IDENTIFICATION OF BERYLLIUM HYDRIDE ISOTOPOMER LINES IN SUNSPOT UMBRAL SPECTRA

R. Shanmugavel¹, S. P. Bagare², N. Rajamanickam¹ and K. Balachandra Kumar³

¹Physics Research Centre, V.H.N.S.N College, Virudhunagar - 626 001 E-mail: nrmanickam@rediffmail.com

²Indian Institute of Astrophysics, Kodaikanal & Bangalore - 560 034 ³Kamaraj College of Engineering and Technology, Virudhunagar - 626 001

(Received: October 13, 2007; Accepted: March 10, 2008)

SUMMARY: A high resolution spectrum of FTS sunspot umbra of NSO/Kitt Peak was used to conduct a search for the molecular absorption lines due to BeH, BeD and BeT isotopomers. Analysis led to estimates of identification of the molecular lines of bands A - X (0,0), (1,1) and (2,2) for BeH, A - X (0,0), (1,1), (2,2) and (3,3) for BeD and of A - X (0,0), (1,1) and (2,2) for BeT. Among the identified lines, those which are well resolved were selected for measurements to calculate equivalent widths. The values of effective rotational temperature T were estimated for bands A - X(1,1) and (2,2) of BeH, A - X(1,1) of BeD and A - X(2,2) of BeT to be 4228K, 4057K, 3941K and 3243K respectively.

Key words. sunspots - Line: identification.

1. INTRODUCTION

The BeH molecule with only five electrons is perhaps of the greatest interest in its group of homologous monohydrides (MgH, CaH, SrH and BaH) which are extensively studied astrophysical molecules. Studies by various authors, from Rowland (1895) to Bagare et al. (2006) have led to identification and confirmation of the presence of many diatomic molecules such as CN, TiO, CaH, CH, MgH, FeH, AlH and AlF in various sunspots umbrae. However, the presence of certain transitions of CN, C₂, MgO, ZrO, VO and CrH are claimed to be uncertain (Wallace et al. 2000) due to various reasons like heavy blending by stronger lines or lack of accurate spectroscopic data. Quite often, a low number of line coincidence, or presence of very weak features makes the identification difficult (Engvold 1970). Nearly 44 molecules have been searched and studied for few selected transitions and an extensive search for a large number of rotational lines was carried out by Wöhl (1971); who classified the molecules studied as either present, or presence questionable, or presence excludable, or not identifiable because of lack of spectroscopic data.

The presence of the rotational lines due to A - X (0,0) band of BeH was first examined by Wöhl (1971); looking for 80 lines, he found wavelength coincidences for 45 lines with a low W-index (0.1 - 0.15). Since the evidence was not convincing, it was concluded that the presence of BeH in umbral spectrum was questionable. This may be due to the fact that the S/N ratio was not high compared to later FTS spectra by Wallace et al. (2000), though the spectral resolutions achieved in their photoelec-

tric scans was claimed to be 40 mÅ. Hence, in the present study, a fresh search for the presence of BeH lines in high resolution FTS umbral spectra (Wallace et al. 2000) was taken up, along with those of its isotopologues BeD and BeT.

In view of the astrophysical significance of BeH, BeD and BeT transitions, the Franck - Condon factors (FCF), which are transition probability parameters, were computed by Shanmugavel et al. (2006) for 5 electronic transitions. In the present paper BeH, BeD and BeT isotopomer lines for a set of selected transitions are identified in sunspot spectra, equivalent widths are deduced and corresponding rotational temperatures are reported.

2. IDENTIFICATION METHODOLOGY

An atlas of sunspots umbral spectra in the visible from 15000 to 20500 cm⁻¹ published by Wallace et al. (2000) was used to search for coincidences with rotational line wavenumbers given by Olsson (1932) for A - X (0,0), (1,1) and (2,2) transition bands of BeH, by Focsa et al. (1998) for A - X (0,0), (1,1), (2,2), (3,3) and (4,4) transition bands of BeD and by DeGreef and Colin (1974) for A - X (0,0), (1,1) and (2,2) transition bands of BeT. The digital spectra downloaded from the NSO website were also plotted and compared with the two formats being identical, magnified prints of the atlas spectra were actually used for identification of the lines. A total of 1371 lines were carefully searched for, and the results were classified as follows.

- (a) Present the line is clearly identifiable,
- (b) Shoulder the line lies on the shoulder of a strong atomic or other molecular line,
- (c) Merged a strong atomic or other molecular line is present at the wavenumber of the line, and
- (d) Doubtful the difference between the laboratory wavenumber and that of the located line is greater than 0.1 cm^{-1} .

The lines which appeared to be almost merging with the local background were treated as absent. However, the number of such lines was very small. Lines classified as present or as shoulder were together taken as lines identified. The total number of lines identified in a given band was noted as the I-parameter of the particular band.

The probability of chance coincidence between laboratory and umbral wavenumbers can be tested by means of the Russell-Bowen formula (Russell and Bowen 1929, Russell and Moore 1944, Engvold et al. 1980). The number of chance coincidences may be expressed as

$$C = N \left[1 - \exp\left(-\frac{2xM}{X}\right) \right] \tag{1}$$

where N is the number of laboratory lines, M/X is the line density in the umbral spectrum and x is the tolerance of wavenumber discrepancy. In order to exclude the possibility of identifying a molecular band by chance, the actual number of line coincidences found should exceed the value of C-index. We examined each of the above band systems of BeH, BeD and BeT for compliance with this condition. We adopted a tolerance of 0.1 cm^{-1} in wavenumber difference to accept the matching to be a coincidence. In addition, a complementary test which can be carried out has to do with the spectral and intensity distribution in P,Q and R branches of the band. This aspect has also been discussed in detail, with illustrations, by Sotirovski (1971). We have used this test for each of the band systems studied by us. In particular, we have looked for maxima in absorption intensity within the P and R branches, following Herzberg (1950)

Several authors (Laborde 1961, Wöhl 1970) used the equivalent widths (W) of molecular lines to determine the temperatures of umbrae. The method of triangular profile approximation was successfully used by Wallace et al. (1999) for MgH lines and by Bagare et al. (2006) for AlF lines. From the lines classified as present, well resolved and isolated lines were selected for measurements to calculate the equivalent width. The effective rotational temperature of the source was evaluated for bands which had a significant number of lines whose equivalent widths were calculated. The equivalent widths of molecular lines in a rotational band depends on the rotational quantum number and the temperature. The relation given by Herzberg (1950) was used:

$$\log(W/J) = \text{const.} - \frac{Bhc}{2.3kT}J(J+1) , \qquad (2)$$

where W is the equivalent width, J is the rotational quantum number, B is the rotational constant, h is Planck's constant, k is Boltzmann's constant, c is the velocity of light and T is the effective rotational temperature of the source.

A plot of $\log(W/J)$ as a function of J(J+1)is a straight line with a slope m, from which one obtains T by

$$T = -hcB/2.3km \tag{3}$$

The results of our search for rotational lines of beryllium hydride isotopomers, calculated equivalent widths and estimated values of T are presented in Section 3.

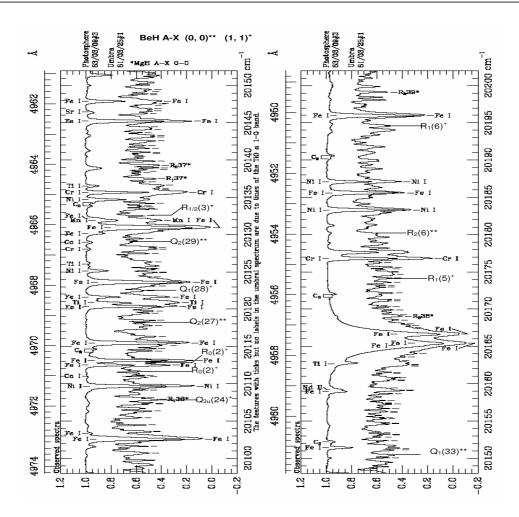


Fig. 1. Section of the sunspot umbral spectrum with identified BeH (1,1) molecular rotational lines.

3. RESULTS AND DISCUSSION

The umbral spectrum is so rich in weak absorption lines that it is essential to establish that the quoted identifications for BeH, BeD and BeT are not simply random coincidences of wavenumbers. Hence, the identified lines were classified into four categories (present, shoulder, merged and doubtful), as described in Section 2. A total of 723 lines were identified, which includes the present and the shoulder categories. A wavenumber discrepancy of not more than 0.1 cm⁻¹ was allowed as the tolerance limit for accepting a line coincidence.

The C-index and the I-parameter were evaluated for each of the bands, as described in Section 2. These results are presented in Table 1¹, together with the reported FCF values, total number of lines searched and wavenumber region for respective bands. The I-parameter is seen to be convincingly higher than the C-index for each of these bands. The test, therefore, supports the presence of BeH, BeD and BeT bands in the observed umbral spectrum. It must be noted that a significant number of lines could have been identified despite of the presence of a large number of other lines, due to MgH, CaH, FeH, TiO and several atomic species, in the region of search. Some examples of sunspot spectra with identified BeH, BeD and BeT molecular rotational lines are shown in Figs. 1-3. The rotational line details and the wavenumber of lines identified in umbral spectra are listed in Tables 2-12 for the eleven bands classified as present.

For the above bands identified as present, those that are clearly resolved and have an absorption intensity of at least one-tenth the maximum of the scale, were selected for the measurements to calculate equivalent widths. A significant number of lines met the requirement in the case of A - X (1,1) and (2,2) for BeH, A - X (1,1) for BeD and A - X (2,2) for BeT. The method of triangular profile approximation described in Section 2 was used to calculate equivalent widths. A list of these values is presented in Tables 13, 14, 15 and 16.

¹Tables are available as http://saj.matf.bg.ac.yu/176/pdf/Tables.pdf

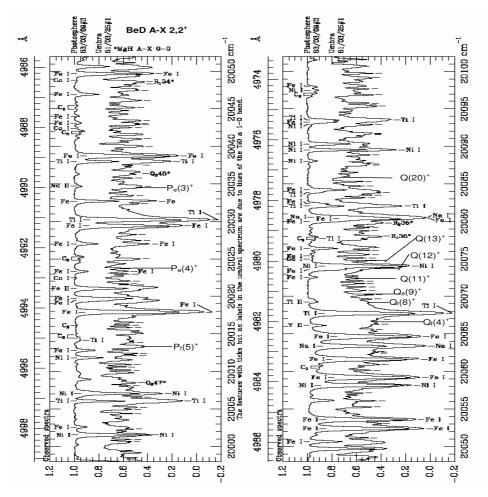


Fig. 2. Section of the sunspot umbral spectrum with identified BeD (2,2) molecular rotational lines.

The variation of equivalent widths with rotational quantum number reflects the rotational temperature of the layers in the umbral atmosphere. In order to evaluate the effective rotational temperature of the umbral region giving rise to the band observed, the procedure of using Eq. (2) was adopted. The values of J(J + 1) were plotted against $\log(W/J)$. Respective plots are shown in Figs. 4-7. The values of slopes being equal to Bhc/2.3kT, values of T were estimated for bands A - X (1,1) and (2,2) of BeH, A - X (1,1) of BeD and A - X (2,2) of BeT to be 4228K, 4057K, 3941K and 3243K respectively. The estimated temperatures are accurate no more than to within 600 to 1000 degrees of the values given.

There is no unique value of the rotational temperature for sunspot umbrae. This has been elaborately discussed by Bagare et al. (2006). Each rotational system observed corresponds to a certain range of rotational temperature in the source, here the sunspot, in which the transitions have high probability of occurrence. Moreover, in the case of sunspots, a range of temperature is to be expected as the systems may be formed at the appropriate temperature range, which can occur at various heights in the sunspot atmosphere. The temperature at the photospheric level above, the sunspot going through the temperature minimum region, varies. The temperature is also known to have a dependence on the strength of the magnetic field. The sunspots being vast regions on the Sun, and having complex magnetic structures, such ranges are to be expected. There are, therefore, 'cold' sunspots with large number of molecular lines and the 'hot' sunspots.

4. CONCLUSION

We have presented evidence for the presence of BeH isotopomers in the sunspot umbral spectra. It is concluded that lines due to eleven bands, A -X (0,0), (1,1) and (2,2) of BeH, A - X (0,0), (1,1), (2,2), (3,3) and (4,4) of BeD and A - X (0,0), (1,1) and (2,2) of BeT, are present in the sunspot spectra.

Further, the rotational lines due to bands of AlF, FeH, TiO, MgH and BeH isotopomers provide a good range of temperatures for the study of absorbing layers in umbral spectra. Hence, these molecular species can, in principle, provide a useful picture of the temperature distribution in umbral atmospheres, that is, the absorbing layers are likely to be present at different heights.

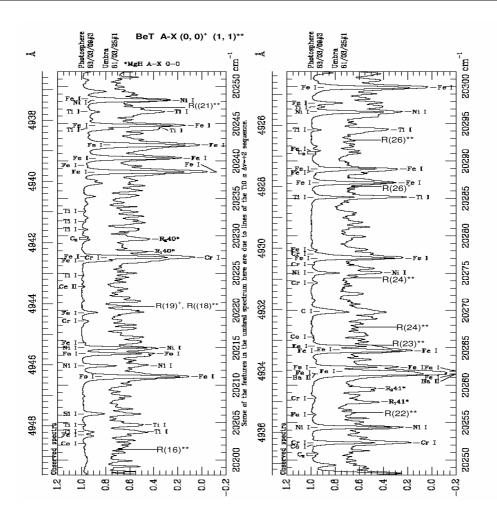


Fig. 3. Section of the sunspot umbral spectrum with identified BeT(0,0) and (1,1) molecular rotational lines.

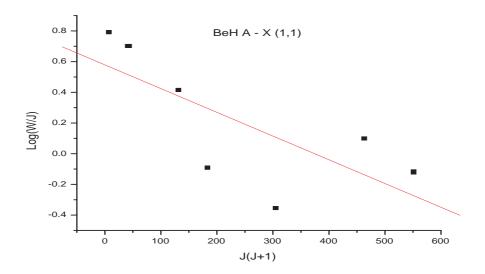


Fig. 4. Plot of log(W/J) vs J(J+1) for BeH A - X (1, 1) band.

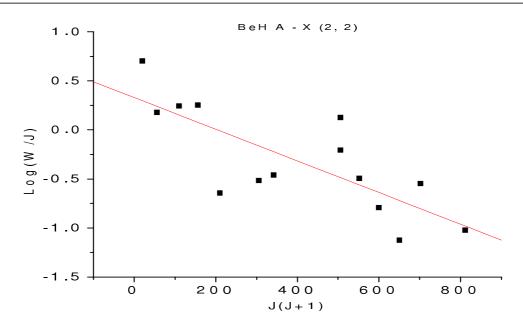


Fig. 5. Plot of log(W/J) vs J(J+1) for BeH A - X (2, 2) band.

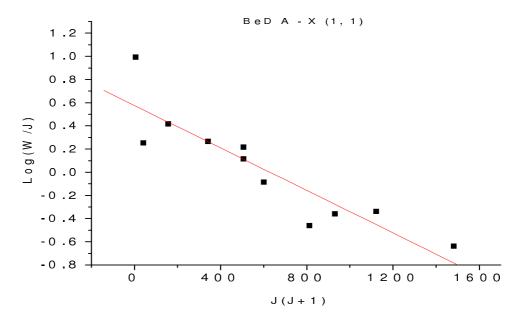


Fig. 6. Plot of log(W/J) vs J(J+1) for BeD A - X (1, 1) band.

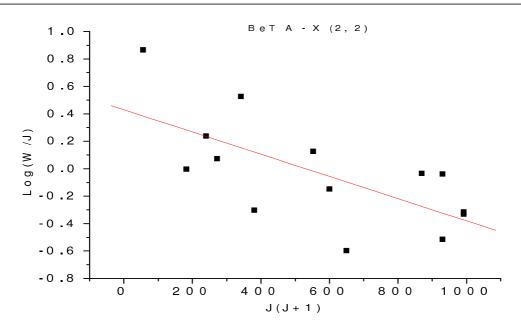


Fig. 7. Plot of log(W/J) vs J(J+1) for BeT A - X (2, 2) band.

Acknowledgements - The sunspot spectra used in this study are taken from the technical reports, and from the site ftp://nsokp.nso.edu/pub/atlas, of the National Solar Observatory, operated by the Association of Universities for Research in Astronomy, Inc. (AURA), under cooperative agreement with the National Science Foundation.

REFERENCES

- Bagare, S. P., Balachandra Kumar, K. and Rajaman-
- ickam, N.: 2006, Solar Phys., **234**, 1. De Greef, D. and Colin, R.: 1974, J. Mol. Spectrosc., **53**, 455.
- Engvold, O.: 1970, Solar Phys., 11, 183. Engvold, O., Wöhl, H. and Brault, J. W.:1980, Astron. Astrophys. Suppl. Series, 42, 209. Focsa, C., Bernath, P. F., Mitzner, R. and Colin.:
- 1998, J. Mol. Spectrosc., 192, 348.

- Herzberg, G.: 1950, Molecular Spectra and Molecular Structures. D. Van Nostrand Company, New York. Laborde, G.: 1961, Ann. Astrophys., 24, 89
- Olsson, V. E.: 1932, Zeitschrift für Physik, 73, 732.
- Rowland, H.: 1895, *Astrophys. J.*, 1, 29. Russell, H. N. and Bowen, I. S.: 1929, *Astrophys. J.*, **69**, 196.
- Russell, H. N. and Moore, C. E.: 1944, Trans. Am. Philos. Soc., **34**, 113. Shanmugavel, R., Bagare, S. P., and Rajamanickam,
- N.: 2006, Serb. Astron. J., 173, 83.
- Wallace, L., Hinkle, K., Li, G., and Bernath, P.: 1999, Astrophys. J., **524**, 454. Wallace, L., Hinkle, K., and Livingston, W.: 2000,
- An Atlas of Sunspots Umbral spectra in the visible from 15,000 to 25,000 $cm^{-1}(3920$ to 6664 Å), Tech.Rep.00-001, National Solar Observatory, Tuscon, AZ. Wöhl, H.: 1970, *Solar Phys.*, **15**, 342.
- Wöhl, H.: 1971, Solar Phys., 16, 362.

ИДЕНТИФИКАЦИЈА ЛИНИЈА ИЗОТОПОМЕРА БЕРИЛИЈУМ ХИДРИДА У СПЕКТРИМА УМБРЕ СУНЧЕВЕ ПЕГЕ

R. Shanmugavel¹, S. P. Bagare², N. Rajamanickam¹ and K. Balachandra Kumar³

¹Physics Research Centre, V.H.N.S.N College, Virudhunagar - 626 001 E-mail: nrmanickam@rediffmail.com

²Indian Institute of Astrophysics, Kodaikanal & Bangalore - 560 034 ³Kamaraj College of Engineering and Technology, Virudhunagar - 626 001

> УДК 523.982.2–355.3 Оригинални научни рад

Спектри умбре сунчеве пеге високе резолуције снимљене спектрографом FTS опсерваторије NSO/Kitt Реак искоришћени су за изучавање апсорпционих линија молекула изотопомера ВеН, ВеD и ВеТ. Извршена је идентификација линија молекула у спектралним тракама A-X(0,0), (1,1) и (2,2) молекуле ВеН, A-X(0,0), (1,1), (2,2) и (3,3) молекуле ВеD, и А-X(0,0), (1,1) и (2,2) молекуле ВеТ. Од идентификованих линија изабране су добро раздвојене линије и измерене су њихове еквивалентне ширине. На основу тих података су процењене ротационе ефективне температуре траке А-X(1,1) и (2,2) молекуле ВеН, А X(1,1) молекуле ВеD и А-X(2,2) молекуле ВеТ и износе редом 4228 K, 4057 K, 3941 K и 3243 K.