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Detection of the mercapto radical SH in the solar atmosphere

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Abstract. We analyze new high-resolution UV observations of the solar photosphere in the disk center and the limb and report the first detection of SH lines in the solar atmosphere. We perform a synthesis of the solar spectrum including many atomic and molecular lines and find a few relatively unblended SH lines from which we determine the (0, 0) band oscillator strength $f_{00} = 2.2 \times 10^{-3}$. We conclude that these lines are excellent indicators of the sulfur abundance and isotope ratio in G and K stars.

Key words. Sun: abundances – Sun: photosphere – molecular data – line: identification – techniques: spectroscopic

1. Introduction

Sulfur is one of the so-called α-elements which are synthesized in the Type II supernovae. Its abundance in stars of different metallicity is therefore important for determining the scenario of the chemical evolution of the Galaxy. For instance, it is expected that there should be an overabundance of α-elements in unevolved stars with metallicities [Fe/H] < -1. The only indicator of the sulfur abundance in oxygen-rich stellar atmospheres used to date is the S I doublet at 8694 Å. In the solar spectrum, equivalent widths of the doublet lines are about 30 and 10 mÅ (Wallace et al. 1993). In spectra of cooler stars, the doublet, because of its high excitation energy, appears several times weaker, down to few mÅ in metal-poor halo stars (Israelian & Rebolo 2001).

Chemical equilibrium calculations suggest that the simplest molecular sulfur compound, SH, the mercapto radical, should be quite abundant in oxygen-rich stellar atmospheres (Tsuji 1973). The first astronomical detection of this molecule was however reported only recently by Yamamura et al. (2000) who identified ro-vibrational SH lines in the infrared spectrum of the S-type star R And, which appeared to be slightly oxygen rich. In the solar atmosphere no sulfur-bearing molecule has been detected to date, although the question of possible presence of SH, CS and SO in the photosphere and sunspot spectra has been theoretically investigated by Sinha et al. (1977) and Joshi & Pande (1979). They calculated equivalent widths of ultraviolet SH absorption lines arising due to transitions between the ground and first excited electronic states, $X^2\Pi$ and $A^2\Sigma$, at about 3280 Å. They showed particularly that the SH equivalent widths increase significantly at the solar limb as compared to the disk center. The principle difficulty with the detection of these lines in the solar spectrum lies in the fact that the UV region is difficult to observe and also is crowded by strong atomic lines which heavily blend weaker SH lines. The predicted equivalent widths were also uncertain due to the absence of the laboratory measured band oscillator strength.

Here we analyze new high-resolution UV observations of the solar photosphere in the disk center and the limb. Using laboratory measured molecular constants, we predict wave numbers of SH lines in the (0, 0) band of the $A-X$ electronic system for highly excited rotational levels and perform a synthesis of the solar spectrum including many atomic and molecular lines. We identify a few relatively unblended SH lines and determine the (0, 0) band oscillator strength. The SH lines can be excellent indicators of the sulfur abundance in G and K stars. They can also be useful for determining the isotope ratio $^{32}S/^{34}S$ in stellar atmospheres. This is important in connection with the recent finding that the interstellar sulfur isotope ratio increases with galactocentric distance (Chin et al. 1996).

2. Observations

The observations were made on the 13.5 m spectrometer of the all reflective McMath-Pierce telescope. Its new grating is very efficient at 3300 Å in the 8th order. A quartz predisperser did the order selection.

Since SH lines are to be rather strong at cooler temperatures, an attempt was first made to observe the 3250–3300 Å region in sunspot spectra. The results were

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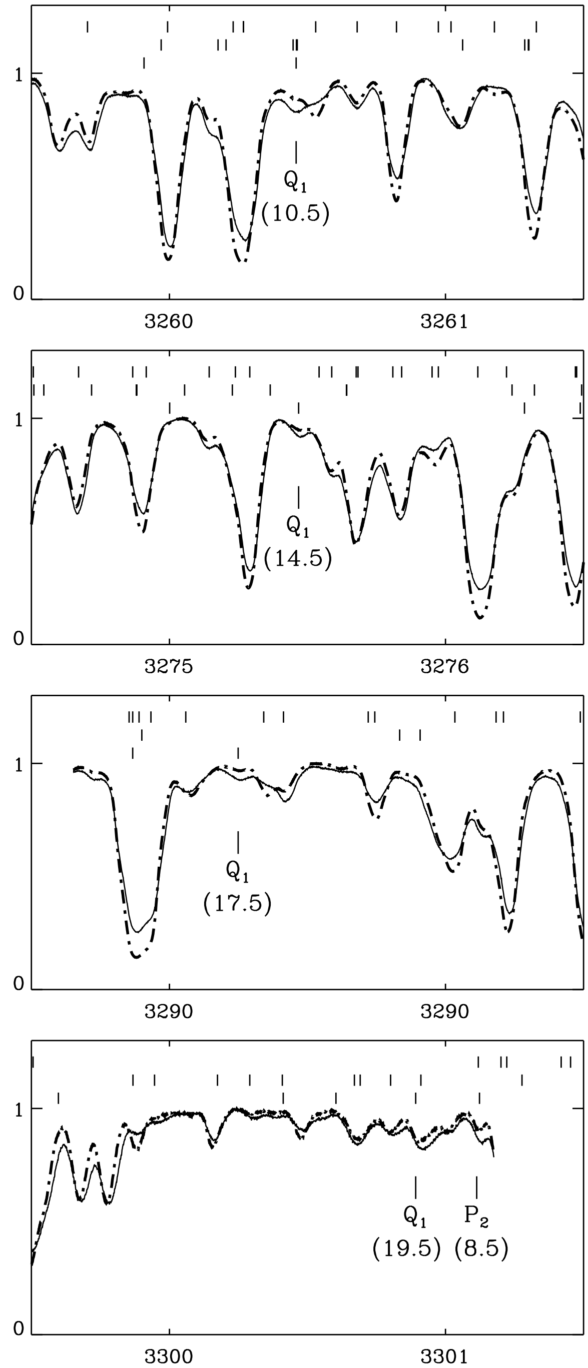

Fig. 1. Center-to-limb variations in the UV spectrum of the solar photosphere. Thick dashed-dotted line represents the spectrum taken at the disk center. Solid thin line indicates the spectrum observed at the solar limb. Three rows of vertical dashes above the spectra indicate positions of atomic lines with central line depths larger than 0.1 (upper row), OH lines with oscillator strengths larger than 10^{-4} (middle row), and all SH lines of the (0, 0) band from the available line list (lower row). Below the spectra, 5 identified SH lines are pointed out.

unsatisfactory because of strong stray light from the photosphere in the UV.

Therefore we switched our attention to a comparison of the limb with disk center. Limb data was acquired under guider control at 5 mm from the limb on the 820 mm diameter image ($\mu = \cos\theta = 0.158$, where θ is the usual line of sight from disc center) at the north geographic pole (which was approximately 20° polar angle from the heliographic pole) and completely free of faculae. Disk center was also facular free. When the two spectra were compared, relatively unblended SH and other molecular lines appeared as noticeably strengthened features in the limb spectrum, as was expected (Fig. 1).

Table 1. Spectroscopic data for the SH (0, 0) band lines identified in the solar spectrum: wavelength λ in Å, dimensionless theoretical strength S_{JJ}, equivalent width of the observed blend $W_{\rm obs}$ in mÅ, and equivalent width of the ^{32}SH lines determined from the synthetic spectrum, $W_{\rm syn}$, in mÅ.

Line	$\lambda_{\rm air}$		$S_{J'J''}$	$W_{\rm obs}$	$W_{\rm syn}$
	^{32}SH	^{34}SH			
$Q_1(10.5)$	3260.459	3260.389	21.905	14.3	5.1
$Q_1(14.5)$	3275.468	3275.371	29.931	7.8	5.0
$Q_1(17.5)$	3289.749	3289.625	35.943	8.5	4.7
$Q_1(19.5)$	3300.892	3300.745	39.949	12.9	4.4
$P_2(8.5)$	3301.112	3301.056	9.412	4.5	2.2

3. SH transitions

Although the first space detection of the mercapto radical has been reported only recently, it was extensively studied in laboratories over the last decades. Ramsay (1952) measured wave numbers of the rotational lines of the (0, 0) band in the $A^2\Sigma - X^2\Pi$ system up to the rotational number $J = 14.5$ and determined molecular constants for both states. Ram et al. (1995) reported the most accurate spectroscopic constants for the ground state $X^2\Pi$ and published term values for its ro-vibrational levels up to $J = 35.5$.

According to calculations of vibrational transition probabilities by Nicholls et al. (1960), the (0, 0) band of the $A - X$ system is at least factor of two stronger than the second strong band (1, 1). We therefore limited ourselves by searching only SH lines from the (0, 0) band. In order to predict wave numbers of rotational lines in this band for $J > 14.5$, we used the data from the studies by Ramsay (1952) and Ram et al. (1995). Errors of the predicted wavelengths are estimated to be not larger than 0.01 Å for $J < 20.5$. Only 5 SH lines were found relatively unblended and sufficiently strong in the solar spectrum. These lines are listed in Table 1 along with their theoretical strengths (Hönl-London factors) which were calculated according to Kovács (1969). A further analysis of the lines via the spectral synthesis showed that only two of them, $Q_1(14.5)$ and $Q_1(17.5)$, are not blended.

4. Analysis of the observations

4.1. Line list

In order to prove the identification of the SH lines, we carried out a synthesis of the corresponding spectral regions.

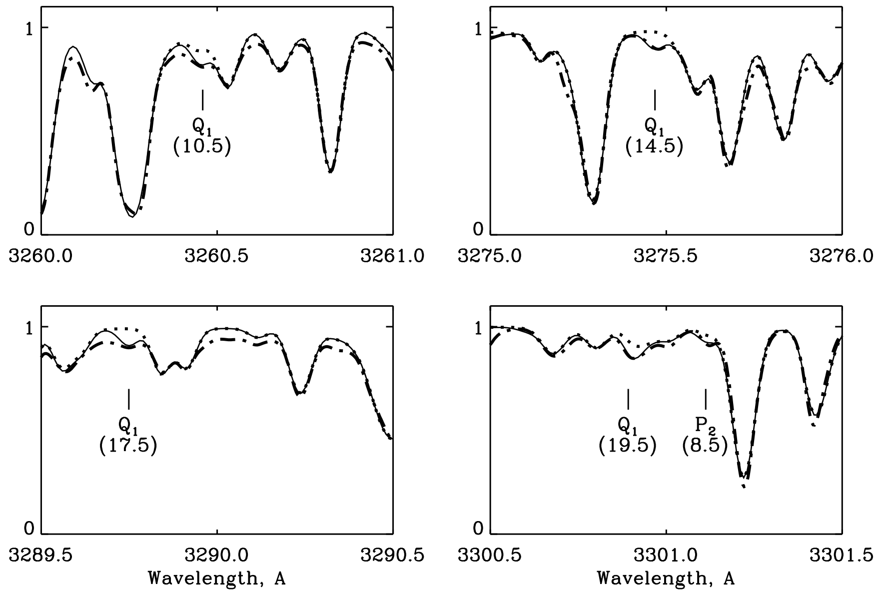

Fig. 2. Synthetic spectra including SH lines (thin solid line) and excluding them (dotted line) compared with the observed spectrum (thick dashed-dotted line) for the solar disk center in the spectral regions of interest.

In the region 3260 Å to 3300 Å major line absorption sources in the solar atmosphere are neutral and singly ionized atoms as well as a number of molecules. A primary list of atomic and molecular lines for the calculation was prepared using the compilation by Kurucz (1993) and the atomic data bases VALD-2 (Kupka et al. 1999) and P. van Hoof (http://www.pa.uky.edu/∼peter/atomic/). In addition to SH lines, the list included transitions of such molecular species as OH, NH, CH and CN, although CH and CN lines in the spectral region under consideration are very weak. Absorption in NH lines starts to be noticeable from about 3280 Å.

A great care has been taken to calculate as many OH lines as possible, since center-to-limb variations in OH and SH lines are quite similar and, also, OH lines of the $A-X$ system are rather numerous in the region. For this purpose, rotational lines of all possible bands arising between upper and lower vibrational levels 0, 1, 2, and 3 have been checked for the presence with the help of the recent calculations by Gillis et al. (2001). This allowed us to update the OH line list based on the Kirucz's data. The strongest atomic and OH lines in the list are indicated in Fig. 1.

Still, after the above updating, a number of weak lines were left unidentified. Their center-to-limb variations suggest, however, that they are atomic lines.

4.2. Spectrum synthesis

The spectrum synthesis was performed with the solar photosphere model by Grevesse & Sauval (1999). Molecular number densities for this model were calculated under the assumption of the chemical equilibrium of 270 compounds consisting of the 33 most abundant atoms (Tsuji 1973; L. Hänni, private communication). A value of the dissociation energy D_0 of the mercapto radical of 3.62 eV was accepted according to measurements by Continetti et al. (1991). A solar sulfur abundance of $\log\epsilon(S) = 7.21$ (on the scale in which $\log\epsilon(H) = 12$) was adopted according to Anders & Grevesse (1989). The spectra were calculated for the disk center and compared with the observations. The results are shown in Fig. 2.

A value of the SH (0, 0) band oscillator strength $f_{00} = 1.63 \times 10^{-3}$ derived by Henneker & Popkie (1971) and used by Sinha et al. (1977) and Joshi & Pande (1979) to predict line equivalent widths in the solar atmosphere appeared to be somewhat small to describe the features which we identified as SH lines. It was therefore varied until a perfect fit to the observed features has been achieved. This is shown in Fig. 2. Our fitting procedure resulted in a value of $f_{00} = 2.2 \times 10^{-3}$. An even larger value of f_{00} was very recently predicted by Resende & Ornellas (2001) who carried out ab initio calculations of SH radiative lifetimes. With the best overall theoretical description of the $A^2\Sigma - X^2\Pi$ system, they determined the Einstein coefficient for the (0, 0) band as large as $1.818 \times 10^6\,\mathrm{s}^{-1}$, which results in $f_{00} = 2.896 \times 10^{-3}$. This is 30% larger than was determined from the solar spectrum.

A pure contribution of the SH lines to the absorption features indicated in Fig. 2 was calculated using the value of $f_{00} = 2.2 \times 10^{-3}$. This is given in Table 1 along with total observed equivalent widths of the blends. There are in fact only two blends whose equivalent widths are more than half due to SH absorption, $Q_1(14.5)$ and $Q_1(17.5)$, so that, for the Sun, probably only these two lines can be used. This however changes significantly for cooler stars where the relative contribution of the SH lines to the blends increases several times (see Fig. 3).

4.3. Sulfur isotope ratio

In the Solar system, sulfur is presented by large amount of the isotope ^{32}S with the second large contamination by ^{34}S: the ^{32}S/^{34}S ratio measured from meteorites equals $95.02{:}4.21 = 22.57$ (Anders & Grevesse 1989). It has never been measured however directly in the Sun as well as in other oxygen-rich stellar atmospheres. As molecules are

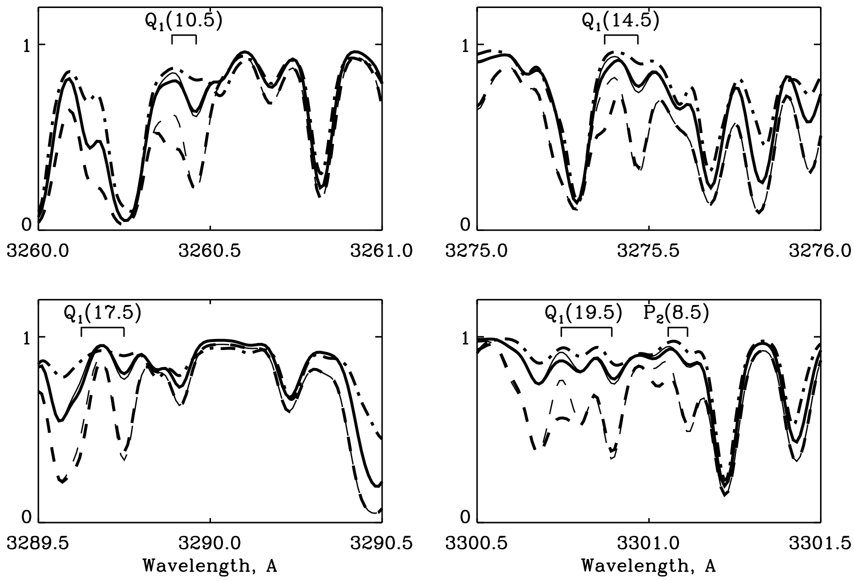

Fig. 3. Synthetic spectra for $T_{\rm eff} = 5250$ K (solid line) and $T_{\rm eff} = 4750$ K (dashed line) compared with the solar spectrum observed at the disk center (dashed-dotted line). Thinner lines indicate spectra calculated with the meteorite sulfur isotope ratio ^{32}S/^{34}S = 22.57, while thicker lines present synthetic spectra for the same temperatures with ^{32}S/^{34}S = 4.

known to be good isotopomers, our identification of SH lines allows us, in principle, to carry out this for the first time. For this purpose, using standard formulas given by Herzberg (1950), we calculated isotope shifts for ^{34}SH lines corresponding to the identified ^{32}SH lines. They are listed in Table 1. The theoretical strengths of corresponding ^{32}SH and ^{34}SH lines are equal, although their vibrational transition probabilities can slightly differ. The latter can be however neglected in the first approximation.

In the spectrum of the solar photosphere, the ^{34}SH isotope lines are rather weak and completely blended by other lines. In other to estimate what the temperature interval must be for the ^{32}SH and ^{34}SH lines to be rather noticeable, we carried out a synthesis of the regions of interest for cooler atmospheres. As seen from Fig. 3, the most favorable temperatures for determining the sulfur abundance using the SH lines is $\leq$5250 K. Even lower temperatures are desired if the sulfur isotope ratio is of interest, namely <5000 K. Thus, in the Sun, the sulfur isotope ratio should be measurable from sunspot spectra, if the the stray light from the photosphere could be successfully eliminated.

5. Conclusions

High-resolution UV observations at the solar disk center and the limb have allowed us to detect the presence of the SH radical in the solar atmosphere. The identification of the 5 relative unblended SH lines was confirmed by the detailed spectrum synthesis. A new value of the (0, 0) band oscillator strength $f_{00} = 2.2 \times 10^{-3}$ was determined from the fit to the observed solar spectrum. A spectral synthesis clearly demonstrated that the new SH lines are excellent indicators of the sulfur abundance and sulfur isotope ratio in stars cooler than the Sun.

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