

Temperature of the disc integrated sunlight from the intensity measurements of rotational lines of the bands of A-X system of CH molecule

Supriya Behere^{a*}, Bhagawan Deshmukh^b, Sunil Patil^a & S H Behere^a

^aDepartment of Physics, Dr Babasaheb Aambedkar Marathwada University, Aurangabad 431 004, India

^bPuranmal Lahoti Government Polytechnic, Latur 413 512, India

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The temperature of the disc integrated sunlight has been calculated by measuring the intensities of 113 rotational lines belonging to the R and P branches of the 0-0, 1-1 and 2-2 bands of the $A^2\Delta_{5/2}-X^2\Pi_{3/2}$ transition and 0-0 and 1-1 bands of $A^2\Delta_{3/2}-X^2\Pi_{1/2}$ transition of a CH molecule. The Fourier transform spectroscopic data has been taken from solar flux Atlas for the visible and near infra-red prepared by Wallace (NSO Technical Report #11-001 2011). The temperature comes out as 3300 ± 121 K, less than the surface temperature of the photosphere of the sun as expected.

Keywords: Solar flux, Disc integrated sunlight, Rotational temperature, Chance of coincidence, CH molecule

1 Introduction

The vibrational and rotational temperatures derived from the band spectra of diatomic molecules are of importance in spectroscopy, chemical physics, thermodynamics and astronomy. There are various types of molecules, atoms and ions observed in spectra in the celestial bodies; whose existence is confirmed by spectroscopic techniques¹. Stars have their own sources of generating brightness and temperature and if the temperatures are related with masses and luminosities, useful information can be obtained. In present work the CH radical is selected as it has astrophysical significance and some part of the spectroscopic information is not known. Most prominent bands of CH molecule are observed in the 'Coma' of a comet.

The intensity distribution in the spectra of CH was earlier reported by Swings^{2,4} and thereafter by McKellar^{5,6}. These studies were made at poor resolution and therefore the measurement of intensities of rotational lines were lacking. The CH molecule is a heterogeneous diatomic molecule, which has seven known excited electronic states viz, $a^4\Sigma^+$, $A^2\Delta$, $B^2\Sigma^-$, $C^2\Sigma^+$, $D^2\Pi$, $E^2\Pi$ and $F^2\Sigma^+$ whereas the ground state is $X^2\Pi$. In absorption the transitions observed with certainty are A-X, B-X and C-X having the common lower $X^2\Pi$ state. Herzberg¹ has given the molecular constants of some systems of CH.

2 The $A^2\Delta - X^2\Pi$ Transition

This electronic transition falls in the region 4300 \AA (23250 cm^{-1}). The first report and partial analysis of the A-X system⁷⁻⁹ was supplemented and extended by Gero¹⁰ in which he analyzed (0-0), (1-1) and (2-2) bands, whereas (0-1) and (1-2) bands were reported by Kies and Broida¹¹ in 1956 through molecular beam experiment. Ubachs *et al.*¹² reported the hyperfine structure in the bands of $A^2\Delta - X^2\Pi$ system. Bernath *et al.*¹³ in 1991 analyzed (0-0), (1-1) and (2-2) bands of A-X system recorded using Fourier Transform Spectrometer. A reliable data were observed by combining these data with earlier data reported by Herzberg¹. In an emission, Zachwieja¹⁴ photographed seven bands viz, (0-0), (1-1), (2-2), (0-1), (1-2), (3-3) and (2-3), of $A^2\Delta - X^2\Pi$ system of CH radical using Geissler tube as source. He has also reported the turning points of RKR curves, FC factors and r centroids of this transitions for $v'=5$, $v''=5$ levels.

3 Bands of CH observed in the Spectrum of Sun

The spectra of various celestial objects like sun, moon, comets, aurorae, planets, stars, interstellar space, etc., are taken by earth based astronomical spectrographs¹⁵⁻¹⁷ and also by space borne instruments like Hubble telescope, Chandra telescope and other orbiting man made satellites. In 1968, Labs and Neckel¹⁸ made an attempt to prepare solar flux atlas but due to poor spectral resolution it was not possible to resolve even major Fraunhofer lines. The first high resolution solar flux atlas was prepared by Beckers

*Corresponding author (E-mail: supriyabehere1987@gmail.com)

*et al.*¹⁹ covering the wavelength range 3800 -7000 Å (26315- 14285 cm⁻¹). In the region 296-1300 nm (33780- 7692 cm⁻¹). Kurucz *et al.*²⁰ recorded the solar flux spectra with high resolution and with high S/N ratio using the Fourier Transform Spectrometer attached to McMath Pierce Solar Telescope, located at Kitt Peak but they faced a problem of presence of telluric spectrum. Ground based astronomical observations suffer from the disturbing effects of earth atmosphere due to presence of ozone, oxygen, water vapors and number of atmospheric trace gases which absorb and emit light at discrete frequencies. Absorption features are referred as telluric features and are prevalent in the IR and visible region of the spectrum. In the mission of Atmospheric Chemistry Experiments (ACE), ATMOS spectrum by Farmer²¹ was obtained. Bernath *et al.*²² obtained exceedingly high resolution solar spectra using FT spectrometer. In the present study we used the solar flux spectrum published by Wallace *et al.*²³ which was taken in 2011 from McMath Pierce Solar Telescope attached with a Fourier transform spectrometer in the region 2958-9250 Å (33800- 10810 cm⁻¹) with the resolution $R=\lambda/\Delta\lambda \sim 350000-700000$ and high S/N ratio. In the region 5680 Å (17600 cm⁻¹) to the violet end of the spectra at 2958 Å (33800 cm⁻¹) there is no need of telluric correction due to either H₂O or O₂ as their absorption range fall in IR region. Wallace *et al.*²³ determined a small multiplicative frequency correction, i.e., Doppler correction 1.000001 for a region 4445- 4015 Å (22490 – 24900 cm⁻¹), 1.00000093 for 4015 –3257 Å (24900 – 30700 cm⁻¹) and 0.99999873 for 3257-2957 Å (30700 – 33800 cm⁻¹). The FeI lines given by Nave, Johansson, Learner, Thorne and Brault²⁴ were used as standards. Doppler correction is necessary because relative radial motion between a wave source and the observer causes a wavelength shift.

4 Intensity Measurements and Rotational Temperature

The intensities of the rotational lines of a particular branch observed in a band show a regular variation unless there are perturbations. The temperature is calculated, using following formulation.

The intensity I of a rotational lines resulting from a transition J to J' can be written as:

$$I_{J, J'} = A S_{J, J'} \exp [-F_{\nu'}(J) hc / kT] \quad \dots (1)$$

where A is a constant, $S_{J, J'}$ is Hönl London factor. $F_{\nu'}(J)$ is a term value in cm⁻¹. h , c , k , and T are Planck's

constant, velocity of light, Boltzmann constant and temperature, respectively.

Taking natural logarithm,

$$\ln (I_{J, J'} / S_{J, J'}) = \text{Constant} - F_{\nu'}(J) hc / kT \quad \dots (2)$$

where $F_{\nu'}(J) = B_{\nu'} J(J+1) - D_{\nu'} J^2(J+1)^2$

But $D_{\nu'}$ is a non-rigidity constant, being too small can be neglected.

The expression therefore is:

$$F_{\nu'}(J) = B_{\nu'} J(J+1) \quad \dots (3)$$

where $B_{\nu'} = B_e - \alpha_e (v + 1/2)$

The Eq. (2) becomes:

$$\ln (I_{J, J'} / S_{J, J'}) = \text{Constant} - B_{\nu'} J(J+1) (hc/kT) \quad \dots (4)$$

Thus, if a graph of Eq. (4) is plotted by taking the L.H.S on y -axis and $J(J+1)$ on x axis, then a straight line with the slope (dy/dx) equal to $(B_{\nu'} hc/kT)$ can be obtained. Using this slope the temperature can be calculated as follows:

$$T = (B_{\nu'} hc/k) (1/\text{slope}) \quad \dots (5)$$

In the present study non overlapped and well resolved 113 rotational lines of A – X system of CH molecule lying in the region 4940 - 4150 Å (20232 to 24091 cm⁻¹) were selected, marked and their intensities were computed. Due to such a enormous high resolution it was easier to assign the J value to these spectral lines. The J assignments are taken from references^{13,14}. 62 lines of P and R branches of three bands, namely (0, 0), (1, 1) and (2, 2) of $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ and 51 lines of P and R branches of (0, 0), (1, 1) bands of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ sub band are measured. The least square fit points are chosen to plot graphs which are straight lines. Slope of these graphs is used to calculate the temperature of disc integrated sunlight. The measurements are shown in Tables 1-5 and corresponding graphs are shown in Figs 1- 5. The average of the temperature and a standard deviation is calculated.

5 Number of Chance of Coincidence

The formula used by Russell–Brown²⁵ and Engvold, Wöhl and Brault²⁶ was used to see the chance of coincidence between laboratory and solar flux measurement. The formula for C , i.e., chance of coincidence is:

$$C = N [1 - \exp (-2xw)] = N.p \quad \dots (6)$$

Table 1 — Intensity measurements of the rotational lines of (0-0) band of $A^2\Delta_{5/2}-X^2\Pi_{3/2}$ System of CH.

Wave number	Rotational line	S_j	Intensity (a.u.)	$\ln(I/S_j)$	Linear regression data
22847.3184	P (15.5)	3.1573	15.4093	1.5853	1.5380
22861.9980	P (14.5)	2.9095	22.1082	2.0280	1.7367
22894.3203	P (12.5)	2.4150	23.7805	2.2872	2.0956
22907.3574	P (11.5)	2.1685	25.8815	2.4795	2.2558
22947.2324	P (9.5)	1.6776	25.0704	2.7043	2.5377
22968.5703	P (8.5)	1.4338	24.0498	2.8198	2.6595
22990.8613	P (7.5)	1.1917	24.2484	3.0130	2.7684
23013.9883	P (6.5)	0.9519	24.7465	3.2580	2.8646
23038.9629	P (5.5)	0.7159	18.2553	3.2387	2.9479
23324.1719	R (4.5)	2.2159	35.7587	2.7811	3.0184
23356.7285	R (5.5)	2.4519	37.2965	2.7220	2.9479
23389.6660	R (6.5)	2.6917	35.4529	2.5780	2.8646
23423.0000	R (7.5)	2.9338	35.4912	2.4930	2.7684
23493.7598	R (9.5)	3.4226	32.8616	2.2619	2.5377
23528.6484	R (10.5)	3.6685	31.8148	2.1602	2.4032
23563.8008	R (11.5)	3.9150	31.4798	2.0845	2.2558
23599.0859	R (12.5)	4.1620	29.7401	1.9665	2.0956
23634.5176	R (13.5)	4.4095	30.7137	1.9410	1.9225
23670.0059	R (14.5)	4.6573	26.3109	1.7316	1.7367
23765.5529	R (17.5)	5.4020	15.5242	1.0556	1.1023
23799.3086	R (18.5)	5.6506	12.9222	0.8272	0.8652
23832.6719	R (19.5)	5.8994	10.4394	0.5707	0.6152
23897.6387	R (21.5)	6.3972	6.5758	0.0275	0.0769

Table 2 — Intensity measurements of the rotational lines of (0-0) band of $A^2\Delta_{3/2}-X^2\Pi_{1/2}$ system of CH.

Wave number	Rotational line	S_j	Intensity (a.u.)	$\ln(I/S_j)$	Linear regression data
22773.8164	P (19.5)	4.1506	11.7808	1.0432	0.9226
22785.1816	P (18.5)	3.9020	14.0095	1.2782	1.1460
22847.3184	P (14.5)	2.9095	16.0780	1.7095	1.9247
22862.5254	P (13.5)	2.6620	18.8340	1.9566	2.0908
22895.2148	P (11.5)	2.1685	20.3878	2.2409	2.3886
22908.1055	P (10.5)	1.9226	19.2626	2.3045	2.5203
22913.0039	P(10.5)	1.9226	27.7072	2.6680	2.5203
22927.8164	P (9.5)	1.6776	24.0438	2.6625	2.6405
22931.9219	P (9.5)	1.6776	22.0832	2.5774	2.6405
22948.4941	P(8.5)	1.4338	23.7799	2.8085	2.7493
22951.9844	P(8.5)	1.4338	22.8669	2.7693	2.7493
22970.1543	P (7.5)	1.1917	22.1695	2.9234	2.8467
22995.0410	P (6.5)	0.9519	20.6890	3.0789	2.9326
23016.4961	P (5.5)	0.7159	19.7962	3.3197	3.0070
23065.8555	P (3.5)	0.2679	16.1111	4.0968	3.1216
23391.8516	R (5.5)	2.4519	50.0846	3.0168	3.0070
23458.0215	R (7.5)	2.9338	48.4448	2.8041	2.8467
23460.8359	R (7.5)	2.9338	42.3864	2.6705	2.8467
23491.6777	R (8.5)	3.1776	40.3503	2.5415	2.7493
23525.5840	R (9.5)	3.4226	38.4469	2.4189	2.6405
23529.8223	R (9.5)	3.4226	32.7728	2.2592	2.6405
23599.0859	R (11.5)	3.9150	29.7401	2.0277	2.3886
23670.0059	R (13.5)	4.4095	28.3109	1.8595	2.0908
23832.0566	R (18.5)	5.6506	19.1844	1.2223	1.1460
23864.7754	R (19.5)	5.8994	17.9559	1.1131	0.9226
23912.0703	R (20.5)	6.1483	12.6122	0.7185	0.6879
23944.5977	R (21.5)	6.3972	10.7592	0.5199	0.4416

Table 3 — Intensity measurements of the rotational lines of (1-1) band of $A^2\Delta_{5/2}-X^2\Pi_{3/2}$ system of CH.

Wave number	Rotational line	S_j	Intensity (a.u.)	$\ln(I/S_j)$	Linear regression data
22856.5566	P (14.5)	2.9095	13.1150	1.5058	1.3598
22875.3730	P (13.5)	2.6620	13.1016	1.5936	1.5372
22910.4219	P (11.5)	2.1685	13.7517	1.8471	1.8555
22914.9395	P (11.5)	2.1685	15.1649	1.9450	1.8555
22935.5879	P (10.5)	1.9226	13.9297	1.9803	1.9962
22953.8457	P (9.5)	1.6776	13.7743	2.1054	2.1247
22956.9551	P (9.5)	1.6776	13.7869	2.1063	2.1247
22978.9688	P (8.5)	1.4338	14.0084	2.2793	2.2410
23023.4336	P (6.5)	0.9519	11.7461	2.5128	2.4369
23024.9277	P (6.5)	0.9519	10.9851	2.4458	2.4369
23048.7441	P (5.5)	0.7159	9.2148	2.5550	2.5164
23262.6504	R (2.5)	1.7679	39.7613	3.1131	2.6817
23381.7324	R (6.5)	2.6917	24.1860	2.1956	2.4369
23413.4531	R (7.5)	2.9338	28.5386	2.2749	2.3451
23505.0527	R (10.5)	3.6685	22.7204	1.8235	1.9962
23535.3809	R (11.5)	3.9150	22.3519	1.7421	1.8555
23595.2578	R (13.5)	4.4095	15.6790	1.2686	1.5372
23624.6914	R (14.5)	4.6573	15.5838	1.2078	1.3598
23749.0957	R (19.5)	5.8994	9.5686	0.4836	0.2888

 Table 4 — Intensity measurements of the rotational lines of (1-1) band of $A^2\Delta_{3/2}-X^2\Pi_{1/2}$ system of CH.

Wave number	Rotational line	S_j	Intensity (a.u.)	$\ln(I/S_j)$	Linear regression data
22793.1152	P (16.5)	3.4053	9.3837	1.0136	0.8512
22811.5059	P (15.5)	3.1573	10.3695	1.1892	1.0540
22830.3223	P (14.5)	2.9095	11.8780	1.4067	1.2445
22849.6504	P (13.5)	2.6620	14.2021	1.6743	1.4226
22911.1270	P (10.5)	1.9226	12.7822	1.8944	1.8835
22932.8008	P (9.5)	1.6776	12.9028	2.0401	2.0125
22980.7578	P (7.5)	1.1917	9.9593	2.1231	2.2337
23003.8105	P (6.5)	0.9519	11.2949	2.4736	2.3259
23025.8965	P (5.5)	0.7159	15.5885	3.0807	2.4058
23076.6973	P (3.5)	0.2679	4.6045	2.8443	2.5287
23077.4883	P (3.5)	0.2679	5.2828	2.9818	2.5287
23269.7930	R (1.5)	1.5750	22.4666	2.6578	2.6024
23354.5430	R (4.5)	2.2159	19.2184	2.1602	2.4734
23415.4766	R (6.5)	2.6917	20.7069	2.0403	2.3259
23443.0039	R (7.5)	2.9338	21.7441	2.0030	2.2337
23475.9121	R (8.5)	3.1776	19.6823	1.8236	2.1293
23502.1055	R (9.5)	3.4226	18.8456	1.7059	2.0125
23506.1816	R (9.5)	3.4226	20.4666	1.7884	2.0125
23536.4062	R (10.5)	3.6685	18.5011	1.6181	1.8835
23566.2500	R (11.5)	3.9150	19.4247	1.6017	1.7422
23625.0137	R (13.5)	4.4095	15.9920	1.2883	1.4226
23645.5156	R (14.5)	4.6573	14.8752	1.1613	1.2445
23724.2969	R (17.5)	5.4020	9.6027	0.5753	0.6361
23748.5527	R (18.5)	5.6506	9.0658	0.4727	0.4088

N is the number of laboratory lines and x is the tolerance for wavenumbers. We have taken it up to $\pm 0.1 \text{ cm}^{-1}$. $W = M/x$ where M is the number of lines in solar flux spectrum in the wavenumber region $x \text{ cm}^{-1}$.

6 Results and Discussion

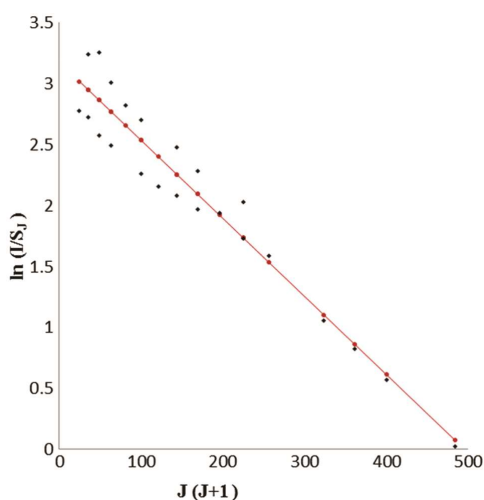
The disc integrated sunlight temperature thus calculated comes out as $3300 \pm 121 \text{ K}$ shown in Table 6 which is lower compared to the surface temperature of photosphere. Similar results are

Table 5 — Intensity measurements of the rotational lines of (2-2) band of $A^2\Delta - X^2\Pi$ system of CH.

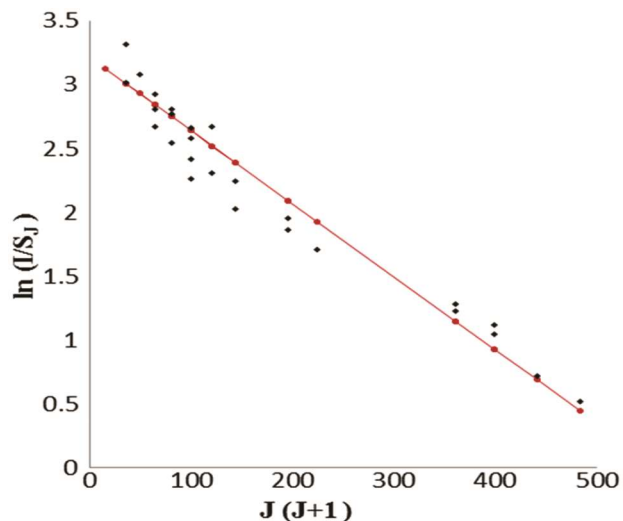
Wave number	Rotational line	S_j	Intensity Arb. Unit	$\ln(I/S_j)$	Linear regression data
22771.5879	P(14.5)	2.9095	8.2949	1.047661	0.928238
22789.8164	P(13.5)	2.6620	11.4633	1.460062	1.112366
22819.3965	P(12.5)	2.4150	10.0375	1.424626	1.283795
22842.5957	P(11.5)	2.1685	10.0257	1.531126	1.442526
22867.4824	P(10.5)	1.9226	9.5006	1.597671	1.588558
22891.6074	P(9.5)	1.6776	9.5582	1.740018	1.721892
22913.6934	P(8.5)	1.4338	9.4374	1.884331	1.842527
22940.5449	P(7.5)	1.1917	9.3640	2.061518	1.950464
22963.8047	P(6.5)	0.9519	8.0844	2.139204	2.045703
22965.3145	P(6.5)	0.9519	7.5545	2.071415	2.045703
22989.2188	P(5.5)	0.7159	6.1196	2.145695	2.128243
23303.1719	R(6.5)	2.6917	15.3879	1.743419	2.045703
23378.3008	R(9.5)	3.4226	15.4398	1.506546	1.721892
23447.668	R(12.5)	4.1620	12.2795	1.081924	1.283795
23468.8887	R(13.5)	4.4095	11.8881	0.991778	1.112366
23488.9329	R(14.5)	4.6573	11.3036	0.886699	0.928238
23507.5449	R(15.5)	4.9053	10.5250	0.763432	0.731412
23515.3477	R(15.5)	4.9053	10.4847	0.759601	0.731412
23533.5469	R(16.5)	5.1536	9.0010	0.557646	0.521887
23550.0449	R(17.5)	5.4020	5.8054	0.072009	0.299664

Table 6 — Rotational temperature of bands of $A^2\Delta - X^2\Pi$ system of CH.

Transition	Band	Temperature (K)	Average temperature
$A - X$	$A^2\Delta_{5/2} - X^2\Pi_{3/2}$ (0,0)	3275	3300±121 K
	(1,1)	3278	
	(2,2)	3017	
$A^2\Delta_{3/2} - X^2\Pi_{1/2}$	(1,1)	3265	
	(0,0)	3665	

Fig. 1 — Plot of $\ln(I/S_j)$ for (0-0) band of $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ system of CH.

obtained by other workers using the Umbral spectra of sun²⁷⁻³⁵. Present study is of solar flux. No other report in literature is available to compare with

Fig. 2 — Plot of $\ln(I/S_j)$ for (0-0) band of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ system of CH.

the temperature calculated using solar flux. This temperature is related to kinetic gas temperature. The environment of the thermal equilibrium at the time of recording the spectra of solar flux plays an important role and this type of equilibrium is always fluctuating; therefore the results of different workers may vary within the limit of an experimental error. The number of chance of coincidences for the 0-0, 1-1 and 2-2 bands of the $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ transition and 0-0 and 1-1 bands of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ transition of a CH molecule have been calculated and entered in Table 7.

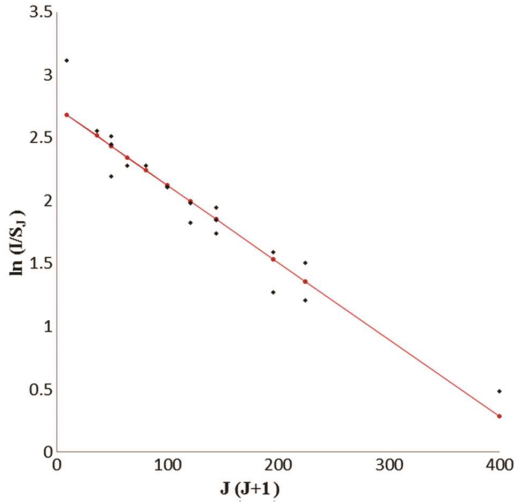
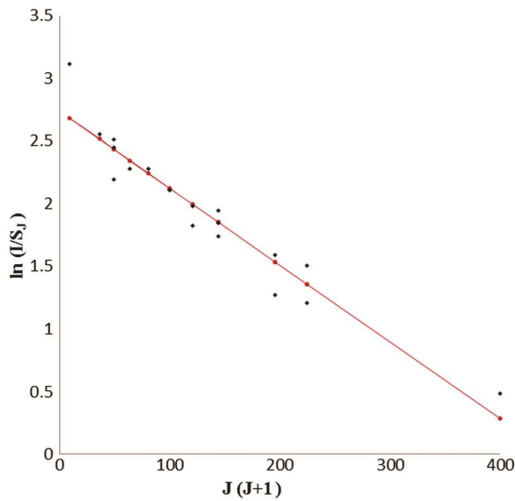
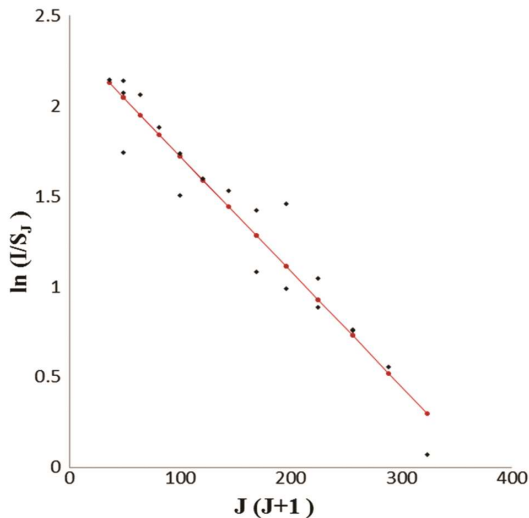

 Fig. 3 — Plot of $\ln(I/S_j)$ for (1-1) band of $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ system of CH.

 Fig. 4 — Plot of $\ln(I/S_j)$ for (1-1) band of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ system of CH.

 Fig. 5 — Plot of $\ln(I/S_j)$ for (2-2) band of A-X system of CH.

Table 7 — Parameters to evaluate the presence of CH transitions.

Transition	Band	C index	I parameter*	
$A - X$	$A^2\Delta_{5/2} - X^2\Pi_{3/2}$	(0,0)	22	23(48)
		(1,1)	16	19(58)
		(2,2)	12	20(33)
	$A^2\Delta_{3/2} - X^2\Pi_{1/2}$	(1,1)	16	24(58)
		(0,0)	22	27(48)

*Total number of lines searched for is given in parentheses

7 Conclusions

Using high resolution solar flux spectra obtained with Fourier transform spectrometer and solar telescope of National Solar Observatory at Kitt Peak. We carefully identified the 0-0, 1-1 and 2-2 bands of the $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ transition and 0-0 and 1-1 bands of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ transition of a CH molecule. The new identification of 113 lines of *P* and *R* branches in the solar flux and calculated the temperature of disc integrated sunlight. We have come to conclusion that the bands of the $A^2\Delta_{5/2} - X^2\Pi_{3/2}$ transition and of $A^2\Delta_{3/2} - X^2\Pi_{1/2}$ transition of a CH molecule are present in the solar flux spectra examined.

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