INFLUENCE OF UNCERTAINTIES OF MOLECULAR DATA UPON THE DETERMINATION OF ABUNDANCES IN COOL STARS

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Abstract. In cool stars, the determination of abundances of elements requires the resolution of the chemical equilibrium for each element even if atomic lines only are used. In the past, several authors have solved the well-known system of equations for a limited number of elements and of molecules. New calculations have been performed with special emphasis on the completeness of the system. Thus, all stable elements (83) have been included and a lot of molecules have been selected in order to omit no abundant compound. Owing to the lack of data (since many molecules are as yet not known spectroscopically), it appeared necessary to estimate many molecular parameters. Approximate equilibrium constants have been determined from analogies found among known molecules.

It has been shown once more that the dissociation energy is by far the most important parameter, which yields alone the final accuracy.

Our calculations include about 1200 molecules, of which more than half are new compounds never introduced in earlier investigations. We have found that, for about twenty elements such as Ti, Zr, La and most of the lanthanides, the new molecules play an important role in the chemical equilibrium. The cases of *titanium, zirconium* and *lanthanum* have been particularly investigated owing to the use of several bands of their oxides in the spectral classification of M- and S-type stars. We have noted that the experimental determinations of the dissociation energy of most monoxides and dioxides are as yet rather inaccurate. Furthermore, neither the spectrum nor the heat of atomization of hydroxides are known in the laboratory. It has appeared that estimating the dissociation energy of hydroxides was particularly difficult in consequence of the lack of data for such molecular compounds.

For oxygen-rich stars, we have investigated the influence of uncertainties of the dissociation energy of the most abundant species on the march of the molecular concentrations. In the case of *titanium*, we have found that the concentration of TiO strongly changes at low temperature (T <2520 K) according to the adopted D_0°- values for TiO, TiOH and TiO_2. Therefore, the interpretation of the TiO bands in the coolest stars has to take this new effect into account. In any way, we have checked that the TiO concentration always increases from early K- to late M-type stars. We have also shown that the depletion factor for Ti presents a final uncertainty of a factor of about ten at 2520 K, which still increases at lower temperature. That is due to the cumulative effect of the inaccuracies of molecular data. Therefore, in late M-type stars, the determination of the abundance of titanium remains rather uncertain even if it is derived from Ti I or Ti II lines. The present inaccuracy will only be reduced from very precise measurements of the dissociation energy of the relevant molecules. For Zr and La, we have found similar results to that for Ti. Furthermore, we have noted that there is no determination of absolute transition probabilities for the ZrO and LaO bands (contrary to TiO bands) which are both of first importance for the spectral classification of cool stars.

For carbon-rich stars as well as for S-type stars (i.e. O/C very near unity), we have checked that the molecules always play a much less important role that in oxygen-rich stars, as it was first noted by Tsuji (*Astron. Astrophys.* **23**, 411, 1973).

Our conclusion is that there is an urgent need of accurate measurements of the dissociation energy of many molecules and also of band oscillator strengths for most of the transitions of stellar interest. Furthermore, several new selected compounds have to be investigated in the laboratory, especially the dioxides and hydroxides. Such accurate molecular data are necessary in order to get a better knowledge of the physical conditions in cool stellar atmospheres.

The detailed account of the present paper will be shortly submitted to *Astronomy and Astrophysics*.

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DISCUSSION

Bidelman: Do you feel that there is some question about the identification of CaOH in M dwarfs? I believe that there is excellent evidence for this polyatomic molecule.

Sauval: The identification of CaOH in dwarf M stars (and not in M III stars) has been proposed by Dr. Pesch (*Astrophys. J.*) and is only based on the criterium of wavelengths coincidence. For me, such a proposed identification has to be checked by other criteria. Moreover, the laboratory analysis of the spectrum of CaOH is rather poor (see Herzberg, 1967: Spectra of polyatomic molecules). Nevertheless, Tsuji's (1973) calculations and my own results show that CaOH is the dominant molecule for $\theta > 2$, adopting D_0^0 (Ca-O-H) = 8.9 eV. All these results make the identification of CaOH probable, but not definitely sure.