low that its spectra show almost no lines features except many CH and OH molecular lines. Thus, the proper modelling of those molecular features represent nearly the only constrain we have to understand this stellar relic and constrain its formation as well as the first stages of the Galaxy formation.

3.2 Stellar evolution and Galactic population studies

Carbon and nitrogen elements have two important specificities: they can be altered by almost any kind of stars - in particular during their giant phase, and they also show proeminant molecular spectral features such as the well-known G-band due to the CH molecule. By measuring the C and N content via those molecular features, we were able to show that a large sample of field giant stars show relatively low C/N ratios compared to their main sequence companion. This is explained by the fact that those stars have undergone the first dredge-up, where the CN cycled material formed during the main sequence in the core of the star is brought to the surface (Masseron & Gilmore 2015). We also show that the C/N ratio is generally even more decreased once the stars evolve along the upper part of the red giant branch. But the mechanism responsible for such an extra-mixing is still debated.
Moreover, we also use the fact that the C+N/Fe ratio is expected to be conserved throughout the live of the star, thus reflect its initial content independently of the stellar evolutionary stage. We show in Fig. 1 the C+N/Fe ratio in two Galactic population: the thin and the thick disk. In this figure, those two population show a distinct C+N/Fe pattern testifying for their different chemical evolution.

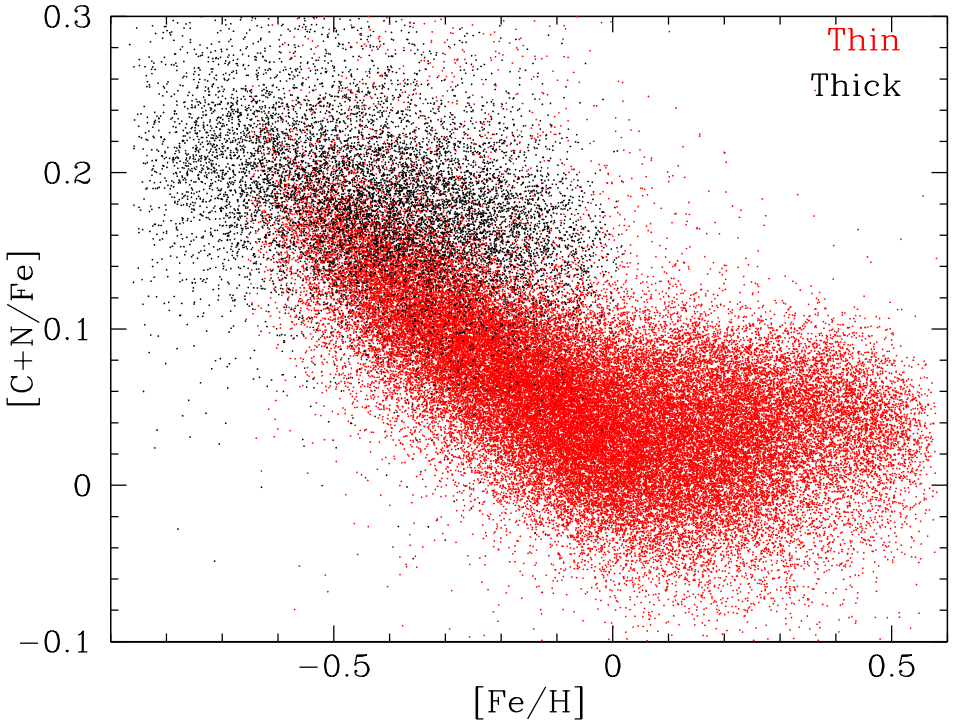

Fig. 1. C+N/Fe ratio in Galactic stars. Red points are thin disk stars while red points are thick disk stars.

4 Conclusions

Despite molecules such as CH and CN are intrinsically very small, their measurement in stars can infer properties of much larger astronomical objects such as stars and our Galaxy. Obviously, the conclusions that can be derive from those molecule are almost entirely dependent on our ability to model them accurately. The examples I

show here are based on recently revised molecular linelists that indeed allow to draw some relatively robust conclusions. Nevertheless, it is still not the case for all the molecules present in stellar atmospheres. As an example, I show in Fig. 2 the current status of the TiO molecular linelist as it could be modelled in Gaia spectra. Despite I show here that there is indeed hope for improvement, this still represent only a small portion of the spectrum.

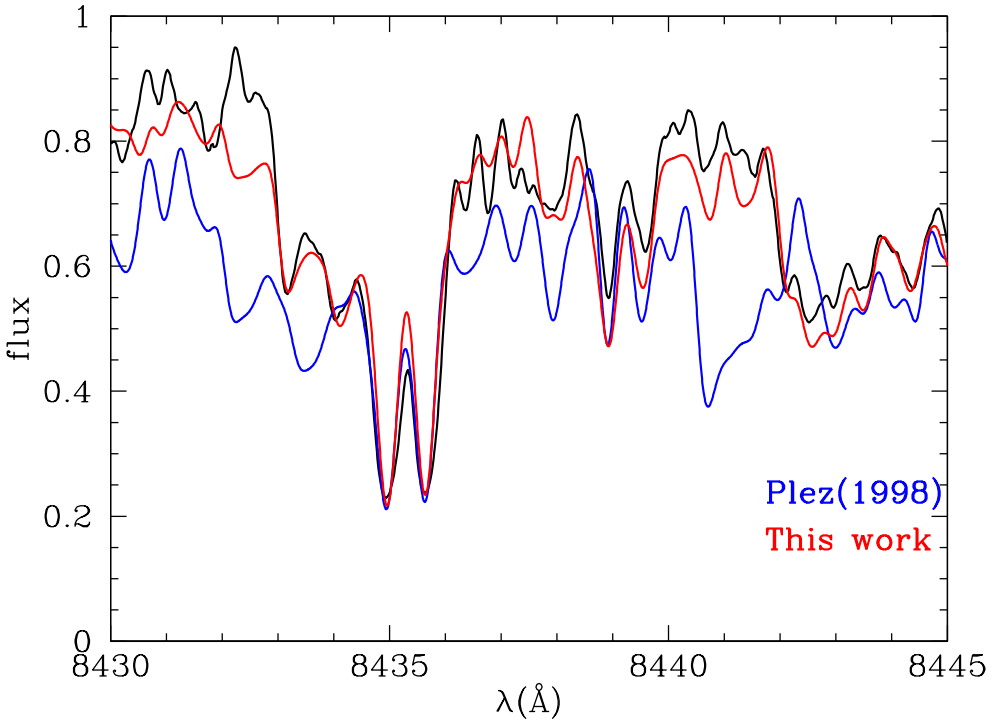

Fig. 2. Example of TiO absorption bands near the Gaia-RVS range. Black: observation. Red: synthesis using my last molecular linelist. Blue: synthesis using the Plez (1998) linelist.

Therefore, in parallel to the efforts made on hydrodynamical stellar simulations, it is crucial to improve fundamental atomic and molecular data. Moreover, molecular measurements in stellar spectra also have the ability to measure more than abundances: they can probe isotopic ratios as well as magnetic field. But for that latter, Lande factors would also need to be calculated via molecular structure programs.

References

Bessell, M. S., Collet, R., Keller, S. C., et al. 2015, ApJ, 806, L16

Brooke, J. S. A., Bernath, P. F., Schmidt, T. W., & Bacskay, G. B. 2013, J. Quant. Spec. Radiat. Transf., 124, 11

Masseron, T. & Gilmore, G. 2015, MNRAS, 453, 1855

Masseron, T., Plez, B., Van Eck, S., et al. 2014, A&A, 571, A47

Plez, B. 1998, A&A, 337, 495

Sneden, C., Lucatello, S., Ram, R. S., Brooke, J. S. A., & Bernath, P. 2014, ApJS, 214, 26