(1) Introduction

During the last decade the spectropolarimetry of diatomic molecules became an important tool for studying stellar atmospheres and magnetism (see review by Berdyugina 2011). At temperatures below 4000 K, a number of diatomic molecules readily exist in the atmospheres of cool stars (see review on molecules of astrophysical interest by Bernath 2009). Because molecules have a more complex energy level structure than atoms, they provide a powerful tool for measuring stellar magnetic fields via the Zeeman and Paschen-Back effects already at 1 G field. This leads to a considerable signal in both circular and linear polarization, up to 30% at the magnetic field strength of $\geq 3$ kG in early L dwarfs. The polarization does not cancel out completely even at very low spectral resolution and is seen as broad-band polarization of a few percent. Since the line asymmetry depends only on the magnetic field strength and not on the filling factor, CrH lines provide a very sensitive tool for direct measurement of the stellar magnetic fields on faint cool objects, such as brown dwarfs and hot Jupiters, observed with low spectral resolution.

1.1 Aims. We investigated the Paschen-Back effect in the (0,0) band of the $A^2\Sigma^+ - X^2\Sigma^+$ system of the CrH molecule, and we examined its potential for estimating magnetic fields on stars and substellar objects, such as brown dwarfs and hot exoplanets.

1.2 Methods. We carried out quantum mechanical calculations to obtain the energy level structure of the electronic-vibrational-rotational states considered both in the absence and in the presence of a magnetic field. Level mixing due to magnetic field perturbation (the Paschen-Back effect) was consistently taken into account. Then, we calculated frequencies and strengths of transitions between magnetic sublevels. Employing these results and solving numerically a set of the radiative transfer equations for polarized radiation, we calculated Stokes parameters for both the individual lines and the (0,0) band depending on the strength and orientation of the magnetic field.

1.3 Results. We demonstrate that magnetic splitting of the individual CrH lines shows a significant asymmetry due to the Paschen-Back effect already at 1 G field. This leads to a considerable signal in both circular and linear polarization, up to 30% at the magnetic field strength of $\geq 3$ kG in early L dwarfs. The polarization does not cancel out completely even at very low spectral resolution and is seen as broad-band polarization of a few percent. Since the line asymmetry depends only on the magnetic field strength and not on the filling factor, CrH lines provide a very sensitive tool for direct measurement of the stellar magnetic fields on faint cool objects, such as brown dwarfs and hot Jupiters, observed with low spectral resolution.

Key words. brown dwarfs – stars: magnetic field – stars: atmospheres – polarization – radiative transfer
which can be seen at lower spectral resolution (cf. the work on the CH molecule in magnetic white dwarfs by Berdyugina et al. 2007). This makes the CrH molecule attractive for polarimetric observations of faint, magnetized substellar atmospheres which cannot yet be observed with high spectral resolution.

The outline of the paper is as follows.

First, we calculate the rotational level structure of the (0, 0) vibrational band of the A$^2\Sigma^+$ and X$^2\Sigma^+$ electronic states using the effective Hamiltonian for a $^2\Sigma$ state given by Ram et al. (1993). Using the rotational energy values obtained and taking into account the matrix elements of the magnetic Hamiltonian represented in the case $b$ wave functions, as in Berdyugina et al. (2005), we calculate the magnetic level structure in both electronic states for different magnetic field strengths (Sect. 2). Strengths of the transitions between the magnetic sublevels are calculated in Sect. 3.

In Sect. 4, we calculate the synthetic Stokes profiles for both the individual transitions and the entire (0, 0) band by employing the results from Sects. 2 and 3 and solving numerically a set of the radiative transfer equations. We employ three model atmospheres from the Phoenix-Drift grid by Witte et al. (2009) with the effective temperatures of 2500 K, 2000 K, and 1500 K. These three models represent roughly the physical conditions in the atmospheres of late M, early and mid-L dwarfs, as well as of a possible hot Jupiter.

We summarize our results in Sect. 5. We conclude that the CrH A$^2\Sigma^+\rightarrow$X$^2\Sigma^+$ system is a sensitive diagnostic tool for studying the magnetic fields in cool substellar objects. Measurable signals can be observed even at fields of a few G and with low spectral resolution, which is advantageous for faint objects, such as brown dwarfs and hot Jupiters. This occurs thanks to the Paschen-Back effect which causes an asymmetry of the magnetic components of a spectral line. This is in contrast to the Zeeman regime (ZR), where splitting of a spectral line and strengths of the individual magnetic components are always symmetric.

2. Energy level structure

2.1. Rotational level structure

We calculate the rotational level structure of the electronic states $X^2\Sigma^+$ and $A^2\Sigma^+$ of the CrH molecule following Ram et al. (1993), who employed the basis wave functions in Hund’s case $a$. Earlier, a similar work was done by Klemm & Uhler (1959), who worked from the basis wave functions in case $b$.

The total Hamiltonian of the CrH molecule in the absence of an external magnetic field, $\hat{H}_0$, can be partitioned as

$$\hat{H}_0 = \hat{H}_{\text{rot}} + \hat{V},$$

where $\hat{H}_0$ represents all the electronic and vibrational terms, and $\hat{V}$ is a perturbation operator. The subscript “$b$” indicates that, after taking account of all interactions contained in $\hat{H}_0$, the electronic states considered occur in case $b$. The perturbation operator $\hat{V}$ is given by

$$\hat{V} = \hat{H}_{\text{cd}} + \hat{H}_{\text{sr}} + \hat{H}_{\text{ss}} + \hat{H}_{\text{so}} + \hat{H}_{\text{sr}} + \hat{H}_{\text{cd}},$$

where $\hat{H}_{\text{cd}}$ is the rotational Hamiltonian of the nuclei; $\hat{H}_{\text{cd}}$ takes into account the centrifugal distortion of the molecule; and $\hat{H}_{\text{sr}}, \hat{H}_{\text{so}}$, and $\hat{H}_{\text{ss}}$ arise respectively from the spin-orbital, spin-rotational, and spin-spin interactions. We note that $\hat{H}_{\text{so}}$ is zero for case $b$.

Representing the total Hamiltonian $\hat{H}_0$ in the wave functions in case $a$, $|\text{a}\rangle$, we have

$$\hat{H}_0 = \langle \text{a}|\hat{H}_0|\text{a}\rangle + \langle \text{a}|\hat{V}|\text{a}\rangle + O\left(\langle \text{a}|\hat{V}^2|\text{a}\rangle\right) + \ldots.$$  \hspace{1cm} (3)

As a result of the perturbation $\hat{V}$, the Hamiltonian matrix $\mathcal{H}_0$ becomes non-diagonal. However, the first term is diagonal with respect to the electronic and vibrational state and gives the unperturbed (and still degenerate) energy level $E_0$. The second and the third terms are the corrections to $E_0$. We considered here up to the third-order and forth-order corrections arising from the spin-rotational and spin-spin interactions, respectively.

We diagonalize numerically the effective Hamiltonian (see, e.g., Brown & Carrington 2003) for the rotational levels of a $^2\Sigma$ state that contains the $V$-dependent terms from the right-hand part of Eq. (3) and that is given by Ram et al. (1993, Table 1). As a result, we obtain the eigenvalues $E_{2Jz}$, and the eigenvectors of $\hat{H}_0$ in the absence of an external magnetic field. The representation $(b|\hat{H}_b|b)$ in the wave functions in case $b$ is then diagonal with respect to the rotational state $(\Sigma J)$.

After the energy values $E_{2Jz}$ in both the upper A$^2\Sigma^+$ and the lower X$^2\Sigma^+$ electronic states have been obtained, one can calculate the energies of all possible electronic transitions in the (0, 0) band allowed by the quantum mechanical selection rules. The line positions calculated are in a good agreement with those analyzed by Ram et al. (1993) and computed by Burrows et al. (2002).

2.2. Magnetic level structure

Now we consider the CrH molecule in the presence of an external magnetic field and examine its impact on the rotational structure calculated in Sect. 2.1.

When neglecting the interaction between the magnetic levels, the energy shift for a level $M$ at the magnetic field strength $\mathcal{H}$, with respect to its energy value in the absence of an external magnetic field, obtains as:

$$\Delta E = g_M\mu_0\mathcal{H},$$  \hspace{1cm} (4)

where $g$ and $\mu_0$ are the Landé factor and the Bohr magneton, respectively. The case, when the expression (4) holds, is called Zeeman regime (see, e.g., Berdyugina & Solanki 2002). However, as we show in Sect. 4.2, the ZR is practically not applicable for the CrH $^2\Sigma^+$ electronic states (especially for the lower state), so the interaction between magnetic levels cannot be neglected.

To take into account the interaction between the magnetic levels, i.e., to calculate the Paschen-Back effect, we consider the total Hamiltonian of the molecule in the form

$$\hat{H}_{\text{mag}} = \hat{H}_0 + \hat{H}_H,$$  \hspace{1cm} (5)

where the interaction of the molecule with an external magnetic field $\hat{H}_H$ is considered to be smaller than the intrinsic molecular interactions $\hat{H}_0$. More precisely, we consider here the case when $\hat{H}_H$ is significantly smaller than the sum $\hat{H}_\text{rot} + \hat{H}_\text{cd}$, but it can be comparable or larger than $\hat{H}_{\text{cd}}$ and $\hat{H}_{\text{ss}}$. This implies that we do not take into account the perturbation $\hat{H}_H$ on the rotational structure, and we consider its impact on the fine level structure only. We note that the values of $\hat{H}_{\text{rot}}, \hat{H}_{\text{cd}}, \hat{H}_{\text{sr}},$ and $\hat{H}_{\text{ss}}$ depend on the angular momentum quantum numbers $J$ and $N$, so the degree of the level mixing for a given magnetic field strength varies within the fine structure (here, it decreases for higher rotational levels).

In other words, for two adjacent rotational levels the mixing occurs at a certain magnetic field strength, which can be deduced from measurements when the entire molecular band is modeled.
To obtain the eigenvalues of $H_{\text{mag}}$, we proceed in the same way as we did for the rotational level structure. Since $H_{\text{b}}$ is diagonal with respect to a rotational state ($\Sigma J$), we express $H_{\text{mag}}$ in the eigenfunctions of $H_{\text{b}}$,

$$
\mathcal{H}_{\text{mag}} = \langle b | \hat{H}_{\text{b}} | b \rangle + \langle b | \hat{H}_{\text{d}} | b \rangle,
$$

where the second term is non-diagonal with respect to the rotational state ($\Sigma J$). We limit our investigation of the molecular level structure to the first-order correction to the energy value $E_{\Sigma J}$, which is given by the second term in the right-hand part of Eq. (6). Thus, the Hamiltonian matrix $\mathcal{H}_{\text{mag}}$ will be specified as

$$
\begin{array}{cccc}
\beta & \gamma & \delta & \epsilon \\
\alpha & i & ii & iii & iv \\
\kappa & v & vi & vii & viii \\
\lambda & vii & viii & i & ii \\
\mu & viii & i & ii & iii \\
\nu & i & ii & iii & iv \\
\xi & ii & iii & iv & v \\
\eta & iii & iv & v & vi \\
\phi & iv & v & vi & vii \\
\theta & v & vi & vii & viii \\
\end{array}
$$

(7)

where the first column and the first row refer to the eigenfunctions in case $b$. The perturbation matrix has a trigonal form because, according to the first-order approximation, only the perturbation of the adjacent levels within the multiplet structure (fine structure) needs to be considered. Consequently, only the matrix elements forming the main and secondary diagonals are distinct from zero. They are (Berdyugina et al. 2005, Table A.4)

$$
i : E_{\Sigma J} + \mu_0 M H \frac{J(J + 1)}{J + 1} - \frac{1}{2} \left[ J(J + 1) + S(S + 1) - N(N + 1) \right],$$

$$ii : E_{\Sigma J} + \mu_0 M \frac{H}{J + 1} \times \frac{(J + 1)^2 - M^2}{(2J + 1)(2J + 3)} \left\{ \sqrt{(J + S + 1)(J + S + 2)} - N(N + 1) \right\},$$

where the quantities $\mu_0$, $M$, $H$, and $S$ are, respectively, the Bohr magneton, the magnetic quantum number, the magnetic field strength, and the total electron spin. The rotational quantum numbers $N$ and $J$ obey the relation $N = J + S$, where $S$ is the projection of $S$ on the inter-nuclear axis. Each rotational level $N$ consists of six fine-structure levels, denoted by $J = N + S/2, N + 3/2, \ldots, N - S/2$, owing to six possible projections of the total spin on the inter-nuclear axis. They are degenerate in the absence of an external magnetic field, while in the presence of a magnetic field each level $J$ splits into $2J + 1$ magnetic levels $M$.

By diagonalizing the Hamiltonian matrix (7) we obtain the eigenvalues $E_{\Sigma J M}$ and the eigenvectors $C_{\Sigma J M}$ of $H_{\text{mag}}$. In Sect. 3.2 we will make use of $C_{\Sigma J M}$ to calculate the strengths of the magnetic transitions.

Figure 1 shows splitting of the fine structure levels of the upper and lower rotational levels $N' = 4$ and $N'' = 3$, respectively\(^1\), depending on the magnetic field strength. At a weak magnetic field ($\lesssim 100$ G for $N' = 4$ and $\lesssim 10$ G for $N'' = 3$), the splitting is linear with the field strength and the interaction between the magnetic levels with the same quantum number $M$ is negligible (ZR). As the field strength increases, the magnetic levels spread out and the levels with the same quantum number $M$ repel each other. As a result, the magnetic levels form a blended structure in the PBR. Subsequently, at stronger magnetic fields ($\gtrsim 300$ kG for $N' = 4$ and $\gtrsim 15$ kG for $N'' = 3$), the $M$ levels are rearranged into a new multiplet structure corresponding to the six spin projections on the magnetic field direction (complete PBR).

Once the energy values $E_{\Sigma J M}$ for both the upper $N'\Sigma$ and the lower $N''\Sigma$ electronic states have been obtained, magnetic transition energies can be calculated as their difference. Transition wavelengths are then obtained by correcting for the air refraction index according to Edlén (1966). We note that in addition to the main branch transitions ($\Delta J = \pm 1$), we also consider here the satellite ($\Delta J = 0$) and forbidden transitions as discussed by Berdyugina et al. (2005).

3. Transition strengths

Intensity of a spectral line is proportional to the Einstein coefficient $A$, which in turn is proportional to the sum of squares of the electric dipole operator matrix elements $R_{J_f J_i}$,

$$A \propto \sum |R_{J_f J_i}|^2,$$

(8)

where the sum is taken over all levels contributing to the transition. Hence, our goal now is to compute the matrix elements $R_{J_f J_i}$ in the PBR.

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\(^1\) Throughout this paper, we use single and double primes to indicate upper and lower levels, respectively.
Following the discussion in Sect. 2, we first express the matrix elements \( R_{\J',\J''} \) in the case \( b \) basis functions, then transform them into case \( a \) to obtain the strengths of transitions in the ZR. Finally, we compute the strengths of transitions in the PBR using the eigenvectors of the magnetic Hamiltonian matrix (7).

### 3.1. ZR transition strengths

We employ the Born-Oppenheimer approximation to express the case \( a \) wave functions \( |\Lambda\Sigma\nu; v; \Omega J M\rangle \) as a product of the electronic \( |\Lambda\Sigma\nu\rangle \), vibrational \( |v\rangle \), and rotational parts \( |\Omega J M\rangle \) (e.g., Schadee 1978):

\[
|\Lambda\Sigma\nu; v; \Omega J M\rangle = |\Lambda\Sigma\nu\rangle |v\rangle |\Omega J M\rangle.
\]

Correspondingly, the right-hand part of Eq. (8) can be expressed as a product of three numbers,

\[
\sum_{\M'} |R_{\J',\J''}\rangle^2 = f_e q_{\J,\nu} \sum_{\M''} \Delta q_{\Omega J M; \J''}^2.
\]

where \( f_e \) is the electronic oscillator strength, \( q_{\J,\nu} \) is the Franck-Condon factor (both are constants for a given vibrational band), and \( \sum_{\M''} \Delta q_{\Omega J M; \J''}^2 \) is the H"{o}nl-London factor. The matrix elements \( q_{\Omega J M; \J''}^2 \) and \( \Delta q_{\Omega J M; \J''}^2 \) are called, respectively, strength and amplitude of a Zeeman component. It is the value of this amplitude that distinguishes the ZR (in both cases, \( a \) and \( b \)) from the PBR.

In the ZR, the matrix elements \( q_{\Omega J M; \J''}^2 \) can be further expressed as a product of two factors to separate the dependence on the quantum number \( \M' \):

\[
q_{\Omega J M; \J''}^2 = q_{\Omega J M; \J''}^2 q_{\nu; \J''}^2.
\]

Expressions for the amplitudes \( q_{\Omega J M; \J''}^2 \) and \( q_{\nu; \J''}^2 \) are given by Schadee (1978, Table 1).

Now we can obtain the matrix elements \( q_{\Omega J M; \J''}^2 \), represented in the case \( b \) wave functions. First, for the \( \M' \)-independent part of the transition amplitude we obtain

\[
q_{\Omega J M; \J''}^2 = \sum_{\Sigma} \sum_{\J''} C_{\Sigma; \J}^T \Delta q_{\Omega J M; \J''}^2 C_{\Sigma; \J''},
\]

where \( C_{\Sigma; \J} \) are the eigenvectors obtained by diagonalizing the Hamilton matrix (3), and \( C_{\Sigma; \J''}^T \) are transposed vectors. Indices \( i \) and \( j \) relate to different spin projections for the level with the total angular momentum quantum number \( \J; \Sigma_i \) and \( \Sigma_j \) take values \(-5/2, -3/2, \ldots, 5/2 \). In contrast to the ZR amplitude (13), the PBR amplitude (15) is no longer a product of two factors, but a linear combination of the ZR transition amplitudes.

### 3.2. PBR transition strengths

The transformation of the amplitudes from the ZR in case \( b \) to the PBR is carried out with the help of the eigenvectors \( C_{\Sigma_i J M} \) obtained by diagonalizing the Hamiltonian matrix (7),

\[
q_{\Omega J M; \J''}^P = \sum_{\Sigma_i} \sum_{\J''} C_{\Sigma_i J M}^T \Delta q_{\Omega J M; \J''}^P C_{\Sigma_i; \J''},
\]

where the indices \( i \) and \( j \) again relate to the different levels \( \J \) that form a fine structure of a rotational level \( \J; \Sigma_i \) and \( \Sigma_j \) take values \(-5/2, -3/2, \ldots, 5/2 \). In contrast to the ZR amplitude (13), the PBR amplitude (15) is no longer a product of two factors, but a linear combination of the ZR transition amplitudes.
In Figs. 3a, 3c, 3e, 3g, and 3i we show the Zeeman patterns for the transition in Eq. (14) in the ZR for the magnetic field strengths 0.001, 0.01, 0.1, 1, and 10 kG, respectively. The Zeeman pattern in Fig. 3a appears quite symmetric; in other words, the upper and lower $N$ levels of the molecule seem to be in the ZR at 0.001 kG. However, the corresponding Stokes $Q/I_c$ profile (Fig. 3b) is clearly asymmetric (see our discussion in Sect. 4.2). As the magnetic field strength increases, the pattern evolves rapidly, because the energy shifts no longer vary linearly, as Eq. (4) predicts. At stronger magnetic fields the shape of the pattern changes dramatically (Figs. 3 e, g, i); the Zeeman shifts change their sign (the pattern appears twisted), and the Zeeman component strengths alter significantly. In this example of the $R$ spectroscopic branch ($\Delta J = 1$), $\sigma^-$ and $\pi$ components become stronger than $\sigma^+$ and $\pi$ components in a strong field regime (cf., Fig. 3g). This is in contrast to the $P$ branch ($\Delta J = -1$), where $\sigma^+$ transitions become dominant (not shown). Thus, considering a great number of rotational transitions we expect a net polarization of the (0, 0) band of the CrH molecule.

4. Radiative transfer calculations
The theoretical line parameters calculated as described in the previous sections have been used to synthesize the Stokes profiles for both individual lines and the entire (0, 0) band with the code STOPRO (described by Solanki 1987; Frutiger et al. 1999; Berdyugina et al. 2003). The code assumes local thermodynamic equilibrium (LTE) and solves numerically a set of polarized transfer equations in a model atmosphere. Furthermore, it is assumed that a magnetized atmosphere acts on a spectral line (both atomic and molecular) through the Zeeman or Paschen-Back effect. The polarization arising from scattering in the atmosphere is neglected. Number densities of about 300 atomic and molecular species are calculated under the assumption of the chemical equilibrium as described in Berdyugina et al. (2003).

4.1. Atmosphere models and condensate opacities
We employ the original Drift-Phoenix atmospheric models calculated by Witte et al. (2009) for $T_{\text{eff}} = 2500$ K, 2000 K, and 1500 K. The solar abundances of the chemical elements and the surface gravity of log $g = 5.0$ is assumed. These three atmospheric models correspond roughly to the physical parameters of late M dwarfs, early and mid-L dwarfs, and hot Jupiters.

In atmospheres of cool brown dwarfs and hot exoplanets dust can considerably contribute to the total opacity. The Drift-Phoenix models, for example in contrast to the Phoenix model grid by Allard & Hauschildt (1995), employ the physics of dust formation and predict abundances of such condensate species as TiO$_2$, Al$_2$O$_3$, Fe, SiO$_2$, MgO, MgSiO$_3$, and Mg$_2$SiO$_4$. Since their significance as opacity sources increases for lower temperature and higher pressure, we want to estimate the effect of dust scattering and absorption on the CrH spectrum in the three selected models. To do this, we make use of an analytical solution of the Mie theory (Mie 1908).

The opacity $\kappa$ caused by the interaction of the radiation with dust particles is related to the interaction cross section $\sigma$ in the relation

$$\kappa = N\sigma,$$

where $\sigma = \sigma_{\text{sca}} + \sigma_{\text{abs}}$ is the sum of the cross sections due to scattering and absorption of the radiation, and $N$ is the number of the dust particles within a unit volume.

To calculate the interaction cross section $\sigma$, we employ an analytical expression obtained for scattering and absorption of electromagnetic waves by small (compared with the radiation wavelength) spherical particles (see, e.g., Landau & Lifshitz 1960),

$$\sigma = \frac{128\pi^5}{3} \left(1 + \frac{1}{2} \frac{k^2}{\lambda^2} \right) \frac{\alpha^6}{\lambda^4} + 24\pi \frac{a_0^2}{\lambda} \left(1 + \frac{4\pi^2}{15} \frac{\rho_{\text{eff}}}{\rho_0} \right),$$

where $a$ is the particle size (radius), $\lambda$ is the wavelength of the incident electromagnetic wave; $\epsilon$ and $\epsilon''$ are the relative dielectric function and its imaginary part of the particle material.

The Drift-Phoenix model grid provides the following deep-dependent dust parameters: average grain size, number of particles in the unit volume, and volume fraction for each dust species. Since we have the average particle size rather than the individual particle sizes of each species, we calculate the corresponding average (volume-fraction-weighted) relative dielectric function according to the effective medium theory (see, e.g., Bohren & Huffman 1998). Thus, Eq. (17) was evaluated using the average grain size and the average relative dielectric function.

We have found that for the chosen model atmospheres the opacity due to light scattering on the dust particles is significantly larger than light absorption by these particles at the CrH band wavelength. Furthermore, the total condensate opacity in Eq. (16) becomes considerable (at a level of a few percent) with the gas opacity only for the $T_{\text{eff}} = 1500$ K model and, respectively, for cooler atmospheres. We note that this condensate opacity contribution is already included in the atmospheric models used.

4.2. Stokes profiles
First we calculate the Stokes profiles for the individual lines at the magnetic field strengths 0.001, 0.01, 0.1, 1, and 10 kG. As an example, the inclination of the magnetic field $\gamma$ is set to 45$^\circ$ and the azimuth $\chi$ to 0$^\circ$ in all calculations presented in this paper. Hence, both Stokes $V$ and $Q$ are distinct from zero, while the Stokes $U$ vanishes. We normalize the Stokes parameters to the continuum intensity $I_c$.

Figures 2 and 3 show the Stokes profiles for the transition in Eq. (14) assuming the ZR and PBR, respectively. A remarkable feature in Figs. 3b, 3d, 3f, 3h, and 3j is that neither of the Stokes profiles vanishes. We normalize the Stokes parameters to the continuum intensity $I_c$.

Indeed, the deviation of the magnetic levels from their degenerate position depends linearly on the magnetic field strength as long as the sub-levels with the same magnetic quantum number do not come close to each other. Otherwise, the sub-levels with the same number $M$ begin to interact (repel), so that the linear dependence from the magnetic field strength, demonstrated by Eq. (4), is no longer guaranteed. Because the separation of the fine structure levels that split in the presence of a magnetic field is not equidistant, and some levels can lie very close together, as shown in Fig. 1, the ZR fails for such levels even at very small magnetic field strengths. Our careful investigation shows that the Stokes $Q/I_c$ is especially sensitive to the shifts of the magnetic transitions with respect to their frequency in the absence of an external magnetic field. In other words, even tiny deviations from Eq. (4) cause a non-symmetric Stokes $Q/I_c$.

Figures 4–6 show the Stokes profiles calculated for the entire (0, 0) band for $T_{\text{eff}} = 2500$ K, 2000 K, and 1500 K, respectively, in the wavelength range 8600–8700 Å at the magnetic field.
Fig. 3. Zeeman patterns and the corresponding Stokes profiles for the transition in Eq. (14) calculated for different magnetic field strengths.

strengths 0.5, 1, 3, 6, and 10 kG. The line list used includes about 500 CrH lines calculated using the theory given in Sect. 2. Very weak forbidden and satellite lines were sorted out from the list. Natural and pressure induced line broadening were included in
Fig. 4. Stokes profiles for the (0, 0) band of the $A^2\Sigma^+ - X^2\Sigma^+$ system of the CrH calculated for $T_e = 2500$ K at different magnetic field strengths. The spectra in the right column are calculated assuming a spectral resolution of 0.8 Å and a stellar rotation $v\sin i = 20$ km s$^{-1}$.

We have found that the Stokes $V/I_c$ spectra show significant signals at the field strengths considered. In general, polarization...
Fig. 5. Same as Fig. 4, but for $T_{\text{eff}} = 2000$ K.

signals increase for stronger magnetic fields from a few percent at 0.5 kG to more than 20% at fields of several kG when observed at high spectral resolution. In addition, the polarization signal arising from some lines or groups of lines (e.g., near 8625...
Fig. 6. Same as Fig. 4, but for $T_{\text{eff}} = 1500$ K.

or 8685 Å) shows a considerable asymmetry due to the Paschen-Back effect in these lines (cf. panels a and b in Figs. 4–6).

Furthermore, the satellite lines ($\Delta J \neq \Delta N$) gain in strength, while the main lines ($\Delta J = \Delta N$) become weaker (cf. Stokes $I/I_c$.)
in Figs. 4a, 4c, 4e, 4g, 4i). Thus, the polarization signal coming from a great number of satellite lines becomes comparable with that coming from the main lines. It reaches 25% in Stokes V/Iₜₕ and 15% in Stokes Q/Iₜₕ at 10 kG (cf. Figs. 4a, 4c, 4e, 4g, 4i). Moreover, while the magnetic field strength increases, the absorption intensity (Stokes I/Iₜₕ) decreases noticeably. This is caused by redistribution of the radiative energy between main and satellite lines.

In the strong field regime, the Stokes V/Iₜₕ undergoes a crucial alteration: it becomes asymmetric over a wide range of wavelengths (cf. panels f, h, and j in Figs. 4–6) leading to a large scale broad-band polarization, which can be detected even at a much lower spectral resolution. For instance, magnetic fields of 6 kG and stronger could be detected on very faint brown dwarfs using this feature.

5. Conclusions

We have explored the magnetic sensitivity of the (0, 0) vibrational band from the A³Σ⁺−X³Σ⁺ system of the CrH molecule and developed a new diagnostic for magnetic field measurements on very cool stars, brown dwarfs, and, potentially, on hot Jupiters.

Our quantum mechanical calculations of the energy level structure of the CrH (0, 0) band in the absence of an external magnetic field reproduce well the results of Ram et al. (1993) and are in a good agreement with the results obtained by Kleman & Uhler (1959) and Burrows et al. (2002).

Employing the approach by Berdyugina et al. (2005) for predicting the magnetic level structure of electronic states of any multiplicity in diatomic molecules, we have calculated for the first time the CrH level structure in the presence of an external magnetic field. Transition frequencies and their strengths are obtained in both the ZR and PBR.

We confirm the following general behavior of transition strengths in the PBR as the magnetic field strength increases (Berdyugina et al. 2005). First, satellite lines become stronger, while the main branch lines weaken. In addition, σ⁺ components (ΔM = 1) become stronger than σ− components (ΔM = −1) in the R branch, while the opposite is true for the P branch.

Our detailed study of a number of Stokes profiles of the individual CrH lines shows that even at weak magnetic fields (~1 G) Eq. (4) for the energy shifts in the ZR becomes inadequate for many of these lines. In general, the energy shifts due to an external magnetic field must be considered non-linear at any magnetic field strength, even though the deviations from the ZR are approaching zero at a very weak magnetic field.

A spectral synthesis of the CrH (0, 0) band at different magnetic field strengths (0.5–10 kG) has revealed the following general behavior of the spectra as the field strength increases:

- the band profile varies with the magnetic field strength;
- absorption in Stokes I/Iₜₕ decreases;
- polarization, particularly Stokes V/Iₜₕ, increases;
- Stokes profiles become asymmetric;
- integral polarization over the band is distinct from zero (broad-band polarization).

The asymmetric shape of the Stokes V/Iₜₕ is the main effect that provides the sensitivity to the magnetic fields on substellar objects. Based on our results, fields of ~100 G and stronger can be detected with existing instruments. This lower limit has two origins: i) at weaker magnetic fields the polarization degree is too small to be detected, and ii) most of lines in the band are not yet in the complete PBR to produce a considerable asymmetry in the Stokes V/Iₜₕ signal.

The calculations presented do not include a filling factor for magnetic regions on the stellar surface because it is not well known for brown dwarfs; however, its effect is linear. Taking into account a filling factor, which is a positive rational number between 0 and 1, will proportionally reduce the intensity of a polarization signal. However, this does not affect the asymmetry and the shape of the signal. Therefore, an analysis of the line (or band) profiles in the PBR can provide unambiguous estimates of both the magnetic field strength and its filling factor. This is in contrast to the ZR, when only a product of these two quantities can be inferred.

The wavelength range considered (8600–8700 Å) includes blends other than CrH lines (e.g., FeH and TiO lines). These have to be taken into account when evaluating and interpreting the observational data.

Overall, we conclude that the CrH A³Σ⁺ − X³Σ⁺ system is a very sensitive magnetic diagnostic for cool substellar objects, and we will employ it for our studies of brown dwarfs in the near future.

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