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Letter to the Editor

Stellar population astrophysics (SPA) with the TNG

Identification of a sulphur line at λ_{air} = 1063.6 nm in GIANO-B stellar spectra*

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ABSTRACT

Context. In the advent of new infrared high-resolution spectrometers, accurate and precise atomic data in the infrared are urgently needed. Identifications, wavelengths, strengths, broadening, and hyper-fine splitting parameters of stellar lines in the near-infrared are in many cases not accurate enough to model observed spectra, and in other cases, these parameters do not even exist. Some stellar features are unidentified.

Aims. The aim with this work is to identify a spectral feature at λ_{vac} = 1063.891 nm or λ_{air} = 1063.600 nm that is visible in spectra of stars of different spectral types that are observed with the GIANO-B spectrometer.

Methods. The search for spectral lines to match the unidentified feature in line lists from standard atomic databases was not successful. However, by investigating the original published laboratory data, we were able to identify the feature and solve the problem. To confirm its identification, we modelled the presumed stellar line in the solar intensity spectrum and found an excellent match.

Results. We find that the observed spectral feature is a stellar line originating from the 4s′–4p′ transition in S I, and that the reason for its absence in atomic line databases is a neglected air-to-vacuum correction in the original laboratory measurements from 1967 for this line only. From interpolation we determine the laboratory wavelength of the S I line to be λ_{vac} = 1063.8908 nm or λ_{air} = 1063.5993 nm, and the excitation energy of the upper level to be 9.74978 eV.

Key words. atomic data – infrared: stars – line: identification – instrumentation: spectrographs – methods: laboratory: atomic – techniques: spectroscopic

1. Introduction

In recent years, several new cross-dispersed near-infrared spectrometers have been developed. These can capture large portions of one or more infrared bands (*Y*, *J*, *H*, *K*, *L* and/or *M* bands) simultaneously, which in principle increases the near-infrared observing efficiency dramatically. Examples of high-resolution ($R > 40\,000$) spectrometers are GIANO-B (Origlia et al. 2014), the Immersion Grating Infrared Spectrograph (IGRINS; Yuk et al. 2010), WINERED (Ikeda et al. 2018), and the CRyogenic InfraRed Echelle Spectrograph (CRIRES+; Follert et al. 2014; Brucalassi et al. 2018). Several medium-resolution ($R \sim$ 20–30 000) spectrometers, such as the Apache Point Observatory Galactic Evolution Experiment (APOGEE; Majewski et al. 2016, 2017) and the Near Infrared Echelle Spectrograph at KECK (NIRSPEC; McLean 2005), can also record large parts of a near-infrared band in one setting. This will also be the case of the Multi Object Optical and Near-infrared Spectrograph (MOONS; Cirasuolo & MOONS Consortium 2016; Taylor et al. 2018), which is under development and will be placed at the Very Large Telescope (VLT). Furthermore, the next generation of extremely large telescopes with their huge apertures will provide enhanced sensitivity in medium-high resolution near-infrared spectroscopy with spectrometers such as Multi-Object Spectrograph (MOSAIC, providing $R \sim 15\,000$; Jagourel et al. 2018) and the High Resolution Spectrograph (HIRES, providing $R \sim 100\,000$; Oliva et al. 2018a) for the Extremely Large Telescope (ELT).

The near-infrared spectral region therefore emerges as a spectral domain for versatile astrophysical use in an efficient way. However, because the near-infrared wavelength region is not as well explored as the optical region for astrophysical

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use, the spectral data, such as line identifications, wavelengths, strengths, broadening, and hyper-fine splitting parameters, are lagging behind. These data are, nevertheless, vitally important for any spectral investigation at both high and low spectral resolution (see e.g. Ruffoni & Pickering 2015).

Experimental and theoretical progress is, however, being made to ameliorate the situation. Recent work includes, for instance, experimental oscillator strengths of 28 Fe I lines in the H band (1.4−1.7 μm), following an urgent need from the APOGEE survey (Ruffoni et al. 2013), and measurements of line strengths of magnesium (Pehlivan Rhodin et al. 2017) and scandium (Pehlivan et al. 2015). These Sc data were vital, for example, in the discussion on K-band Sc abundances in the Nuclear Star Cluster by Thorsbro et al. (2018). Other examples are the works on WINERED spectra by Kondo et al. (2019), who investigated Fe lines at 0.9−1.3 μm in spectra of red giants and their usefulness for determining the metallicity and microturbulence, and the work by Fukue et al. (2015) on the development of the line-depth ratio method to determine effective temperatures of classical Cepheids in the H band. Furthermore, in the K band, not many measurements on relevant atomic data, such as wavelengths and lines strengths, exist at all from laboratory spectra, and the line wavelengths in the Vienna Atomic Line Database (VALD; e.g. Piskunov et al. 1995) are often uncertain. An example taken from Thorsbro (2016) is a Si I line at 2114.4 nm with theoretically estimated atomic physics parameters (Kurucz 2007). This line can be identified in the solar spectrum to have a wavelength shift of as much as 0.1 nm. When we correct the wavelength and compare it with other stars like Arcturus, its identification is shown to be correct. Thorsbro (2016) furthermore showed a clear difference in the wavelength accuracy in the K band for different elements, sulphur having the smallest spread, and silicon and calcium requiring the largest corrections in order to match the solar spectrum.

In the same spirit, we present in this paper the identification of an unidentified feature at $\lambda_{\rm vac}$ = 1063.891 nm in a range of stellar spectra that were observed at high spectral resolution with the GIANO-B spectrometer. We discuss the line behaviour with stellar effective temperature and finally identify it as an S I line. We also discuss why it was missed in earlier works.

2. Observations and spectral analysis

Six giants and supergiants of spectral types from A to K were observed with GIANO-B, the high-resolution ($R \simeq 50\,000$) infrared (950–2450 nm) spectrometer (Oliva et al. 2012a,b; Origlia et al. 2014) of the Telescopio Nazionale *Galileo* (TNG). The stars and their stellar parameters are provided in Table 1.

GIANO was designed for direct feeding of light at a dedicated focus of the TNG. In 2012 the instrument was provisionally commissioned and used in the GIANO-A configuration: the spectrometer was positioned on the rotating building and fed through a pair of fibers that were connected to another focal station (Tozzi et al. 2014). In 2016 the spectrometer was eventually moved to the originally foreseen configuration (called GIANO-B), where it can also be used in the GIARPS mode for simultaneous observations with High Accuracy Radial velocity Planet Searcher-North (HARPS-N; Tozzi et al. 2016).

GIANO provides a fully automated online data reduction pipeline based on the GOFIO reduction software (Rainer et al. 2018) that processes all the observed data; from the calibrations (darks, flats, and U-Ne lamps taken in day-time) to the scientific frames. The main feature of the GOFIO data reduction is the optimal spectral extraction and wavelength calibration based on a physical model of the spectrometer that accurately matches instrumental effects such as the variable slit tilt and orders curvature over the echellogram (Oliva et al. 2018b).

The spectra presented here were collected in November 2018 with the spectrometer in the GIARPS configuration. For an optimal subtraction of the detector artifacts and background, the spectra were collected by nodding the star along the slit; that is, with the target alternatively positioned at 1/4 (position A) and 3/4 (position B) of the slit length. Integration time was 5 min per A,B position. The nodding sequences were repeated to achieve a total integration time between 40 and 60 min per target.

The telluric absorption features were corrected using the spectra of a telluric standard (O-type star) taken at different airmasses during the same nights. The normalized spectra of the telluric standard taken at low and high airmass values were combined with different weights to match the depth of the telluric lines in the stellar spectra.

Figure 1 shows the normalized GIANO-B spectra of stars with different temperatures. The telluric correction applied is shown as a dashed line; it is negligible in the spectral region of interest here. The positions of the stronger atomic lines are marked. The wavelength scale is in the rest frame of each star, determined using standard cross-correlation techniques including the full GIANO-B spectrum (970−2450 nm). The final accuracy in the spectral region of interest here is 0.001 nm rms.

3. Discussion and conclusions

The unidentified feature at $\lambda_{\rm vac}$ = 1063.891 nm ($\lambda_{\rm air}$ = 1063.600 nm) resembles a single spectral line, broadened similarly as nearby spectral lines, especially in the four cooler stars (see Fig. 1). Because the telluric spectra do not show appreciable features in this region and because the feature is at the same stellar rest-wavelength in all stars, the possibility of it being a telluric line is excluded. It therefore has to be a stellar feature.

The feature becomes very shallow at temperatures below 5000 K and above 8000 K. This is the typical behaviour of a highly excited spectral line of a neutral ion; it disappears at high temperatures due to the ionization equilibrium, and at lower temperatures, the line becomes weaker as a result of the lower degree of excitation. However, no known line lies at this wavelength according to the NIST (Kramida et al. 2018) and VALD (Piskunov et al. 1995) databases. The closest lines are much farther away than any reasonable uncertainty of measured laboratory wavelengths of any known atom or the uncertainty of the wavelength scale of the observed spectra.

A first clue as to the origin of the spectral feature can be found in the similar behaviour of the close-by sulphur-line triplet at 1046 nm. These are lines with an excitation energy of $\chi_{\rm exc}$ = 6.9 eV. These lines originate from the $3s^2 3p^3 4s\,^3S^o_1 – 3s^2 3p^3 4p\,^3P_{0,1,2}$ transitions, have been measured in the laboratory by Zerne et al. (1997), and were successfully used in a work on the galactic chemical evolution of sulphur in the galaxy (e.g. Caffau et al. 2007; Jönsson et al. 2011). They change in strength in a similar way as the feature at $\lambda_{\rm vac}$ = 1063.891 nm, see Fig. 1. We have therefore searched for measured S I lines in the literature.

The NIST database indeed includes an S I line at $\lambda_{\rm vac}$ = 1063.599 nm ($\lambda_{\rm air}$ = 1063.308 nm). The excitation energy of this line is only slightly higher than that of the triplet at 1046 nm, that is, $\chi_{\rm exc}$ = 8.6 eV, and it would fit in nicely with the line strength variation with effective temperatures of the observed stars. The wavelength of the line is too far away for being accommodated within a random uncertainty in the wavelength measurement, however.

Table 1. Stellar parameters.

Name	Spectral type	$T_{\rm eff}$	$\log g$	[Fe/H]	Reference
HD 15316	A2Iab	8770	1.7	–	Verdugo et al. (1999)
HD 13784	F0II2	7080	2.1	0.0	Luck (2014)
HD 40457 (CO Aur)	~F5Ib (Classical Cepheid)	6620	2.5	−0.1	Luck (2014)
HD 187921 (SV Vul)	~F8Ia (Classical Cepheid)	4900−6330	0.29−1.28	0.0	Luck (2018)
HD 12650	G2II	5325	2.7	–	Hohle et al. (2010)
HD 14346	K0II	4585	2.2	–	Hohle et al. (2010)

Notes. The effective temperatures of the Cepheids depend on the phase at which the spectrum was collected. The same holds for the spectral type.

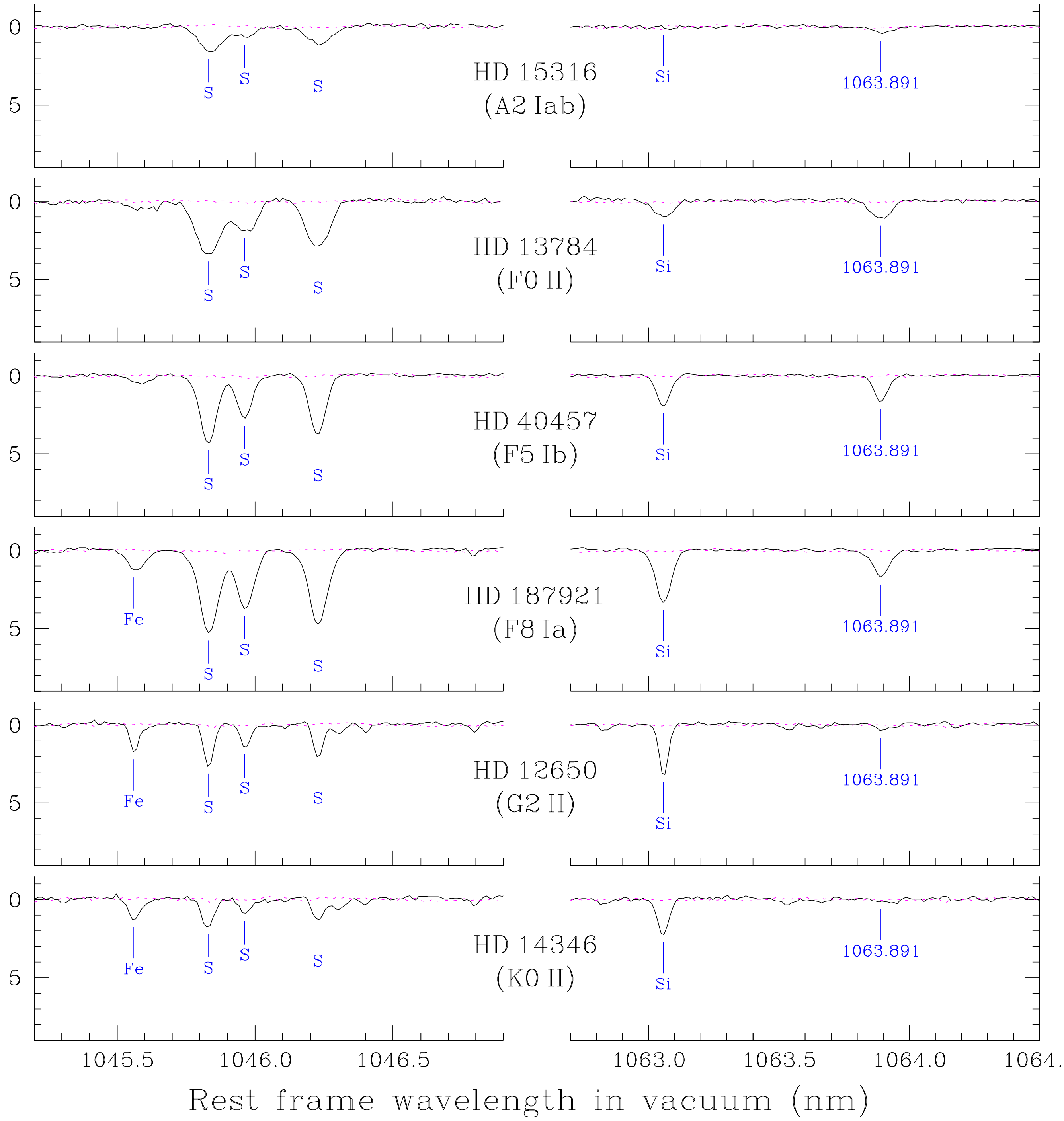

Fig. 1. Sections of the GIANO spectra including the unidentified feature at $\lambda_{\rm vacuum}$ = 1063.891 nm, which is identified as a sulphur line in this paper. The sulphur triplet at 1046 nm is also shown.

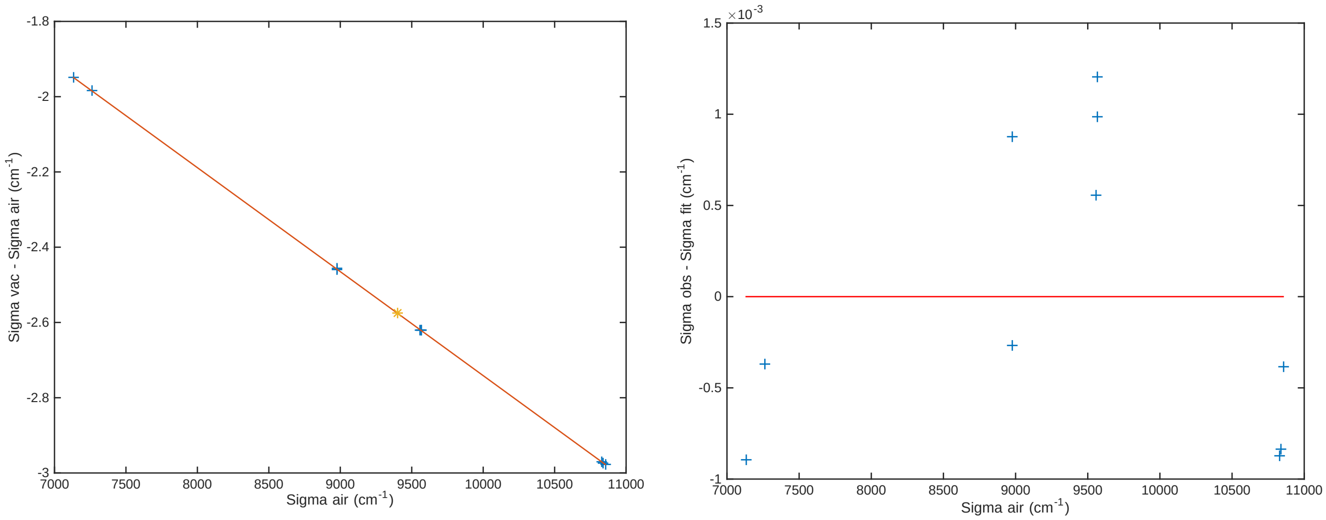

Fig. 2. Correction to air wave numbers. *Left*: difference between air and vacuum wave numbers, and a linear fit to the existing values. *Right*: difference between the reported wave numbers by Jakobsson (1967) and the values from the linear fit. The difference is about 0.001 cm^{-1}, which is less than the stated uncertainty in the study by Jakobsson (1967).

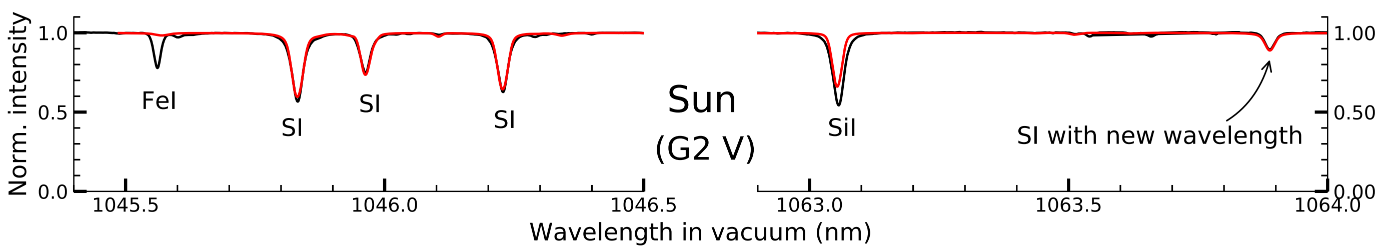

Fig. 3. Intensity spectrum of the solar centre around the S I triplet at 1045 nm and the moved S I line. No further adjustments to the line strengths in the line lists from VALD have been made. Solar abundances (Grevesse et al. 2007) are assumed, and the $\log gf$ values of the S I lines are those that are listed in NIST, i.e. Zerne et al. (1997) and Zatsarinny & Bartschat (2006). The Fe I and Si I lines obviously have incorrect $\log gf$ values and can be adjusted to solar astrophysical values if required.

The relevant laboratory data for S I on which the NIST spectral data are derived is taken from the work by Jakobsson (1967). They used a high-frequency discharge with sulfur dioxide as a light source to produce the sulfur lines. Because the wavelength region studied was the "extraphotographic infrared", the light was fed into a 1 m scanning grating spectrograph operated with a nitrogen-cooled PbS-detector that fed a pen recorder producing the spectrum. Their primary data are the air wavenumbers, $\sigma_{\rm air}$, subsequently converted into air wavelengths, $\lambda_{\rm air}$, and vacuum wavenumbers, $\sigma_{\rm vac}$, in their Table 1. This table shows that for the 4s′ $^1D_2$–4p′ $^1F_3$ line the vacuum wavenumber, denoted by $\sigma_{\rm obs}$, was not corrected for the refractive index to provide $\lambda_{\rm air} = 1063.5993$ nm ($\sigma_{\rm air} = 9402.037\,{\rm cm}^{-1}$), while the correction has been properly applied to all the other lines. The correction amounts to about 2.6 cm^{-1}, which can fully account for the observed wavelength mismatch.

Unfortunately, neither the procedure for the conversion into vacuum data nor the value used for the refractive index n is presented in the paper. Because n slowly varies with wavenumber, we used the laboratory data of the neighbouring lines to interpolate the true laboratory data for the missing line, as presented in Fig. 2. We find a wavenumber shift ($\sigma_{\rm vac} - \sigma_{\rm air}$) of $-2.576\,{\rm cm}^{-1}$. We thus derive a new value of $\sigma_{\rm vac} = 9399.461\,{\rm cm}^{-1}$ ($\lambda_{\rm vac} = 1063.8908$ nm).

The right panel of Fig. 2 shows that the difference between the laboratory value and the fitted value is around 0.001 cm^{-1} or less, corresponding to 1 mÅ. This is an order of magnitude smaller than the stated uncertainty of the laboratory data and clearly justifies the linear interpolation. For the discussed lines, measured by Jakobsson (1967) with a photoelectric setup, they estimate the wavenumber accuracy to be better than 0.01 cm^{-1}, corresponding to 10 mÅ or 0.001 nm at these wavelengths. We estimate the uncertainty in our new values to be of the same magnitude. In addition, we choose to report the same number of digits for the numbers as the original reference. The new atomic wavelengths and wavenumber are reported in Table 2, along with the oscillator strength as listed in the NIST database (Kramida et al. 2018) from the calculations by Zatsarinny & Bartschat (2006). The uncertainty of this value, quoted by the authors, is 2%.

The energy of the $^1F_3$ level (upper level of the transition) is derived only from one line (i.e. the one under investigation in this paper) because only few lines are available. Because the current value is based on the incorrect wavenumber, we used the new wavenumber to derive a corrected energy of the $3s^23p^3(^2D)4p$ $^1F_3$ level. The new excitation energy of the level is $E_{\rm exc} = 78\,637.303\,{\rm cm}^{-1} = 9.7497830(10)$ eV.

Being confident that the published wavelength of the S I line from the original reference (Jakobsson 1967) is incorrect because of an air-to-vacuum conversion mistake, we finally checked our new wavelength by synthesizing the solar centre intensity spectrum observed with the Fourier Transform Spectrometer at the McMath/Pierce Solar Telescope at Kitt Peak (Wallace et al. 1993) for the wavelength region around the S I

Table 2. New atomic line data for the S I line ($3p^3(^2D)4s\ ^1D_2$–$3p^3(^2D)\ 4p\ ^1F_3$).

Spices	S I
Wavelength (in vacuum)	1063.8908(11) nm
Wavelength (in air)	1063.5993(11) nm
Wavenumber	9399.461(10) cm^{-1}
log gf (NIST: Zatsarinny & Bartschat 2006)	0.391(10)
E_{exc} (lower) (Jakobsson 1967)	8.5844037(10) eV
E_{exc} (upper)	78 637.303(10) cm^{-1}
E_{exc} (upper)	9.7497830(10) eV
Lower level term	$3s^2 3p^3(^2D^o)\ 4s\ ^1D^o_2$
Higher level term	$3s^2 3p^3(^2D^o)\ 4p\ ^1F_3$

Notes. Uncertainties are given in brackets.

line. To do this we used the spectral synthesis code spectroscopy made easy (SME; Valenti & Piskunov 1996, 2012), in which the radiative transfer and line formation is calculated for a model atmosphere defined by the fundamental stellar parameters of the Sun. SME uses a grid of model atmospheres in which the code interpolates for a given set of fundamental parameters of the analysed star. We use 1D MARCS models, which are hydrostatic model photospheres in plane-parallel geometry, computed assuming local thermodynamic equilibrium, chemical equilibrium, homogeneity, and conservation of the total flux (radiative plus convective, the convective flux being computed using the mixing-length recipe) (Gustafsson et al. 2008). We calculated the synthetic spectrum of the solar spectrum as an intensity spectrum of the solar centre.

In Fig. 3 we show our synthesised solar spectra together with the observed intensity spectrum of the solar centre. The previously unidentified line fits well and agrees with the sulfur triplet at 1046 nm. We therefore confidently move the S I line in the NIST database to its correct wavelength as determined from the GIANO-B spectra. The final parameters of this S I line are summarized in Table 2.

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