Abundances and search for vertical stratification in the atmospheres of four HgMn stars

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ABSTRACT

Using high-resolution, high-signal-to-noise ratio archival UVES (Ultraviolet-Visual Echelle Spectrograph) spectra, we have performed a detailed spectroscopic analysis of four chemically peculiar HgMn stars (HD 71066, HD 175640, HD 178065 and HD 221507). Using spectrum synthesis, mean photospheric chemical abundances are derived for 22 ions of 16 elements. We find good agreement between our derived abundances and those published previously by other authors. For the five elements that present a sufficient number of suitable lines, we have attempted to detect vertical chemical stratification by analyzing the dependence of derived abundance as a function of optical depth. For most elements and most stars, we find no evidence of chemical stratification with typical $3\sigma$ upper limits of $\Delta \log N_{\text{elem}}/N_{\text{tot}} \sim 0.1–0.2$ dex per unit optical depth. However, for Mn in the atmosphere of HD 178065 we find convincing evidence of stratification. Modelling of the line profiles using a two-step model for the abundance of Mn yields a local abundance varying approximately linearly by $\sim 0.7$ dex through the optical depth range $\log \tau_{5000} = -3.6$ to $-2.8$.

Key words: stars: abundances – stars: chemically peculiar – stars: individual: HD 71066 ($\kappa^2$ Vel) – stars: individual: HD 175640 (HR 7143) – stars: individual: HD 178065 (HR 7245) – stars: individual: HD 221507 ($\beta$ Scl).

1 INTRODUCTION

Chemically peculiar (CP) stars are A- and B-type stars exhibiting peculiar chemical abundances and slow rotation. With effective temperatures ranging between 10 000 and 15 000 K, the late B-type HgMn stars belong to the third group of CP stars defined by Preston (1974). They are characterized spectroscopically by large overabundances of Hg (possibly up to 6 dex; Heacox 1979; Cowley et al. 2006) and Mn (possibly up to 3 dex; Aller 1970). Overabundances greater than 2 dex of Be, Ga, Y, Pt, Bi, Xe, Eu, Gd, W and Pb are frequently observed in these stars, while He, N, Mg, Al, Ni and Zn often are underabundant by more than 0.5 dex (Takada-Hidai 1991). The elements C, O, Si, S, Ca, V, Cr and Fe usually show only modest peculiarities, with abundances within 0.5 dex of their solar abundances (classified as ‘normal type’ elements by Takada-Hidai 1991).

HgMn stars rotate slowly in comparison to ‘normal’ late-B stars, with $v \sin i < 100 \text{ km s}^{-1}$. Their average rotation velocity is estimated to be 29 km s$^{-1}$ (Abt, Chaffee & Suffolk 1972). These stars present a high rate of binarity: Gerbaldi, Floquet & Hauck (1985) estimate that 51 per cent are members of binary systems. Most of these binary systems have relatively small separations, with 41 per cent belonging to SB1 systems, while 59 per cent belong to SB2 systems. Some authors (Mathys & Hubrig 1995; Hubrig, Castelli & Wahlgren 1999; Hubrig & Castelli 2001) have reported the presence of weak magnetic fields in the atmospheres of some HgMn stars. However, attempts to confirm these claims for other HgMn stars have been unsuccessful (Landstreet 1982; Shorlin et al. 2002; Wade et al. 2006). In light of the lack of convincing evidence, we assume for the purposes of this study that HgMn stars are non-magnetic objects. Because of their high effective temperatures, the HgMn stars should not host hydrogen convective zones in their envelopes, and their low He abundances may reduce the importance of He convection zones as well. Indeed, Adelman (1994) showed that HgMn stars have small microturbulent velocities. Atmospheric velocity fields are estimated to be less than 1 km s$^{-1}$ for stars with $T_{\text{eff}}$ ranging between 10 200 and 12 000 K (Landstreet 1998).

The slow rotation and weak microturbulence of HgMn stars suggest that their atmospheres should be hydrodynamically stable. Atomic diffusion (Michaud 1970), resulting from the competition between local gravitational settling and radiative acceleration, may therefore play an important role in determining the chemical properties of their outer layers. A natural consequence of diffusion is the presence of non-uniform vertical distributions of chemical abundances (chemical stratification). Detecting and

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characterizing such stratification are the primary goals of this study.

Several investigations aimed at the detection of chemical stratification in atmospheres of HgMn stars were undertaken in the past. Savanov & Hubrig (2003) reported stratification of Cr in a sample of 10 HgMn stars. Their method involved the derivation of the abundance of Cr from eight lines of Cr II multiplet 30 located in the Stark-broadened wings of the Hβ line. According to these authors, the average chromium abundance from nine stars of their sample increases towards the core of Hβ and therefore presumably towards the upper atmosphere by 0.34 ± 0.12 dex. The difference of 0.2 dex in the average abundances between Cr I and Cr II in the HgMn star HD 175640, obtained by Castelli & Hubrig (2004), is interpreted by these authors as a confirmation of Cr stratification found by Savanov & Hubrig (2003). An increase of Mn towards the upper atmosphere of HgMn stars was reported by Alecian (1982) and Sigut (2001). Evidence of the stratification of Ga has also been published by Lanz et al. (1993).

Meanwhile, Dubaj et al. (2004) modelled Fe lines in the spectrum of the HgMn star HD 143807A shortwards and longwards of the Balmer jump. They found no conclusive evidence of Fe stratification. This suggests that if stratification of these elements is present in the atmospheres of HgMn stars, it is relatively weak (in comparison to that frequently observed in magnetic Ap stars, e.g. Ryabchikova, Leone & Kochukhov 2005).

Additional evidence for the presence of chemical stratification in HgMn stars has also been published. Sigut, Landstreet & Shorlin (2000) signalled the discovery of Mn II, P II and Hg II emission lines in the spectrum of the HgMn star 46 Aql. Sigut (2001) interpreted these emission lines as the result of interlocked non-local thermodynamic equilibrium (NLTE) processes in the presence of chemical stratification. Wahlgren & Hubrig (2000) also identified several emission lines of other elements, mostly Cr II and Mn II, in the spectra of some HgMn stars. They postulated that the emissions of the aforementioned elements in the red spectral region arise from a selective excitation process involving Lyα photon energies.

Very recently, Khalack et al. (2007, 2008) have detected stratification of several elements including Fe in Blue Horizontal Branch (BHB) stars, evolved objects with effective temperatures similar to those of HgMn stars. These authors found that the iron abundance increases towards the lower atmosphere in three BHB stars. They also reported nitrogen and sulphur stratification in the hot BHB star HD 135485. In this star, the abundances of those elements increase towards the upper atmosphere. The method used to detect vertical stratification in BHB stars in the aforementioned papers is applied here to HgMn stars.

The aim of this paper is to search for vertical stratification of elements in the atmospheres of HgMn stars. Our approach is to model a large number of absorption lines of many different elements and to examine the variation of the derived abundances as a function of optical depth. The mean abundances of the various elements analyzed will also be obtained.

### 2 OBSERVATIONS AND SPECTRAL REDUCTION

Spectra of the HgMn stars HD 71066 (κ² Vel), HD 175640 (HR 7143), HD 178065 (HR 7245) and HD 221507 (β Scl) were obtained from the European Southern Observatory (ESO) Science Archive. The Heliocentric Julian Date and program ID of these stars are summarized in Table 1. The spectra were obtained with the Very Large Telescope UV (ultraviolet)-Visual Echelle Spectrograph (UVES) on the UT2 unit telescope. This instrument covers a wide spectral region from λ = 3040 to 10000 Å. The slit widths for the two arms of the UVES were 0.4 arcsec for the blue and 0.3 arcsec for the red. The resultant resolving power is approximately λ/Δλ = 80000 in the blue and 110000 in the red. The recorded spectra exhibit gaps which are located between 5730–5840 and 8510–8660 Å.

Spectral reduction was performed using the UVES pipeline Data Reduction Software (version 2.2.0) for the 346 (304–388 nm) and 437 (373–499 nm) settings. Each order of these spectra was normalized using the IRAF ‘continuum’ procedure. The signal-to-noise ratio (S/N) after normalization ranges between S/N = 200 and 600. For the 580 (476–684 nm) and 860 (660–1040 nm) settings, we used a software provided by Tsymbal (private communication) for spectral reduction and normalization, because it works faster and has convenient interface.

Before adopting Tsymbal’s code, we applied it to reduce the 580 settings for two stars of our sample. The same procedure was also performed using the UVES pipeline. A comparison of the resulting reduced spectra yields excellent agreement. After spectral normalization, observed and synthetic line profiles were compared to determine the radial velocities of our sample of stars. The radial velocity obtained for each star is reported in Column 8 of Table 1.

### 3 SPECTRUM SYNTHESIS

In our analysis, we have adopted the stellar atmosphere parameters derived for the investigated stars by Hubrig et al. (1999) and Dolk, Wahlgren & Hubrig (2003). The adopted atmospheric and spectroscopic parameters, including the effective temperature, surface gravity and projected rotational velocity, are reported in Table 1. The atmosphere models used for spectrum synthesis are computed with ATLAS9 (Kurucz 1993). They are calculated with a solar metallicity and a microturbulent velocity ξ = 2.0 km s⁻¹. For atomic data, we used primarily the Vienna Atomic Line Data base² (VALD) (Martin, Fuhr & Weise 1988; Kurucz 1993, 1994; Kupka et al. 1999; Ryabchikova et al. 1999). We also extracted some phosphorus and mercury atomic data from the National Institute of Standards and Technology³ (NIST) (Martin, Zalubas & Musgrove 1985; ²http://vald.astro.univie.ac.at
³http://physics.nist.gov/PhysRefData/ASD/lines_form.html
Ralchenko et al. 2007). The NIST data base was used because the VALD does not provide a large number of P and Hg atomic data. Meanwhile, titanium atomic data from Pickering, Thorne & Perez (2001) have been used to compare the derived abundances from different sources. The lines and associated atomic data used in our analysis are summarized in Table A4 (online material – see Supporting Information).

To determine elemental abundances and to characterize the optical depth of line formation, we used the ZEEMAN2 local thermodynamic equilibrium (LTE) spectrum synthesis code (Landstreet 1988; Wade et al. 2001a). Although developed for spectrum synthesis of magnetic stars, this code is also able to reproduce stellar spectra in the non-magnetic case, including the effects of non-solar and vertically stratified abundances.

As shown by Adelman (1994) and Landstreet (1998), and implicitly confirmed in the study of Dolk et al. (2003), HgMn stars have small microturbulent velocities. In this study, line profiles were synthesized assuming $\xi = 0$ km s$^{-1}$, an assumption that will be verified a posteriori in Section 4. Since we desire high-precision results, we carefully pre-selected lines to avoid blends and misidentifications. We also only selected lines located within spectral orders longwards of the Balmer jump, in the 437 and 580 settings, for which $S/N \geq 300$. For our spectral analysis, each line profile of a particular species is fitted independently, while assuming a vertically uniform abundance of the element in the atmosphere.

Hyperfine and isotopic splittings are respectively important for Mn (Jomaron, Dworetsky & Allen 1999) and Hg (White et al. 1976; Smith 1997; Dolk et al. 2003) line profile synthesis in HgMn stars. When modelling these lines, we include the data of Mn hyperfine structure (hfs) and Hg isotopic splitting, when they are available. The data for Mn hyperfine structure are taken from Holt, Scholl & Rosner (1999), while those of the Hg isotopic splitting are from Dolk et al. (2003). These data are summarized respectively in Tables A1 and A2 (online material – see Supporting Information). Otherwise, lines are synthesized without these data. This leads us to ignore lines with a large reduced $\chi^2$, related to the difference between the observed and synthesized lines. The same procedure is used for all analyzed elements. Fig. 1 shows the Mn $\lambda$4206 line with the hfs data of the line taken into account and without it. These results show that the synthetic Mn $\lambda$4206 line is better fitted when the hfs data are taken into account, except for the fast-rotating star HD 221507. For this star, no significant difference is observed between the fits with and without hfs data. Nevertheless, the abundance obtained from the hfs data of this line for HD 221507 is closer to the mean abundance of Mn measured in the atmosphere of this star. The consideration of the isotopic composition of Hg $\lambda$3984 agrees with observed lines (see Fig. 2). Both the core and wings of this line are better fitted by taking into account the isotopic composition. The isotopic mixture of mercury for the peculiar Hg $\lambda$3984 line is presented in Table A3 (online material – see Supporting Information).

During the spectral synthesis, the continuous opacities for H, H$^-$ and He I bound-free and free–free transitions are computed. Photon scattering by free electrons and H I atoms are also taken into account in the opacity calculations, as well as line broadening due to the natural, Doppler and pressure broadenings. For more details, see Wade et al. (2001a). To fit a line, we simultaneously determine the element’s abundance $\log(N_{\text{ion}}/N_{\text{tot}})$, the stellar radial velocity $V_r$ and projected rotational velocity $v\sin i$ by minimizing the deviation between the simulated and observed line profiles. The optical depth of formation of the line is defined as the continuum optical depth $\tau_{5000}$ where the monochromatic optical

![Figure 1. The Mn $\lambda$4206 line observed (dots) for HD 71066, HD 175640, HD 178065 and HD 221507. This line is fitted by assuming a single-line component (dashed curve) and the hfs data (solid curve). The vertical lines represent the hfs line positions.](image-url)
Abundances and stratification in HgMn stars

Table 2. Effective temperature, luminosity, mass and age of studied stars. The approximate errors in effective temperatures and luminosities are, respectively, ±5 per cent and ±0.1 dex.

<table>
<thead>
<tr>
<th>HD</th>
<th>$T_{\text{eff}}$ (K)</th>
<th>log($L/L_{\odot}$) (dex)</th>
<th>M/$M_{\odot}$</th>
<th>log$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>71066</td>
<td>12 010</td>
<td>2.05</td>
<td>3.09</td>
<td>8.11</td>
</tr>
<tr>
<td>175640</td>
<td>11 958</td>
<td>2.08</td>
<td>3.21</td>
<td>8.16</td>
</tr>
<tr>
<td>178065</td>
<td>12 193</td>
<td>2.26</td>
<td>3.31</td>
<td>8.21</td>
</tr>
<tr>
<td>221507</td>
<td>12 476</td>
<td>1.88</td>
<td>3.07</td>
<td>6.09</td>
</tr>
</tbody>
</table>

Figure 3. The positions of HD 71066 (filled circle), HD 175640 (empty square), HD 178065 (filled square) and HD 221507 (empty circle) in the HR diagram assuming that their temperatures and luminosities are respectively known within ±5 per cent and ±0.1 dex. These positions are determined using the standard evolution track $Z = 0.02$ (Schaller et al. 1992).

Two stars studied here are SB1 and the others are non-binary (see Table 1). Since the contribution of the companion star for SB1 systems is not observed in the spectra, in this paper the SB1 stars are treated as single stars. The position in the Hertzsprung–Russell (HR) diagram of each star was determined photometrically. The effective temperature and surface gravity used are those from Table 1. The Johnson magnitude and Strömgren indices in the $ubvy$ photometric system are extracted from the General Catalogue of Photometric Data. Stars’ parallax values are extracted from the Hipparcos catalogue. The bolometric correction was calculated as in Balona (1994). The parameters such as log($L/L_{\odot}$), M/$M_{\odot}$ and log$\tau$ presented in Table 2 are determined using the evolutionary model calculations of Schaller et al. (1992) with $Z = 0.02$. The position of stars in the HR diagram [log($L/L_{\odot}$), log($T_{\text{eff}}$)] is presented in Fig. 3. As shown in this figure, all stars studied here belong to the main sequence. HD 221507 is the youngest star, while the others appear to be somewhat older.

4 AVERAGE ABUNDANCES

The mean abundances log($N_{\text{ion}}/N_{\text{tot}}$) measured in the atmospheres of the HgMn stars HD 71066, HD 175640, HD 178065 and HD 221507 are reported in Table 3. Several error sources have to be taken into account. For example, Khan & Shulyak (2007) show

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4 http://obswww.unige.ch/gcpd/gcpd.html
5 http://cadcwww.hia.nrc.ca/astrocat/hipparcos/
that by using an atmospheric model calculated with iron abundance [Fe/H] between 1 and 10 times its solar value, the derived abundances for elements can change by up to ±0.25 dex. Uncertainties in atmospheric parameters (T\text{eff} and log g) and in the atomic data can also modify abundances. NLTE effects may also play a role. The errors in the average abundances in Table 3 are obtained by calculating the standard deviation relative to the mean abundances for elements with a large number of lines. The uncertainties in the atmospheric parameters are not included in error calculations for these elements. For those species for which abundances are derived from a unique line, we took the formal error derived from the line profile fit. This error arises from the uncertainties in stellar atmospheric parameters and atomic data. The solar abundances used in this study are those used in Kurucz (1993) (see [A] of Table 3). In the same table, we present the solar abundances determined by Grevesse, Asplund & Sauval (2007) ([B]). The differences between these two sets of abundances are summarized in Column 8 ([C]) of Table 3 and are within ~0.2 dex.

### 4.1 HD 71066

The elements He, C, O, Mg, Si, P, S, Ca, Ti, Cr, Mn, Fe, Ni, Sr and Hg were investigated to determine their abundances in the atmosphere of HD 71066. The abundances are given in Column 2 of Table 3. Comparing these abundances to those of the Sun, the elements C, O, Si, Ca, Ti, Cr and Fe are within 0.5 dex of solar values. He, Mg and S are deficient by more than 0.5 dex, while P, Mn, Sr and Hg are overabundant by more than 0.5 dex.

Comparing the Cr abundance derived in this paper to the log(N/C)/N(H) = −6.23 ± 0.10 obtained by Savanov & Hubrig (2003), we find a good agreement. The enhanced Fe abundance of 0.11 dex obtained by Hubrig et al. (1999) is consistent with our measurement when taking into account the error bars. Concerning the abundance of Hg, no significant difference is observed between that derived from this study and the value reported by Dolk et al. (2003), namely, log(N(H)/N(H)) = −6.35 ± 0.26.

### 4.2 HD 175640

Chemical abundances of a large number of elements were determined for HD 175640 by Castelli & Hubrig (2004). In this paper, we diagnosed abundances of He, C, O, Mg, Si, P, S, Ca, Ti, Cr, Mn, Fe, Ni, Sr and Hg. The measured abundances are presented in Column 3 of Table 3. The elements C, O, Mg, Si, P and Ca show abundances within 0.5 dex of solar values. Helium, iron and nickel are underabundant by more than 0.5 dex, while Ti, Cr, Mn, Sr and Hg are enhanced by more than 0.5 dex.

The abundances obtained in this study are generally in agreement with those derived by Castelli & Hubrig (2004). However, our abundance of Ni is 0.37 dex lower than reported by those authors log(N(Ni)/N(H)) = −6.09 ± 0.16. The abundance log(N(Ni)/N(H)) = −6.5 ± 0.15 derived by Dolk et al. (2003) is close to that reported in this paper. Disagreements are observed between mean abundances derived from the analysis of neutral and singly ionized Hg (0.25 dex) lines. These differences are greater than the error bars associated with these abundances. Potential sources of these differences in the abundances inferred from different ions of an element, which are observed in several of the stars in this study, will be explored in Section 6.

Unlike the other stars presented in this paper, the spectrum of HD 175640 does not show any absorption (or emission) line at the location of the Hg II λ5677 line.

### 4.3 HD 178065

Lines of the elements He, C, O, Mg, Si, P, S, Ca, Sc, Ti, Cr, Mn, Fe, Ni, Sr and Hg were analyzed to determine their abundances in...
the atmosphere of HD 178065. The abundances of the elements C, O, Mg, Si, Ca, Sc, Ti, Cr, Fe and Sr are within 0.5 dex of their corresponding solar values. He, S and Ni are deficient by more than 0.5 dex, while P, Mn and Hg are enhanced by more than 0.5 dex.

The Cr abundance is close to the log(N_{Cr}/N_{H}) = −5.99 ± 0.10 obtained by Savanov & Hubrig (2003). A slight difference of 0.14 dex is obtained between the iron abundance derived in this study and the log(N_{Fe}/N_{H}) = −4.43 obtained by Hubrig & Castelli (2001). The mean abundance of Hg is in good agreement with log(N_{Hg}/N_{H}) = −6.65 ± 0.12 derived by Dolk et al. (2003).

As mentioned above, differences of 0.16 and 0.53 dex are respectively observed between the abundances of neutral and singly ionized states of both Mg and Hg.

4.4 HD 221507

For the more rapidly rotating (v sin i = 25 km s⁻¹) star HD 221507, we analyzed abundances of He, C, O, Mg, Si, P, S, Ca, Ti, Cr, Mn, Fe, Ni, Sr and Hg. We find that C, O, Mg, Si, S, Ti, Cr, Fe and Ni are within 0.5 dex of the solar abundance. Helium is the only underabundant element, while P, Ca, Mn, Sr and Hg are overabundant by more than 0.5 dex.

As observed in other stars, a difference (of 0.33 dex) is observed between abundances of neutral and singly ionized magnesium. The abundance derived from the Hg I 5460.731 line is enhanced by 1.02 dex with respect to that obtained from Hg II lines.

The Si abundance agrees very well with log(N_{Si}/N_{H}) = −4.5 ± 0.10 obtained from the UV analysis by Smith (1993). Our result for Mn abundance is consistent with the value log(N_{Mn}/N_{H}) = −4.5 ± 0.05) found by Jomaron et al. (1999) for this star. The iron abundance is in excellent agreement with log(N_{Fe}/N_{H}) = −4.35 ± 0.10 obtained by Smith & Dworetsky (1993). Although the Hg II abundance obtained by Dolk et al. (2003) differs by 0.21 ± 0.43 dex compared to our analysis, the values are still within the error bars.

5 STRATIFICATION

For elements exhibiting a sufficiently large number of suitable lines in our spectra, we have examined the dependence of their abundance versus the optical depth of line core formation. To evaluate vertical stratification, we have calculated the slope a of the abundance versus τ to by performing a linear fit to the data by the least squares method (LSM): log(N_{ion}/N_{tot}) = a log τ + b. The slopes a obtained for investigated elements are summarized in Table 4. For the confirmation of vertical stratification, we require that the following three conditions be met:

1. More than 10 lines, formed at different optical depths, must be present in the spectra.
2. The slope a should be statistically significant in comparison to the uncertainties.
3. The chemical abundance should change significantly (by more than ~0.5 dex) in the diagnosed range of optical depth.

This last condition is related to the fact that several factors such as errors in atmospheric parameters (T_{eff} and log g), NLTE effects and uncertainties in the model atmosphere can cause errors in abundance determination. For example, as discussed by Takada-Hidai (1991), an error of ±1000 K in T_{eff} causes errors in abundances derived from resonance lines by ±0.08 dex and [−0.19, +0.25] dex for lines with high excitation energy. Furthermore, an error of ±0.3 dex in log g introduces uncertainties in abundance calculations of ±0.1 dex. The uncertainty in the metallicity can account for an error of ~0.25 dex for abundance calculations (Khan & Shulyak 2007). Requiring a significant change in abundance helps to ensure that any abundance gradient is real and not generated by poorly quantified uncertainties.

5.1 HD 71066

In the spectrum of HD 71066, lines of Ti, Cr and Fe were studied for vertical stratification. We found that titanium lines are formed over a small range of optical depth, between log τ_{5000} ≈ −5.9 and −5.3 (see Fig. 4a). The slope a is relatively small compared to the formal uncertainty (see Table 4). We conclude that the titanium abundance does not show a significant dependence on optical depth for HD 71066.

As reported in Table 4, the linear fit of chromium abundance versus optical depth reveals a slope smaller than the error. No significant variation of Cr abundance in the optical depth range from log τ_{5000} ≈ −5.9 to −4.8 is detected (see Fig. 4b).

From log τ_{5000} ≈ −5.5 to −1, the iron abundance (derived from 22 Fe I, 134 Fe II and 2 Fe III lines) does not show a clear dependence on depth (see Fig. 4c). The LSM gives a slope which is marginally significant compared to the error (a ≈ 3σ_a). However, the variation of the abundance versus the optical depth is too weak to confidently conclude that Fe is stratified in the atmosphere of HD 71066.

5.2 HD 175640

In the spectrum of HD 175640, lines of S, Ti, Cr, Mn and Fe were studied for vertical stratification. With 15 S II lines, we were able to evaluate the possibility of stratification of this element in the atmosphere of HD 175640. As the slope a is lower than the corresponding error, sulphur shows no sign of stratification between log τ_{5000} ≈ −2.4 and −1.2 (see Fig. 5a).

The linear fit of Ti abundance versus the optical depth of HD 175640 reveals a weak (negative) slope. No significant variation of Ti abundance is observed in the optical depth range from log τ_{5000} ≈ −5.9 to −4.6 of HD 175640 in Fig. 5(b).

### Table 4. The slope a obtained from a linear regression of abundance versus optical depth: log(N_{ion}/N_{tot}) = a log τ + b.

<table>
<thead>
<tr>
<th>Element</th>
<th>HD 71066</th>
<th>HD 175640</th>
<th>HD 178065</th>
<th>HD 221507</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>a</td>
<td>n</td>
<td>a</td>
<td>n</td>
</tr>
<tr>
<td>S</td>
<td>+0.050 ± 0.061</td>
<td>28</td>
<td>-0.069 ± 0.025</td>
<td>41</td>
</tr>
<tr>
<td>Ti</td>
<td>+0.045 ± 0.065</td>
<td>19</td>
<td>-0.010 ± 0.046</td>
<td>45</td>
</tr>
<tr>
<td>Mn</td>
<td>-</td>
<td>-</td>
<td>+0.008 ± 0.038</td>
<td>62</td>
</tr>
<tr>
<td>Fe</td>
<td>+0.035 ± 0.012</td>
<td>158</td>
<td>+0.061 ± 0.018</td>
<td>57</td>
</tr>
</tbody>
</table>

*Note. The number of lines investigated is represented by n.*
Figure 4. Dependence of (a) Ti, (b) Cr and (c) Fe abundance in the atmosphere of HD 71066 against the line (core) formation optical depth calculated at $\lambda = 5000$ Å. The optical depth range between $-6$ and $-0.5$ is approximately associated to the physical depth from $\sim 0$ to $9.58 \times 10^3$ km. The filled circles, open circles and filled squares correspond to abundances derived from the neutral, singly and doubly ionized ions, respectively. The error bars correspond to formal uncertainties derived from the fits of line profiles. The linear fit of the data using the LSM $\log(N_{\text{ion}}/N_{\text{tot}}) = a \log \tau_{5000} + b$ is represented by the solid line.

45 Cr lines were studied in the spectrum of HD 175640, of which two are from the neutral ion. The chromium abundance presented in Fig. 5(c) does not show any variation with optical depth ranging between $\log \tau_{5000} \approx -5.9$ and $-3.6$. The slope $a \approx 0.2 \sigma_a$ is not statistically significant and is very weak. No stratification is thus observed.

Fig. 5(d) shows the variation of Mn abundance with optical depth between $\log \tau_{5000} \approx -4.1$ and $-1$. The slope obtained from the linear fit of Mn abundance in the atmosphere of HD 175640 is relatively weak and is statistically not significant ($a \approx 0.2 \sigma_a$). Manganese is not stratified in the atmosphere of HD 175640.

The investigation of 6 Fe I and 51 Fe II lines yields a weak slope (see Table 4) between $\log \tau_{5000} \approx -5$ and $-1.8$. We conclude that iron is not detectably stratified in the diagnosed optical depths of the atmosphere of HD 175640 (see Fig. 5e).

5.3 HD 178065

In the spectrum of HD 178065, lines of Ti, Cr, Mn and Fe were studied for vertical stratification. Fig. 6(a) shows that the titanium lines observed are formed in a small range of optical depth (between $\log \tau_{5000} \approx -5.9$ and $-4.8$). The slight slope (see Table 4) leads us to conclude that Ti is not significantly stratified in the diagnosed optical depths of HD 178065.

As presented in Table 4, the linear fit of Cr abundance in the investigated optical depth of HD 178065 reveals a negative slope. However, this slope is weaker than the associated error ($a \approx 0.6 \sigma_a$). The chromium abundance does not show a systematic dependence on optical depth from $\log \tau_{5000} \approx -5.9$ to $-4.2$ (see Fig. 6b).

The abundance obtained from 5 Fe I and 89 Fe II lines also does not reveal a significant variation at optical depths between $\log \tau_{5000} \approx -5$ and $-2$ (see Fig. 6d). The slope $a$ is relatively small (see Table 4), and we conclude that iron is not detectably stratified in the atmosphere of HD 178065 in the diagnosed optical depths.

In contrast to the behaviour observed for Ti, Cr and Fe, Fig. 6(c) shows a strong increase of the Mn abundance with optical depth.
Secondly, we analyzed Mn lines using ATLAS9 atmosphere models with $T_{\text{eff}} = 12,000$ K, calculated with different metallicities from $\pm 0.1$ to $\pm 1$ dex. These metallicities correspond to both deficiencies (negative) and enrichments (positive) of metals relative to the Sun denoted by $[+0.0]$. The Mn abundances determined with different metallicities are not very different in comparison to those obtained with the solar metallicity model. The slopes of the regression of Mn abundance versus optical depth increase when metallicity increases. As an example, for $[-1.0]$, the slope obtained is $+0.240 \pm 0.066, +0.289 \pm 0.060$ for $[+0.0]$ and $+0.326 \pm 0.058$ for $[+1.0]$. These remain both statistically and quantitatively significant for all investigated metallicities.

Thirdly, we have analyzed the Mn lines using a model atmosphere computed with a different code: an LTE model obtained with the PHOENIX code (Hauschild, Baron & Allard 1997). This model is calculated by assuming $T_{\text{eff}} = 12,193$ K, log $g = 3.54$ while using the abundances given in Table 3. Mean abundances derived from Mn i and Mn ii lines are, respectively, $-5.17 \pm 0.18$ and $-5.08 \pm 0.23$. No disagreement is observed between abundances derived from Mn ii lines using the two different atmosphere models, while for Mn i the difference is within the error bars. The slope $a = +0.296 \pm 0.061$ obtained from the regression of Mn versus the optical depth using the Phoenix atmosphere model is close to those obtained with ATLAS9.

We therefore conclude that the Mn stratification remains statistically significant for both ATLAS9 and Phoenix model atmospheres, at all investigated effective temperatures and metallicities. As the variation of Mn abundance is substantial, we can confidently claim that Mn is stratified in the atmospheric layers of HD 178065.

Following the detection and modelling of stratification in magnetic Ap stars by Babel (1994), vertical abundance profiles were subsequently parametrized assuming a simple two-step (or two-zone) model (Wade et al. 2001b; Ryabchikova, Wade & LeBlanc 2003). In an attempt to characterize the vertical distribution of Mn in the atmosphere of HD 178065, we have selected the best line profile candidates to fit simultaneously using synthetic profiles computed assuming the two-step model. We assume an abundance $\log(N_{\text{ion}}/N_{\text{tot}})$ deep in the atmosphere, below optical depth $\tau_1$. The abundance in the upper atmospheric layers (above optical depth $\tau_2$) is given by $\log(N_{\text{ion}}/N_{\text{tot}}) + \Delta \epsilon$, where $\Delta \epsilon$ is the difference in abundance between the deeper and upper zones. The atmospheric layers between $\tau_1$ and $\tau_2$ (the ‘transition zone’) are assumed to have abundances given by a linear interpolation between that of the deep layers and of the upper layers. In our fitting of the line profiles, this method operates with six free parameters $[\log(N_{\text{ion}}/N_{\text{tot}}), \Delta \epsilon, \tau_1, \tau_2, V_r$ and $\psi$] which are simultaneously fitted to all selected lines. More details concerning this method are provided by Khalack et al. (2007).

We simultaneously analyzed the selected Mn line profiles, and the results of the line synthesis are presented in Table 5 and the derived stratification profile is represented in Fig. 8. Fig. 7 shows some Mn ii lines formed at different optical depths. These line profiles are fitted by assuming an uniform abundance (dashed curve) and a stratified abundance (solid curve). The reduced $\chi^2$ for the uniform and stratified models are summarized respectively in Columns 7 and 8 of Table 5. As represented in Fig. 8, the abundance of Mn increases deep in the atmosphere of HD 178065 by $0.74 \pm 0.21$ dex in the optical depth range between $-3.79 \pm 0.20$ and $-2.92 \pm 0.10$. The abundance of Mn is larger in the lower atmosphere as compared to the shallower atmosphere. The Mn transition zone observed in HD 178065 dominates the stratified profile. This profile differs strongly from those of Ap stars where the transition

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**Figure 6.** Same description as in Fig. 4 but for (a) Ti, (b) Cr, (c) Mn and (d) Fe for HD 178065, but where we have added 3σ regression curves (dash) for Mn.

The slope $a \approx 5\sigma_a$ is statistically significant, and the inferred Mn abundance increases by $\sim 0.7$ dex in the diagnosed range of optical depth between $\log \tau_{5000} \approx -4.5$ and $-2.5$. Therefore, Mn satisfies all three of our criteria required for the detection of stratification.

To confirm the presence of Mn stratification, several tests have been undertaken. We began by verifying the effect on the derived stratification of modifying $T_{\text{eff}}$ and the metallicity.

First, we determined the abundance and stratification of Mn using ATLAS9 model atmospheres with different effective temperatures centred on the adopted effective temperature of HD 178065 (11 000, 11 500, 12 500 and 13 000 K). Neutral Mn lines are sensitive to the change of $T_{\text{eff}}$. A difference of $\pm 1000$ K (three to four times larger than our estimate of the uncertainty associated with $T_{\text{eff}}$) changes the abundance by approximately $\pm 0.6$ dex. In contrast, the difference is less than $\sim 0.2$ dex for Mn ii lines. At each adopted effective temperature, the slopes remain statistically significant for Mn i (larger than $3\sigma_a$) and Mn ii (larger than $4\sigma_a$), as well as for all Mn lines (at least $4\sigma_a$). The increase of the Mn abundance is also large enough (more than 0.5 dex) to be considered numerically significant.
zone has a very small extent (Ryabchikova et al. 2005). The radial \( V_r \) and rotational \( v \sin i \) velocities are similar to those adopted from the individual line analysis discussed in Section 3.

### 5.4 HD 221507

In the spectrum of HD 221507, lines of Ti, Cr, Mn and Fe were studied for vertical stratification. The linear fit of the abundance derived from 14 Ti lines reveals a large slope. However, this slope is heavily weighted by a few lines which are concentrated close to the log \( \tau_{5000} \approx -5.9 \). Also, the lines studied here are formed in a small range of optical depth from log \( \tau_{5000} \approx -5.9 \) to \( -5 \) (see Fig. 9a). Therefore, it is not possible to conclude from these results that Ti is stratified.

From log \( \tau_{5000} \approx -5.9 \) to \(-4.5\), the Cr abundance does not show dependence on depth (see Fig. 9b). The slope obtained \((a \approx 0.9\sigma_a)\) is not statistically significant. Chromium does not show any stratification in the studied optical depth range.

From MnI and MnII lines, we obtain no significant slope from the regression. Manganese does not appear to be stratified in the optical depths between log \( \tau_{5000} \approx -4.4 \) and \(-2.2 \) in HD 221507 (see Fig. 9c).

The investigated Fe lines are formed between log \( \tau_{5000} \approx -5.9 \) and \(-2.3 \) (see Fig. 9d). The linear fit of iron abundance reveals a weak slope (see Table 4) that is not statistically significant.

### 6 DISCUSSION AND CONCLUSION

In this paper, we determined the abundances of 16 elements in the atmospheres of the HgMn stars HD 71066, HD 175640, HD 178065 and HD 221507. Mean abundances of elements, relative to the Sun, are presented for each star in Fig. 10. The abundances of most of these elements had never been determined in the past for these stars. However, for the elements previously investigated and discussed in Section 4, the mean abundances obtained are generally in good agreement with past studies.

As expected (see Fig. 10), He is underabundant while Mn and Hg are overabundant in all the investigated stars. Phosphorus, which is generally overabundant in HgMn stars, is solar in HD 175640. Titanium and chromium, which are typically present in their solar abundances in HgMn stars, are strongly enhanced in the atmosphere of HD 175640. We also note that the more rapidly rotating star HD 221507 presents the highest abundances of Sr and Hg of our sample.

We have examined the dependence of the mean abundances of each element as a function of the physical parameters \( T_{\text{eff}} \) and \( v \sin i \). As the results we obtained are derived from only four data points with highly clustered \( T_{\text{eff}} \) and \( v \sin i \), we decided to use data from published papers. We used Ryabchikova (1998) for P and Sr, Smith & Dworetsky (1993) for Cr and Smith (1997) for Hg. We can definitely confirm the correlation of the abundance of Cr versus \( T_{\text{eff}} \) (see Fig. 11), with a large dispersion of abundances for \( T_{\text{eff}} \geq 13\,000 \,\text{K} \) (Smith & Dworetsky 1993). However, we cannot confidently affirm any trends of the abundance of P with respect to \( T_{\text{eff}} \), and Sr and Hg with respect to \( v \sin i \).

The synthesis of elements represented by a large number of lines in our spectra allowed us to track vertical stratification of elements in the atmospheres of these stars. As shown in Section 5, an attempt to detect stratification for Ti, Cr and Fe in HD 71066, S, Ti, Cr, Mn and Fe in HD 175640, Ti, Cr, Mn and Fe in HD 178065 and Ti, Cr, Mn and Fe in HD 221507 was undertaken. Most of these elements’ abundances do not show any significant tendencies in the diagnosed optical depths.

The study of Savanov & Hubrig (2003) that reports the vertical stratification of Cr in 10 HgMn stars is performed in the spectral region 4812.34–4864.33 Å. They did not evaluate the depth of line formation. The spectra used in our study do not appear to be of sufficient quality to confidently detect the chromium abundance variation claimed by those authors. Therefore, it is difficult to compare their data with the results presented here.

An interesting finding is that Fe increases slightly (\( \sim 0.25 \,\text{dex} \)) with optical depth for the four stars (HD 71066, HD 175640, HD 178065 and HD 221507). This systematic trend for Fe might suggest stratification. However, the increase in abundance is too small to confidently conclude to the detection of stratification.

Strong evidence of Mn stratification in the atmosphere of HD 178065 is observed. The abundance of Mn increases by \( \sim 0.7 \,\text{dex} \) in diagnosed optical depth range. The simultaneous fit of lines assuming a two-step model also shows that Mn increases towards the deep atmosphere. If such stratification can be confirmed (for Mn or for other elements), this would provide important new quantitative constraints on diffusion in the atmosphere of HgMn stars. Such observed vertical stratification profiles could then be compared to theoretical model atmospheres which include elemental stratification such as those of Hui-Bon-Hoa, LeBlanc & Hauschildt (2000).

Differences observed between the abundance of neutral and ionized Mg ions are greater than 0.1 dex in HD 178065 and HD 221507. The largest discrepancies are observed between Mg I and Hg II in HD 175640, HD 178065 and HD 221507, where they are greater than 0.25 dex. This result remains the same even when not using the isotopic data for the Hg II λ 3984 line shown in Fig. 2. The fact that differences are observed for some stars and not for others led us to conclude that they may not be only attributed to uncertainties surrounding atomic data and/or small number of lines observed. The sources of these differences might be attributed to NLTE effects. Takada-Hidai (1991) showed that neutral ions are more affected by NLTE corrections than ionized ones in HgMn stars. However, NLTE corrections are smaller for the heavier ions (Takada-Hidai 1991).

Basing on the aforementioned paper, the magnitudes of NLTE corrections for some elements are \(-0.4 \,\text{dex} \) for Be II, from \(-2.00 \,\text{dex} \) to \( 0.00 \,\text{dex} \) for O I, \(-0.02 \,\text{dex} \) for Mg I, \(-0.04 \,\text{dex} \) for Mg II, from \(-0.45 \,\text{dex} \) to \(+0.70 \,\text{dex} \) for Ca II, \(+0.20 \,\text{dex} \) for Sr II and from \(-0.3 \,\text{dex} \) to \(+0.3 \,\text{dex} \) for Ba II. The corrections are given to indicate possible uncertainties in our results. After the discovery of Ga ionization anomalies in HgMn stars by Smith (1995), this author suggested stratification as the possible cause of these anomalies.
Abundances and stratification in HgMn stars

Figure 7. A sample of manganese lines observed (dots) for HD 178065. These lines are fitted by assuming an uniform abundance (dashed curve) and a stratified one (solid curve). The optical depth of line core formation is also given for each line.

In this paper, we reported for the first time the detection of Mn stratification in an HgMn-type star. However, the attempt to detect element stratification failed for most of the investigated elements. The investigation of HgMn stars could be complicated by several physical processes, which should be taken into account. Sigut (2001) suggested that the emission lines present in spectra of some HgMn stars are photospheric in nature. After the first discovery of Mn II emission lines in the spectra of the HgMn star HD 186122 (46 Aql)
Figure 8. The manganese stratification profile in the atmosphere of HD 178065.

Figure 9. Same description as in Fig. 4 but for (a) Ti, (b) Cr, (c) Mn and (d) Fe for HD 221507.

Figure 10. The catalogue of the abundances measured in the atmospheres of HD 71066, HD 175640, HD 178065 and HD 221507. These abundances are relative to the Sun, which is represented by the horizontal line.
The abundance of Cr against the effective temperature of several HgMn stars. The filled circles and the filled squares correspond respectively to the abundances derived in our study and those of Smith & Dworetsky (1993).

by Sigut et al. (2000), emission lines of several elements were also discovered (Wahlgren & Hubrig 2000). These authors observed titanium and chromium emission lines in the spectra of HD 71066, HD 175640 and HD 178065. As interpreted by Sigut (2001), the presence of emission lines is caused by interlocked NLTE effects in the region where the element is stratified. When doing LTE analysis such as done in this paper, the presence of such emission lines increases the uncertainty of their results.

Possible presence of spots and weather in the atmosphere of HgMn stars also add complications to the investigation of these stars. The variability of Hg ii λ3984 in the spectra HgMn stars is interpreted as inhomogeneous distribution of this element on the stellar surface (Adelman et al. 2002; Kochukhov et al. 2005). To properly study this line, isotopic consideration is critical. Several line profile variations are found in other HgMn stars, such as the strong line variations of Pt, Hg, Sr, Y, Zr, He and Nd in the eclipsing binary AR Aur by Hubrig et al. (2006).

We note here the absence of the mercury line (Hg ii λ5677) in the spectrum of HD 175640. This means that the conditions required for the formation of the absorption or the emission Hg ii λ5677 line are not met in the specific layers. On the other hand, it could also mean that the absorption line is formed in deeper layers, but the emission line forms in upper layers and fills in the line. This adds a constraint to the hypothesis that NLTE effects probably act in the atmosphere of HD 175640. In future studies, improvements must be brought to the characterization of the optical depth of line formation and inclusion of NLTE effects. The study of spectral regions covering the UV and infrared may allow to diagnose deeper and shallower regions of the atmospheres. Also, spectra with a high S/N and accurate atomic data might permit us to detect weaker stratification.

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SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this article:

Table A1. The hyperfine structure of the Mn II $\lambda$4206 line taken from Holt et al. (1999).
Table A2. The isotopic composition of the Hg II $\lambda$3984 line taken from Dolk et al. (2003).
Table A3. Isotopic mixture of the Hg II $\lambda$3984 line for the studied stars.
Table A4. Atomic data used for the spectral synthesis.

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