

*Letter to the Editor***Successful spectral synthesis of Zeeman-split molecular bands in sunspot spectra**S.V. Berdyugina<sup>1</sup>, C. Frutiger<sup>2</sup>, S.K. Solanki<sup>3</sup>, and W. Livingston<sup>4</sup><sup>1</sup> University of Oulu, Astronomy Division, P.O. Box 3000, 90014 Finland<sup>2</sup> ETHZ, Institut für Astronomie, Scheuchzerstrasse 7, 8092 Zürich, Switzerland<sup>3</sup> Max-Planck-Institut für Aeronomie, Max-Planck-Strasse 2, 37191 Katlenburg-Lindau, Germany<sup>4</sup> National Solar Observatory, AURA, P.O. Box 26732, Tucson, AZ 85726, USA

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**Abstract.** We present the first spectral synthesis of Zeeman-split Stokes profiles of the MgH  $A^2\Pi-X^2\Sigma$  green system and TiO  $\gamma$ -system. The calculations involve different regimes of the molecular Zeeman effect, up to the complete Paschen-Back effect for individual lines. The synthetic spectra are compared with observations of Stokes  $I$  and  $V$  in sunspot umbrae. We find that although the Stokes  $I$  spectra are reasonably reproduced, some lines are obviously still missing from the employed line lists. The Stokes  $V$  spectra turn out to be much cleaner since the missing lines do not appear to be Zeeman-split. We thus provide the first good fit to Zeeman-split molecular lines, including profiles with unconventional Stokes  $V$  shapes, determined by the Paschen-Back effect.

**Key words:** Sun: magnetic fields – Sun: sunspots – line: formation – polarization – molecular processes

**1. Introduction**

A study of molecular lines in sunspots is of particular interest because of their high temperature and pressure sensitivity. Many of them are also magnetically sensitive, but this has not yet been investigated in detail.

Earlier investigations of molecular lines in sunspots generally concentrated on line identification, determination of temperatures (rotational and vibrational) and pressure as well as elemental and isotopic abundances (e.g. Sotirovski 1971, Boyer 1978). Wöhl (1969) demonstrated that molecular lines in spectra of sunspots show the Zeeman effect. He found that the magnetic field strength derived from molecular lines was smaller than that derived from iron lines. Only few reports of polarimetric observations of molecular lines in sunspots can be found in the literature (e.g. Harvey 1973, 1985; Rüedi et al. 1995). They reported a puzzling reversal of the circular polarization and unconventional Stokes  $V$  profile shapes of some molecular

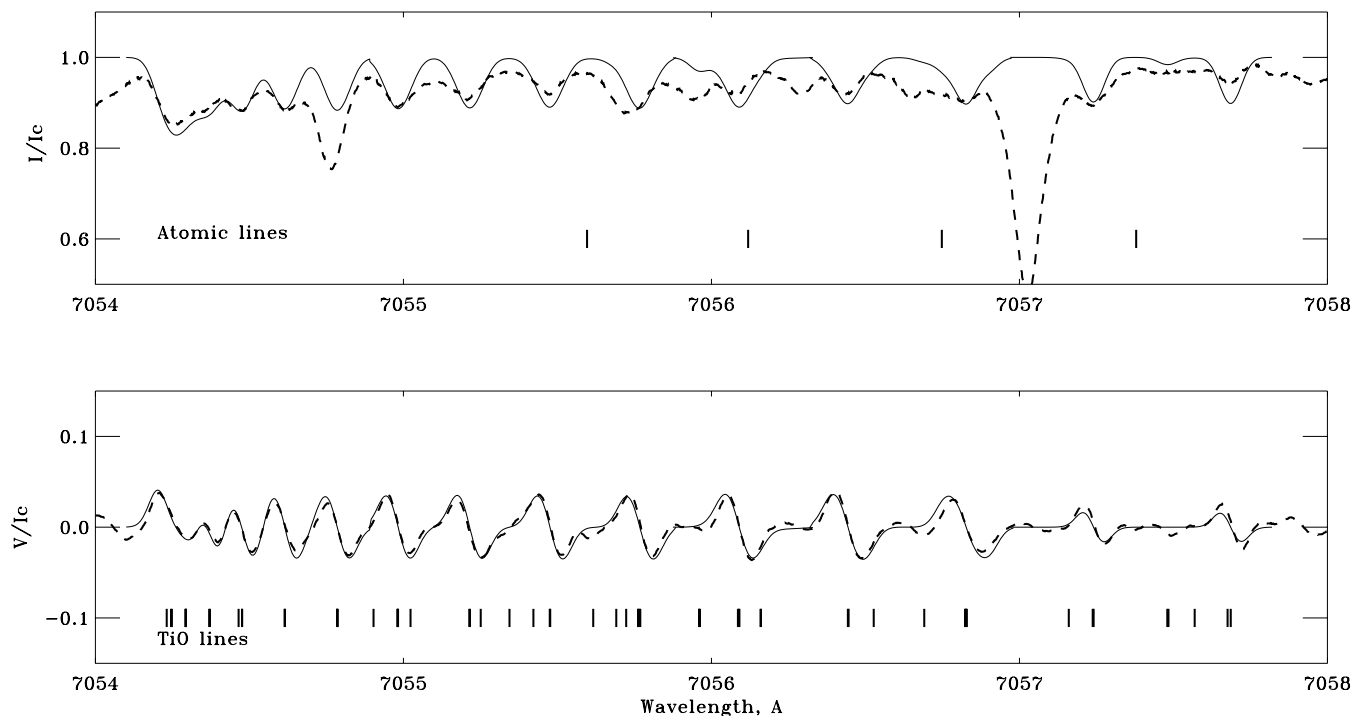
lines compared to atomic or other molecular lines. No in-depth analysis of those observations has been carried out as yet.

The problem of the molecular Zeeman and Paschen-Back effects was addressed by Schadee (1978). In spite of the major advance which Schadee's work represents, there seems to have been only a single attempt to utilize this theory, namely to explain the broad-band circular polarization in sunspots (Illing 1981). However, only a part of the effect could be attributed to molecular bands, and asymmetries of atomic Stokes profiles turned out to be a more suitable explanation for the effect (e.g. Sánchez Almeida & Lites 1992; Solanki & Montavon 1993; Martínez Pillet 2000). Hence the theory of the Zeeman splitting of molecular lines of interest for the study of solar and stellar magnetism has remained largely untested.

In this paper we present calculations of splitting and the Stokes parameters for the green system of MgH and TiO  $\gamma$ -system, which are the most studied band systems in sunspot spectra. We present the first spectral synthesis calculations and, also for the first time, confront synthetic molecular Stokes profiles with low-noise observations. Here we demonstrate that the synthetic spectra successfully reproduce the observations for reasonable atmospheric parameters. This opens the door to use these lines to recover the thermal, magnetic and dynamic properties of sunspots, and eventually for novel investigations of stellar spots.

**2. Observations**

The 1.5-meter McMath-Pierce Telescope, with its 13.5 meter spectrometer, is employed. A 1 mm (2.4x2.4 arcsec) Bowen-type image slicer serves as the entrance slit. In front of this slicer is a 50 khz Morvue quartz modulator. A few angstroms of the spectrum are rapidly scanned with the spectrometer photomultiplier output, being phase detected by a lockin amplifier to yield Stokes  $V$ . Scans are averaged by the photometry system until the desired S/N is obtained. Stokes  $I$  results by placing a circular polarizer before the Morvue. An interesting aspect of the above scheme is that the Stokes  $V$  signal is, to first or-



**Fig. 1.** Calculated (solid line) and observed (dashed line) Stokes  $I$  and  $V$  for the TiO  $\gamma(0,0)R_3$  band head. The field strength is 3000 G and the filling factor is 0.75 for an angle between the magnetic vector and the line of sight of  $0^\circ$ . Vertical dashes indicate positions of lines included in the spectral synthesis. The two strongest absorption features seen in Stokes  $I$  are atmospheric water lines.

der, seeing independent (since non-umbral scattered light is not polarized).

### 3. Molecular Stokes profiles

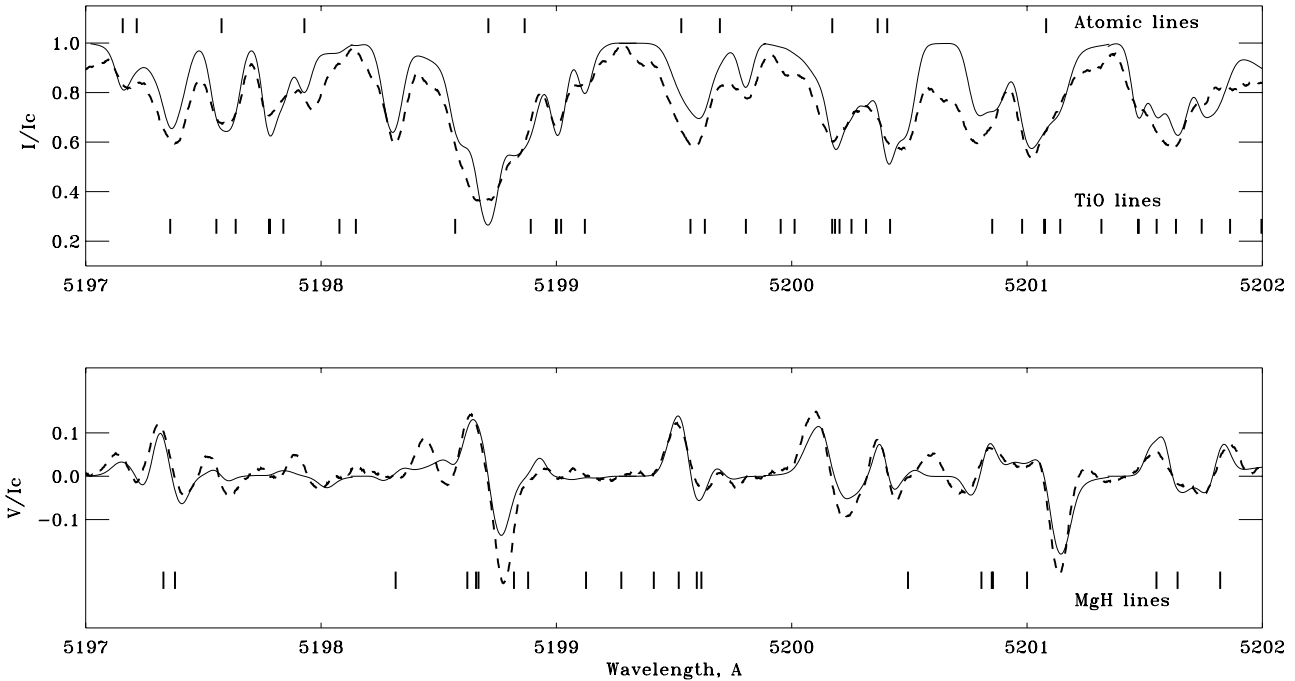
Here we present the forward spectral synthesis of the Stokes parameters of the MgH and TiO transitions. The set of radiative transfer equations is solved using the formulation given by Rees et al. (1989) as implemented in the code STOPRO (in an extended and improved version relative to that described by Solanki et al. 1992, cf. Frutiger et al. 2000). The code has been further updated to allow for molecular line computations. Calculations of the wavelength shifts of the Zeeman components and their theoretical strengths were included in accordance with the theory by Schadee (1978). Also, molecular number densities are calculated under the assumption of the chemical equilibrium of 270 compounds consisting of the 33 most abundant atoms (Tsuji 1973; L. Hänni, private communication). The code has also been extended to include the influence of blends (important near band heads), so that we can carry out the first spectral synthesis calculations of molecular and atomic Zeeman-split lines.

As in the case of atomic lines, the magnetic splitting of molecular lines depends on the strength of the interaction of the internal magnetic moment of the molecule with the external magnetic field. It is sufficient to consider the molecular Zeeman effect if the coupling between internal angular momenta is strong, i.e. the magnetic splitting is less than rotational and multiplet splitting. If the relevant angular momentum interacts

stronger with the external field than with the molecular fields, i.e. decoupling of the momenta takes place, the molecular Paschen-Back effect must be taken into account. In the following subsections we present calculations of the TiO and MgH band systems, whose splittings at the strengths reached by sunspot magnetic fields are good examples of the Zeeman and Paschen-Back effects, respectively. Here we concentrate on the results of the spectral synthesis and on their comparison with the data. Details about the code and the molecular physics of the considered bands are given in a separate paper (Berdyugina et al. 2000).

#### 3.1. The TiO $\gamma$ -system

The electronic states of the TiO  $\gamma$ -system  $A^3\Phi - X^3\Delta$  are under strong spin-orbit coupling, and, thus, the system is a good example of the ordinary molecular Zeeman effect up to very strong fields. The splitting of the levels is symmetrical and proportional to the field strength for a given total angular momentum number  $J$ . It is larger for low  $J$  and decreases with increasing  $J$ . The splitting is also proportional to the sum of the projections of the orbital and spin quantum numbers. Larger splitting is therefore expected for the  $^3\Phi$  state, especially for the third multiplet level. Our calculations show also that lines of the Q- and R- branches show Stokes  $V$  profiles polarized in the same sense as atomic lines, while lines of the P-branch show reverse polarization, which could be interpreted as lines having negative Landé factors. This behaviour is peculiar to molecular lines and results from different changes of the total angular momentum numbers in the transitions of different branches.



**Fig. 2.** The same as Fig. 1 for the MgH (0,0) band. The field strength is 3000 G and the filling factor is 0.95 for an angle between the magnetic vector and the line of sight of  $0^\circ$ .

Since the largest Zeeman effect is expected for lines with small values of  $J$ , the best spectral region for studying molecular magnetic splitting is at the beginning of rotational branches. The strongest and least blended band head of the TiO  $\gamma$ -system observed in the spectrum of sunspot umbra is (0,0) $R_3$  at  $\lambda$  7054.4 Å. The wavelength separation between rotational lines in the band is small and lines of low rotational numbers (larger splitting) almost coincide with those of high numbers (smaller splitting) in the band head. Nonetheless, a clear Stokes  $V$  signal is measured. In Fig. 1 we present the observed Stokes  $I$  and  $V$  profiles compared with the synthetic spectrum. The calculations were carried out with the molecular constants and line positions from Ram et al. (1999) and band oscillator strengths from Davis et al. (1986). Along with the TiO (0,0) $R_3$  lines, the line list included a number of atomic lines and weak TiO lines from higher vibrational bands of the  $\gamma$ -system. The maximum number of the Zeeman components of a single line considered was 939 (for  $J=156$ ). As a model umbra we used a radiative equilibrium atmosphere by Kurucz (1993) having  $T_{\text{eff}} = 3750\text{K}$  and  $\log g = 4.5$ , with the magnetic field strength of 3000 G. Since the observations of Stokes  $I$  are affected by stray light from the photosphere, we combined calculated spot and photospheric spectra using a spot filling factor of 0.95 prior to plotting them.

The Stokes  $V$  observations are excellently reproduced. This suggests that our current understanding of molecular Zeeman splitting underlying this calculations is adequate for this band. The main contribution to the polarization is due to the TiO (0,0) $R_3$  lines. Other TiO lines, from higher vibrational bands and rotational levels, are not Zeeman sensitive. Stokes  $I$  however suggests that our spectral synthesis does not include all

lines and that some of the blends are not identified (some are telluric lines). Nonetheless, we expect this band to be very useful for future investigations of cool magnetic structures in the solar photosphere, since Stokes  $V$  is the important quantity.

### 3.2. The MgH green system

The MgH  $A^2\Pi-X^2\Sigma$  system is an example of the partial Paschen-Back effect at moderate field strengths. The orbital angular momentum of the electrons in the lower electronic state ( $X^2\Sigma$ ) is zero, and this results in decoupling of the electron spin from the internuclear axis. Also, the electron spin interacts very weakly with the angular momentum of nuclear rotation in the lower state. Therefore, at low rotation the decoupling of the spin starts at rather moderate field strengths, less than 1000 G.

Because of shifts of magnetic sublevels in the lower electronic state, the line splitting is no longer symmetrical with respect to the zero field wavelength, and the strengths of the Zeeman components are not balanced (Schadee 1978; Illing 1981). This results in wavelength shifts of lines. The imbalance of the transition probabilities of single rotational lines leads to increased strengths of lines of the satellite branches. Therefore, it is essential to consider a rotational transition and its satellite transition as a single line. The main rotational line and its satellite line have a common upper level and similar energies of the lower levels. At field strengths above 1000 G, the Zeeman components of the two lower levels start to merge and the satellite line gains strength. The two lines thus start to imitate a normal Zeeman splitting. This effect must be taken into account when interpreting molecular line splittings in terms of magnetic

field strengths. Since the splitting is not linearly proportional to the field strength, it is not surprising that Wöhl (1969), who assumed proportionality, obtained significantly lower magnetic field strengths from MgH lines than from iron lines.

The strongest lines of the MgH green system are observed in the (0,0) band. We find that early rotational lines of the P-branch are less blended in sunspot spectra and, thus, more suitable for study. The calculations of Stokes  $I$  and  $V$  in the region with the P-branch lines were made in the same way as for the TiO band and include as many blends as possible. This region is plagued by many TiO  $\alpha$ -system lines as well as a number of strong atomic lines. The former, fortunately, do not contribute to Stokes  $V$  because of the special symmetry of the splitting (Schadee 1978). They do, however, make themselves felt in that they reduce and distort polarization signals of any line which they blend. The present calculations were carried out with the molecular constants and band oscillator strengths from Bernath et al. (1985) and Kirby (1979). The MgH line list and identifications were taken from Bernath et al. (1985) and Balfour & Cartwright (1976). The TiO lines of the  $\alpha$ -system are from Phillips (1973).

Four MgH features are found to be useful for future investigations: 5197.3, 5199.6, 5200.9, 5201.7 Å. Although they are all blended by atomic and TiO lines, the MgH transitions dominate the Stokes  $V$  signals of these lines. In particular, the unusual shapes of their Stokes  $V$  profiles are due to their intrinsic Zeeman patterns (partial Paschen-Back effect). A satisfactory fit of the observed Stokes  $V$  profiles of these features by the present calculations suggests that the employed theory of the molecular Paschen-Back effect is adequate. We expect further improvements from the inclusion of further lines and improved atomic and molecular data.

#### 4. Conclusions

In addition to the well-known strong temperature sensitivity of molecules, molecular transitions are sensitive to the presence of magnetic fields in sunspots. By comparing synthetic with observed Stokes  $I$  and  $V$  spectra we test (for the first time in detail) the use of the theory of the molecular Zeeman and

Paschen-Back effects for solar and stellar studies. We find that the current theory of the molecular Zeeman effect when combined with spectral synthesis (including as many blending lines as possible) and the best molecular data reproduces the data rather well for both spectral regions considered. These contain two of the best-studied solar molecular bands which are rather different from each other with respect to their Zeeman properties. This opens new perspectives for using molecular lines to investigate cool magnetic features in the solar photosphere and on other stars, including those of later spectral type.

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