

# Molecular Lines as Diagnostics of Solar and Stellar Magnetic Fields

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## Abstract.

Thanks to recent advances in theory we can now calculate molecular line profiles in the presence of magnetic fields with high accuracy, both in the Zeeman and Paschen-Back regimes (Berdyugina et al. 2000; Berdyugina & Solanki 2001a). The synthetic Stokes profiles of various molecular species (e.g. TiO, OH, MgH, CN, FeH) have been compared with profiles observed in sunspots. The agreement between the theory and observations is remarkable. For example, the mutually opposite polarities of different OH lines are reproduced without invoking any free parameters, except the magnetic field strength and sunspot temperature. Introducing molecular lines into the inversion of sunspot spectra leads to significant improvements in the deduced magnetic field vector. Here we investigate how molecular lines can be used to deduce magnetic parameters of cool stars. We find that such lines are of great interest for measuring magnetic fields on cooler stars and in starspots.

## 1. Introduction

The spectra of sunspots and of cool stars contain a rich collection of molecular lines (e.g. Wallace et al. 1998). Lines of diatomic molecules observed in sunspot spectra are good temperature and pressure indicators. They are also useful for determining elemental and isotopic abundances. Recently we performed an overview of the magnetic properties of molecular band systems observed in visible and near infrared spectra of sunspots and cool stars. We showed that many molecular lines are also good indicators of solar and stellar magnetic fields (Berdyugina et al. 2000; Berdyugina & Solanki 2001a).

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. Simultaneous inversions of Stokes profiles of atomic and molecular lines observed in spectra of solar umbrae and penumbrae can significantly improve the current models of sunspots. 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 at field strengths of 1 – 3 kG.

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On cool stars with magnetic activity, such as T Tauri stars, solar type G-K dwarfs, RS CVn- and FK Com-type stars, molecular lines can provide measurements of magnetic fields directly in spatially unresolved spots, wherein they are formed. Also, since molecular lines dominate spectra of cool Me and brown dwarfs, their magnetic fields can be measured only by means of the molecular Zeeman effect (e.g. Valenti et al. 2001). This will help in understanding how strong the magnetic fields in fully convective stars can be.

Here we discuss a sample of molecular bands and lines which represent the most powerful diagnostics for stellar and solar studies. Using the theoretical Zeeman patterns calculated as described by Berdyugina & Solanki (2001a), we carried out the forward spectral synthesis of Stokes parameters of molecular transitions of interest. The radiative transfer calculations were performed with an extended and improved version of the code STOPRO (Solanki et al. 1992; Frutiger et al. 2000), which solves the set of radiative transfer equations in the formulation given by Rees et al. (1989). This code has been updated to enable computations of lines of diatomic molecules in the presence of a magnetic field, i.e. calculate the wavelength shifts of the Zeeman components and their theoretical strengths as well as molecular number densities. As a model umbra we used a radiative equilibrium atmosphere tabulated by Kurucz (1993) having  $T_{\text{eff}} = 3750\text{K}$  and  $\log g = 4.5$ , into which we introduced a height-independent magnetic field of an appropriate strength.

### 1.1. TiO

*Sunspots.* TiO lines are observed in spectra of sunspots and cool stars. In sunspots, the (0,0)  $R_3$  band head of the  $\gamma$ -system ( $A^3\Phi - X^3\Delta$ ) at 7054 Å is the strongest molecular absorption feature in the visible. It is remarkable that lines of this system are also strongly magnetically sensitive, especially in the  $P_3$  and  $R_3$  branches: their effective Landé factors  $|g_{\text{eff}}| \leq 2.1$  (Berdyugina & Solanki 2001a). 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. Recently, we presented the first Stokes  $V$  observation of the  $\gamma$  (0,0)  $R_3$  band head in a sunspot and successfully reproduced it with our current calculation technique (Berdyugina et al. 2000). In Fig. 1 we present the observed Stokes  $I$  and  $V$  profiles compared with the synthetic spectrum. 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  $J=156$ ). 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 0.75 prior to plotting them.

The Stokes  $V$  observations are excellently reproduced. This suggests that our current understanding of molecular Zeeman splitting underlying this calculation 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

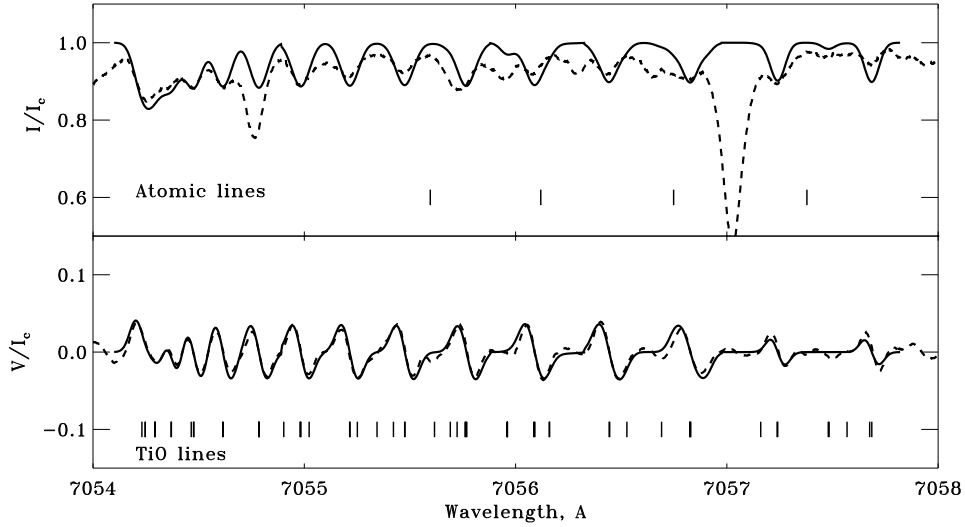


Figure 1. The TiO  $\gamma(0,0)R_3$  band head in a sunspot. Calculated and observed Stokes  $I$  and  $V$  are represented by solid and dashed lines, respectively. The field strength is 3 kG, the filling factor is 0.75, and the magnetic vector is directed along the line of sight. Vertical dashes indicate positions of lines included in the spectral synthesis. The two strongest absorption features seen in Stokes  $I$  are atmospheric water lines.

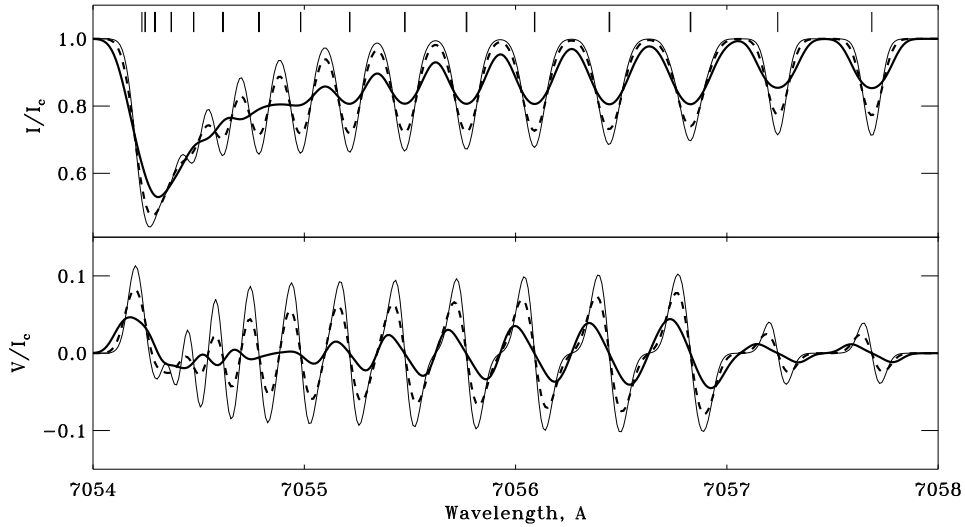


Figure 2. The TiO  $\gamma(0,0)R_3$  band head in a starspot with a field strength of 3 kG. The thin solid line represents synthetic Stokes  $I$  and  $V$  with only instrumental broadening of  $0.07 \text{ \AA}$  ( $R=100\,000$ ), while thick dashed and solid lines show the spectra broadened in addition by the effect of the stellar rotation with  $v \sin i$  of  $2.5$  and  $5 \text{ km s}^{-1}$ , respectively.

be very useful for future investigations of cool magnetic structures in the solar photosphere, since Stokes  $V$  is the important quantity.

*Starspots.* The idea that TiO bands could be used to measure starspot properties was first stated by Ramsey & Nations (1980). They observed a TiO band in the spectrum of the active G5 IV + K1 IV system V711 Tau (HR1099) near its photometric minimum. The spectral classes of the binary components excluded the possibility for the band to be formed in the unspotted photosphere, so that the TiO feature must be produced in spot regions that are at least 1000 K cooler than the photosphere of the K1 IV star. Further observations revealed the TiO bands in starspot spectra of other active stars which allowed to measure the spot area and temperature (e.g. Neff et al. 1995; O’Neal et al. 1996).

The  $\gamma(0,0)R_3$  band head is among other band heads observed in starspots. It is interesting therefore to estimate the significance of the Stokes  $V$  signal from the band under stellar conditions. The most important factors are then the spectral resolution, stellar rotation, ratio of the continuum surface flux between the spot and the photosphere, and filling factor of spots of the same polarity at the visible stellar disk. In Fig. 2 we present the synthesis of the band head at a resolution of  $0.07 \text{ \AA}$  (resolving power  $R=100\,000$ ) broadened with two rates of stellar rotation:  $v \sin i$  of  $2.5$  and  $5 \text{ km s}^{-1}$ . The resulted Stokes  $V$  amplitudes are of  $0.08$  and  $0.05$ , respectively. Recall that the calculation was done for the model with  $T_{\text{spot}} = 3750\text{K}$  and  $\log g = 4.5$ . At lower temperatures, the signal is stronger. Then, the amplitudes should be reduced in accordance with the continuum flux ratio ( $0.3$  for  $T_{\text{phot}} = 4750\text{K}$  at  $7054 \text{ \AA}$ ) and the spot filling factor, which is normally within  $20\%$  to  $50\%$ , while little is known about the polarity of starspots. An estimate can be made from the fact that the observed central depth of the band can be as large as  $0.1$  from the total continuum level in some very active stars. It is therefore clear that with current stellar spectropolarimetric facilities the registration of the Stokes  $V$  signal from starspots in this band head is achievable for a sample of active stars and, thus, the analysis of these observations can provide the first direct measurements of the magnetic field strength inside spatially unresolved starspots and, thus, provide the first probe of the internal structure of starspots.

## 1.2. OH

*Sunspots.* A particularly interesting case is presented by OH transitions in the infrared H-band. They belong to the Meinel system and are observed in sunspot spectra as two main band sequences extending up to  $4.2 \mu\text{m}$  and starting at  $1.4 \mu\text{m}$  and  $3.1 \mu\text{m}$ , for the difference between the upper and lower vibrational state numbers  $\Delta v = 2$  and  $\Delta v = 1$ , respectively (Wallace & Livingston 1993).

In the spectrum of a sunspot umbra Harvey (1985) discovered that lines of the same OH band and of approximately the same strength exhibit opposite polarities. A portion of an FTS (Fourier Transform Spectrometer) spectrum of a sunspot umbra is plotted in Fig. 3, where 4 OH lines from the  $(2,0)$  band are marked. The complete data set is described and discussed by Rüedi et al. (1995). Note that the pair on the right has  $V$  profiles of opposite polarity compared with those on the left. The fact that two lines each have  $V$  profiles of the same polarity, the  $V$  profiles are antisymmetric and all lines are otherwise similar

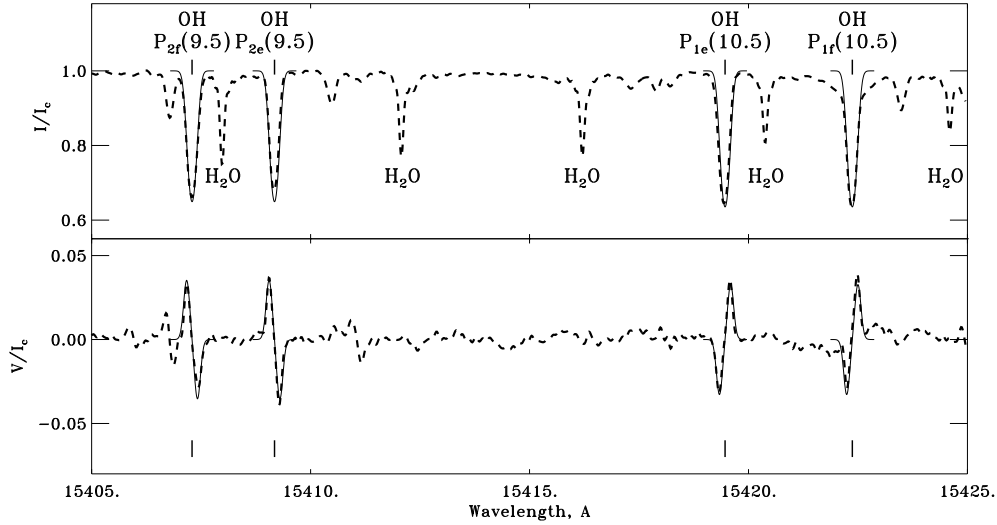


Figure 3. Stokes  $I$  and  $V$  spectra of the two pairs of OH lines pointed out by Harvey (1985). Dashed lines: observed in a sunspot, solid lines: synthesized. The field strength is 2.5 kG, and the filling factor is 0.8. Note that the magnetic field in the spot is directed away from the observer and, thus, the reversed polarization is present in the left pair of lines. The weaker reversed-polarity  $V$  profiles, e.g. at 15407 Å, are also due to OH.

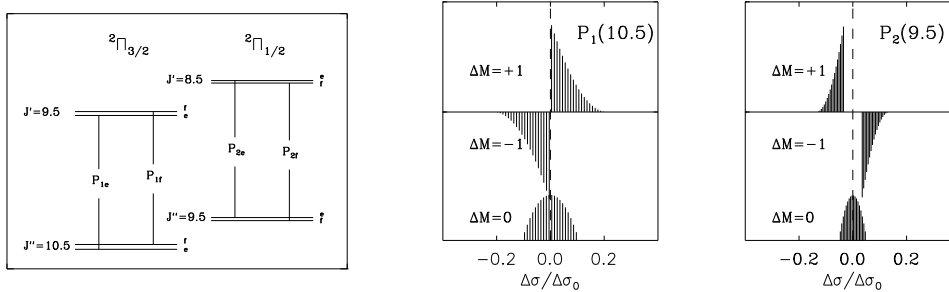


Figure 4. In the left panel is shown a schematic representation of the transitions underlying the two pairs of OH lines, for one of which the puzzling reversed polarization was reported by Harvey (1985). The small  $\Lambda$ -type doubling intervals between levels denoted by  $e$  and  $f$  are exaggerated for clarity. The other two panels show the Zeeman patterns of the two pairs of OH lines. In spite of rather different Zeeman patterns, the two plotted lines have almost identical absolute values of the effective Landé factors: 0.11 and  $-0.12$  for  $P_1(10.5)$  and  $P_2(9.5)$ , respectively.

cannot be explained any other way than that they have equal but opposite effective Landé factors (Berdyugina & Solanki 2001b). This is demonstrated in Fig. 4, which reveals that reversed polarity is exhibited by the lines belonging to the  $P_2$  sub-branch ( $g_{\text{eff}} > 0$ ), while the  $P_1$  transitions have normal sign polarity ( $g_{\text{eff}} > 0$ ). Our calculations show that the same occurs for the  $R_1$  and  $R_2$  transitions and such a behavior is typical for all OH lines from the Meinel system and pure rotational transitions in the ground state.

The synthesis of Zeeman-split OH lines also helps to improve the diagnostic capability of atomic lines. In sunspots, strong OH lines from the (3,1) band are observed in the vicinity of the Zeeman sensitive Fe I 15648.5 Å line and are blended with Fe I 15652.9 Å. Together, these two Fe I lines are the premier infrared diagnostics of the solar magnetic field (e.g. Solanki et al. 1992) and are being increasingly widely used. Inverting the Stokes parameters of the blending OH lines along with the Fe I lines greatly improves the reliability of magnetic, thermal and dynamic quantities deduced from these lines in sunspot umbrae.

With the inversion code described by Frutiger et al. (2000), we carried out the inversion of Stokes parameters observed in the central part of an umbra where the strength of molecular lines was the largest. These observations are fully described by Lagg et al. (in preparation). Our simplified model included two components, magnetic and nonmagnetic, the first representing the umbra itself, while the second describing the contribution from the photospheric stray light. Two inversions were made: one disregarding the blending OH lines, the other including them. As the Fe I and OH lines are formed in different parts of the umbral atmosphere, the effect of including of the OH lines was the largest in the upper layers, at optical depths  $\log \tau \leq -1$ . Without OH lines, the non-magnetic component is too cool, the field strength in the magnetic component unreasonably grows towards smaller optical depths, and the vector of the field changes its direction with respect to the line of sight (Fig. 5). Also, the fit to the Stokes parameters is not satisfactory (Fig. 6). If the OH lines are included in the calculations, the behaviour of the magnetic component is stabilized, i.e. the field strength smoothly drops towards higher layers and the field direction corresponds well to the observed position of the sunspot on the solar disk. Also, the nonmagnetic component becomes as hot as the photosphere (Fig. 7). Finally, the fit to the profiles becomes acceptable for such a simple model (Fig. 8).

*Starspots.* The first detection of infrared OH lines from starspots was reported by O’Neal & Neff (1997). They observed an excess of OH absorption in the blend of the  $\Lambda$ -type doublet  $P_2(5.5)$  at 15627 Å and interpreted it as a contribution from cool starspots. In order to see the effect of the starspot magnetic field in this blend, we synthesized the Stokes  $I$  and  $V$  profiles of the OH lines contributing to this blend. This is shown in Fig. 9. The calculation was done for a model with  $T_{\text{spot}} = 3750\text{K}$  and  $\log g = 4.5$  with a height-independent magnetic field strength of 3 kG. Plotted are the profiles for a spectral resolution of 0.15 Å (resolving power  $R=100\,000$ ) and stellar rotation broadening of 0, 2.5 and 5  $\text{km s}^{-1}$ . Again, the resulting Stokes profiles should be scaled by the continuum flux ratio (0.6 for  $T_{\text{phot}} = 4750\text{K}$  at 15627 Å) and the spot filling factor, which results in a rather measurable signal even in Stokes  $V$ . In fact, the Stokes  $V$

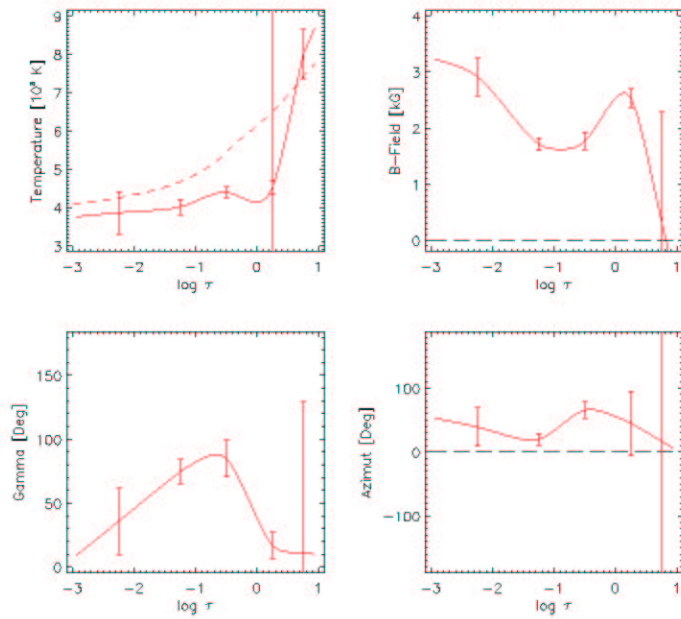


Figure 5. The umbra atmosphere deduced from the inversion of the Fe I profiles only. The solid curves represent the magnetic component of the model, while the dashed curve shows the temperature distribution in the nonmagnetic component.

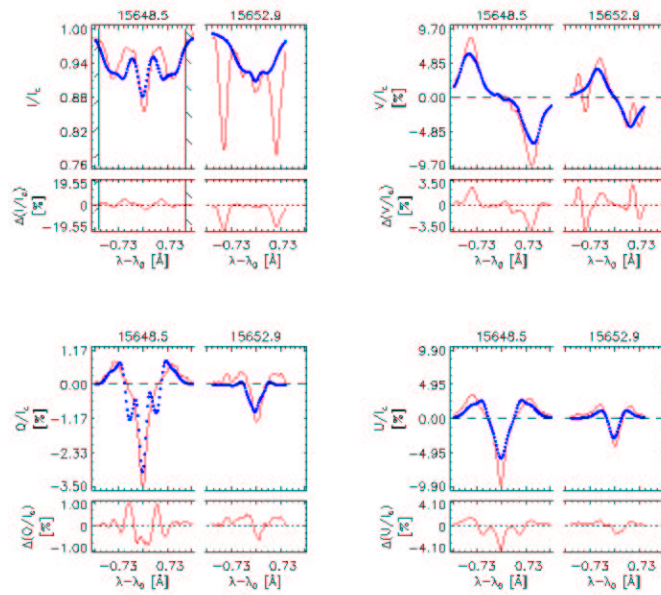


Figure 6. The fits (dots) to the observed Stokes profiles (solid lines) for the model presented in Fig. 5.

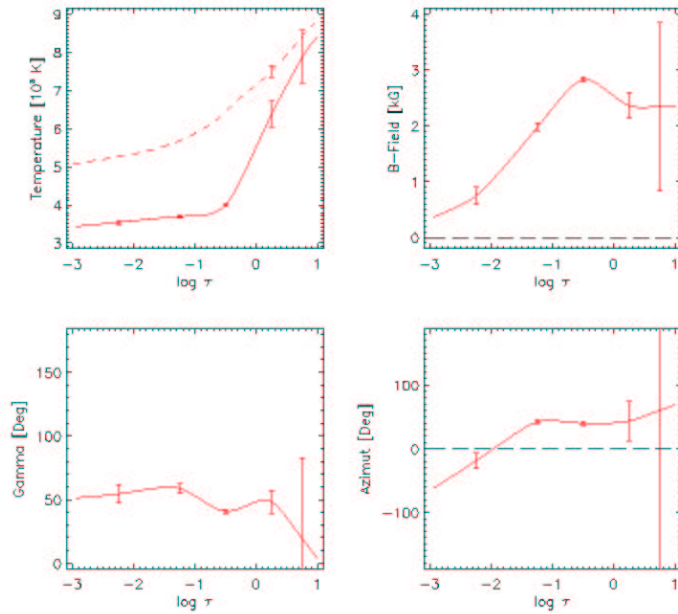


Figure 7. The same as Fig. 5 for the inversion including both Fe I and OH lines.

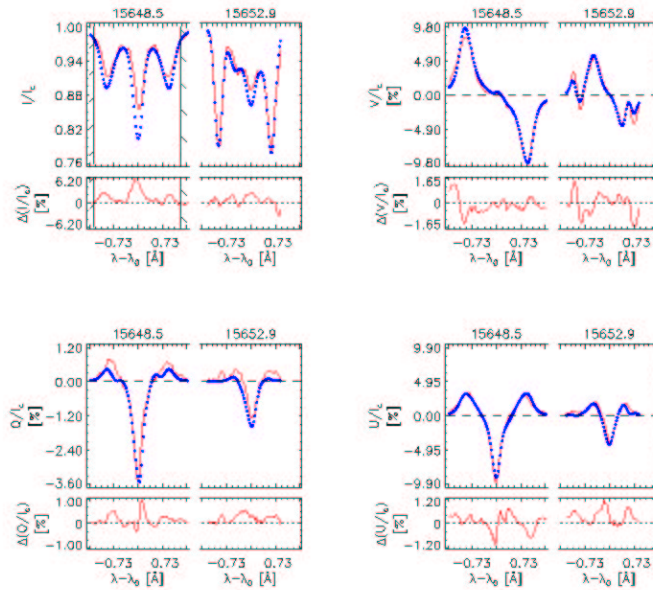


Figure 8. The fits (dots) to the observed Stokes profiles (solid lines) for the model presented in Fig. 7.



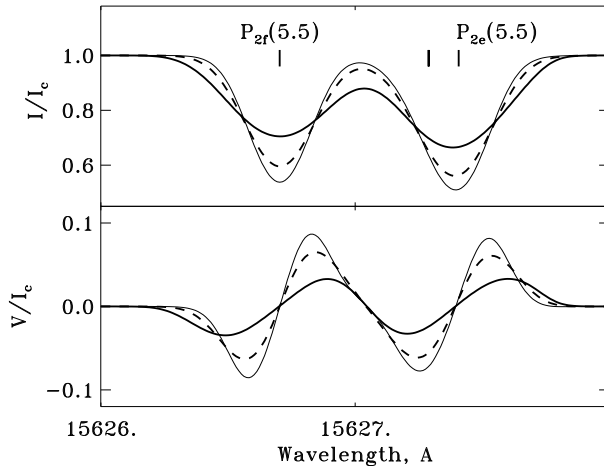


Figure 9. The same as Fig. 2 for the OH lines from the (3,1) band at a spectral resolution of  $0.15 \text{ \AA}$  ( $R=100\,000$ ) and different  $v \sin i$ .

signal could be even larger than in the TiO band head discussed above. So, infrared OH lines can also be a useful diagnostic of stellar magnetic fields.

### 1.3. FeH

*Sunspots.* The calculation of the Zeeman effect in FeH lines of the infrared  $^4\Delta - ^4\Delta$  system is made difficult by the fact that the required spin-orbit coupling constants of the two electronic states were not determined. Their magnetic sensitivity is, however, remarkable, for which sunspot observations by Wallace et al. (1998) provide evidence. With appropriate spin-orbit coupling constants we can reproduce these observations as shown in Fig. 10 and predict the Stokes V signal as well. The fully split  $Q_1(3.5)$  line at  $10062.7 \text{ \AA}$ , for instance, is potentially an excellent diagnostic of the umbral upper atmosphere.

*Starspots.* The power of the FeH lines as stellar magnetic field diagnostics was clearly demonstrated by Valenti et al. (2001). They detected the Zeeman broadening of FeH lines in an active M dwarf and, using the sunspot spectrum by Wallace et al. (1998), performed simple modeling of the stellar spectrum. Nevertheless, accurate laboratory analysis is urgently needed.

### References

- Berdyugina, S.V., Frutiger, C., Solanki, S.K., & Livingston, W. 2000, *A&A*, 364, L101  
 Berdyugina, S.V., & Solanki, S.K. 2001a, *A&A*, submitted  
 Berdyugina, S.V., & Solanki, S.K. 2001b, *A&A*, submitted  
 Frutiger, C., Solanki, S.K., Fligge, M., & Bruls, J.H.M.J. 2000, *A&A*, 358, 1109  
 Harvey, J.W. 1985, in *Measurement of Solar Vector Magnetic Fields*, M.J. Hagyard (ed.), NASA CP-2374, p.109

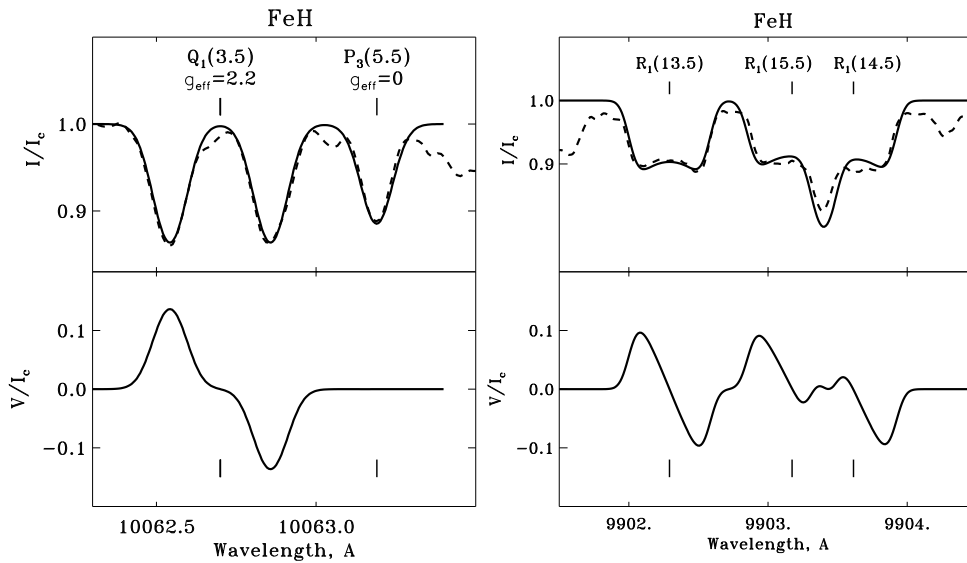


Figure 10. Stokes  $I$  and  $V$  of the FeH lines. Observations (dashed) are from Wallace et al. (1998). Synthetic Stokes profiles (solid) are calculated for a field strength of 3 kG. The zero-field positions of lines are indicated by vertical dashes.

Kurucz, R.L. 1993, CDROM No. 13

Neff, J.E., O'Neal, D., & Saar, S.H. 1995, *ApJ*, 452, 879

O'Neal, D., & Neff, J.E. 1997, *AJ*, 113, 1129

O'Neal, D., Saar, S.H., & Neff, J.E. 1996, *ApJ*, 463, 766

Rees, D.E., Murphy, G.A., & Durrant, D.J. 1989, *ApJ*, 339, 1093

Rüedi, I., Solanki, S.K., Livingston, W., & Harvey, J. 1995, *A&AS*, 113, 91

Solanki, S.K., Rüedi, I., & Livingston, W. 1992, *A&A*, 263, 312

Valenti, J.A., Johns-Krull, C.M., Piskunov, N. 2001, in *The 11th Cool Stars, Stellar Systems and the Sun*, eds. R.J. García López, R. Reboló, M.R. Zapatero Osorio, ASP Conf. Ser., Vol. 223, p. 1579

Wallace, L., & Livingston, W.C. 1993, *An Atlas of a Dark Sunspot Umbral Spectrum in the Infrared from 1970 to 8640 cm<sup>-1</sup> (1.16 to 5.1 μm)*, NOAO, <ftp://ftp.noao.edu/fts/spot1at1>

Wallace, L., Livingston, W.C., Bernath, P.F., & Ram, R.S. 1998, *An Atlas of the Sunspot Umbral Spectrum in the Red and Infrared from 8900 to 15,050 cm<sup>-1</sup> (6642 to 11,230 Å)*, NOAO, <ftp://ftp.noao.edu/fts/spot3at1>