THE SEARCH OF CH_3CN IN INTERSTELLAR MEDIUM

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ABSTRACT: We present the binding energy, rotational constant, rotational frequency and rotational temperature of CH_3CN in different basis sets using Gaussian03. A systematic search of the emission region at 115 GHz is carried out using SkyView Virtual Observatory. A region is selected and studied in the context of rotational temperature of CH_3CN using ALADIN2.5 software. From the ab-initio (First principle) calculation of CH_3CN in the Hartree Fock level of approximation it is found that there is a strong binding between H, C and N in CH_3CN, minimum value of the binding energy being 12.79 eV in the basis set 6-311G which agrees within around 8% to the maximum value of 13.74 eV obtained in the basis set 6-31G*. The estimated value of rotational frequency in the Hartree Fock level of approximation is found to be 322.62 GHz in the basis set 6-31G* which agrees with the values of rotational frequency obtained in other basis sets within around 4%. Similarly, value of rotational temperature in the same basis set 6-31G* is found to be 7.74 K which agrees within around 4% to the corresponding values obtained in other basis sets. The investigation region is a huge (7° × 4°) structure having east to west elongated emission pattern in the *CO* - survey (115 GHz). We classified this region into three parts (Upper Wing, Lower Wing and Third Region) and study the variation of relative flux density in each pixel. We found that the minimum dust color temperature 8.15 K, 8.04 K and 7.99 K respectively at Upper Wing, Lower Wing and Third Region which are almost 4% differs from rotational temperature CH_3CN. This implies that there is strong evidence of possibility of finding CH_3CN in the investigated region. But the conformation can only be done by spectral analysis. It is found that the flux density increase from 12 µm to 25 µm and then decreases sharply on moving from 25 µm to 60 µm in the maxima of Upper Wing and Lower wing. The flux density increases but not at significant level when moving from 60 µm to 100 µm. We estimated the dust mass of the three different regions. We found that the mass of Upper Wing, Lower Wing and Third Region are 4273.50 $M_{È,}$ 4778.79 M_{Θ} and 2026.75 M_{Θ} respectively. The total mass of the investigated region has to obtain 11079.04 M_{Θ}. The mass of the gas found in the investigated structure is almost 200 times the dust mass. Thus the mass of the investigated structure is found to be 2.22×10^6 M_{Θ}.

Key Words: Interstellar Medium; Flux density; Dust color temperature; Solar mass; Cyanogens.

INTRODUCTION

Dense interstellar clouds harbor a rich and exotic chemistry. Many interstellar molecules have been identified in such clouds, from small and stable species like carbon monoxide to reactive radicals and long carbon chains such as C_8H or $HC_{11}N$. Despite the extremely low temperatures (10 K above zero) and densities (at most a million particles per cubic centimeter), chemical reactions both in gas and solid phase, enable the synthesis of the known interstellar molecules. It was considered up to now that most interstellar species in dark clouds were either reactive or unsaturated species, in accordance with the detected molecular species. The presence of saturated molecules was expected in the solid phase, but not in the gas phase as the gas phase chemical networks led mostly to the production of reactive and unsaturated species.

Measurements of the absorption line spectra of the interstellar lines of CN contained the first direct evidence for the cosmic background radiation (CBR) (McKellar, 1940)[1]. Unfortunately these were not recognized as such until after the discovery of the cosmic background radiation by Penzias & Wilson (1965)[2] and its interpretation by Dicke et al. (1965)[3]. Subsequently several observers have determined the cosmic background radiation temperature from the CN absorption lines. These have been reviewed by Thaddeus (1972), by Meyer & Jura (1985) and by Crane et al. (1986). It now appears possible that the CN lines may provide the most precise measurement of the CBR temperature at the wavelengths sampled by CN (Crane et al., 1986)[4].

In 1940 McKellar first measured the absorption-line spectrum of interstellar CN molecules and found that they were in a heat bath of about 3K. Discovery of cosmic background radiation by Penzias and Wilson in 1965 made it clear that McKellar had not only measured the CN absorption-line spectrum but had actually determined the temperature of the cosmic background radiation. Since then many scientists have used the absorption-line spectrum of CN molecules to find the CBR temperature which has already been described

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above. Here we are searching for the possible region consisting of CN^- which is the possible source of CH_3CN.

THEORY

The basic method to describe the Hartree Fock theory is similar to Szabo & Ostlund (1989)[5] and Foresman & Frisch (1996)[6]. The stability of molecule is checked by finding its binding energy. The rotational frequency and rotational temperature can be calculated using the relations

5Øß = 2B(J+1); J= 0,1,2,... and $T_{Rot} = \frac{hB}{K}$

The basic method to calculate the dust color temperature and column density from the IRAS 60 µm and 100 µm flux densities is similar to Schnee et al. (2005)[7]. The temperature is determined by the ratio of the 60 µm and 100 µm flux densities. The dust temperature T_d in each pixel of a FITS image can be obtained by assuming that the dust in a single beam is isothermal and that the observed ratio of 60 µm to 100 µm emissions is due to blackbody radiation from dust grains at T_d, modified by a power law emissivity spectral index. The dust temperature estimation formula is

$T_d = \frac{-96}{\ln\{R \times 0.6^{(3+\beta)}\}}$ Where R = F (60µm) / F (100 µm), F (60µm) and F (100 µm) are the flux densities in 60 µm and 100 µm respectively and â is the spectral index takes the values 0, 1 and 2. In our case, we take â =2 (Dupac et al. 2003)[8].

The mass of the investigated structure is measured by measuring the temperature of the region. The formula toestimate the mass is

$$M_{dust} = \frac{4}{3}\frac{a\rho}{Q\upsilon}\left[\frac{S\upsilon \times D^2}{B(\upsilon,T)}\right]$$

where,

a = Weighted grain size = 0.1µm , ρ = Grain density = 1000 kg/m[2], Q_ = Grain emissivity = 0.0010 (for 100µm) (Young et al. 1989)[9] = 0.0046 (60 µm) (Young et al. 1993)

$S\upsilon$ = Flux density at wavelength υ, D = Distance = 20 pc (Odenwald & Richard, 1989).

$B(\upsilon; T)$ = Intensity of the black body temperature at T K

METHOD

The methods we are adopting are theoretical calculation of CH_3CN and its observation is performed using Gaussian 03 and Gaussview softwares. The observation is guided by theoretical calculation. Survey frequency is the rotational frequency of CH_3CN obtained from the theoretical calculation. We are confined to the rotational parameters because the energy corresponding to 7.5 K temperature is less than 0.005 eV. With the quantum of energy less than 0.005 eV, electronic and vibrational energy states will not be excited or in other words transitions that are purely rotational in character will appear (Gupta et al., 2003)[10]. We plan to search a region in which the possible existence of CH_3CN can be justified. From ab-initio calculations we have obtained the rotational frequency for CH_3CN to be 322.624 GHz. Therefore, to search a region consisting of CH_3CN we need to perform all sky survey in this frequency range. But there is no any survey in this range of frequency till January 2009 (htpp: // www.skyiew.gsf.nasa.gov). Among surveys available in the SkyView virtual observatory, one survey named CO under the heading of radio survey is found to have the frequency of 115 GHz. Since the frequency of the CO survey is within the rotational frequency of CN^- by less than 1.5% we have selected this survey for searching the possible source of CN^- which is the possible source of our investigated molecule CH_3CN in the interstellar medium. The FITS image is thus downloaded from the SkyView and studied it in ALADIN2.5.

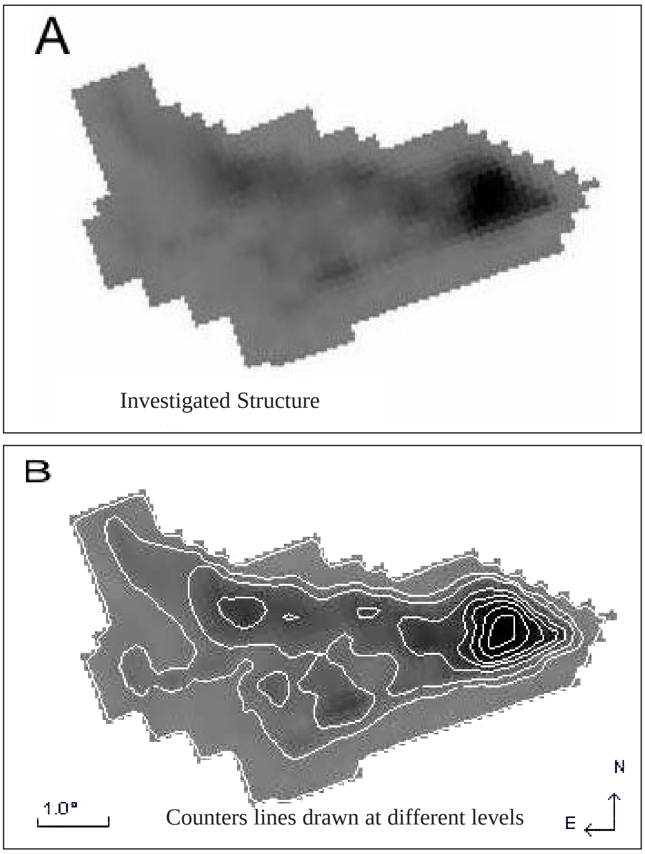

Fig. 1: A shows the investigated structure in CO survey and B shows the different counter lines drawn at different level in the unit of relative flux density. This image is centered at RA (J2000): $19^h12^m01.09^s$, Dec (J2000): −37°362 31.702 2†.

RESULT

From the ab-initio (First principle) calculation of CH_3CN in the Hartree Fock level of approximation. It is found that there is a strong binding between H, C and N in CH_3CN, minimum value of the binding energy being 12.7947 eV in the basis set 6-311G which agrees within around 8% to the maximum value of 13.7352 eV obtained in the basis set 6-31G*. We found the value of rotational frequency for CH_3CN obtained in the basis set 6-31G* as the rotational frequency for CH_3CN which is 322.62 GHz, and the rotational temperature corresponding to the same basis set is also taken as the rotational temperature for CH_3CN which is 7.74 K. (Table 1)

Table 1: Rotational frequency and rotational temperature in various Basis Sets

Basis set	Binding Energy (eV)	Rotational frequency (GHz)	Rotational temperature (K)
3-21G	13.06	323.56	7.76
3-21G*	13.06	323.56	7.76
6-31G	12.94	324.90	7.80
6-31G*	13.74	322.62	7.74
6-311G	12.79	326.45	7.83
6-311G*	13.60	323.26	7.76
6-311G(3df)	13.70	322.65	7.74
6-311++G(3df)	13.66	322.67	7.74

In the second part we have carried out observation in the SkyView virtual observatory (www.skyiew.gsf.nasa.gov). There are 52 different surveys available in the SkyView. Due to the unavailability of the survey in the range of rotational frequency of the CH_3CN, one of the radio surveys named CO has frequency of 115 GHz which is the survey having frequency nearest to that of CN (within 1.5%). Therefore, we performed a systematic search in CO survey and explored a huge extended (~7°×4°) emission at RA (J2000): 19^h16^m Dec. (J2000): – 37°37'.

The whole structure is like a flying bird, the most emissive part behaves as the head part and backside forms two different wings shaped structure (Fig. 1A). The region of interest is an isolated structure in CO survey. The structure is extended from east to west. The two ends are at and the central part is bulged. The eastern end is broader than the western end and the structure has more or less a slipper shape. We sub divide the downloaded image into three regions namely Upper Wing, Lower Wing and Third Region (where huge emission seen) (see Fig 2A).

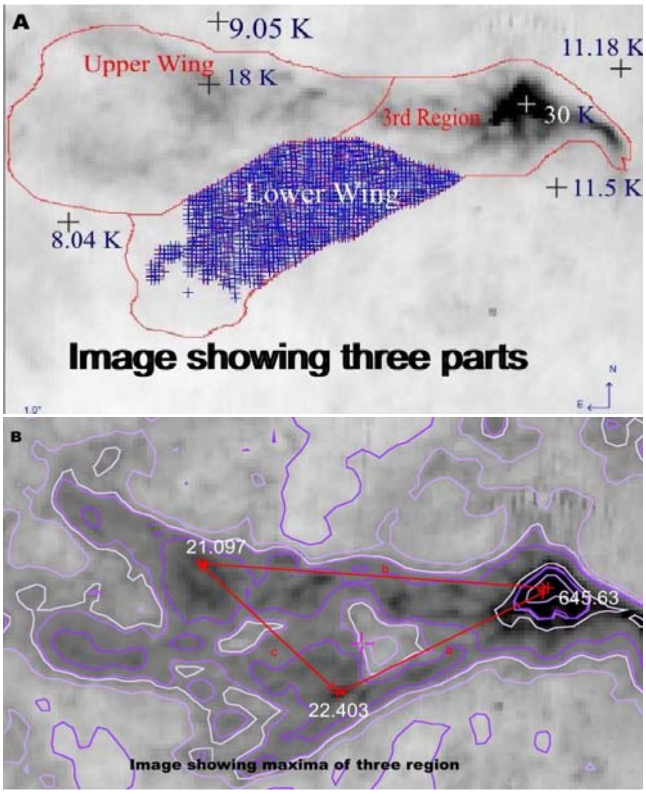

Figure 2: (A) Three different regions of ROI at 100 μm and (B) Maxima in three different regions at 100 μm IRAS image.

We have identified three significant emission region, one towards the west with relative flux density 645.63, another peak observed towards north-east, designed as the Upper Wing, with relative flux density 21.097 and the other towards the South-east, designed as Lower Wing, with relative flux density 22.403. These three points of emission is designated as the principal maxima of three different regions. Calculation of the flux density change along the line of two maxima shows that there are several knots in between the two maxima of either path whose contribution appears to be relatively small.

In order to estimate the temperature at different region we have studied the emission structure in 12 μm, 25 μm, 60 μm, and 100 μm IRAS surveys. In all four IRAS surveys shape of the emission in the ROI is similar. Although the structure in IRAS bands are not isolated as in CO survey, the pattern of emissions within the region of interest are similar in nature with that of CO emission. The object appears more clear with the increasing wavelength. This close association of CO and IRAS emission in the region of interest confirms that the object is intense in the interstellar medium. With the help of ALADIN 2.5 we have taken the reading of relative flux density at the points of principal and secondary maxima in each of the four IRAS surveys. Interestingly, we have found that the value of relative flux density decreases on moving from 25 μm to 60 μm and then increases on moving to 100 μm.

Here, we compare our result with other published works. Fig. 2 shows a comparison of spectral distribution of the maxima (Upper Wing, Lower Wing and Third Region) with other published works. Aryal & Weinberger's (2006) skeleton nebula (Fig. 3) does not have a strong 12 μm and 25 μm spectral components. This lack of emission at 12 μm and 25 μm suggests that the dust population may be relatively devoid of a small grain component as compared to the cirrus material (Puget et al. 1985)[11], or perhaps that the small dust grain are not being adequately excited by the ambient radiation field (Mebold et al. 1985)[12]. The strength of the stellar radiation field near the Draco cloud is estimated to be about 10× lower than in the Galactic plane (Mebold et al. 1985). The Draco cloud is at 38° latitude, at slightly higher latitude than the skeleton nebula (32°). It is estimated that the stellar radiation field for the skeleton nebula is also weaker (~10–12×) with respect to a position in the Galactic plane not only because of its high latitude but also due to the smaller number of stars in this region due to the longitude of ℓ = 197°.

We have compared results of Aryal & Weinberger (2006)[13], Weiland et al. (1986)[14] and Odenwald & Rickard (1987)[15] by considering their respective estimated mass, size and the position of the emission and found that the stellar radiation field, in our case, is ~8 –10× weaker with respect to a position in the Galactic plane. As for as the temperature is concerned, we rule out that the temperature never pass the limit of 10 K because of the steeper slope from 60 to 100 micron plot in Upper Wing (see Fig. 2). The average slope from 12 to 25 micron is much less than the slope from 60 to 100 micron. The usual decrease in the range 25 µm to 60 µm can be seen. But for Third Region this unusual behavior disappears. This indicates that the dust color temperature lie in between 10 to 20 K in the emission region. The temperatures never cross the 30 K limit, if we adopt the result obtained by Odenwald & Rickard (1987) as a correct one. Thus our emission region is relatively colder than other infrared clouds.

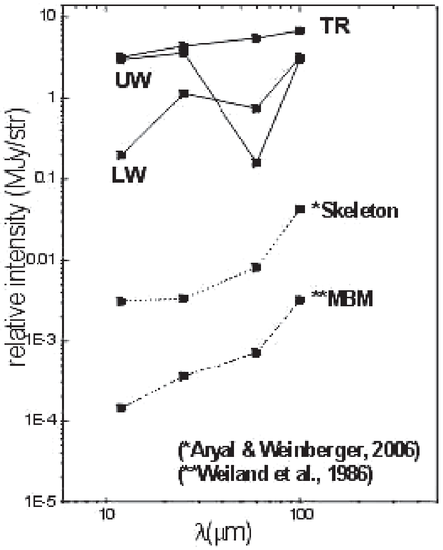

Figure 3: Far-IR spectral distributions of the maxima Upper Wing (UW), Lower Wing (LW) and the Third Region (TR) of our ROI. A comparison with the Skeleton nebula (Aryal & Weinberger 2006) and MBM 20 cirrus cloud" (Weiland et al. 1986)[16] is shown. All intensities have been background subtracted and colour corrected for 240 K blackbody emission.

To investigate for the presence of CH_3CN, we need the temperature profile of the ROI which can be estimated from the data of relative flux density observed in the four IRAS surveys - 12 µm, 25 µm, 60 µm and 100 µm. The 12 µm and 25 µm FITS image are not very clear. So we chose 60 µm and 100 µm image to evaluate the temperature. (Table 2)

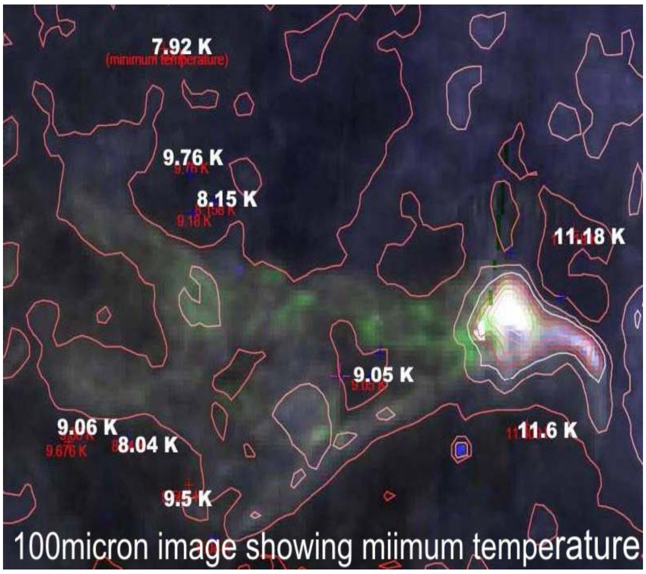

Figure 4: 100 µm IRAS image showing minimum temperature in investigated Region. The white part shows huge emissive part.

As for as the dust color temperature is concerned, it is well known that the IRAS 100 µm wavelength corresponds less than 40 K temperature in any case. By use of the 60 µm and 100 µm fluxes of this region (after subtraction of the background infrared emission) we adopt a dust color temperature of T ~ 25 ±5 K, using the paper by Henning et al. (1990)[16]. The distance of our huge emission is primarily unknown. In order to study how massive our huge structure, we estimate the mass range by assuming 20 pc (Odenwald & Richard, 1989) which is shown in Table 3.

Table 2: Relative flux density and temperature at various pixels in three different regions.

Region	RA (J2000)	Dec. (J2000)	Relative	flux density	Temperature
	(hr: min: sec)	(deg: min: sec)	100 µm	60 µm	K
Upper	19:21:30.61	35:34:17.0	8.170	0.005	9.71
Wing	19:20:01.58	35:54:54.3	7.950	0.0007	8.15
	19:13:54.03	37:08:10.1	12.670	0.5818	17.03
Lower	19:29:11.41	38:06:01.8	9.206	0.014	9.6
Wing	19:25:52.71	38:14:12.6	9.418	0.756	8.04
	19:12:55.99	37:35:53.6	12.970	0.856	22.78
	19:13:06.31	37:28:38.3	10.777	0.6189	17.74
Third	19:09:53.39	37:32:53.1	9.824	0.2819	15.72
Region	19:01:14.89	36:24:10.9	10.244	0.0009	7.99
	18:55:59.43	37:38:46.1	13.960	1.3998	19.78
	18:58:18.20	36:44:01.4	8.904	0.3889	16.89

Table 3: Mass of three different regions, in solar mass unit.

Region	Temperature (K)	Flux at 100 µm $(S\upsilon)$ (Kg s^2)	Distance (Pc)	Planks function (B) (J m^2)	Mass (solar mass)
Upper Wing	17	1.17079×10^{-20}	20	8.39×10^{-17}	4273.50
Lower Wing	17	1.3087×10^{-20}	20	8.39×10^{-16}	4778.78
Third Region	19	1.3512×10^{-20}	20	2.04×10^{-16}	2026.75

CONCLUSION

We have calculated the binding energy, rotational constant, rotational frequency and rotational temperature of CH_3CN in different basis sets are calculated using Gaussian03. We searched emission region at 115 GHz and studied the investigated structure using data reduction software ALADIN2.5. We summarize our results as follows:

(1) From the ab-initio (First principle) calculation of CH_3CN in the HF level of approximation it is found that there is a strong binding between H, C and N in CH_3CN, minimum value of the binding energy being 12.79 eV in the basis set 6-311G which agrees within around 8% to the maximum value of 13.73 eV obtained in the basis set 6-31G*.

(2) The estimated value of rotational frequency in the HF level of approximation is found to be 322.62 GHz in the basis set 6-31G* which agrees with the values of rotational frequency obtained in other basis sets within around 4%. Similarly, value of rotational temperature in the same basis set 6-31G* is found to be 7.74 K which agrees within around 4% to the corresponding values obtained in other basis sets.

(3) The investigated region in CO survey (frequency 115 GHz) is a huge (~7° × 4°) structure having east to west elongated emission pattern. There are three different regions named as Upper Wing, Lower Wing and Third Region. We estimated the relative flux density and temperature of each pixel. We found that the minimum dust color temperature at Upper Wing is 8.15 K which is almost 5% differs from rotational temperature CH_3CN. Similarly, we found that the minimum dust color temperature at

Lower Wing is 8.04 K which is almost 4% differs from rotational temperature CH_3CN. And we found that the minimum dust color temperature at Third Region is 7.99 K which is almost 5% differs from rotational temperature CH_3CN. This implies that there is strong evidence of possibility of finding CH_3CN in the investigated region. But the confirmation can only be done by spectral analysis.

(4) We have suspected that the vibrational band in the infrared region is the main cause for the observed excess temperature for CH_3CN background. The vibrational and electronic bands in optical region, however, also cannot be denied as the cause of excess temperature.

(5) It is found that the flux density increases from 12 µm to 25 µm and then decreases sharply on moving from 25 µm to 60 µm in the maxima of Upper Wing. This is unusual if we compare with previous published works. In addition, the flux density increases but not at significant level when moving from 60 µm to 100 µm. This is also noticeable. Similarly, It is also found that the flux density increase from 12 µm to 25 µm and then decreases sharply on moving from 25 µm to 60 µm in the maxima of Lower Wing. This is also unusual if we compared with previous published works.

(6) We estimated the dust mass of the three different regions. We found that the mass of Upper Wing, Lower Wing and Third Region are 4273.504 $M_{È}$, 4778.786 $M_{È}$ and 2026.75 $M_{È}$ respectively. The total mass of the investigated region has to obtain 11079.04 $M_{È}$.

(7) The mass of the gas found in the investigated structure is almost 200 times the dust mass, so the mass of the investigated structure is found to be 2215808 $M_{È}$.

ACKNOWLEDGEMENTS

This research has made use of NASA Extragalactic Database under contract with the National Aeronautics and Space Administration. We acknowledge the B. P. Koirala Memorial Planetarium, observatory and Science museum Development Board, Singha Durbar, Kathmandu, Nepal, which provides the scholarship to complete this work. One of the authors (U. P. Chaulagain) acknowledges Central department of physics, TU for providing various supports for his M.Sc. thesis.

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