Accuracy of atmospheric parameters of FGK dwarfs determined by spectrum fitting

T. Ryabchikova1*, N. Piskunov2, Yu. Pakhomov1, V. Tsymbal3, A. Titarenko1,4, T. Sitnova1,4, S. Alexeeva1, L. Fossati5, L. Mashonkina1

1 Institute of Astronomy, Russian Academy of Sciences, Pyatnitskaya 48, 119017 Moscow, Russia
2 Department of Physics and Astronomy, Division of Astronomy and Space Physics, Uppsala University, Box 516, 751 20 Uppsala, Sweden
3 Physical Technical Institute, Crimea Federal University, Vernadsky’s Avenue 4, 95007 Simferopol, Crimea
4 Department of Astronomy, Physics Faculty, M.V.Lomonosov Moscow State University, GSP-1, 1-2 Leninskie Gory, 119991 Moscow, Russia
5 Space Research Institute, Austrian Academy of Sciences, Schmiedlstrasse 6, A-8042 Graz, Austria

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ABSTRACT
We performed extensive tests of the accuracy of atmospheric parameter determination for FGK stars based on the spectrum fitting procedure Spectroscopy Made Easy (SME). Our stellar sample consists of 13 objects, including the Sun, in the temperature range 5000–6600 K and metallicity range $-1.4 – +0.4$. The analysed stars have the advantage of having parameters derived by interferometry. For each star we use spectra obtained with different spectrographs and different signal-to-noise ratios (S/N). For the fitting we adopted three different sets of constraints and test how the derived parameters depend upon the spectral regions (masks) used in SME. We developed and implemented in SME a new method for estimating uncertainties in the resulting parameters based on fitting residuals, partial derivatives, and data uncertainties. For stars in the 5700–6600 K range the best agreement with the effective temperatures derived by interferometry is achieved when spectrum fitting includes the H$_\alpha$ and H$_\beta$ lines, while for cooler stars the choice of the mask does not affect the results. The derived atmospheric parameters do not strongly depend on spectral resolution and S/N of the observations, while the uncertainties in temperature and surface gravity increase with increasing effective temperature, with minima at 50 K in $T_{\text{eff}}$ and 0.1 dex in log $g$, for spectra with S/N=150–200. A NLTE analysis of the Ti I/Ti II and Fe I/Fe II ionisation equilibria and abundances determined from the atomic C I (NLTE) and molecular CH species supports the parameters we derived with SME by fitting the observed spectra including the hydrogen lines.

Key words: stars: fundamental parameters – stars: abundances – methods: observational – methods: data analysis – stars: individual: Procyon, HD 49933, v And, β Vir, HD 149026, HD 209458, Sun, HD 1461, 61 Vir, HD 69830, HD 189733, δ Eri, HD 10395

1 INTRODUCTION
The discovery of exoplanets, the results of the Kepler space mission, and the expected huge amount of information from the Gaia mission have attracted special attention to the problem of accurately determining atmospheric parameters for a large number of stars. Accurate atmospheric parameters are essential for exoplanet studies to best derive the planet parameters (e.g., mass, radius, and equilibrium temperature) and to characterise their atmospheres. The Gaia mission will provide unprecedented positional and proper motion measurements for about one billion stars in our Galaxy and throughout the Local Group and, thus, accurate parallaxes needed to improve stellar surface gravities. Accurate kinematic properties together with accurate atmospheric parameters will allow one to constrain Galactic stellar populations and chemical evolution more accurately than ever been possible before. This space mission is supported by ground-based spectroscopic observations within the Gaia-ESO Survey (GES) project (Gilmore et al. 2012)...

* E-mail: ryabchik@inasan.ru

1 http://sci.esa.int/gaia/
nation of atmospheric parameters for the GES benchmark and program stars was discussed by Smiljanic et al. (2014) and Heiter et al. (2015). Determining atmospheric parameters for a large number of stars requires the development of automatic procedures capable of quickly producing reliable results. Following this reasoning, several different automatic spectral analysis procedures were developed during the last decades. All of them are essentially based on either the fit of synthetic to observed spectra or the measurement and analysis of equivalent widths (EW) of metal lines. For F-, G-, and K-type stars and for both techniques various authors claimed a very high accuracy of the order of 20–40 K in effective temperature, 0.02–0.06 dex in surface gravity, and 0.02–0.05 dex in metallicity derived in the spectral analysis with S/N \( > 150 \)–400 (Valenti & Fischer 2005; Sousa et al. 2006). Nevertheless, it has been shown that analysis of the spectra obtained using the same spectrograph, but in different observational runs may lead to results that differ in effective temperature by 70 K, though the spectra had been analysed using the same technique (e.g., see Table 3 of Gonzalez et al. 2010). The situation is getting worse, when analysing the same technique (e.g., see Table 3 of Gonzalez et al. 2010). The situation is getting worse, when analysing the same spectra with different techniques. Torres et al. (2012) compared atmospheric parameters derived by the spectrum fitting and the EW techniques, and for stars hotter than 6000 K they found that the values from the spectrum fitting method are systematically lower compared to those from the EW method. Smiljanic et al. (2014) showed the presence of a large spread in the atmospheric parameters derived by thirteen different groups using different techniques for 11 bright F-, G-, and K-type main-sequence stars (the Gaia FGK benchmark stars). The Gaia spectral library collects spectra for these stars (Blanco-Cuaresma et al. 2014). Most of them have S/N>200. The average difference between the recommended effective temperatures and gravities and individual determinations from the six different spectrum fitting and seven EW methods ranges between 46 K and 186 K and 0.09 dex and 0.28 dex, respectively. The largest discrepancies are probably caused by a systematic component, which is usually difficult to accurately estimate. It is worth noting, the difference in parameters reaches 100 K in effective temperature and 0.16 dex in surface gravity even between the two groups using a common technique based on EW. The analysis of the results for all groups of FGK dwarfs led to a method-to-method dispersion of \( \pm 150 \) K in \( T_{\text{eff}} \), \( \pm 0.30 \) dex in log \( g \), and \( \pm 0.10 \) dex in [Fe/H]. The situation is even worse for giant and metal-poor stars. These examples show how far the actual uncertainties may differ from the adopted ones.

This paper presents an extensive analysis of the uncertainties in atmospheric parameter determination made with the fitting procedure Spectroscopy Made Easy (SME, Valenti & Piskunov 1996). The investigated stars and their spectra are described in Section 2. A short description of the SME tool, the implemented modifications, and the error analysis are given in Section 3. We tested the best recommended atmospheric parameters and their uncertainties in Section 4 by inspecting the Ti i/Ti ii and Fe i/Fe ii ionisation equilibrium and element abundances from the atomic C i and molecular CH lines. Section 5 summarises our conclusions.

2 OBSERVATIONS

For the spectroscopic analysis we choose the 13 main-sequence (MS) stars including the Sun (Table 1) in the 4900–6600 K temperature range and with metallicity between [Fe/H] = -1.5 and +0.3 dex. All the stars, except HD 149026, have, at least, one interferometric determination of radius and effective temperature. Our methods of atmospheric parameter determination were first applied to the Sun that is the only star with a directly measured effective temperature and surface gravity.

Spectra of the program stars were obtained with different spectrographs. Most data were extracted from the following archives: the UVES/VLT and HARPS/3.6 m spectrographs at ESO3, the ELODIE/1.93-m spectrograph at the Observatoire de Haute Provence, and the ESPoDOns spectrograph at the Canada-France-Hawaii Telescope (CFHT). Spectra of \( \beta \) Vir and HD 103095 were obtained with the FOCES spectrograph at 2.2-m telescope of the Calar Alto Observatory (Fuhrmann 1998). One of the spectra of 61 Vir was obtained with the Hamilton Echelle Spectrograph attached to the Shane 3-m telescope of the Lick Observatory (Sinić et al. 2013). Spectra of few stars, including that of the Sun reflected from Gaumyeode, were obtained with the HiReS/Keck spectrograph (Howard et al. 2014). All the retrieved spectra have been reduced with the standard reduction pipelines available for each spectrograph. For the Sun, we used the National Solar Observatory (NSO) solar flux spectrum (Kurucz et al. 1984).

For each star we tried to find an archival spectrum with as high as possible signal-to-noise ratio (S/N). All observed spectra have a resolving power R>40 000 with a peak resolution of R\~{}110 000 obtained with the UVES and HARPS spectrographs. Most ESPoDOns spectra have been collected in spectropolarimetric mode, which provides spectra with a resolution of R = 65 000 instead of R = 80 000 reached with the “object only” mode. Rather large range of S/N and R for the collected spectra allows us to thoroughly explore the uncertainties in the atmospheric parameters as a function of the basic spectral characteristics. Detailed information on the spectral resolution and S/N along with the program ID is given in Table 1 for each analysed spectrum. Continuum rectification was performed using low-order polynomials, giving special attention to the regions covered by the H\( \beta \) and H\( \alpha \) lines, which play a crucial role in the atmospheric parameter determination.

3 ATMOSPHERIC PARAMETER DETERMINATION

We determined the stellar atmospheric parameters with the SME package (Valenti & Piskunov 1996). The tool SME was designed to perform an analysis of stellar spectra using spectrum fitting techniques in a consistent and reproducible way. The fit can be done in several spectral intervals simultaneously. The data points can further be masked to avoid observational defects and/or spectral regions with uncertain
Table 1: List of investigated stars and spectrographs used to collect the spectra. The first column lists also the resolving power of each spectrum. Column 2 gives the average S/N calculated in the three wavelength ranges discussed in Sect. 3.1. The atmospheric parameters derived with SME are given in columns 4, 5, and 6, while columns 7 and 8 list the atmospheric parameters derived from interferometry. The last four columns indicate the spectroscopic atmospheric parameters from the literature and their source. The uncertainties are given in parentheses.

| Observations | SME | Interferometry | Other spectroscopy |
|--------------|-----|----------------|--------------------|
| Spectrograph | S/N | T eff,K | log g | [M/H] | T eff,K | log g | [M/H] | Reference |
| Resol. power | mask | (7) | (8) | (9) | (10) | (11) | (12) | |
| Program ID   |     |       |       |       |       |       |       |         |
| (1) | (2) | (3) | (4) | (5) | (6) | (7) | (8) | (9) | (10) | (11) | (12) |
| HD 61421 = Procyon |
| UVES | 500 m6 | 6615(89) | 3.89(33) -0.05(05) | 6597(18) | 4.00(02) | Bovajian et al. (2013) | 6485(80) | 3.89(09) | 0.01(07) | Bruntt et al. (2010) |
| (80000) | m5 | 6579(37) | 3.84(37) -0.07(05) | 6573(42) | 4.00(02) | Bovajian et al. (2013) | 6593(50) | 3.90(01) | 0.02(03) | Gonzalez et al. (2010) |
| UVES POP | m4 | 6690(89) | 3.85(25) -0.02(05) | 6563(33) | 4.00(02) | Bovajian et al. (2013) | 6660(95) | 4.05(06) | 0.02(09) | Doyle et al. (2013) |
| (Bagnulo et al. 2003) | VF | 6602(112) | 3.98(17) -0.11(07) | 6562(32) | 4.00(02) | Bovajian et al. (2013) |
| HD 49933 |
| HARPS | 350 m6 | 6582(115) | 4.00(52) -0.48(09) | 6635(90) | 4.21(05) | Bovajian et al. (2013) | 6570(60) | 4.28(06) | -0.44(03) | Bruntt (2009) |
| (110000) | m4 | 6653(143) | 4.08(33) -0.44(08) |  |  |  | 6600(80) | 4.15(05) | -0.47(07) | Sitnova et al. (2015) |
| 076.C-0279 | VF | 6512(120) | 4.13(20) -0.57(10) |  |  |  |  |  |  |  |
| ESPaDONs | 300 m6 | 6546(100) | 4.04(52) -0.50(08) |  |  |  |  |  |  |  |
| (65000) | m4 | 6706(149) | 4.22(33) -0.41(08) |  |  |  |  |  |  |  |
| 05bf6a | VF | 6567(107) | 4.17(15) -0.54(08) |  |  |  |  |  |  |  |
| HD 9826 = υ And |
| ESPaDONs | 700 m6 | 6145(39) | 4.06(12) 0.05(02) | 6177(25) | 4.13(03) | Bovajian et al. (2013) | 6170(48) | 4.00(08) | 0.08(04) | Gonzalez et al. (2010) |
| (65000) | m4 | 6323(38) | 4.25(12) 0.15(03) | 6027(26) | 4.10(02) | Bovajian et al. (2013) | 6239(37) | 4.19(03) | 0.14(03) | Gonzalez et al. (2010) |
| 05BO2 | VF | 6292(27) | 4.22(04) 0.07(03) |  |  |  |  |  |  |  |
| ELODIE | 250 m6 | 6132(84) | 4.03(30) 0.14(06) |  |  |  |  |  |  |  |
| (42000) |  |  |  |  |  |  |  |  |  |  |
| HiReS | 200 m4 | 6354(103) | 4.33(28) 0.13(07) |  |  |  |  |  |  |  |
| (69000) | VF | 6278(76) | 4.20(09) 0.08(07) |  |  |  |  |  |  |  |
| HD 102870 = β Vir |
| ESPaDONs | 1000 m6 | 6122(27) | 4.07(10) 0.10(02) | 6054(13) | 4.11(04) | Bovajian et al. (2013) | 6050(80) | 3.98(07) | 0.12(07) | Bruntt et al. (2010) |
| (65000) | m4 | 6232(27) | 4.18(09) 0.18(02) |  |  |  | 6111(28) | 4.00(05) | 0.16(02) | Gonzalez et al. (2010) |
| 05bf6a | VF | 6214(21) | 4.13(03) 0.12(02) |  |  |  | 6180(36) | 4.15(05) | 0.21(03) | Gonzalez et al. (2010) |
| FOCES | 250 m6 | 6122(85) | 4.02(30) 0.13(11) |  |  |  | 6170(80) | 4.14(04) | 0.11(06) | Sitnova et al. (2015) |
| (60000) | m4 | 6242(81) | 4.14(23) 0.21(06) |  |  |  |  |  |  |  |
| VF | 6218(75) | 4.10(13) 0.14(04) |  |  |  |  |  |  |  |  |
| (1)  | (2)    | (3)    | (4)    | (5)    | (6)    | (7)    | (8)    | (9)    | (10)   | (11)   | (12)   | (13)   |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| HD 149026 |
| ESPaDOns  | 200 m6  | 6074(82) | 4.18(29) | 0.24(06) | 6131 | 4.22(05) | 0.31(03) | Gonzalez et al. (2010) |
| (65000) | m4 6239(74) | 4.33(23) | 0.33(06) | 6103(66) | 4.27(05) | 0.24(07) | Torres et al. (2012) |
| 07ah28a | VF 6183(62) | 4.22(09) | 0.27(05) |  |
| HiReS  | 300 m4  | 6285(95) | 4.46(31) | 0.37(07) | 6137(85) | 4.23(17) | 0.28(07) |  |
| (69000) | VF 6137(85) | 4.23(17) | 0.28(07) |  |
| HD 209458 |
| ESPaDOns  | 1250 m6  | 6033(28) | 4.28(08) | -0.05(02) | 6092(103) | 4.28(10) | Bovajian et al. (2015) |
| (80000) | m4 6160(27) | 4.39(07) | 0.02(07) | 6118(25) | 4.50(04) | 0.03(02) | Santos et al. (2008) |
| co-added | VF 6145(15) | 4.41(02) | -0.05(02) | 6065(50) | 4.42(04) | 0.00(05) | Torres et al. (2008) |
| HARPS  | 300 m6  | 6010(74) | 4.23(22) | -0.08(05) |  |
| (110000) | m4 6116(65) | 4.35(16) | -0.01(04) |  |
| co-added | VF 6112(45) | 4.38(06) | -0.07(04) |  |
| UVES  | 300 m6  | 5987(70) | 4.25(23) | -0.09(05) |  |
| (110000) | m4 6106(67) | 4.38(17) | -0.02(05) |  |
| co-added | VF 6093(42) | 4.38(06) | -0.07(04) |  |
| HiReS  | 170 m4  | 6174(140) | 4.43(39) | 0.02(10) |  |
| (69000) | VF 6181(103) | 4.42(18) | -0.03(08) |  |
| ELODIE  | 170 m6  | 5980(123) | 4.19(40) | -0.08(09) |  |
| (42000) | m4 6152(120) | 4.36(33) | 0.02(09) |  |
| Sun  |
| Atlas  | 1000 m6  | 5757(24) | 4.41(06) | -0.03(02) | 5777 | 4.44 |  |
| (550000) | m4 5787(22) | 4.44(05) | -0.01(02) |  |
| HiRes  | 200 m4  | 5778(67) | 4.43(18) | -0.00(06) |  |
| (690000) | VF 5792(42) | 4.46(06) | -0.06(04) |  |
| HD 1461 |
| UVES  | 270 m6  | 5732(55) | 4.31(17) | 0.14(05) | 5386(60) | 4.23(05) | von Braun et al. (2014) |
| (115000) | m4 5764(51) | 4.35(16) | 0.16(04) | 5751(50) | 4.33(07) | 0.18(04) | Ramírez et al. (2009) |
| 076.B-0055 | VF 5798(38) | 4.36(06) | 0.13(04) | 5765(44) | 4.41(06) | 0.18(03) | Valenti & Fischer (2005) |
| HiRes  | 150 m4  | 5805(80) | 4.41(23) | 0.18(07) |  |
| (690000) | VF 5837(53) | 4.40(09) | 0.16(06) |  |
| ELODIE  | 150 m6  | 5757(92) | 4.31(28) | 0.12(08) |  |

5 05BC16, 05BH32A, 06AC12, 06AH20A
6 076.C-0878, 183.C-0972, 074.C-0012, 60.A-9036
7 265.C-5038, 067.C-0206, 077.C-0379, 087.D-0010, 088.C-0879
Table 1: continue.

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| (42000) | m4 | 5815(89) | 4.36(25) | 0.17(08) |   |   |   |   |   |   |   |   |
| HD 115617 = 61 Vir

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| ESPaDons | 700 | m6 | 5567(27) | 4.42(07) | -0.03(02) | 5538(13) | 4.42(03) | von Braun et al. (2014) | 5558(19) | 4.36(03) | -0.02(01) | Sousa et al. (2008) |
| (65000) | m4 | 5595(23) | 4.45(06) | -0.01(02) |   |   |   |   |   |   |   |   |
| 11AC04 | VF | 5588(12) | 4.46(02) | -0.06(02) |   |   |   |   |   |   |   |   |
| Lick | 200 | m4 | 5559(69) | 4.42(18) | -0.02(06) |   |   |   |   |   |   |   |
| (60000) | VF | 5617(54) | 4.45(09) | 0.02(07) |   |   |   |   |   |   |   |   |

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| ESPaDons | 650 | m6 | 5422(43) | 4.47(12) | -0.04(04) | 5394(62) | 4.46(04) | Tanner et al. (2015) | 5402(28) | 4.40(04) | -0.06(02) | Sousa et al. (2008) |
| (65000) | m4 | 5436(39) | 4.49(10) | -0.03(04) |   |   |   |   |   |   |   |   |
| 14AF14 | VF | 5419(23) | 4.48(05) | -0.09(04) |   |   |   |   |   |   |   |   |
| HiRes | 200 | m4 | 5424(60) | 4.58(17) | 0.04(07) |   |   |   |   |   |   |   |
| (69000) | VF | 5415(45) | 4.49(10) | -0.09(07) |   |   |   |   |   |   |   |   |

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| ESPaDons | 1500 | m6 | 5049(10) | 4.53(03) | -0.02(01) | 4875(43) | 4.56(03) | Bovajian et al. (2015) | 5051(47) | 4.53(08) | -0.03(05) | Sousa et al. (2006) |
| (65000) | m4 | 5076(8) | 4.58(03) | -0.00(01) |   |   |   |   |   |   |   |   |
| co-added8 | VF | 5016(6) | 4.64(02) | -0.05(01) |   |   |   |   |   |   |   |   |
| HiRes | 180 | m4 | 5056(68) | 4.53(18) | -0.02(10) |   |   |   |   |   |   |   |
| (69000) | VF | 5019(62) | 4.57(16) | -0.06(09) |   |   |   |   |   |   |   |   |

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| HARPS | 500 | m5 | 5040(28) | 3.73(07) | 0.05(03) | 4955(30) | 3.77(03) | Bovajian et al. (2013) | 5150(51) | 3.89(08) | 0.13(04) | Sousa et al. (2008) |
| (110000) | m4 | 5037(21) | 3.73(06) | 0.05(02) |   |   |   |   |   |   |   |   |
| 60-A-9036 | VF | 5053(15) | 3.87(05) | 0.05(03) |   |   |   |   |   |   |   |   |
| HiRes | 200 | m4 | 5052(48) | 3.76(14) | 0.07(06) |   |   |   |   |   |   |   |
| (69000) | VF | 5085(27) | 3.78(07) | 0.05(05) |   |   |   |   |   |   |   |   |

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| FOCEs | 150 | m6 | 4958(46) | 4.52(17) | -1.38(10) | 4771(18) | 4.56(03) | Bovajian et al. (2013) | 5130(65) | 4.66(06) | -1.26(08) | Sitnova et al. (2015) |
| (60000) | m4 | 4944(43) | 4.48(15) | -1.36(09) | 4831(25) | 4.58(04) | Bovajian et al. (2013) | 5110(80) | 4.66(10) | -1.35(05) | Fuhrmann (1998) |
| VF | 4904(27) | 4.49(07) | -1.52(06) |   |   |   |   |   |   |   |   |

8 06AF34, 06bd01, 06bf27, 07AC27
atomic/molecular data. Since the first version of SME, a number of modifications and improvements were made to the original version. They include new molecular and negative hydrogen ion partition functions and equilibrium constants in the equation-of-state (EOS) package, a new algorithm for solving the radiative transfer (the Fournier algorithm was replaced with a Bezier attenuation operator scheme; see de la Cruz Rodríguez & Piskunov 2013), and a modification of the interpolation procedure in the model atmosphere grid. Further details of the current version of SME can be found in the upcoming paper by Piskunov & Valenti (2013). In this work, we use the sme_443 package version.

The SME package is working with various grids of model atmospheres: ATLAS9 and ATLAS12 (Castelli & Kurucz 2004), MARCS (Gustafsson et al. 2008) for dwarfs, and Llnmodels (Shulyak et al. 2004). All these models assume plane-parallel one-dimensional (1D) geometry and the local thermodynamical equilibrium (LTE). Our calculations were performed with the MARCS models.

### 3.1 Choice of spectral windows

For stars hotter than 6000 K Torres et al. (2012) found that the SME and SPC (Stellar Parameter Classification, Buchhave et al. 2012) spectrum fitting procedures produce systematically lower effective temperatures and surface gravities compared to the results based on the EW measurements and analysis of the Fe i excitation and Fe i/Fe ii ionisation equilibria. These authors used spectral intervals similar to those adopted by Valenti & Fischer (2005), which include the 5163–5190 Å spectral region and few small windows in the 6000–6180 Å wavelength range. The first region contains the Mg ii lines, whose extended wings are sensitive to surface gravity variations in G- and K-type stars, while being less sensitive for F-type stars. Most of the other lines belong to Fe-peak elements. The strong Ca i lines in the 6100–6180 Å spectral range were not included in the fitting.

For the present analysis we have selected four spectral regions to be fitted by SME: 4485–4590 Å, 5100–5200 Å, 5600–5700 Å, and 6100–6200 Å. They include the spectral features, which are sensitive to a variation in different atmospheric parameters. The 4485–4590 Å spectral range includes numerous Ti i-Ti ii and Fe i-Fe ii lines with accurate laboratory data, making this region very sensitive to gravity variations. The 5100–5200 Å spectral range covers the molecular C2 (C2 Swan system) and MgH lines, which are strongly temperature dependent in cool stars. The 5167–5183 Å and 6100–6200 Å intervals include the Mg ii and strong Ca i lines with Lorentz wings induced by the collisional broadening sensitive to gravity variations.

However, in spectra of stars hotter than the Sun the line broadening due to collisions with hydrogen atoms (i.e., Van der Waals broadening) becomes smaller and the molecular lines disappear. Therefore, the degeneracy between different atmospheric parameters increases, resulting in biases in temperature, gravity, and metallicity. To solve this problem, one needs to use features that are strongly sensitive to one of the parameters, for example the hydrogen Balmer line wings, which are temperature indicators in F-, G-, and K-type stars (Fuhrmann et al. 1998; Cayrel et al. 2011). When dealing with hydrogen lines, the major problem is a correct continuum normalisation, in particular for high-resolution echelle spectra. We included the Hβ (4820–4880 Å) and Hα (6520–6580 Å) lines in the SME fitting, excluding the ±1.5 Å regions around the line centers. Also the cores of the strong Mg i and Ca i lines were not considered in the fit because of departures from LTE.

The SME mask was used to remove unidentified features and spectral lines with uncertain atomic parameters. The mask was verified using the solar atlas and then applied to all stars. For individual observations the mask was further corrected to exclude regions showing spectral defects (e.g., dead pixels), remaining cosmics, and telluric lines, particularly in the wings of the Hα line. The use of new/extended spectral regions was made possible thanks to a new version of the Vienna Atomic Line Database (VALD3, Ryabchikova et al. 2015) that includes a new extensive set of atomic line calculations by R. Kurucz and his collection of molecular lines. Also the new data for the C2 Swan system from Brooke et al. (2013) were included. For lines of Sc, V, Mn, Co, and Cu the full hyperfine structure (HFS) was taken into account (see references on Kurucz’s web site). Hydrogen line profiles were calculated with the code described in Barklem et al. (2000), and references therein. For comparison purposes we also run SME using the mask adopted by Valenti & Fischer (2003), including their atomic and molecular line parameters.

We analysed the stars using the four following masks:

(i) the four regions covering the metal lines (hereafter, m4),
(ii) m4 plus the Hα line (hereafter, m5),
(iii) m4 plus the Hα and Hβ lines (hereafter, m6), and
(iv) the mask used by Valenti & Fischer (2003, hereafter, VF)

In total, our masks consist of 331 spectral intervals from six large regions. The masks are available at Table A1 in Appendix. For each star the best fit solution was searched for a set of six free parameters: effective temperature $T_{eff}$, surface gravity log $g$, metallicity [M/H], microturbulence velocity $V_{mic}$, macroturbulence velocity $V_{mac}$, and projected rotational velocity $V_{rot} \sin i$. The final $T_{eff}$, log $g$, and [M/H] values are listed in Table 4.

### 3.2 Error analysis

The newly implemented method for estimating uncertainties in the free parameters within SME is based on the fit residuals, partial derivatives, and data uncertainties. We construct a cumulative distribution using all data pixels for a given free parameter $p$. This distribution describes the fraction of spectral pixels that requires a change of $\delta p$ or less to achieve a "perfect" fit. Examples of such distributions for different parameters in HD 1461 (UVES spectrum) are given in Figure A. The position of the data pixels on the z-axis is estimated from the residuals and the partial derivative of the synthetic spectrum over the particular parameter. Probability density distributions for such uncertainty estimate have

9. http://vald.astro.univie.ac.at/vald3/php/vald.php
10. http://kurucz.harvard.edu/atoms.html
11. http://www.astro.uu.se/~barklem/hilinop.html
The fact that the central part is not too far from a Gaussian confirms that we can still apply normal distribution standard deviation concept for assessing parameter uncertainties for a bulk of observations; this is anyway more easily done with a cumulative distribution because it does not require an a priori knowledge of the bin size and of the clipping range for the central part. The final parameter uncertainty includes both systematic uncertainty (model limitations) and the observational one. While our method still ignores the cross-talk between different parameters it shows massive improvement over the uncertainties based on the covariance matrix (also evaluated by SME). The uncertainties derived from the diagonal of the covariance matrix are effectively a projection of the observational errors onto the model parameter space using partial derivatives averaged over all data pixels. For high S/N observations the contribution of the observational errors is negligible in comparison to model limitations, and the resulting uncertainty estimates are unrealistically small. The mathematical background of the new approach can be found in the upcoming paper by Piskunov & Valenti (2015).

Note that the estimated median values in Fig. 1 are close to, but not exactly matching, the SME result. The reason is that the error estimate procedure presented here is not taking into account the degeneracy/correlation between parameters. The final estimated errors are listed in Table 1. The starting points used for the SME’s optimisation algorithm were taken close to the previously published parameters. We check the robustness of the convergence algorithm implemented in SME by performing 1000 runs for the ESPaDONS spectrum of HD 69830 (mask4) with initial guesses for \( T_{\text{eff}} \), \( \log g \), and \([M/H]\) equally spaced across the volume: \([4972:5872; 4.015:4.915; -0.4945:0.4055]\). The solutions were found to converge within 3 K in \( T_{\text{eff}} \), 0.005 dex in \( \log g \), and 0.002 dex in \([M/H]\).

The influence of the continuum rectification on the final atmospheric parameters was checked in the following way. For three stars of different effective temperature and grav-
Figure 2. Example of density distributions for the same parameters as in Figure 1. Best fit Gaussians of the central peaks are shown by gray colour. Dashed and dash-dotted lines indicate the median and the ±σ range estimated from the cumulative distributions.

ity, HD 9826, HD 69830, and HD 23249, we run SME with the m4 and m6 masks using observations with the continuum rectification independently made by three of us, i.e. T. Ryabchikova, Yu. Pakhomov, and L. Fossati; we did not find any systematic bias in our parameter determinations caused by the different continuum placements. The differences in the derived gravity and metallicity did not exceed 0.03 dex and 0.01 dex, respectively. For the effective temperature, a maximum difference of 20 K was obtained for HD 69830, but this value is smaller than the uncertainty.

A close look at the results presented in Table 1 shows that the spectral resolution of the observations does not significantly affect the derived parameters: the overall difference in the effective temperature, surface gravity, and metallicity does not exceed the error bars. For the effective temperature, a maximum difference of 20 K was obtained for HD 69830, but this value is smaller than the uncertainty.

We further checked a dependence of the derived parameters and their uncertainties on the spectrum quality (i.e., S/N). We took the ESPaDOns spectrum of HD 69830 and introduced an additional white noise component in order to decrease the S/N. In the SME analysis we used the common initial parameters for each spectrum. The results are shown in Fig. 4. The $T_{\text{eff}}$ values derived from different spectra agree within ±20 K, while the log $g$ values range between 4.38 and 4.53, not centering at log $g = 4.49$ that was derived from the spectrum with the highest S/N. A similar behaviour was also found for the metallicity. For the effective temperature, surface gravity, and metallicity SME finds solutions in a range much smaller than the typical error estimates. Our conclusion is therefore that the S/N should not have a great influence on the derived parameters even though the error bars increase dramatically with decreasing S/N.

For high S/N spectra the derived uncertainty is driven by model limitations (systematic error). In our case these
Figure 3. Uncertainty in the effective temperature (top) and surface gravity (bottom) as a function of the effective temperature. The solid line shows the quadratic polynomial fit to the data.

systematic errors are ±20-30 K in \( T_{\text{eff}} \), ±0.05-0.08 dex in \( \log g \), and ±0.02 dex in \([\text{M/H}]\), if we consider spectra with \( S/N \geq 1000 \). We also checked the possible effect of the model grids used in SME on the derived parameters. For a few, including the Sun, we run SME with ATLAS9 and LLmodels grids of stellar atmospheres. LLmodels give effective temperatures of 10-15 K higher than MARCS models for stars cooler than the Sun and of 10-20 K lower for hotter stars. Surface gravity changes by less than +0.02 dex for stars with \( T_{\text{eff}} > 5700 \) K and by +0.03–+0.05 dex for cooler stars. Metallicity is practically unaffected. With ATLAS9 models the corresponding changes are −30 K to +50 K in \( T_{\text{eff}} \) and −0.03 dex or less in surface gravity. All these changes lie within the error limits obtained with MARCS models. The comparison for the solar spectrum allows us to evaluate possible offsets, because the Sun is then only star with a direct, model independent determination of the effective temperature and surface gravity. We obtain possible offsets of −20 K, −0.03 dex, −0.03 dex for effective temperature, surface gravity and metallicity. All these values are compatible with the corresponding errors given by spectrum fitting.

4 ANALYSIS OF THE DERIVED ATMOSPHERIC PARAMETERS

We compare here the obtained atmospheric parameters with those present in the literature and based on interferometric and spectroscopic methods.

4.1 Comparison with the interferometric parameters

From interferometric data, the effective temperature is derived from the measured angular diameter and bolometric flux. The interferometric \( T_{\text{eff}} \) for Procyon, HD 49933, \( \upsilon \) And, \( \beta \) Vir, \( \delta \) Eri, and HD 103095 were extracted from Bovajian et al. (2013, and references therein). For other stars the corresponding data were taken from Bovajian et al. (2013, HD 209458 and HD 189733), von Braun et al. (2014, HD 1461 and 61 Vir), and Tanner et al. (2013, HD 69830). These values are listed in Table 1. Bolometric fluxes for all stars were calculated using the spectral energy distribution (SED) fitting code presented by van Belle et al. (2008). For the solar atmosphere we used the canonical parameters Christensen-Dalsgaard et al. (1996). Three stars have two or more independent measurements of the angular diameter (see Bovajian et al. 2013, and references therein).

For Procyon the angular diameter measurements lead to effective temperatures that agree within the quoted uncertainties. For the other two stars, with quoted uncertainties of ~25 K or less, the interferometric temperatures differ by 60 K to 150 K. While the effective temperature is a measured parameter, though indirect, the surface gravity is only inferred from the stellar radius measured with interferometry and the star’s mass, derived on the basis of evolutionary tracks. There are two stars, HD 209458 and HD 189733, for which the surface gravities have been derived from the binary solution obtained from the analysis of the transit and radial velocity curves of their planets Bovajian et al. (2013). We estimated the uncertainty in \( \log g \) assuming a 5 % un-
Figure 5. Differences between the SME and interferometric $T_{\text{eff}}$ (left) and $\log g$ (right) values as a function of the interferometric effective temperature. The differences are shown on the basis of the adopted masks for the SME analysis: m6/m5 (top), m4 (middle), and VF (bottom). The Sun is shown by a filled circle.

The only outlier is HD 1461: we believe that its measured angular diameter is too high resulting in lower effective temperature. Plenty of different modern methods of parameter determination provide results for HD 1461 which agree with each other, but not with the interferometric ones (see the PASTEL catalogue of stellar parameters; Soubiran et al. 2010). When excluding this particular star, the average temperature differences between the SME and interferometric values are 50 K, 80 K, and 120 K for m6, VF, and m4 masks, respectively. When considering instead only stars hotter than 5100 K, the corresponding average differences are 18 K, 60 K, and 110 K. In all comparisons the standard deviation in $T_{\text{eff}}$ varies from 60 K (m6) to 90 K (m4, VF). The difference in $\log g$ varies...
from -0.04 dex (m6) to +0.04 dex (m4, VF) with a standard deviation of 0.08 dex.

4.2 Comparison with other spectroscopic studies

Table I lists the atmospheric parameters derived in the literature using various spectroscopic methods, together with their sources, and Fig. 6 displays the differences in temperature, gravity, and metallicity between the SME analysis with the m6/m5 masks and the corresponding literature data. No significant trends and offsets are found. Using the VF and m4 masks leads to an overestimation of all three parameters for the hottest stars. Instead, using the mask including the hydrogen lines (m6/m5) removes this offset.

The average difference between the stellar parameters derived with SME (m6/m5 masks) and other spectroscopic methods was found to be 12±66 K for the effective temperature, 0.04±0.12 dex for the surface gravity, and 0.04±0.04 dex for the metallicity. It may be considered as method-to-method dispersion. The dispersion values correspond to the error estimates derived by SME for S/N=200.

4.3 Micro- and macroturbulent velocities

When deriving atmospheric parameters for a large number of stars by means of a spectrum fitting technique, both micro and macroturbulent velocities \( V_{\text{mic}} \) and \( V_{\text{mac}} \) are usually not directly estimated, but are either fixed (e.g., \( V_{\text{mic}} \) in Valenti & Fischer 2005) or estimated on the basis of analytical approximations (e.g., \( V_{\text{mac}} \) in Torres et al. 2012). Our SME analysis allowed us to derive both these parameters, with the corresponding error bars, for each star. Figure 7.
shows stellar \( V_{\text{mic}} \) and \( V_{\text{mac}} \) parameters as a function of the effective temperature.

In general, our measurements agree with those given by previous studies. The analytical expression by Bruntt et al. (2010) for \( V_{\text{mic}} \) seems to fit our data in a reasonable way, while using a fixed value of \( V_{\text{mic}} \) would be inappropriate for stars hotter than 6000 K. The analytical formula proposed by Valenti & Fischer (2005) underestimates \( V_{\text{mac}} \) for the hottest stars, while it reasonably represents our measurements for stars cooler than 5500 K. The Gray (1984) formula seems to be a good approximation for \( V_{\text{mac}} \) in stars hotter than the Sun.

5 ABUNDANCES

We test the atmospheric parameters obtained with the m6 mask by inspecting abundances from two ionisation stages for Ti and Fe and from the atomic C i and molecular CH species. The elements Ti and Fe were chosen because of the large number of lines with precise laboratory atomic data available at optical wavelengths. For Ti i and Ti ii we used the homogeneous set of laboratory transition probabilities by Lawler et al. (2013) and Wood et al. (2013), while for Fe i and Fe ii the line parameters were extracted from the third version of the VALD database (Ryabchikova et al. 2013). We also considered the C abundance derived from atomic C i and molecular CH lines that are known to be sensitive to \( T_{\text{eff}} \) variations. Line parameters were also extracted from VALD. While the C2 Swan system lines were included in fitting procedure, for abundances we employed the CH lines in 4200-4400 Å region because these lines are strong and are easily measured in spectra of all stars of our program. Unblended C2 lines suitable for abundance determinations practically disappeared in spectra of stars hotter than 6000 K. A list of the lines used for the abundance determination, together with the adopted line parameters, is given in Table 2 (online material). In total we used 8 lines of C i in the visible and near IR regions, 8 bands of CH, 21 lines of Ti i, 10 lines of Ti ii, 73 lines of Fe i, and 28 lines of Fe ii.

Element abundances from the atomic lines were calculated based on the non-local thermodynamic equilibrium (NLTE) line formation. To solve the coupled radiative transfer and statistical equilibrium (SE) equations, we used a revised version of the DETAIL code (Butler & Giddings 1983). The update was described by Mashonkina et al. (2011). In the atmospheric parameter range covered by the analysed stars, departures from LTE are negligible for Ti i and Fe ii lines and small for lines of Ti ii and Fe i lines and lines of C i in the visible spectral range. The molecular CH lines are considered to be free of NLTE effects. For Ti i and Ti ii the NLTE calculations were performed using a comprehensive model atom constructed by Sitnova et al. (2013). For cool stars the main source of uncertainty in NLTE calculations for Ti i (as well as for Fe i) is poorly known inelastic collision with hydrogen atoms. In this study they are treated employing the Drawinian (Drawin 1968, 1969) rates scaled by a factor of \( S_H = 0.5 \). It is worth noting that for HD 49933 (\( T_{\text{eff}} = 6580 \) K; \( log g = 4.0; [M/H] = -0.48 \) dex) using \( S_H = 0.5 \) leads to 0.019 dex higher average abundance from the Ti i lines compared to that for \( S_H = 1.0 \).

| Wavelength, Å | Ion | \( E_1, \text{eV} \) | \( \log gf \) | Reference |
|---------------|-----|-----------------|-----------------|-----------|
| 4218.7130     | CH  | 0.411           | -1.339          | 1         |
| 4218.7340     | CH  | 0.411           | -1.361          | 1         |
| 4489.7391     | Fe i| 0.121           | -3.966          | 2         |
| 4491.3971     | Fe ii| 2.856         | -2.700          | 3         |
| 4493.5220     | Ti ii| 1.080           | -2.780          | 4         |

Effect of varying \( S_H \) is even smaller for the Sun, with a difference of 0.008 dex between applying \( S_H = 0.5 \) and 1.0. For iron, we used a comprehensive Fe i-Fe ii model atom treated by Mashonkina et al. (2011) and employed \( S_H = 0.5 \), as deduced by Sitnova et al. (2013) from analysis of the nearby dwarf stellar sample. The NLTE calculations for the C i lines were performed with the method from Alexeeva & Mashonkina (2015).

The departure coefficients (the ratios of NLTE to LTE level populations) calculated for each atmospheric model with the DETAIL code were then implemented in the SYNTH_NLTE code. This software, presented in (Tsymhal 1996), calculates the spectrum emerging from the static, 1-D model atmosphere, and it was tuned for the modelling of early B- to late M-type stars. The code was originally employing the LTE approximation, and in this study it was modified to take into account the pre-computed departure coefficients for various chemical species. We further integrated it within the IDL BINGMAG3 code written by O. Kochukhov, finally allowing us to determine the best fit to the observed line profiles with the inclusion of the NLTE effects. The spectrum synthesis code adopted by SME and the SYNTH_NLTE code use different algorithms for the radiative transfer solution, which may result in systematic differences in the derived abundances. We compared the two codes as follows. We used the synthetic spectrum computed by SME for HD 69830 (ESPADONS spectrum) in the 5640-50 Å wavelength region as the “observed spectrum” for (SYNTH_NLTE + BINGMAG3). In the latter code, abundances of eight elements listed in Table 3 were allowed to vary, when fitting the SME ’observed spectrum’. Table 3 shows the LTE abundances from calculations with SME and SYNTH_NLTE + BINGMAG3. The SME code returns an overall element abundance based on all the lines of each given element in the SME spectral windows, while SYNTH_NLTE + BINGMAG3 provides abundances from individ-

References: (1) Jorgensen et al. (1996); (2) Fuhr et al. (1988); (3) Kroll & Kock (1979); (4) Wood et al. (2013); (5) Raassen & Uylings (1998); (6) Lawler et al. (2013); (7) Ryabchikova et al. (1999); (8) Baschek et al. (1970); (9) Kurucz (2013); (10) O’Brian et al. (1991); (11) Rachchenko et al. (2010); (12) Blackwell et al. (1980) (corrected); (13) Bard et al. (1991); (14) Hannaford et al. (1992); (15) Bard & Kock (1994); (16) May et al. (1973); (17) Allende Prieto et al. (2004).

Table 2. Atomic and molecular line parameters

| Wavelength, Å | Ion | \( E_1, \text{eV} \) | \( \log gf \) | Reference |
|---------------|-----|-----------------|-----------------|-----------|
| 4218.7130     | CH  | 0.411           | -1.339          | 1         |
| 4218.7340     | CH  | 0.411           | -1.361          | 1         |
| 4489.7391     | Fe i| 0.121           | -3.966          | 2         |
| 4491.3971     | Fe ii| 2.856         | -2.700          | 3         |
| 4493.5220     | Ti ii| 1.080           | -2.780          | 4         |

References: (1) Jorgensen et al. (1996); (2) Fuhr et al. (1988); (3) Kroll & Kock (1979); (4) Wood et al. (2013); (5) Raassen & Uylings (1998); (6) Lawler et al. (2013); (7) Ryabchikova et al. (1999); (8) Baschek et al. (1970); (9) Kurucz (2013); (10) O’Brian et al. (1991); (11) Rachchenko et al. (2010); (12) Blackwell et al. (1980) (corrected); (13) Bard et al. (1991); (14) Hannaford et al. (1992); (15) Bard & Kock (1994); (16) May et al. (1973); (17) Allende Prieto et al. (2004).

Table 2 shows the LTE abundances from calculations with SME and SYNTH_NLTE + BINGMAG3. The SME code returns an overall element abundance based on all the lines of each given element in the SME spectral windows, while SYNTH_NLTE + BINGMAG3 provides abundances from individ-

http://www.astro.uu.se/~oleg/download.html
Abundances differences between the atomic C and molecular CH lines (stars), between lines of Ti i and Ti ii (filled circles), and between lines of Fe i and Fe ii (open circles). The solar values are shown by larger size symbols. The solid line shows the perfect ionisation balance, while the dashed lines indicate the \( \sigma = \pm 0.05 \) dex level.

We compared our results with those obtained with interferometry arriving at the following conclusions.

- Atmospheric parameters derived with SME on the basis of different masks agree within the uncertainties for stars cooler than 5500 K, while for hotter stars we recommend to include the H\( \beta \) and/or H\( \alpha \) lines to the spectrum fitting procedure.
- The uncertainty in the effective temperature is 50–70 K for the S/N = 200 spectra of the main-sequence F-, G-, K-type stars.
- Given the spectral ranges, spectral resolution, and S/N values explored here, we were unable to measure surface gravity with an accuracy of log \( g \) better than 0.1 dex using SME.
- The typical uncertainty in the metallicity derived with SME is 0.05-0.06 dex.

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**Table 3.** LTE abundances derived by SME for HD 69830 (second column) and by synthV\_NLTE + binnmag3 for the SME ‘observed spectrum’ (third column). See text for more details.

| Element | Abundance log([N]/[N_{tot}]) |
|---------|-------------------------------|
|         | SME synthV\_NLTE+ binnmag (LTE) |
| Si      | -4.57(0.17) -4.56 |
| Sc      | -8.87(0.04) -8.87 |
| Ti      | -7.11(0.07) -7.11 |
| V       | -8.11(0.06) -8.10 |
| Cr      | -6.44(0.07) -6.42 |
| Fe      | -4.60(0.06) -4.59 |
| Co      | -7.23(0.10) -7.22 |
| Ni      | -5.87(0.05) -5.86 |

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6 CONCLUSIONS

We used a sample of well studied F-, G-, and K-type stars to perform an extensive test of the accuracy of atmospheric parameters derived with the fitting procedure SME, widely applied in the literature for late-type stars. In our analysis we used high-quality and high-resolution spectra obtained with a wide range of different instruments and telescopes. We adopted three different masks for the spectral analysis and implemented a new, more accurate scheme for the determination of the uncertainties in the atmospheric parameters. We would like to emphasise that our approach provides self-consistent spectroscopic results without any external constraints on any of five atmospheric parameters: \( T_{eff} \), log \( g \), [M/H], \( V_{mic} \), and \( V_{mac} \).
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Table 4. NLTE abundances of C, Ti, and Fe derived from the atomic lines and the LTE abundances from the molecular CH lines together with their standard deviations given in parentheses.

| Name/HD  | Teff, K | log g | CH | C i | Ti i | Ti ii | Fe i | Fe ii |
|----------|---------|-------|-----|-----|------|-------|------|-------|
| Sun      | 5777    | 4.44  | −3.60(02) | −3.62(01) | −7.09(03) | −7.06(04) | −4.55(05) | −4.57(06) |
| Procyon  | 6615    | 3.89  | −3.59(02) | −3.66(01) | −7.12(06) | −7.09(08) | −4.57(05) | −4.57(08) |
| HD 49933 | 6582    | 4.00  | −4.09(05) | −4.09(02) | −7.52(06) | −7.55(04) | −5.08(06) | −5.08(06) |
| HD 9826  | 6145    | 4.06  | −3.62(01) | −3.59(02) | −7.04(05) | −7.01(06) | −4.48(07) | −4.50(06) |
| HD 102870| 6122    | 4.07  | −3.53(03) | −3.51(03) | −6.96(04) | −6.94(05) | −4.40(06) | −4.41(06) |
| HD 149026| 6074    | 4.18  | −3.42(03) | −3.41(02) | −6.87(06) | −6.81(06) | −4.27(06) | −4.31(06) |
| HD 209458| 6033    | 4.28  | −3.78(02) | −3.71(02) | −7.14(04) | −7.08(05) | −4.58(06) | −4.62(05) |
| HD 1461  | 5732    | 4.31  | −3.50(02) | −3.49(02) | −6.95(06) | −6.94(06) | −4.38(06) | −4.43(05) |
| HD 115617| 5567    | 4.42  | −3.72(02) | −3.71(03) | −7.09(04) | −7.05(06) | −4.58(07) | −4.62(06) |
| HD 69830 | 5422    | 4.47  | −3.72(02) | −3.66(05) | −7.07(05) | −7.08(06) | −4.57(07) | −4.63(06) |
| HD 189733| 5065    | 4.55  | −3.74(03) | −3.75(04) | −6.98(06) | −7.10(06) | −4.53(10) | −4.60(09) |
| HD 23249 | 5052    | 3.76  | −3.61(03) | −3.60(03) | −6.89(07) | −7.00(06) | −4.45(09) | −4.55(07) |
| HD 103095| 4958    | 4.52  | −5.17(05) |          | −8.23(08) | −8.22(06) | −5.94(06) | −5.92(05) |

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Parameters determination in FGK dwarfs

APPENDIX A:

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| First and last wavelengths, Å | 4511.144–4551.445 | 4865.521–4886.407 | 5193.964–5199.393 | 6105.670–6111.972 | 6524.252–6525.690 |
|-------------------------------|--------------------|-------------------|-------------------|-------------------|-------------------|
| 4551.114–4551.445            | 4865.521–4886.407 | 5193.964–5199.393 | 6105.670–6111.972 | 6524.252–6525.690 |
| 4551.114–4586.101            | 4865.521–4866.407 | 5193.964–5199.393 | 6105.670–6111.972 | 6524.252–6525.690 |
| 4866.101–4866.407            | 5193.964–5199.393 | 6105.670–6111.972 | 6524.252–6525.690 |
| 5193.964–5199.393            | 6105.670–6111.972 | 6524.252–6525.690 |
| 6112.000–6113.743            | 6526.200–6526.773 |
| 6526.200–6526.773            | 6529.184–6530.333 |
| 6113.955–6115.053            | 6530.137–6530.433 |
| 6133.966–6135.276            | 6530.137–6530.433 |
| 6157.740–6174.092            | 6530.137–6530.433 |
| 6176.792–6177.098            | 6530.137–6530.433 |
| 6176.792–6177.098            | 6530.137–6530.433 |
| 6176.792–6177.098            | 6530.137–6530.433 |

**Table A1.** Laboratory wavelengths of the mask m6. The beginning of each region marked by bold face.