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# Magnetic Splitting of Molecular Lines in Sunspots

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Abstract. We investigate the magnetic sensitivity of molecular lines observed in sunspot umbrae and briefly discuss their major differences compared to atomic lines.

## 1. Introduction

With high-resolution, high signal-to-noise spectroscopy in four Stokes parameters now available, the use of molecular lines for studying the structure of sunspots brings real gains. One is the extension of spot models, including the magnetic field, to layers, where atomic lines suffer from NLTE effects but molecules can still be treated in LTE. Another is that since molecular lines are extremely temperature sensitive they can be used to probe the thermal and magnetic structure of the coolest parts of sunspots. However, the magnetic properties of molecular lines observed in the sunspot spectrum has not yet been investigated in detail. Here we present our first calculations of the Stokes profiles of some molecular lines and discuss their most important peculiarities.

#### 2. The Molecular Stokes Profiles

The magnetic moment associated with the orbital and spin angular momenta of the electrons is the largest contributor to the magnetic moment of a diatomic molecule (Herzberg 1950). The relative strengths of the interactions between the external field and the magnetic moment of a molecule result in two exteme cases of the molecular Zeeman effect.

Case a: For an external magnetic field weaker than any internal molecular coupling, the total dipole moment of the molecule J interacts with the field giving 2J + 1 magnetic sublevels, as for the atomic Zeeman effect. With increasing J the maximum splitting decreases as J + 1.

Case b: The spin is uncoupled from the sum of other angular momenta even by a small field. This is the molecular Paschen-Back effect. Then, momenta are



Figure 1. Stokes profiles for different branches of the TiO  $\gamma$ -system.

independently space quantized in the field direction. With increasing J, the splitting becomes dependent only on the field strength.

It often happens that a molecule in a magnetic field is described by an intermediate coupling case. Then, it is necessary to calculate the Zeeman effect in detail and not rely on the results of limiting cases. Here we present calculations for the TiO  $\gamma$ -system (case a) and the MgH green system (intermediate case) following the theory of the molecular Zeeman effect developed by Schadee (1978). Our calculations are the forward spectral synthesis of the Stokes parameters carried out with the code STOPRO (Solanki, Rüedi, & Livingston 1992; Frutiger et al. 2000), which solves the set of radiative transfer equations for Zeeman-split lines.

The TiO  $\gamma$ -system. Both electronic states of the TiO  $A^3\Phi - X^3\Delta$  system are under strong spin-orbit coupling which holds up to very strong fields (case a). Also, the multiple substate  ${}^3\Phi$  shows the largest splitting among all triplet states of TiO. Lines of the  $\gamma$ -system are therefore the best features for studying sunspot magnetic fields with TiO. In Fig. 1 we present Stokes profiles of some TiO lines from different rotational branches for longitudinal and transverse fields of different strengths. One can see that the strongest effect is expected from the  $R_3$  branch. Also, it is clear that while lines of the Q- and R- branches show Stokes profiles polarized in the same sense as atomic lines, lines of the P-branches shows reverse polarization as if they would have negative Landé factors. This results from different changes of the total angular momentum numbers in the transitions of different branches.

The green MgH system. Because of a weak spin-rotation interaction in the lower electronic state, lines of the MgH  $A^2\Pi - X^2\Sigma$  system show a prominent Paschen-Back effect, even in the presence of rather moderate magnetic fields of 1000 G. As a consequence, the strengths of the Zeeman components become unbalanced, lines of main branches weaken, while lines of satellite branches strengthen (Schadee 1978; Illing 1981). Therefore, it is essential to consider a rotational transition and its satellite transition as a single line. This is illustrated in Fig. 2, where we present Stokes profiles for selected MgH lines. Because of merging of the transitions of the main and satellite lines, the resulting Stokes profiles are unconventional in shape. At stronger fields, however, the two lines imitate a normal Zeeman splitting. The line shapes are therefore sensitive to



Figure 2. Stokes profiles for selected lines of the MgH green system.

the field strength. This can provide a novel diagnostic of the magnetic field strength.

## 3. Conclusions

The reversal of circular polarization and unconventional Stokes V profiles of some molecular lines compared to atomic or other molecular lines were puzzling subjects for a long time (e.g. Nicholson 1938; Harvey 1973, 1985; Rüedi et al. 1995). With the help of TiO and MgH lines, we have demonstrated that the roots of such behaviour lie either in the molecular Paschen-Back effect or in the specific changes of the total angular momentum in the molecular transitions.

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