H$^{13}$CN–HN$^{13}$C Intensity Ratio as a Temperature Indicator of Interstellar Clouds

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Abstract—With the 30-m IRAM radio telescope, we observed several massive star forming regions at wavelengths of 3–4 and 2 mm. The temperature of the gas in the sources was estimated from the lines of CH$_3$CCH and from the transitions of the NH$_3$ molecule obtained during observations at the 100-m radio telescope in Effelsberg. As a result, a correlation between the integrated intensity ratios of the $J = 1$–0 transitions of H$^{13}$CN–HN$^{13}$C and the kinetic temperature has been obtained. The obtained results allow us to propose the use of the intensity ratio H$^{13}$CN–HN$^{13}$C as a possible temperature indicator of interstellar clouds. We also compared the obtained estimates of the kinetic temperature with the dust temperature $T_{dust}$. As a result, no significant correlation was found.

Keywords: star formation, interstellar medium, molecular clouds, temperature

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1. INTRODUCTION

The hydrogen cyanide molecule HCN and the isomer HNC are widely distributed in the interstellar medium. It is known that the HCN/HNC abundance ratio strongly depends on the kinetic temperature, for example, it was found in [1] that the abundance ratio in high mass protostellar objects is 4, in hot ultracompact H II regions the average value is 9. In [2] it was proposed to use the intensity ratio of HCN to HNC line as a temperature indicator based on observations of the integral shaped filament in Orion.

The main pathway for the formation of HCN and HNC isomers is the dissociative recombination of the HCNH$^+$ ion with an electron:

$$\text{HCNH}^+ + e^- \rightarrow \begin{cases} 
\text{HCN} + H, \\
\text{HNC} + H.
\end{cases}$$

This reaction has an approximately equal branching ratio [3], and the abundance differences between HCN and HNC are largely determined by the destruction and isomerization reactions of HNC.

These include the following reactions (see details in [4]):

$$\text{HNC} + \text{H} \rightarrow \text{HCN} + \text{H},$$

$$\text{HNC} + \text{O} \rightarrow \text{CO} + \text{NH}.$$  

The energy barrier for the reaction (2) is 200 K [4], for the reaction (2) is 20 K, which determines the dominant role of reaction (3) at low temperatures of the order of 50 K [2]. However, the classical calculated energy barriers are 1200 and 2000 K, respectively (see details in [4]).

2. OBSERVATIONS AND DATA REDUCTION

2.1. Observations at the 30-m Radio Telescope of the Institute of Millimeter Radio Astronomy (IRAM)

In September 2019, with the 30-m radio telescope of the Institute of Millimeter Radio Astronomy (IRAM), we observed several massive star forming regions at wavelengths of 2 and 3–4 mm (as part of project 041-19). The list of sources is given in Table 1. In this paper, a part of the obtained data is discussed. Table 2 contains the corresponding list of molecular
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Table 1. List of source

| Source    | $\alpha$ (2000), h m s | $\delta$ (2000), deg arcmin | $V_{\text{lsr}}$, km s$^{-1}$ | $d$, kpc | Note          |
|-----------|------------------------|-----------------------------|-------------------------------|---------|---------------|
| L 1287    | 00 36 47.5             | 63 29 02.1                  | −17.7                         | 0.93    | G121.30+0.66, IRAS 00338+6312 |
| S 187     | 01 23 15.4             | 61 49 43.1                  | −14.0                         | 1.0     | G126.68−0.81, IRAS 01202+6133 |
| S 231     | 05 39 12.9             | 35 45 54.0                  | −16.6                         | 2.3     | G173.48+2.45, IRAS 05358+3543 |
| DR 21(OH) | 20 39 00.6             | 42 22 48.9                  | −03.8                         | 1.5     | G81.72+0.57   |
| NGC 7538  | 23 13 44.7             | 61 28 09.7                  | −57.6                         | 2.8     | G111.54+0.78, IRAS 23116+6111 |

Distances to sources are quoted from [5–7].

Table 2. Observed molecular lines

| Molecule | Transition | Frequency, MHz | $E_u/k$, K |
|----------|------------|---------------|------------|
| NH$_3$   | (1, 1)     | 23694.495     | 23.4       |
|          | (2, 2)     | 23722.634     | 64.9       |
| CH$_3$CCH| 5$^2$−4$_1$ | 85442.601     | 77.3       |
|          | 5$^2$−4$_2$ | 85450.766     | 41.2       |
|          | 5$^1$−4$_1$ | 85455.667     | 19.5       |
|          | 5$^0$−4$_0$ | 85457.300     | 12.3       |
| H$^{13}$CN| 1−0        | 86339.921     | 4.1        |
| HN$^{13}$C| 1−0        | 87090.825     | 4.2        |
| HCN      | 1−0        | 88631.602     | 4.3        |
| HNC      | 1−0        | 90663.568     | 4.4        |
| CH$_3$CCH| 9$^3$−8$_3$ | 153790.772    | 101.9      |
|          | 9$^2$−8$_2$ | 153805.461    | 65.8       |
|          | 9$^1$−8$_1$ | 153814.276    | 44.1       |
|          | 9$^0$−8$_0$ | 153817.215    | 36.9       |

The transition frequency and upper level energy are taken from the CDMS$^1$ catalogue.

The full beam width at half maximum at the discussed frequencies ranged from ~30" to ~16". The antenna temperature $T_A^*$ was reduced to the main beam temperature $T_{\text{mb}}$, using the beam efficiency $B_{\text{eff}}$, which was determined by the Ruse’s equation in accordance with the IRAM recommendations and ranged from 0.72 to 0.82. The minimum system noise temperature was ~100 K in 3 mm range and ~200 K in 2 mm range.

Observations were carried out by the method of continuous mapping (OTF, On The Fly) of a 200" × 200" area in full power mode. The reference position was chosen with a shift of 10" in right ascension. In some extended sources DR 21(OH), NGC 7538 two partially overlapping areas were observed. The pointing precision was checked periodically by observations of nearby continuum sources.

$^1$ http://cdms.de

2.2. Observations at the Max-Planck-Institute for Radio Astronomy with the Effelsberg 100-m Radio Telescope

On December 9, 2019 we observed with the 100-m telescope near Effelsberg (Germany) the H$_2$O maser transition at a frequency of 22 GHz, as well as the ammonia inversion lines (1,1), (2,2), and (3,3). The full beam width at half maximum was ~40". The measurements were carried out by the method of continuous mapping using a $K$-band receiver in a secondary focus with a dual bandwidth of 300 MHz, including the aforementioned H$_2$O lines in one band and NH$_3$ in the other band. 5′ × 5′ maps were obtained at a scanning rate of 20″ per second in right ascension; intervals between scans were 15″. The reference position was shifted by +15″ in azimuth. Weather conditions included light rain with low wind speeds (~2 m s$^{-1}$).

The source NGC 7027 was used for calibration with a flux density of 5.5 Jy at 22 GHz [8]. The antenna temperature $T_A^*$ was obtained by multiplying the observed intensities by $T_{\text{cal}}$ and taking into account atmospheric absorption.$^2$

2.3. Data Reduction

The GILDAS/CLASS$^3$ software was used for data reduction. The IRAM-30m and Effelsberg-100m datasets were reduced to the same spatial resolution of 40″. After baseline subtraction and smoothing, the spectral resolution for the Effelsberg-100m data was ~0.46 km s$^{-1}$.

In the analysis, integrated intensity maps ($I = \int T_{\text{mb}} dV$ in units [K km s$^{-1}$]) were used in the velocity range [$V_{\text{lsr}}−10$, $V_{\text{lsr}}+10$] for HCN, H$^{13}$CN and [$V_{\text{lsr}}−4$, $V_{\text{lsr}}+4$] for HNC, HN$^{13}$C. It should be noted that two velocity components about −4 and 0 km s$^{-1}$ are observed in the source DR 21(OH) (see details in [9]). In the reduction, the components were separated, and only about −4 km s$^{-1}$ component has

$^2$ http://eff100mwiki.mpifr-bonn.mpg.de

$^3$ http://www.iram.fr/IRAMFR/GILDAS
been used for the analysis, since it is stronger and is detected throughout the source.

3. RESULTS

3.1. Kinetic Temperature from Observations of CH$_3$CCH

In [10, 11] it was shown that the rotational temperature of CH$_3$CCH gives a good estimate of the gas kinetic temperature at gas density $n \approx 10^{3-4}$ cm$^{-3}$ (transitions $J = 5-4$ and $6-5$ were considered). It is explained by the fact that, due to the low dipole moment ($\mu = 0.78$ D), the CH$_3$CCH molecule is easily thermalized under such conditions. Gas density in our sources are above this threshold (Pazukhin et al., in preparation). Thus, the CH$_3$CCH lines in our data can be a good gas kinetic temperature indicator. Rotational (and, accordingly, kinetic) temperature is determined by the population diagrams method:

$$\ln \left( \frac{3k}{8\pi} \frac{T_{mb}dv}{\nu^2} \right) = -\frac{E_u}{T_{\text{kin}}} + \ln \left( \frac{N_{\text{tot}}}{Q} \right),$$  \hspace{1cm} (4)

where $S$ is the line strength equal to $J^2 - K^2$, $\nu$ is the transition frequency, $E_u$ is the upper energy level in temperature units, $\mu$ is the dipole moment, $T_{mb}dv$ is the integrated line intensity, $N_{\text{tot}}$ is the total column density, $Q$ is the partition function, $g_K$ is the $K$ degeneracy associated with the internal quantum number $K$ due to the projection of the total angular momentum onto a molecule axis, $g_j$ is the statistical weight associated with the nuclear spin. It is assumed here that the emission is optically thin and the background radiation can be neglected.

The rotational diagrams were constructed using the $J = 5-4$ and $9-8$ transitions of the CH$_3$CCH molecule. The spectra were fitted with Gaussian profiles, assuming that the widths of each component are equal, and the spacings between them are known. Then a graph was built, where the upper energy level $E_u$ was plotted along the abscissa axis, and the left part of the Eq. (4) was plotted along the ordinate axis. Then, $T_{\text{kin}}$ is proportional to the inverse of the slope. In Fig. 1 in the direction IRAS 23116+6111 and DR 21(OH) the spectra of the CH$_3$CCH molecule and rotational diagrams are plotted. Figure 2 (left) shows a comparison of the kinetic temperature estimates for the $J = 5-4$ and $9-8$ CH$_3$CCH transitions. In general these estimates are close to each other, therefore, the population diagram can be plotted using both transitions.

It should be noted that for the L 1287, estimates of the kinetic temperature were obtained only at two points ($0''$, $0''$) and ($-14''$, $-14''$) and are equal 21.5 ± 1.9 and 20.4 ± 1.8 K, respectively. For objects S 187, S 231, the CH$_3$CCH lines turned out to be too weak to estimate the kinetic temperature.

3.2. Kinetic Temperature from NH$_3$ Observations

Transitions of the NH$_3$ molecule were observed in sources S 187, DR 21(OH) with the Effelsberg-100m radio telescope. For S 231, we used the estimate of the kinetic temperature with ammonia from [12].

The optical depth and rotational temperature were determined using the methods described in [13]. The spectra were fitted with Gaussian profiles, in the transition (1,1) the widths of each component were assumed to be equal, and the spacings between them are known. Assuming that hyperfine components are under LTE conditions, the optical depth $\tau(1,1,m)$ can be determined from the ratio of the main and satellite line intensities:

$$\frac{T^*_A(m)}{T^*_A(s)} = 1 - \exp(-\alpha(1,1,m)), \hspace{1cm} (5)$$

where $T^*_A$ is the antenna temperature, $\alpha$ is the ratio of the main and satellite line intensities, equal to $\alpha = 0.28$ for inner satellites and $\alpha = 0.22$ for outer satellites. The optical depth $\tau(1,1,m)$ was determined numerically from Eq. (5).

Thus, the rotational temperature can be obtained from the ratio of the main component intensities of (1,1) and (2,2) transitions using the equation:

$$T_{\text{rot}} = -41.5/\ln \left[ \frac{0.282}{\tau(1,1,m)} \times \ln \left( \frac{1 - T^*_A(2,2,m)}{T^*_A(1,1,m)} \right) \right]. \hspace{1cm} (6)$$

The kinetic temperature values were obtained using the equation from [14]:

$$T_{\text{kin}} = \frac{T_{\text{rot}}}{1 - \frac{T_{\text{rot}}}{41.5} \ln \left[ 1 + 1.1 \exp \left( \frac{-16}{T_{\text{rot}}} \right) \right]}. \hspace{1cm} (7)$$

4. DISCUSSION

Figure 2 (right) shows a comparison of the kinetic temperature estimates from ammonia and CH$_3$CCH transitions for the DR 21(OH) source. In general, there is a fairly good agreement between them, although the estimates for the CH$_3$CCH transitions result in slightly higher values than the estimates for ammonia. This is probably due to the fact that methylacetylene is observed in a denser gas, where the temperature is higher.

In addition, for the sources L 1287, DR 21(OH), and NGC 7538, there are maps of dust temperature...
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Fig. 1. Spectra (left) and population diagrams (right) for IRAS 23116+6111 (upper panels) and DR 21(OH) (lower panels). CH$_3$CCH $J = 9$–8 and 5–4 spectra are indicated in black; the red and blue lines are the Gaussian profile fitting. The lines in the population diagrams are plotted by the least squares method. In the lower left corner of the diagrams, the obtained value of the kinetic temperature is given. For DR 21(OH), the Gaussian profiles are plotted for the velocity components about $-4$ and 0 km s$^{-1}$, and the population diagram are plotted for about $-4$ km s$^{-1}$ component.

$T_{\text{mb}}^{98}$, K

$T_{\text{kin}}^{54}$, K

$T_{\text{kin}}$ (CH$_3$CCH), K

$T_{\text{kin}}$ (NH$_3$), K

Fig. 2. Comparison of estimates of the kinetic temperature from $J = 5$–4 and 9–8 CH$_3$CCH transitions (left) and for the source DR 21(OH) from ammonia and CH$_3$CCH transitions (right). Lines of the form $y = x$ are plotted diagonally.
and column density $N(H_2)$ according to data from the Herschel telescope taken from the open database,\footnote{http://www.astro.cardiff.ac.uk/research/ViaLactea} which were obtained using the PPMAP \cite{15, 16} algorithm. We compared the dust temperature $T_{\text{dust}}$ estimates with the kinetic temperature estimates (Fig. 3). As a result, no significant correlation was found. $T_{\text{dust}}$ values are in the range $\sim$18–25 K, while $T_{\text{kin}}$ increase to 35 K. It is possible that the lack of correlation is due to the insufficient density of our sources. Thus, in \cite{14} demonstrated that the dust temperature approaches the gas temperature at a gas density $n \approx 10^{7-8} \text{ cm}^{-3}$, which is much higher than the gas density estimates in our sources, which, according to our data, is $n \sim 10^4–10^6 \text{ cm}^{-3}$ (Pazukhin et al., in preparation).

We estimated the optical depths in the HCN and HNC lines. To do this, we used the intensity ratio of the isotopologues HCN/H$^{13}$CN and HNC/HN$^{13}$C in Eq. (5) and the value $a$ from the abundance ratio of carbon isotopes \cite{18}

$$\frac{^{12}\text{C}}{^{13}\text{C}} = 4.7R_{\text{GC}} + 25.05,$$

where $R_{\text{GC}}$ is the Galactocentric distance of the source. Figure 4 (left) shows a comparison of the obtained optical depth values. The optical depths in both lines are large. The optical depth in the HCN line is on average higher than in the HNC line and reaches $\sim$20. In this case, a rather large spread in the ratio of optical depths in these lines is observed. This makes it preferable to use the lines of their rare isotopologues H$^{13}$CN and HN$^{13}$C, in which the optical depth is obviously small. In \cite{2} it was came to the conclusion that the optical depth in the HCN and HNC lines does not significantly affect the relation between the intensity ratio of these lines and the gas temperature. Our data cast doubt on this. In Fig. 4 (right) shows the dependence of the ratio $R_{12}/R_{13}$ [$R_{12} = I(\text{HCN})/I(\text{HNC})$, $R_{13} = I(\text{H}^{13}\text{CN})/I(\text{HN}^{13}\text{C})$] on the optical depth $\tau$(HCN), as well as the values of the column density $N$(HCN), as well as the values of the column density $N(H_2)$. It can be seen that at large optical depths, which are typical for HCN lines, the ratio $R_{12}/R_{13}$ is much less than unity. As the optical depth decreases, this ratio, as expected, tends to 1. The hydrogen column density, at which the optical depth in the lines becomes small, is $N(H_2) \sim 10^{22} \text{ cm}^{-2}$.

Variations of the $R_{12}$ ratio can be caused by different excitation temperatures $T_{\text{ex}}$ of HCN and HNC. However, on the dependence of $T_{\text{kin}}$ on $R_{2}$ plotted using the RADEX \cite{19} program under the conditions...
$n = 10^5 \text{ cm}^{-3}$ and $N = 10^{12} \text{ cm}^{-2}$ it can be seen that the ratio changes only slightly with increasing temperature and amounts to $\lesssim 1$ (Fig. 5).

As a result of the analysis of our data, the dependence of the ratios $R_2$ and $R_3$ on the gas kinetic temperature was plotted (Fig. 6). The value of $R_3$ increases from 1 to 10, and the intensity ratio of the main isotopologues increase from 1 to 4 in the temperature range $\sim 15-45$ K.

Thus, as a result of the linear least squares fit, the following dependencies were obtained:

$$T_{\text{kin}} = \begin{cases} 2.4R_3 + 19.1, \\ 8.7R_2 + 6.4. \end{cases} \quad (8)$$

The line obtained for HCN and HNC agrees with the line $T_{\text{kin}} = 10 \frac{I(\text{HCN})}{I(\text{HNC})}$ obtained in [2], which is valid for the intensity ratio $\leq 4$ and up to temperatures $T_{\text{kin}} \sim 40$ K.

In addition, Fig. 6 shows an approximation by a function of the form $A \exp \left(\frac{-\Delta E}{T_{\text{kin}}}\right)$ which is chosen based on the population ratio expressed in terms of the Boltzmann distribution. As a result, the following dependencies were:

$$R_{13} = 179 \exp \left(\frac{-109}{T_{\text{kin}}}\right), \quad (9a)$$

$$R_{12} = 8.4 \exp \left(\frac{-34}{T_{\text{kin}}}\right). \quad (9b)$$

The energy barrier for the ratio $R_{13}$ is $\Delta E \sim 109$ K, and for the main isotopologues $\Delta E \sim 34$ K. The results from other publications are somewhat different, the energy barrier at low temperatures is $\Delta E \sim 20$ K [2], with a further increase with temperature $\Delta E \sim 200$ K [4, 20].

In general, the data for HCN and HNC agree with the results from [2]. However, the results for $R_{12}$ are noticeably different. The main reason for the discrepancy between the results is probably the large optical depth of the HCN and HNC lines, as well as the presence of anomalies in the hyperfine structure of the HCN molecule.

The use of the $^{13}$HCN and $^{15}$HN lines for temperature estimation was also recently proposed and demonstrated in [21]. However, in this paper, to estimate the temperature, the correlation dependence of $R_{12}$ on temperature found in [2] is used. As shown above, the dependence of $R_{13}$ on temperature differs from it.

We suppose that it is preferable to use Eq. (9a) for the ratio $R_{13}$ as a temperature indicator. Temperature estimates for NGC 7538 and DR 21(OH) are shown in Fig. 7. The plotted maps demonstrate good agreement with the estimates obtained from lines of CH$_3$CCH and NH$_3$. The temperature gradient is visible, the peaks coincide with the emission of the continuum and the emission of the IR source. In addition, maps extend further than plotted temperature maps obtained from CH$_3$CCH and NH$_3$. 

Fig. 4. Dependence on the optical depth estimates $\tau(\text{HCN})$ for HCN and HNC molecules of the $\tau(\text{HNC})$ (left) and of the ratio $\tau_{12}/\tau_{13}$ (right). The color-coded indicates the column density $N(\text{H}_2)$ values.

Fig. 5. Dependence of the optical depth estimates $\tau(\text{HCN})$ for HCN and HNC molecules of the $\tau(\text{HNC})$ (left) and of the ratio $\tau_{12}/\tau_{13}$ (right). The color-coded indicates the column density $N(\text{H}_2)$ values.
Fig. 5. Dependence of the kinetic temperature $T_{\text{kin}}$ on the ratio $R_{12}$ plotted using the RADEX program for $n = 10^5$ cm$^{-3}$ and $N = 10^{12}$ cm$^{-2}$.

Fig. 6. Dependence of the kinetic temperature on the integrated intensity ratio of the molecules $^{13}$CN and $^{13}$C (left) and HCN and HNC (right). The fitting results are represented by the blue straight line $ax + b$ and the red curve describes a function $A \exp \left( -\frac{\Delta E}{T_{\text{kin}}} \right)$. The green curve corresponds to $\Delta E = 20$ K from [2]. The parameters of the fits ($a$, $b$, $A$, $\Delta E$) are shown in each of the figures.
It is worth noting that temperature maps can be further expanded by combining the observational data from isotopologues H$^{13}$CN and HN$^{13}$C with observations from the main isotopologues, for example, as suggested in [21]. In this paper, in those source regions where the H$^{13}$CN and HN$^{13}$C lines become too weak, the intensity ratio of the main isotopologues $R_{12}$ is used.

5. CONCLUSIONS

Based on observations of five massive star forming regions obtained with the IRAM–30m and Effelsberg-100m radio telescopes, as well as using estimates of the dust temperature $T_{dust}$ from the Herschel telescope data, we obtained following results.

(1) A correlation between the integrated intensity ratios of the $J = 1-0$ transitions of H$^{13}$CN and HN$^{13}$C and the kinetic temperature has been found. The intensity ratio increases from 1 to 10 in the temperature range ~15–45 K was found. Since these lines can be detected in observations of most sources, the results obtained allow us to propose using the H$^{13}$CN/HN$^{13}$C intensity ratio as a possible temperature indicator of interstellar clouds.
(2) For the low-temperature reaction $\text{HNC} + \text{O} \rightarrow \text{CO} + \text{NH}$, the energy barrier obtained from the ratio $\text{H}^{13}\text{CN}/\text{HN}^{13}\text{C}$ was $\Delta E \approx 109$ K, and from the ratio of the main isotopologues is $\Delta E \approx 34$ K. The main reason for the discrepancy between the results is probably the large optical depth of the HCN and HNC lines, as well as the presence of anomalies in the hyperfine structure of the HCN molecule.

(3) We compared the obtained estimates of the kinetic temperature with the estimates of the dust temperature $T_{\text{dust}}$. As a result, no significant correlation was found. $T_{\text{dust}}$ values are in the range $\sim 18$–$25$ K, while $T_{\text{kin}}$ grows up to $35$ K. It is possible that the lack of correlation is due to the insufficient density of the observed sources.

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CONFLICT OF INTEREST
The authors declare that they have no conflicts of interest.

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