

**INSTITUTE OF THEORETICAL ASTROPHYSICS
BLINDERN - OSLO**

REPORT No. 45

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SOLAR ATMOSPHERE DETERMINED FROM CH-LINES
IN THE PHOTOSPHERIC SPECTRUM.**

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ABSTRACT

The R-branch of the (0,0) vibrational band of the violet electronic transition $A^2\Delta - X^2\Pi$ of CH is analysed. Isotope wavelength shifts are measured on laboratory spectrograms. The method of synthesizing the spectrum is used, and the molecular dissociation equilibrium through the photosphere is computed. ^{13}CH is not definitely identified in the photospheric spectrum and only upper limits of the ^{13}C abundance are deduced. The upper limits are sensitive to the local continuum level. A photospheric abundance ratio $^{12}\text{C}/^{13}\text{C}$ greater than the terrestrial value of 90 seems highly probable.

1. INTRODUCTION

It is generally accepted today that the solar system originated from contracting interstellar material (Reeves 1972). In a work on the origin of the solar system, Fowler, Greenstein and Hoyle (1962) suggest that nuclear reactions have taken place in the preplanetary material. The nuclear reactions were due to high-energetic charged particles ejected from a magnetically active, contracting sun. Fowler et al. points out that possibly all terrestrial ^{13}C may be due to such an irradiation of the preplanetary material, and that ^{13}C was practically absent in the original interstellar material.

The theory of Fowler et al., therefore, predicts that the solar abundance ratio $^{12}\text{C}/^{13}\text{C}$ may be much greater than elsewhere in the solar system, and equal to the original, interstellar value of $^{12}\text{C}/^{13}\text{C}$. On the other hand, theories not including the assumption of an irradiation by high-energetic particles, predict approximately the same ratio $^{12}\text{C}/^{13}\text{C}$ throughout the solar system.

The isotopic ratio $^{12}\text{C}/^{13}\text{C}$ in different objects in the solar system is given in Table 1-1. From Table 1-1 it is evident that the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ in the preplanetary material, after possible nuclear reactions have taken place, was about 90. This value is referred to as the terrestrial value.

It is interesting to establish the solar abundance ratio $^{12}\text{C}/^{13}\text{C}$ in order to support or reject the theory of Fowler et al.

Table 1-1. The isotopic ratio $^{12}\text{C}/^{13}\text{C}$ in the solar system.

Object	$^{12}\text{C}/^{13}\text{C}$	References
Earth	89±2	Rankama (1963)
Moon	90±2	Epstein and Taylor (1970) Friedman, O'Neil, Adami, Gleason and Hardcastle (1970) Kaplan and Smith (1970)
Meteorites	91±2	Rankama (1963) Mason (1971) Begemann and Heinzinger (1969) Belsky and Kaplan (1970)
Venus	100	Connes, Connes, Kaplan and Benedict (1968)
Mars	100	Kaplan, Connes and Connes (1969)
Jupiter	110±40	Fox, Mantz, Owen and Rao (1972)
Comet	70±15	Stawikowski and Greenstein (1964)

To determine the ratio $^{12}\text{C}/^{13}\text{C}$ in the solar atmosphere, it is necessary to analyse absorption lines from carbon compounds. Molecules with strong absorption bands in the solar spectrum are CH, CN, CO and C_2 .

Table 1-2 shows earlier determinations of the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ in the solar atmosphere.

Use of the CN-lines P(57) and P(58) by various authors results in widely different solar isotopic ratio $^{12}\text{C}/^{13}\text{C}$. The ratio, or alternatively its upper limit, is very sensitive to the assumed continuum intensity level, since the isotopic ^{13}CN lines are barely detectable in the ultraviolet part of the photospheric spectrum.

The two works on the CH (0,0)-band also lead to different conclusions. From the three least blended isotopic lines,

Table 1-2. The isotopic ratio $^{12}\text{C}/^{13}\text{C}$ in the solar atmosphere.

Molecule	Band/lines	Wavelength ⁽ⁱ⁾	$^{12}\text{C}/^{13}\text{C}$	References
CN	$\text{B}^2\Sigma^+ - \text{X}^2\Sigma^+$, (0,0) P(57), P(58)	3874-75 ph	>15	Mc Kellar (1948)
CN	$\text{B}^2\Sigma^+ - \text{X}^2\Sigma^+$, (0,0) P(57), P(58)	3874-75 ph	>36	Greenstein, Richardson and Schwarzschild (1950)
CN	$\text{B}^2\Sigma^+ - \text{X}^2\Sigma^+$, (0,0) P(58)	3874.34 ph	1000	Righini (1956)
CN	$\text{B}^2\Sigma^+ - \text{X}^2\Sigma^+$, (0,0) P(58)	3874.34 ph	>200	Ganiari., Bashkin and Waddell (1966)
CN	$\text{B}^2\Sigma^+ - \text{X}^2\Sigma^+$, (0,0) P(57), P(58)	3874-75 ph	>40-120	Herzberg, Delbouille and Roland (1967)
CH	$\text{A}^2\Delta - \text{X}^2\Pi$, (0,0) R-branch	4315 ⁽ⁱⁱ⁾ ph	100±30	Richter and Tonner (1967)
CH	$\text{A}^2\Delta - \text{X}^2\Pi$, (0,0) R(13)	4231.43 ph	>150±30	Lambert and Mallia (1968)
CO	Infrared vibration-rotation bands	22880 -24750 sp/ph	90±13	Hall, Noyes and Ayres (1972)
CO	Infrared vibration-rotation bands	22880 -24750 sp/ph	84±9	Hall (1973)

(i) ph=photospheric spectrum
sp=spot spectrum

(ii) band head

Richter and Tonner (1967) find a mean value of 100 for the isotopic ratio. Lambert and Mallia (1968), however, emphasize that even the least blended ^{13}CH identification of Richter and Tonner may be spurious, and they find a lower limit of 150 for the isotopic ratio $^{12}\text{C}/^{13}\text{C}$.

According to Hall, Noyes and Ayres (1972) and Hall (1973) the presence of $^{13}\text{C}^{16}\text{O}$ in the infrared umbral spectrum is unquestionably established. They find a $^{12}\text{C}/^{13}\text{C}$ abundance ratio that agrees well with the terrestrial value. This result deviates from the isotopic ratio derived from the photospheric spectrum by Lambert and Mallia and others.

From the preceding, the abundance ratio $^{12}\text{C}/^{13}\text{C}$ is not unambiguously established. It is not yet clear whether the solar $^{12}\text{C}/^{13}\text{C}$ ratio is greater than or equal to the terrestrial value.

In this investigation a reanalysis of the R-branch of the (0,0)-vibrational band of the ultraviolet electronic transition $A^2\Delta - X^2\Pi$ of CH is carried out with better spectral resolution than before, and more accurate reduction methods are used.

The observations were obtained at the R.R. McMath Solar Telescope, Kitt Peak National Observatory, Arizona (Brault, Slaughter, Pierce and Aikens 1971) by O. Engvold in the period december 13, 1968 to september 25, 1969. The spectral scans cover the rotational lines R(16) to R(7) at the centre of the solar disk with the exception of R(11) and R(9).

For each spectral region two simultaneous scans were obtained. The difference in intensity between two such simultaneous, restored and averaged spectra (see Brault et al. 1971) reflects the uncertainty due to the recording of the spectra

and to an imperfect averaging of an inhomogeneous and non-stationary photosphere. The uncertainty according to this criterion is about 0.1% of the continuum intensity on most spectra, in all cases less than or equal to 0.2%.

In this investigation, the line profiles are computed by a model atmosphere. The complete spectral appearance is synthesized by including also the formation of absorption lines other than the CH-lines. The abundance of CH molecules through the solar atmosphere is computed.

2. THE ISOTOPE SHIFT

Richter and Tonner (1967) have published laboratory wavelengths of ^{13}CH lines in the R-branch of the violet (0,0)-band.

A preliminary survey of the solar spectrum showed that some of the ^{13}CH wavelengths of Richter and Tonner coincide with weak spectral lines. In other cases a possible identification of ^{13}CH is ambiguous, or no weak line can be detected at the ^{13}CH position. To obtain reliable identifications of ^{13}CH -lines, isotope shifts of the ^{13}CH lines were remeasured on laboratory spectrograms.

Experimental

A glass container filled with a mixture of hydrogen (H_2) and methane (CH_4), under low pressure was used as a spectral lamp. The methane was enriched with the ^{13}C isotope, and the gas mixture excited with a microwave oscillator to produce an emission spectrum. The spectral lamp was constructed at the Institute of Physics, University of Oslo.

A CH-spectrum in emission and a photospheric spectrum in absorption (Fig. 2-1) were exposed on the same film with the spectrograph at Oslo Solar Observatory.



Fig. 2-1. Photospheric and laboratory spectrum of CH. Upper marks refer to the photospheric spectrum, lower marks refer to the laboratory spectrum.

Measurements

The least blended photospheric ^{12}CH -line in each rotational group is selected as reference line. The resulting wavelengths are tabulated in Table 2-1 and compared to the measurements of Richter and Tonner.

The total uncertainty in the laboratory wavelengths of the ^{12}CH and ^{13}CH lines is estimated to 10mÅ.

The wavelengths of the ^{12}CH lines from the two works agree within the uncertainty of the measurements. Some of the ^{13}CH wavelengths, however, deviate more than the uncertainty. The deviation varies systematically with the rotational quantum number K, indicating an error in one of the investigations.

Table 2-1.

The wavelengths of ^{12}CH and ^{13}CH in the solar spectrum⁽ⁱ⁾.

Rotational transition	Present ⁽ⁱⁱ⁾ (Å)		Richter and Torner (Å)	
	$\lambda(^{12}\text{CH})$	$\lambda(^{13}\text{CH})$	$\lambda(^{12}\text{CH})$	$\lambda(^{13}\text{CH})$
R(16)			4210.977 4212.622 4212.663	4211.51 4213.15 4213.19
R(15)			4217.207 4217.257 4218.725	4217.69 4217.74 4219.22
R(14)			4223.488 4223.575 4224.861	4223.94 4224.02 4225.31
R(13)	4229.800 4229.914 4231.032	4230.236 4230.344 4231.440	4229.787 4229.908 4231.028	4230.22 4230.32 4231.43
R(12)	4236.116 4236.263 4237.172 4237.241	4236.501 4236.651 - -	4236.121 4236.263 4237.160 4237.220	4236.49 4236.64 4237.54 4237.60
R(11)	4242.445 4242.604 - 4243.446	4242.787 4242.965 (4243.660) 4243.790	4242.448 4242.615 4243.348 4243.460	4242.79 4242.96 4243.69 4243.81
R(10)	4248.731 4248.944 4249.501 4249.647	4249.040 4249.251 4249.799 4249.945	4248.739 4248.945 4249.498 4249.649	4249.05 4249.26 4249.81 4249.96
R(9)	4255.003 - 4255.637 4255.833	(4255.241) 4255.524 4255.898 4256.094	4254.996 4255.252 4255.632 4255.834	4255.28 4255.53 4255.91 4256.11
R(8)	4261.223 4261.530 4261.736 4261.991	4261.461 4261.741 4261.970 4262.208	4261.229 4261.533 4261.732 4261.994	4261.48 4261.78 4261.98 4262.24
R(7)	4267.389 4267.773 4268.112	4267.589 (4267.951) 4268.306	4267.389 4267.753 4267.801 4268.108	4267.60 4267.97 4268.01 4268.33

Table 2-1 continued.

Rotational transition	Present(ii)		Richter and Tonner	
	(Å)		(Å)	
	$\lambda(^{12}\text{CH})$	$\lambda(^{13}\text{CH})$	$\lambda(^{12}\text{CH})$	$\lambda(^{13}\text{CH})$
R(6)	4273.480	4273.647	4273.476	4273.66
	4273.788	4273.935	4273.787	4273.97
	4273.925	4274.082	4273.927	4274.11
	4274.193	4274.346	4274.192	4274.38

- (i) it is supposed that the isotope wavelength shifts in the solar and laboratory spectra are equal.
(ii) - the wavelength is not measurable, due to blend.
() the wavelength is uncertain, due to blend.

Calculations

The total isotope wavelength shift is composed of the electronic, vibrational and rotational shift. The vibrational and rotational energy formulae are obtained from Herzberg (1950, p. 92 and p. 232). Isotopic molecular constants are calculated from the formulae in Herzberg's book, p. 152 and p. 144, which for ^{13}CH are very good approximations to the expressions of Dunham (1932). The electronic shift is neglected. However, as the electronic shift is independent of the rotational quantum number K , the variation of the isotope shift with K should essentially be correct.

Theoretical and observed isotope shifts are plotted as a function of the rotational quantum number K in Fig. 2-2.

Considering the variation of the isotope wavelength shift with K , neither the present laboratory measurements nor that of Richter and Tonner (1967) agree perfectly with the computed shifts. The ^{13}CH wavelengths chosen in this investigation are discussed in Ch. 4.

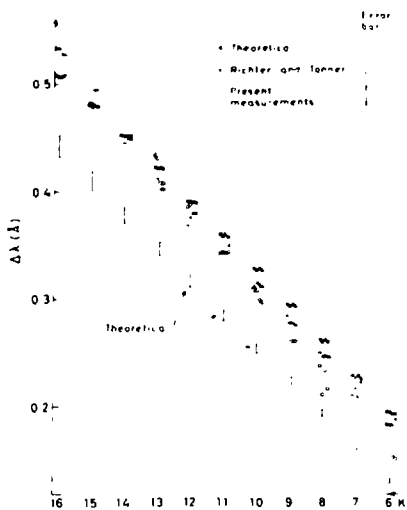


Fig. 2-2. Theoretical and observed isotope shift $\Delta\lambda = \lambda(^{13}\text{CH}) - \lambda(^{12}\text{CH})$.

3. THE ABUNDANCE OF CH IN THE SOLAR PHOTOSPHERE

The strength of CH absorption lines is determined by the relative abundance of CH molecules as function of depth in the atmosphere. Computations of the CH abundance involve (i) a model atmosphere, (ii) the relative abundances of all elements that influence the equilibrium of dissociation of the CH molecule, (iii) dissociation constants of the participating molecules.

The dissociation constant $K(AB)$ of the molecule AB is defined by

$$K(AB) = p(A) p(B)/p(AB) \quad (3.1)$$

where the p's are the partial pressures of the atoms A and B and the molecule AB.

The dissociation equilibrium is determined by the partial pressures of the atoms which constitute the molecules (Schadee 1964, Tsuji 1964).

The partial pressure of CH is determined directly from the partial pressures of C and H (equation 3.1). Every molecule that influences the partial pressures of C and H have to be included in the dissociation equilibrium equations. A test calculation shows that only the molecules CO, H₂, CN and OH may affect the CH abundance in the solar photosphere. Of these four molecules, only CO seriously affects the CH-abundance.

The dissociation equilibrium is therefore calculated for the molecules ¹²CH, ¹³CH, ¹²CO, ¹³CO, ¹²CN, ¹³CN, H₂, OH. The equations for the partial pressures are then:

$$\begin{aligned}
 p(^{12}\text{C}) &= p'(^{12}\text{C}) / (1 + S(^{12}\text{C}) + p(\text{H}) / K(^{12}\text{CH}) + p(\text{O}) / K(^{12}\text{CO}) + p(\text{N}) / K(^{12}\text{CN})) \\
 p(^{13}\text{C}) &= p'(^{13}\text{C}) / (1 + S(^{13}\text{C}) + p(\text{H}) / K(^{13}\text{CH}) + p(\text{O}) / K(^{13}\text{CO}) + p(\text{N}) / K(^{13}\text{CN})) \\
 p(\text{H}) &= p'(\text{H}) / (1 + S(\text{H}) + p(\text{C}) / K(\text{CH}) + 2p(\text{H}) / K(\text{H}_2) + p(\text{O}) / K(\text{OH})) \\
 p(\text{N}) &= p'(\text{N}) / (1 + S(\text{N}) + p(\text{C}) / K(\text{CN})) \\
 p(\text{O}) &= p'(\text{O}) / (1 + S(\text{O}) + p(\text{C}) / K(\text{CO}) + p(\text{H}) / K(\text{OH}))
 \end{aligned}
 \tag{3.2}$$

where S is the quotient of the number of ionized and neutral atoms computed by the Saha equation, and p' are the partial pressures corresponding to the total number of nuclei of the element.

Given the temperature, gas pressure, electron pressure and the relative abundances of the elements, the equations (3.2) may be solved by iteration, inserting p' for p the first time.

The dissociation constants are calculated in Appendix A.

The total abundances of the elements involved in the calculation of the dissociation equilibrium are given in Table 3-1.

Table 3-1. Abundances of the elements

Element	log ε	References
C	8.60	Nicolaides and Sinanoglu (1973)
H	12.00	reference value by definition
N	7.93	Lambert (1968)
O	8.93	Nicolaides and Sinanoglu (1973)

Some of the results of the equilibrium calculation are presented in Fig. 3-1. τ_c is the optical depth in continuum at 4240Å. The abundances are calculated with Harvard Smithsonian Reference Atmosphere (HSRA) (Gingerich, Noves, Kalkofen and Cuny 1971) and with Holweger's model atmosphere (Holweger 1967).

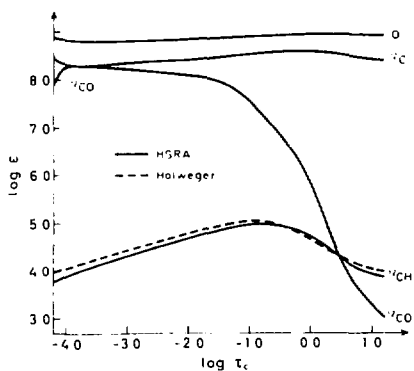


Fig. 3-1. The dissociation equilibrium in the solar photosphere.

4. LINE FORMATION IN THE SOLAR PHOTOSPHERE

The calculation of the line spectrum was performed with a computer program, assuming LTE, originally made by O. Engvold and O. Kjeldseth Moe. The present calculation of the dissociation equilibrium is incorporated in this program.

The observed spectra are synthesized by adjusting the oscillator strengths and wavelengths of the spectral lines and the continuum intensity. The model atmosphere including the turbulent velocity is fixed during this procedure.

In reproducing the observed spectral regions, absorption features other than CH-lines are accounted for. Most of the reasonably strong absorption features are identified in the tables of Moore, Minnaert and Houtgast (1966).

The continuum intensity

The observed spectra are normalized to the largest intensity level on each spectral scan. In virtually no cases the observed intensity maxima provide realistic continuum levels. The observed, and hereafter called local continua, are depressed relative to the true continuum levels by absorption from many very faint atomic and molecular lines which overlap each other.

Here, the continuum depression is described by the additional absorption

$$\eta_{\lambda}(\tau_c) = \eta_D e^{-(\log \tau_c + 3.2)} \quad (4.1)$$

at various optical depths τ_c . $\eta_{\lambda} = \frac{\kappa_{\lambda}}{\kappa_c}$ where κ_{λ} is the line absorption coefficient, and κ_c is the continuum absorption

coefficient. The exponential represents a mean of the variation of η_λ with depth for faint lines, arising under different excitation and ionization conditions. η_D is a free parameter, adjusted to give the desired value of the continuum depression.

The local continuum depression due to faint lines may be wavelength dependent, or the spectral region to be reproduced may be situated in the wing of a strong line far from the line centre. In both cases the parameter η_D is computed from

$$\eta_D = \frac{\alpha}{(\lambda - \lambda_0)^2} \quad (4.2)$$

where the constants α and λ_0 are determined from the observed depression.

Unidentified lines

For weak unidentified lines with central depths less than about 2% of the continuum intensity, arbitrary line parameters have a negligible effect on the computed profiles. For stronger lines the atomic weight of the element is the most critical parameter for the line profile.

The turbulent velocity

Variations of the turbulent velocities will influence the line profiles and the deduced abundances, but the influence on the abundance ratio $^{12}\text{C}/^{13}\text{C}$ is negligible.

The profile function

The majority of lines are computed with the Gauss profile. The effect of using the more accurate Voigt profile for the wing of the ^{12}CH lines is minor. The determination of the oscillator strengths of ^{12}CH is not influenced.

CH-lines and LTE

In LTE there is a strong coupling between the radiation field and the gas particles. In the solar atmosphere this coupling is secured by the photons being destructed by ionization of the atoms (a continuum process).

Athay (1972, p. 18-27 and p. 175-176) defined a quantity δ as the probability that a photon in a given spectral line be destructed by a continuum process, as defined above.

The ^{12}CH lines have a typical value of $\delta = 0.3$ in the line-forming layers. It is therefore doubtful if ^{12}CH -lines are formed in LTE. It is not known how this will influence the population of the levels.

Reproduction of the ^{12}CH lines

Observed and theoretical spectra of two of the ^{12}CH regions are shown in Fig. 4-1 and 4-2. Each ^{12}CH line has a designation of the form $R_{2d}(K)$ (see Herzberg 1950, p. 227 and p. 232). The notations refer to the lower level of the transition.

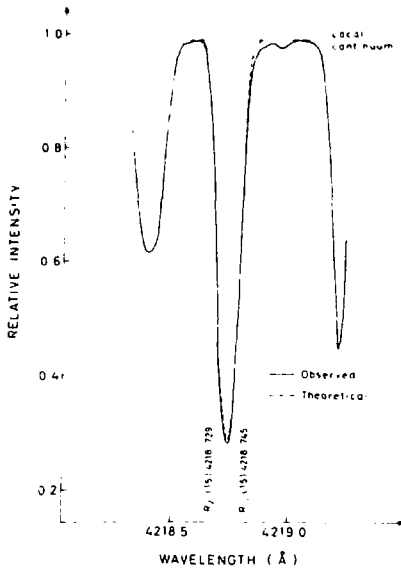


Fig. 4-1. Observed and theoretical spectrum, R(15), 4218.8 Å.

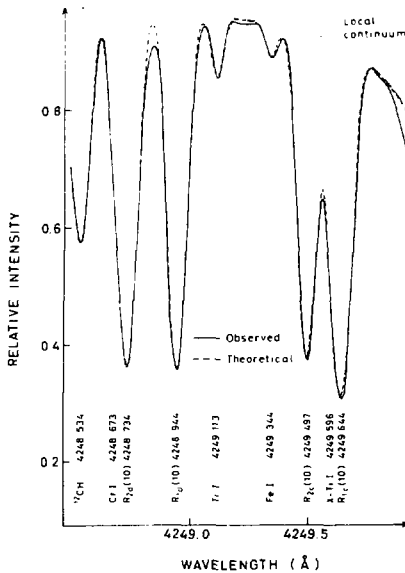


Fig. 4-2. Observed and theoretical spectrum, R(10), 4249 Å.

Unidentified spectral lines are marked with X and the "identification" used.

A number of the ^{12}CH lines are doublets that are not resolved neither in the solar spectrum nor in the laboratory spectra. To a certain extent it is possible to account for the observed width and asymmetry of these doublets by using slightly different wavelengths and oscillator strengths for the two line components.

Theoretical oscillator strength

To deduce a ^{13}CH abundance, it is necessary to know the oscillator strengths f_J of the (0,0) band. The oscillator strength for a single rotational line is given by

$$f_J = f_{el} f_{00} \frac{S_J}{2J+1} \quad (4.3)$$

The electronic oscillator strength f_{el} is determined by Kuzmenko, Kuzyakov, Kuznetsova, Kudryumova and Chuev (1971), who recommend the value $f_{el} = (2.3 \pm 0.4) \cdot 10^{-3}$.

The vibrational strength f_{00} for the (0,0) band is $f_{00} = 0.9996$ according to Childs (1964). The Hönl-London factors S_J for the R branch of the $^2\Delta-^2\Pi$ transition of CH is given by Kovacs (1969, p. 61 and p. 130). $2J+1$ is the statistical weight g of the lower level.

Empirical oscillator strength

The gf values of the ^{12}CH lines resulting from the fitting of theoretical spectra to the observed ones together with theoretical values are shown in Fig. 4-3. The scattering

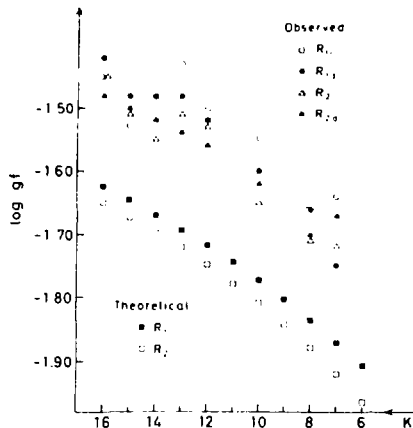


Fig. 4-3. $\log(gf)$ values for ^{12}CH .

in the observed gf values is probably mainly due to blends which are so close to the line centres that they cannot be discovered. The observed gf values may therefore be considered as upper limits to the correct values which result if all blends in the ^{12}CH lines are incorporated in the calculation. A lower limit of $\Delta = 0.16$ for the difference between observed and theoretical $\log gf$ values may be deduced, neglecting rather uncertain results due to nonsatisfactory reproduction of the ^{12}CH lines. The theoretical $\log gf$ values increased by $\Delta = 0.16$ are the empirical $\log gf$ values used in the calculation of the ^{13}CH lines.

The difference Δ may be due to (i) an erroneous band oscillator strength $f_{el} f_{00}$, (ii) an erroneous carbon abundance $\epsilon(^{12}\text{C})$, (iii) erroneous model atmosphere or turbulent velocities and (iv) deviations from LTE.

The effect of all reasonable errors in the carbon abundance on the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ is negligible.

However, the ^{13}C abundance is proportional to Δ . The uncertainty of Δ is hard to estimate because the results shown in Fig. 4-3 include few spectral lines, and several lines are unresolved doublets for which the gf values depend on the wavelength splitting.

Reproduction of the ^{13}CH lines

Observed and theoretical spectra of some of the ^{13}CH spectral regions are shown in Fig. 4-4 to 4-8. The two simultaneously observed spectral scans (see Ch. 1) are shown in the figures. The ^{13}CH lines are indicated with the notations for each single rotational line, as the ^{12}CH lines were previously.

The ^{13}CH laboratory wavelengths of Richter and Tonner (1967) and the present measurements are given in Table 4-1, together with the accepted wavelengths used in the reproduction of the spectra.

The wavelengths of Richter and Tonner are slightly adjusted so that the present ^{12}CH reference lines have the same wavelength in both investigations. The positions of the ^{13}CH lines in the solar spectrum according to the two investigations are then comparable.

The unresolved doublets of ^{13}CH are calculated with the same wavelength splitting as the corresponding ^{12}CH doublets, retaining the laboratory isotopic wavelength displacement of the line centres of the doublets.

Table 4-1. Wavelengths of ^{13}CH .

^{13}CH -line	Richter and Tonner $\lambda(\text{Å})$	Present $\lambda(\text{Å})$	Accepted $\lambda(\text{Å})$
R(16) 2d	4211.468		4211.458
1d	4211.518		4211.508
R(15) 2d	4217.682		4217.682
1d	4217.749		4217.749
R(14) 2d	4223.940		4223.960
1d	4224.020		4224.040
R(13) 2d	4230.226	4230.236	4230.226
1d	4230.326	4230.344	4230.326
2c	4231.421	4231.425	4231.425
1c	4231.451	4231.455	4231.455
R(12) 2d	4236.490	4236.501	4236.475
1d	4236.640	4236.651	4236.655
2c	4237.540		4237.520
1c	4237.600		4237.600
R(10) 2d	4249.049	4249.040	4249.040
1d	4249.259	4249.251	4249.270
2c	4249.809	4249.799	4249.790
1c	4249.959	4249.945	4249.945
R(8) 2d	4261.474	4261.461	4261.461
1c	4262.234	4262.208	4262.244
R(7) 1c	4268.330	4268.306	4268.325

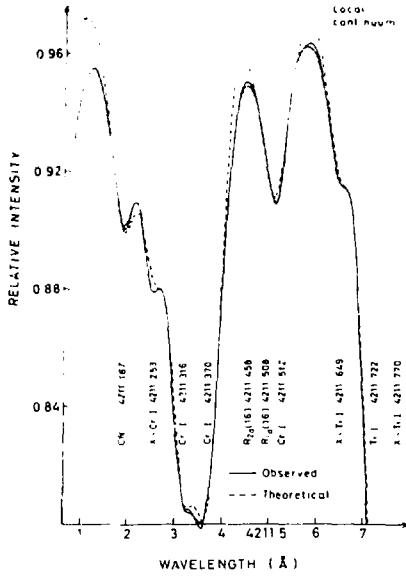


Fig. 4-4. Observed and theoretical spectrum, R(16), 4211Å.

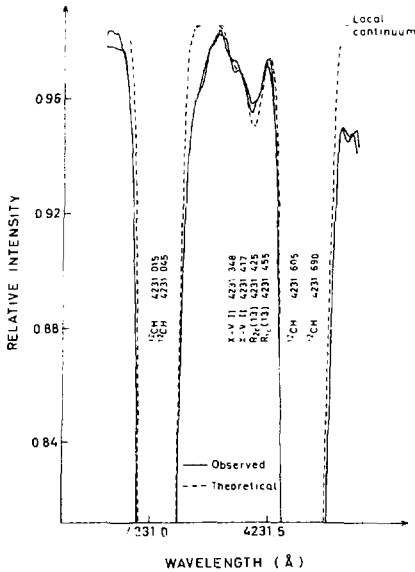


Fig. 4-5. Observed and theoretical spectrum, R(13), 4231Å.

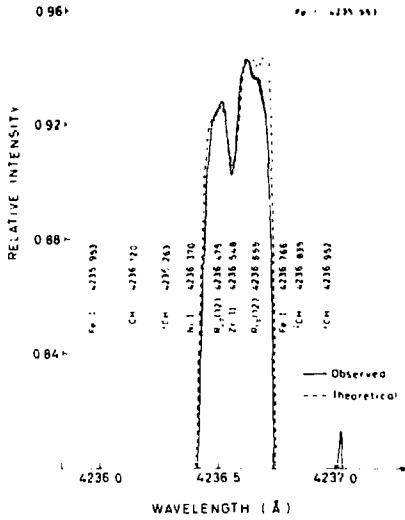


Fig. 4-5. Observed and theoretical spectrum, R(12), 4236Å.

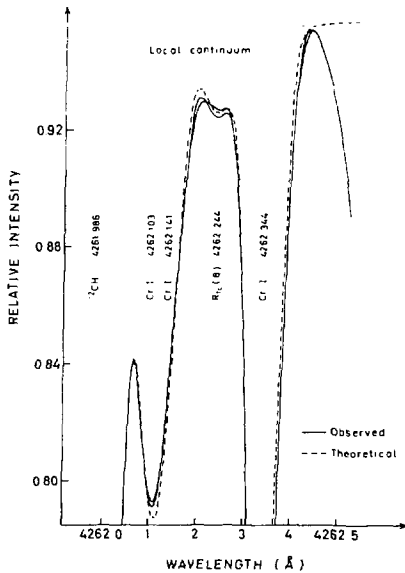


Fig. 4-7. Observed and theoretical spectrum, R(8), 4262Å.

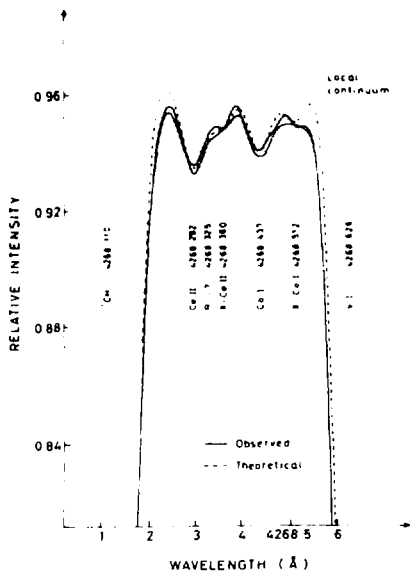


Fig. 4-8. Observed and theoretical spectrum, R(7), 4268Å.

The accepted wavelength of a ^{13}C line is defined as the wavelength of the strongest unidentified absorption feature within the interval

$$\lambda_{\min} - 0.020\text{Å} < \lambda(^{13}\text{C}) < \lambda_{\max} + 0.020\text{Å}$$

where λ_{\min} is the least of the two laboratory wavelengths in Table 4-1 and λ_{\max} is the greater.

The local and depressed continuum varies irregularly with wavelength. The amplitude of this irregularity is estimated to 0.4% of the continuum intensity. Using an upper limit of the local continuum, the ^{13}C abundance is increased until the calculated ^{13}C line depth is below the observed one by the amount of the uncertainty. This will result in an absolute upper limit to the abundance of ^{13}C .

In the figures 4-4 to 4-8 the theoretical spectra are calculated with the upper limit of the local continuum and the absolute upper limit of the ^{13}C -abundance.

A probable value of the abundance of ^{13}C is found by reducing the central depth of ^{13}CH lines by about 0.4% of the continuum intensity. This value is also considered to be an upper limit, since blends and erroneous identifications may contribute to the absorption.

Upper limits of the ^{13}C abundance and the corresponding lower limits of the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ are given in Table 4-7.

The difference between an absolute lower limit and a probable lower limit of the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ reflects the uncertainty of the ratio due to the uncertainty in the local continuum level.

The spectra were first calculated using the HSRA model atmosphere (Gingerich et al. 1971). The fitted spectra were recalculated with the model atmosphere of Holweger (1967). A slightly lower value of the ^{13}C abundance results from Holweger's model. The absolute lower limits of $^{12}\text{C}/^{13}\text{C}$ given in Table 4-2, calculated with the HSRA model, are therefore absolute lower limits with respect to the uncertainty of the model atmosphere, too.

Comments to the figures 4-4 to 4-8:

R(16), 4211Å (Fig. 4-4): The ld component is very near the line centre of CrI 4211.512Å, and the strength of this component cannot be determined unambiguously. However, to attribute all the observed absorption in the violet wing of CrI to the

Table 4-2. The abundance of ^{13}C and the isotopic ratio $^{12}\text{C}/^{13}\text{C}$.

^{13}CH -line	$\log \epsilon(^{13}\text{C})$		$\epsilon(^{12}\text{C})/\epsilon(^{13}\text{C})$	
	Absolute upper limit	Probable upper limit	Absolute lower limit	Probable lower limit
R(16) 2d 1d	6.73	6.65	75	89
R(15) 2d 1d	6.88		53	
R(14) 2d 1d	6.60	6.45	100	142
R(13) 2d 1d	6.81	6.72	62	76
2c 1c	6.66	6.58	87	105
R(12) 2d 1d	6.72	6.61	76	98
2c 1c	6.96	6.90	44	50
R(10) 2d 1d	6.79	6.69	65	81
2c 1c		6.58		105
R(8) 2d	6.65	6.51	89	124
1c	6.95	6.88	45	53
R(7) 1c	6.39	6.12	163	302

1d and 2d components of ^{13}CH will produce an unreasonably broad absorption line.

R(13), 4231Å (Fig. 4-5): The line feature at 4231.42Å is a possible identification of the ^{13}CH doublet. The line 4231.42Å has a weak blend in the red wing. However, in all the unresolved doublets of ^{12}CH from R(15) to R(6), the red component is the strongest one. The same conclusion is drawn from the theoretical gf values of ^{12}CH . All the absorption of the 4231.42Å feature may therefore not be attributed to ^{13}CH .

R(12), 4236Å (Fig. 4-6): An absorption at the ^{13}CH positions is clearly detected.

R(8), 4262Å (Fig. 4-7): Here, also, a spectral line is detected at the ^{13}CH position.

R(7), 4268Å (Fig. 4-8): The laboratory wavelength of the 1c component from Richter and Tonner's and the present measurements do not coincide (Table 4-1). The solar line 4268.292Å is situated 14 mÅ to the violet of the shortest laboratory wavelength, and the line is thus a possible identification of ^{13}CH according to the defined criterion.

However, the laboratory wavelength 4268.298Å for CeII (Corliss 1973) agrees well with the solar line 4268.292Å.

This line is not identified by Moore et al. (1966).

The identification CeII is adopted here. The line feature X-CeII 4268.360Å is discarded as ^{13}CH , since it deviates too much in wavelength.

5. DISCUSSION AND CONCLUSIONS

The main contribution to the uncertainty of the ^{13}C abundance is the uncertainty in the local continuum. To a less extent the uncertainty in the model atmosphere and in the empirical $\log gf$ values of ^{12}CH may contribute to the uncertainty of the ^{13}C abundance. The effect of deviations from LTE on the formation of ^{12}CH lines is not known.

The first two uncertainty contributions are accounted for by the definition of an absolute upper limit of the ^{13}C abundance.

Considering that the tentative ^{13}CH absorption partly may be due to other weak spectral lines not included in the calculations, the notation "absolute" upper limit for $\epsilon(^{13}\text{C})$ certainly is an appropriate one.

According to this analysis, ^{13}CH is not definitely identified in the photospheric spectrum. In all spectral regions, if not seriously blended, a very small absorption is present at the positions of the ^{13}CH lines, after the observed spectra has been reproduced with all spectral lines in the region apart from ^{13}CH . However, the resulting abundances of ^{13}CH if all the absorption is attributed to ^{13}CH are not at all consistent. (Table 4-2).

Since ^{13}CH is not definitely identified, it is only possible to indicate upper limits of the ^{13}C abundance and the corresponding lower limits of the isotopic abundance ratio $^{12}\text{C}/^{13}\text{C}$. Four of eleven regions result in absolute lower limits of the ratio $^{12}\text{C}/^{13}\text{C}$ of about 90 and greater. Seven of eleven regions result in probable lower limits of

the ratio $^{12}\text{C}/^{13}\text{C}$ of about 90 and greater (Table 4-2). It therefore seems highly probable that the isotopic abundance ratio $^{12}\text{C}/^{13}\text{C}$ in the solar photosphere is greater than the terrestrial value of 90.

It is not possible to say whether the abundance ratio $^{12}\text{C}/^{13}\text{C}$ is much greater than the terrestrial value, as proposed by Fowler et al. (1962). But in the sense that the isotopic ratio $^{12}\text{C}/^{13}\text{C}$ is different from the terrestrial value, this investigation supports the theory of Fowler et al. that terrestrial ^{13}C may have been produced by irradiation of the preplanetary material.

There is still a discrepancy between the isotopic ratio derived from spot spectra and photospheric spectra (see Ch. 1).

It is two main causes that ^{13}CH was not identified and only lower limits of the ratio $^{12}\text{C}/^{13}\text{C}$ were obtained. One is that ^{13}CH lines under all circumstances are very faint. This makes the deduced abundances sensitive to the local continuum level. The other is that the spectral region in which this CH-band is situated, contain a great number of overlapping spectral lines, which makes it difficult to identify possible ^{13}CH -lines.

To obtain more precise results for the abundance ratio $^{12}\text{C}/^{13}\text{C}$ in the solar photosphere, it is necessary to consider molecular bands in other spectral regions, with smaller spectral line density than the violet part of the solar spectrum. Fay and Wyller (1970) suggest favourable regions for ^{13}CN in the infrared.

APPENDIX A. CALCULATION OF THE DISSOCIATION CONSTANTS

The method used for computing dissociation constants of diatomic molecules is that of Tatum (1966). In local thermodynamical equilibrium (LTE) the dissociation constant is given by

$$K(AB) = \left(\frac{2\pi\mu kT}{h^2} \right)^{3/2} kT \frac{Q(A)Q(B)}{Q(AB)} \exp(-D_0/kT) \quad (A.1)$$

where μ is the reduced mass of the molecule, k is Boltzmann's constant, T is the temperature, D_0 is the dissociation energy of the molecule and the Q 's are the partition functions.

The partition function Q of an atom or a molecule is defined by

$$Q = \sum_i g_i \exp(-E_i/kT) \quad (A.2)$$

where g_i is the statistical weight and E_i is the energy above the ground level for energy level i .

Atomic partition functions are computed by de'Galan, Smith and Winefordner (1968) for the temperature range 3000K to 7000K. They represent their results by the series

$$Q = a + b \left(\frac{T}{10^3} \right) + c \left(\frac{T}{10^3} \right)^2 + d \left(\frac{T}{10^3} \right)^3 + e \left(\frac{T}{10^3} \right)^4 + f \left(\frac{T}{10^3} \right)^5 \quad (A.3)$$

where a, b, c, d, e and f are constants tabulated for neutral and ionized atoms.

Molecular partition functions are computed from Tatum's (1966, p. 5) expression

$$Q(AB) = \exp \frac{hc}{kT} \left(\frac{1}{2} \omega_e - \frac{1}{4} \omega_e x_e \right) \cdot \quad (A.4)$$

$$\sum_{T_e=0}^{40000 \text{ cm}^{-1}} \sum_{v=0}^{v_{\text{max}}} \frac{\tilde{\omega} kT}{\sigma h c} \frac{1}{E_e - \alpha_e (v + \frac{1}{2})} \exp \left[- \frac{hc}{kT} (\omega_e (v + \frac{1}{2}) - \omega_e x_e (v + \frac{1}{2})^2 + T_e) \right]$$

Analogous to the atomic partition functions, the molecular partition functions are represented by the polynomial (A.3). The partition functions calculated from equation (A.4) deviate less than 0.01% from the polynomial values computed from equation (A.3) in the temperature range 3000K to 9000K.

The partition functions being known, the dissociation constants K may be tabulated as function of temperature from equation (A.1).

To facilitate further calculations involving the dissociation constants, the results are fitted to the expression

$$\log K = A - B/T + C \log T \quad (\text{A.5})$$

where A, B and C are constants determined analytically from three values of T and $\log K$. In the temperature range 4200 to 8000K the dissociation constants calculated from equation (A.5) deviate less than 0.2% from the values calculated from equation (A.1).

The molecular data used in the calculation of partition functions and dissociation constants of the molecules CH , CO , H_2 , CN and OH are obtained from Rosen (1970). For the CH molecule, a low-lying electronic state $^4\Sigma^-$ was recently found to be stable. Molecular constants for this state are calculated by Lie and Hinze (1972), and the electronic energy is obtained from Liu and Verhaegen (1970). Table A-1 shows the influence of the new state $^4\Sigma^-$ on the dissociation constant of CH , and the fitting of the dissociation constant to formula (A.5).

Table A-1. Dissociation constant of ^{12}CH .

T (K)	$\log K^{(i)}$ (N/m)	$\log K^{(ii)}$ (N/m)	$\log K^{(iii)}$ (N/m)
4000	6.138	6.114	6.112
4500	6.667	6.635	6.635
5000	7.092	7.052	7.052
5500	7.440	7.392	7.392
6000	7.731	7.675	7.675
6500	7.976	7.914	7.913
7000	8.186	8.117	8.116
7500	8.367	8.292	8.292
8000	8.525	8.444	8.445

- (i) calculation without the new state $^4\Sigma^-$
(ii) calculation including the new state $^4\Sigma^-$
(iii) calculated from equation (A.5)

For isotopic molecules, the molecular constants are changed according to the relations given by Herzberg (1950, p. 192 and p. 194), and the reduced mass is changed.

The coefficients that are used in the calculation of partition functions and dissociation constants of the molecules from equation (A.3) and (A.5), are given in Tables A-2 and A-3.

Table A-2. Coefficients for the fitting of the partition functions.

Mole- cule	a	b	c	d	e	f
¹² CH	2.25549 E2	-7.40250 E1	1.16745 E2	-1.23734 E1	1.68463 E0	-4.77841 E-2
¹³ CH	2.24984 E2	-7.25551 E1	1.16783 E2	-1.22915 E1	1.68324 E0	-4.78471 E-2
¹² CO	7.96030 E1	1.90187 E2	1.13466 E2	1.31769 E0	-3.42438 E-2	2.06749 E-3
¹³ CO	8.18515 E1	1.98484 E2	1.21572 E2	1.38051 E0	-3.44204 E-2	2.14240 E-3
H ₂	3.77392 E0	1.51570 E0	1.62796 E0	-1.26180 E-1	1.37190 E-2	-3.09725 E-4
CN	-4.99365 E2	1.25889 E3	-1.88945 E2	8.88587 E1	-3.90464 E0	1.03877 E-1
OH	8.75761 E1	4.32863 E1	4.24645 E1	-2.22890 E0	2.30309 E-1	-2.77160 E-3

Table A-3. Coefficients for the fitting of the dissociation constants.

Molecule	A	B	C
¹² CH	12.03237	19383.26	-0.29830
¹³ CH	12.01861	19374.54	-0.29493
¹² CO	9.06310	55952.87	0.85697
¹³ CO	9.06784	55943.19	0.85589
H ₂	11.12065	24237.76	0.10525
CN	10.28369	38086.45	0.32905
OH	9.97360	23408.23	0.28955

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