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Note

Is CH$^+$ Present in the Solar Spectrum?

Krishnanand SINHA and Bhuwan Mohan TRIPATHI

Uttar Pradesh State Observatory,
Manora Peak, Naini Tal-263 129, India

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Abstract

Identification of the $A^1\Pi$–$X^1\Sigma$ transitions of the CH$^+$ molecules in the solar spectrum was reinvestigated by using new laboratory data on molecules, standard photospheric models, the KPNO and the Liège solar atlases. We believe that CH$^+$ lines may not be detectible in the solar spectrum, though the predicted upper limits of equivalent widths exceed the observed upper limit by a factor of 6. A possible explanation for the absence of CH$^+$ lines is also suggested.

Key words: CH$^+$ molecules; Oscillator strength; Photosphere; Solar models; Solar spectrum.

1. Introduction

The molecule CH$^+$ has been observed in the spectra of comets (Arpigny et al. 1986) and interstellar medium (Lambert and Danks 1986). The difficult task of detecting the $A^1\Pi$–$X^1\Sigma$ transition of CH$^+$ in the crowded blue region of the solar spectrum was attempted by Grevesse and Sauval (1971), and they concluded that if it is present the equivalent widths (EWs) of the most intense lines cannot exceed 2 mÅ. Also, to explain large predicted EWs, these authors suggested that the only estimate of the oscillator strength, $f_{0,0} = 6.8 \times 10^{-2}$, then available (Smith, 1971) could be in error by as large a factor as sixty. Subsequent theoretical and experimental investigations by Yoshimine et al. (1973), Brzozowski et al. (1974), Elander et al. (1977), Erman (1977), Saxon et al. (1980), Mahan and O'Keefe (1981), and Larsson and Siegbahn (1983) support this view. However, the *solar* value $f_{0,0} = 1.2 \times 10^{-3}$ due to Grevesse and Sauval (1971) is still lower by a factor of about 5 than the currently available *theoretical* [$f_{0,0} = 5.45 \times 10^{-3}$, Larsson and Siegbahn (1983)] and *experimental* [$f_{0,0} = 5.57 \times 10^{-3}$, Mahan and O'Keefe (1981)] values. Hinkle et al. (1973) and Sneden and Lambert (1982) have also discussed the solar CH$^+$ problem briefly.

For the $A^1\Pi$–$X^1\Sigma$ transition of CH$^+$ molecules, fairly reliable estimates of $f_{0,0}$ (uncertainty $< 20\%$) and of D_0^0 (uncertainty < 0.02 eV) are available

(E. F. van Dishoeck 1987, private communication; M. Larsson 1987, private communication). This circumstance coupled with the availability of accurate wavenumbers for a large number of vibrational bands (Carrington and Ramsay 1982) prompted us to take a fresh approach to the above problem. We used the KPNO (Brault and Testerman 1972) and the Liège (Delbouille et al. 1973) solar atlases for line identifications.

2. Method

The method of weighting functions was used by us for EW calculations for the HM (Holweger and Müller 1974) and the MACKKL (Maltby et al. 1986) photospheric model atmospheres. The molecular constants from Huber and Herzberg (1979) and the sources of continuum opacity from Tsuji (1966) were borrowed. We depended on Tsuji (1973) and Irwin (1981) for calculations of the atomic partial pressures and atomic partition functions. The dissociation constants used for calculations of partial pressures of CH^+ were taken from Tarafdar (1977). The CNO abundances were from Lambert (1978). Larsson and Siegbahn (1983) oscillator strengths were used to compare the EWs of the CH^+ lines in different bands. For the EW calculation of all the lines of the (0–0) band, the oscillator strengths were taken from Mahan and O'Keefe (1981). It is noted that the $f_{0,\,0}$ values in Larsson and Siegbahn (1983) as well as in Mahan and O'Keefe (1981) are in excellent agreement with each other. A depth-independent microturbulence was assumed [2.1 km s^{-1}, Porfireva (1986)] for the HM model. However, uncertainties in this value do not appreciably affect the EWs predicted here.

3. Results and Discussions

The HM model is unanimously thought to be the most successful LTE model for representing the solar atmosphere (Chmielewski 1984; Grevesse 1984; Sinha 1984). The only objection, that this model does not include the chromospheric part of the atmosphere, is taken care of by the MACKKL model considered here. Our preliminary analysis based on rotational temperature calculations of the C_2 lines shows that for calculations for the centre on the solar disc there is practically no difference between these two models.

Following Larsson (1983) and Lambert and Danks (1986), appropriate expressions for the Hönl-London factors and $f_{v',v''}$ were written. At photospheric temperatures, the lines originating from the J $\simeq$ 11 level should be the most intense amongst other CH^+ lines. Calculations were carried out for $\mu = 1.0$ and $\mu = 0.2$ for one line each of the P, Q, and R branches of the (0–0), (1–0), (0–1), (1–1), (2–1), (3–1), (1–2), and (1–3) bands, i.e., for all the bands studied by Carrington and Ramsay (1982). The (0–0) and the (1–0) bands were found to possess appreciable intensity and were worth a search in the solar atlas.

The vacuum wavenumbers from Carrington and Ramsay (1982) were converted to wavelengths in dry air with the help of the NBS monograph (Coleman et al. 1960). The method of line coincidences for solar identifications requires that the difference between a laboratory wavelength and the solar wavelength must not exceed a value, $\Delta\lambda$, which depends upon the accuracy of the laboratory wavelengths in question and on the uncertainty of the wavelength scale of the atlas being used. Since we are not too sure about what value of $\Delta\lambda$ should be used, we persisted with the conservative approach of Schadee (1964) who gave it as ± 0.05 mÅ which, however, being on the higher side, has the effect of increasing wavelength coincidences. The identification atlas due to Moore et al. (1966) served as a reference. The KPNO atlas includes observations at $\mu = 1.0$ and $\mu = 0.2$, whereas the Liège atlas with a better signal-to-noise ratio gives the same for $\mu = 1.0$ only. The following notations were used in our identification programme:

A: No feature at these wavelengths. The line is *absent.*
P: There is an unidentified solar feature at this wavelength. The line may possibly be *present.*
M: The CH$^+$ line is *masked* (?) by some known or unknown lines.

When we say a solar feature, it may be taken to mean a resolved line core, an inflection in a wing of a strong line or a weak, but broader than average, line. We expect the CH$^+$ lines to stay constant in EW towards the limb and to be absent in sunspots. The result of our search for the (0–0) and the (1–0) bands is summarised below:

(0–0) band, 34 lines:
P branch : A = 1, P = 0, M = 7 a total of 8 lines,
Q branch : A = 4, P = 1, M = 6 a total of 11 lines,
R branch : A = 6, P = 1, M = 8 a total of 15 lines,
A = 11, P = 2, M = 21.

(1–0) band, 33 lines:
P branch : A = 2, P = 2, M = 4 a total of 8 lines,
Q branch : A = 2, P = 1, M = 9 a total of 12 lines,
R branch : A = 6, P = 2, M = 5 a total of 13 lines,
A = 10, P = 5, M = 18.

Thus, in both the (0–0) and the (1–0) bands the lines absent outnumber the lines present. The large value for the number of masked lines may be a consequence of our search in a crowded spectral region. In a private communication Prof. David L. Lambert advised us against the use of the (1–0) band because of a highly depressed continuum in the region of its occurrence. We now proceed to closely examine only the (0–0) band.

The EWs of all the lines of the (0–0) band for which a search was made in the solar spectrum were calculated. We used here Mahan and O'Keefe's (1981) value for $f_{0,\,0}$.

The first question attempted was whether we can detect a solar line as weak as the CH$^+$ lines in the Liège atlas. It is interesting to note that there is an unidentified solar feature in the Liège atlas with EW = 4.3 mÅ at a wavelength 4245.787 Å, where the $Q(4)$ line with the expected EW = 7.9 mÅ should occur. Moore et al. (1966) give its EW = 3.5 mÅ. If this feature can be identified as the $Q(4)$ line of CH$^+$ it is then clear that the other lines of this molecule, which are stronger, can be easily detected. Considering the difference in the predicted EW of the $Q(4)$ line and that of this unidentified feature in the solar spectrum, we should be prepared to reduce the predicted values by half if a large number of CH^+ lines are found present. We carefully noted the positions where the CH^+ lines with EW > 6 mÅ could occur in the solar atlas and it was found that the $Q(5)$, $Q(7)$, and $Q(8)$ lines, all stronger than the above $Q(4)$ line, fall on the wings of already identified lines; however, they are not able to produce even a kink, whereas the $Q(6)$ and $Q(10)$ lines are masked. Similarly, the $R(5)$, $R(7)$, $R(8)$, and $R(12)$ lines are not traceable and $R(13)$ is masked. However, the above should not be taken to mean that a line marked absent is always weaker than a line marked present. In such cases the anomaly needs to be explained in terms of known physical causes.

We are thus faced with a situation in which the lines of CH^+ with detectible predicted EWs seem to be absent in the solar photospheric spectrum. A few remarks concerning the D_0^0 and the $f_{0,\,0}$ values used here would be pertinent. We used $D_0^0(CH^+) = 4.08$ eV from Huber and Herzberg (1979). This is in perfect agreement with a recent experiment by Helm et al. (1982) which gives $D_0^0(CH^+) = 4.080 \pm 0.003$ eV and utilizes a fast ion-beam technique which allows a direct measurement of D_0^0. Also, the results due to Graff et al. (1983) give firm lower and upper bounds of 4.077 and 4.091 eV, meaning that $D_0^0(CH^+)$ is known with an accuracy better than 0.02 eV. The measured lifetime by Mahan and O'Keefe (1981) from which the $f_{0,\,0}$ values are derived is considered to be by far the best experimental determination of the CH^+ $A^1\Pi$ state lifetime (M. Larsson 1987, private communication). Also, a recent theoretical study based on a coupled cluster polarization propagator method by Geersten and Oddershede (1986) supports this view. The oscillator strengths used here are based on large basis set calculations by Larsson and Siegbahn (1983) which, in turn, are in excellent agreement with Mahan and O'Keefe (1981), Erman (1977), and Lambert and Danks (1986). Larsson (1987, private communication) investigated the effect of the rotational dependence of the CH^+ $A^1\Pi$–$X^1\Sigma$ oscillator strength. He calculated $f_{v'=0\ J'=10,\ v''=0\ J''=10}$ with the same transition moment function used to derive $f_{v'=0\ J'=0,\ v''=0\ J''=0} = 5.45 \times 10^{-3}$; the result was 4.68×10^{-3}. Obviously, the values chosen here are very reliable and the solar value $f_{0,\,0} < 1.2 \times 10^{-3}$ due to Grevesse and Sauval (1971) should be in error.

In brief, it can be stated that a reliable CNO abundance (Lambert 1978), a standard model atmosphere (Holweger and Müller 1974; Maltby et al. 1986), accurate dissociation energy and oscillator strengths used here seem to indicate that it is difficult to argue that a solution to the solar CH^+ problem is to be found in the basic molecular data for this molecule. We now move to a discussion of another area which might provide a solution.

To test the hypothesis of an additional source of opacity which may weaken the CH^+ lines (Hinkle et al. 1973; Sneden and Lambert 1982), one may feel tempted to use the violet system of the CN bands e.g. the (0–1) band which occupy about the same spectral region as that discussed above. However, such an effort may not succeed because of different depths of formation for the two molecules and their lines. D. Lambert (1988, private communication) believes that because of a veil of weak absorption lines the solar continuum around the wavelengths in question is depressed. The effect of this veil on the analysis of weak absorption lines depends, among other things, on the depth of formation of the typical lines producing the veil. Weak lines formed above the veil should preserve their EWs, whereas those formed with it should have diluted EWs. We suspect that the CH$^+$ lines could be formed with the veil in view of a large concentration of this molecule in deeper layers, corresponding to the same quantities of CN. Additionally, the model-based predicted photospheric rotational temperatures for CN and CH$^+$ are 5000 and 5950 K respectively.

However, a possible importance of the veil opacity is already known (cf. Holweger 1970) and the problem now is to clarify the nature of this opacity on the basis of weakening in well detected lines.

In conclusion we infer that the discrepancy in the calculations and observations cannot be attributed to errors in the molecular data, such as $f_{0,0}$ and D_0^0. It is supposed that it may have been caused by a failure of the model atmosphere calculations to represent the opacity due to both weak and overlapping lines.

3.1. Limitations of the Present Work

It has been pointed out by one of the referees that the weighting function method provides correct estimates of EW only for weak lines that are found in a spectral region with a clear continuum. Otherwise, this method provides upper estimates of the EWs. It is probably worth while comparing the synthetic spectrum, including all of the known line absorption with the observed one. Then, the effect of other overlapping lines can be taken into account in estimating EW. Even in this method, however, the difficulty to define the true continuum in the observed spectrum will remain but, because of the high S/N ratio of the solar spectral atlases, deformation of line profiles due to different sources can perhaps be detected.

Without extremely helpful comments from Professors Ewine F. van Dishoeck, N. Grevesse, David Lambert, Mats Larsson, and A. J. Sauval on a preliminary version of this paper, it was not possible to prepare this paper in its present form. We express our sincere gratitudes to them. Also, the discussions and comments by the referees were extremely helpful in improving both the contents and the presentation of the paper. We thank Dr. M. C. Pande for useful suggestions.

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Erratum

In the paper “Asymmetric Distribution of Gas in the Large Magellanic Cloud and Dynamical Condition for Globular Cluster Formation” by Mitsuaki FUJIMOTO and Masafumi NOGUCHI [*Publ. Astron. Soc. Japan* **42**, 505 (1990)], figures 1 (page 507) and 5 (page 511) were not clearly presented, and they should be replaced with the following:

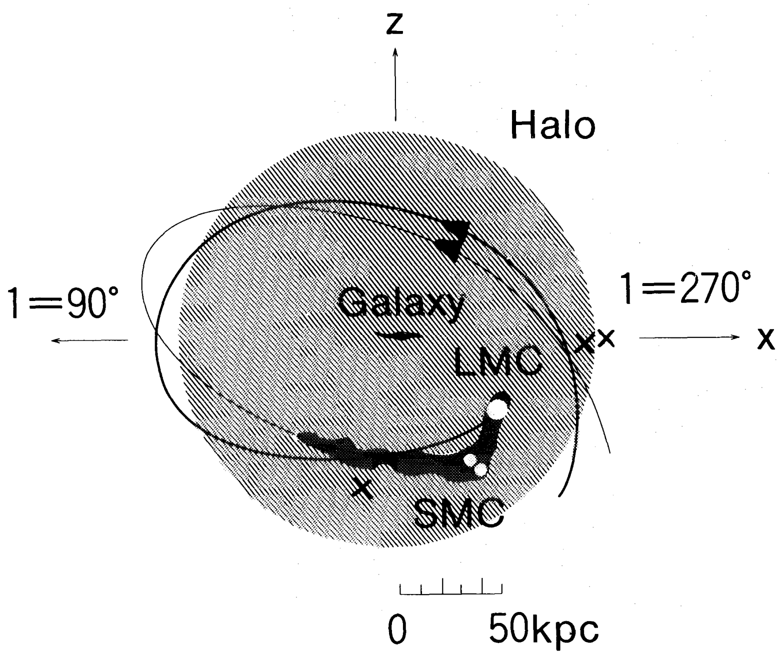

Fig. 1. Past orbits of LMC and SMC around the Galaxy with a massive halo of 10^{12} $M_{\odot}$, reproduced from the tidal model of the Magellanic Stream by Murai and Fujimoto (1980). The orbits satisfy the observed positions and radial velocities of LMC and SMC, and their orbital planes are approximately perpendicular to the line of $l = 180°$ and $b = 0°$. LMC and SMC made close encounters at the symbols $\times$ and $\times\times$, respectively, $\sim$ 0.2 Gyr and 1.7 Gyr ago. The Magellanic Stream was generated by H I gas torn off tidally from SMC during a latter encounter, or at $\times\times$. The x-axis is applied as being parallel to the direction $l = 270°$ and $b = 0°$, the y-axis to $l = 0°$ and $b = 0°$, and the z-axis coincides with the rotation axis of the Galaxy. The origin is, therefore, taken at the Galactic center. A massive halo of 10^{12} $M_{\odot}$ is shown by a gray sphere and the Magellanic Stream by a dark smoke.

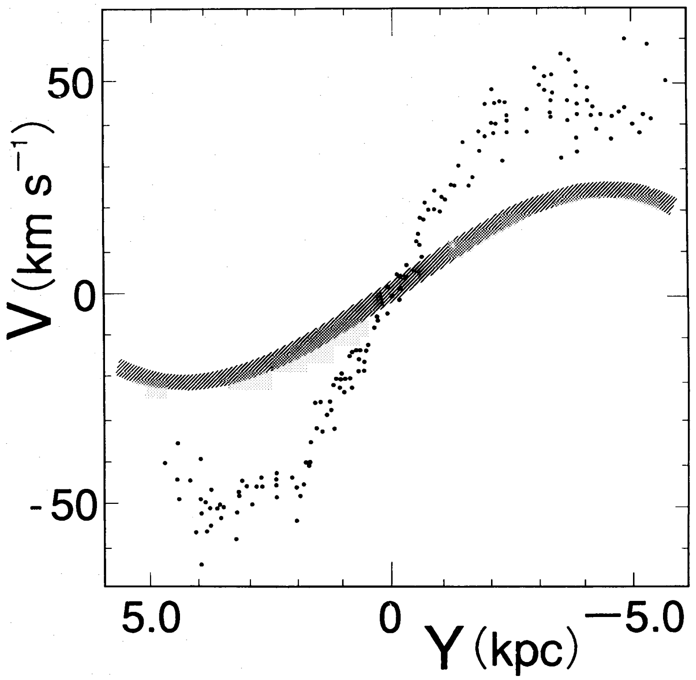

Fig. 5. Rotation law of particles (gas clouds) in figures 4a and b. The rotation plane is approximately on the y-z plane in figure 1 and thus its inclination angle i is $\sim 35°$ against the line-of-sight. The line-of-node of the rotation plane is nearly the same as the apparent major axis of LMC, or along the line of $\alpha = 5^{\mathrm{h}}25^{\mathrm{m}}$. A wavy gray belt of small amplitude is a rotation curve, averaged in an ensemble way over the orbits of gas clouds in hydrodynamical collision with SMC gas. Since the abscissa is taken along the major axis of LMC, these two curves correspond to the two-valued rotation curves of H I gas in LMC discovered by McGee and Milton (1966).