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# Calculating the Excitation Temperature for $H_2CO$ Absorption Lines in Molecular Clouds

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## Abstract

The excitation temperature $T_{ex}$ for molecular emission and absorption lines is an essential parameter for interpreting the molecular environment. This temperature can be obtained by observing multiple molecular transitions or hyperfine structures of a single transition, but it remains unknown for a single transition without hyperfine structure lines. Earlier $H_2CO$ absorption experiments for a single transition without hyperfine structures adopted a constant value of $T_{ex}$, which is not correct for molecular regions with active star formation and H II regions. For $H_2CO$, two equations with two unknowns may be used to determine the excitation temperature $T_{ex}$ and the optical depth $\tau$, if other parameters can be determined from measurements. Published observational data of the 4.83 GHz ($\lambda = 6$ cm) $H_2CO$ ($1_{10}-1_{11}$) absorption line for three star formation regions, W40, M17 and DR17, have been used to verify this method. The distributions of $T_{ex}$ in these sources are in good agreement with the contours of the H110$\alpha$ emission of the H II regions in M17 and DR17 and with the $H_2CO$ ($1_{10}-1_{11}$) absorption in W40. The distributions of $T_{ex}$ in the three sources indicate that there can be significant variation in the excitation temperature across star formation and H II regions and that the use of a fixed (low) value results in misinterpretation.

*Key words:* ISM: molecules – (ISM:) HII regions – ISM: clouds

## 1. Introduction

$H_2CO$ is the first organic poly-atomic molecule discovered in the interstellar medium, which was first detected and reported by Snyder et al. (1969). The regions of $H_2CO$ production may be associated with the dense clumps along the line of sight (Prasad & Huntress 1980), and the $H_2CO$ absorption provides a tool for analyzing the distribution of dense interstellar gas (Scoville et al. 1972). In addition, Downes et al. (1980) reported that $H_2CO$ absorption is found against most of the H II regions and provides a good probe of star formation regions. $H_2CO$ absorption against a background continuum source serves as a probe of the physical conditions of the foreground clouds and gives constraints for mm and sub-mm spectral lines, both in front and behind the region. For clouds near H II regions, the $1_{10}-1_{11}$ transition of $H_2CO$ also provides a tool for identifying motions (Gardner et al. 1984).

The excitation state of the $H_2CO$ may be expressed as the excitation temperature. This excitation temperature $T_{ex}$ determines the level populations using the Boltzmann equation when in local thermodynamic equilibrium and is a reflection of the environmental conditions such as temperature and density.

The excitation temperature for the $H_2CO$ absorption may be determined from line intensity ratios of two transitions or hyperfine structure of a single transition. The work of Heiles (1973) demonstrates the accurate determination of $T_{ex}$ using $H_2CO$ hyperfine structure lines. This is reasonable because of the very close energy separations for the 6 cm line of $H_2CO$ which consists of six hyperfine components, but this method is suitable only for cases in which the Doppler line width is small enough that the hyperfine structure is not excessively smeared. In some cases, such as spectra from molecular clouds with H II regions, the Doppler line widths are so large that the hyperfine structure lines are obscured.

In the absence of multiple transitions or hyperfine structures of a single transition, the distribution of the excitation temperature is difficult to be determined and a constant excitation temperature is usually assumed for the entire area, such as in Tang et al. (2013), Komesh et al. (2019) and Gong et al. (2023). In a star formation region with varied environmental conditions, the assumption of a fixed value of $T_{ex}$ may result in under- or over-estimates of other physical parameters. For extended molecular clouds with a relatively small variation range of the excitation temperatures, a relatively low value for $T_{ex}$ may be acceptable, but for regions with active star formation and H II regions, the excitation temperatures for the $H_2CO$ absorption lines would be much higher than those of the surroundings (Komesh et al. 2019).

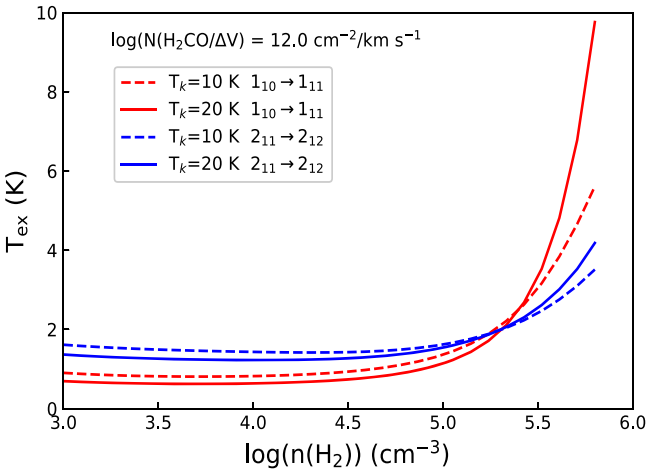


**Figure 1.** RADEX calculations of $H_2CO$ excitation temperatures as a function of molecular hydrogen density at an $H_2CO$ column density per velocity gradient of $10^{12.0}$ cm$^{-2}$ (km s$^{-1}$)$^{-1}$ and kinetic temperature of 10 K and 20 K for $1_{10}\rightarrow1_{11}$ and $2_{11}\rightarrow2_{12}$ transitions.

Figure 1 presents RADEX calculations of $H_2CO$ excitation temperatures as a function of molecular hydrogen density at kinetic temperatures of 10 K and 20 K for the $1_{10}\rightarrow1_{11}$ and $2_{11}\rightarrow2_{12}$ transitions of formaldehyde. This shows that in regions with higher density in the neighborhood of star formation hubs and H II regions, the increased temperature may substantially raise the value for $T_{\rm ex}$ for both the lowest transitions. While in previous studies the assumption of a fixed $T_{\rm ex}$ temperature is acceptable for lower density regions, this is not correct for regions with molecular hydrogen densities above $10^{4.5}$ cm$^{-3}$.

In this work, we put forward a pragmatic method of calculating the excitation temperature for $H_2CO$ absorption lines in molecular clouds, and we take the 4.83 GHz ($\lambda = 6$ cm) $1_{10}-1_{11}$ transition as an example. Especially for molecular clouds near H II regions, this method can effectively overcome the drawback that the excitation temperature differs from a pre-assumed average value. In Section 2 of this paper, we describe the practical method of calculating excitation temperatures for the $H_2CO$ ($1_{10}-1_{11}$) absorption line in molecular clouds. In Section 3, we exemplify the feasibility of this method. Our conclusions and discussion are presented in the last section.

## 2. The Method of Calculating the Excitation Temperature

Mangum & Shirley (2015) present a method for calculating the column density of molecules in the upper transition state ($N_u$) of the $H_2CO$ $1_{10}-1_{11}$ and give a formula

$$N_u = \frac{3h}{8\pi^3|\boldsymbol{\mu}_{\rm lu}|^2}\left[\exp\left(\frac{h\nu}{kT_{\rm ex}}\right)-1\right]^{-1}\int\tau dv, \qquad (1)$$

where $h$ is the Planck constant, $\mu_{\rm lu}$ is the dipole moment of 2.33 Debye, $k$ is the Boltzmann constant, and $\tau$ is the optical depth of the absorption line. Assuming the observed $H_2CO$ absorption is optically thin, the variation of the optical depth is very small within a small velocity range. Although the $1_{10}-1_{11}$ transition of $H_2CO$ has hyperfine structure lines, in some cases, such as in spectra from molecular clouds with H II regions, the Doppler line widths are so large that the hyperfine structure lines are obscured. For this case, a single component Gaussian profile can be adopted and the variation of the optical depth $\tau$ follows the Gaussian profile. So, as an approximation, the integral in the above formula reduces to $(1.064\,\tau\,\Delta V)$.

The second relation relates the excitation temperature $T_{\rm ex}$ to this optical depth $\tau$ and may be expressed as (Heiles 1973)

$$T_L = (T_{\rm ex} - T_c)[1 - \exp(-\tau)], \qquad (2)$$

where $T_L$ is the measured brightness temperature, $T_c$ is the continuum brightness temperature plus the Cosmic Microwave Background, and continuum emissions originate from behind molecular clouds.

The two unknowns, the excitation temperature $T_{\rm ex}$ and the optical depth in the line $\tau$ may be solved from Equations (1) and (2) if the four independent variable parameters $T_L$, $T_c$, $\Delta V$ and $N_u$ may be determined by measurement.

The column density of $H_2CO$ in the upper energy level, $N_u$, may be estimated from the total $H_2CO$ column density $N_{\rm tot}$. For the $H_2CO$ ($1_{10}-1_{11}$) absorption in the H II region of Cygnus X, Gong et al. (2023) adopted an empirical relation between $N_u$ and $N_{\rm tot}$: $N_u/N_{\rm tot} \simeq 0.39$ for a representative kinetic temperature of 10 K. This ratio may be different for different regions, but it should not vary too much under similar physical conditions. While there can be a 13% uncertainty in the derived column densities based on the above empirical relation, we have estimated the uncertainty in $T_{\rm ex}$ caused by this 13% uncertainty using Monte Carlo simulations and found that the uncertainty in $T_{\rm ex}$ is less than 0.1 K.

In addition, the total $H_2CO$ column density can be estimated from the column density of $H_2$ by the relation: $N_{\rm tot} = 3\times10^{-9}{\rm N(H_2)}$ (Evans et al. 1975), or it can be estimated from the column density of $^{13}$CO by the relation: $N_{\rm tot} = 1.25\times10^{-3}{\rm N(^{13}CO)}$ (Komesh et al. 2019). Of course, the ratio of column densities between $H_2CO$ and $H_2$ may not be equal everywhere, and the ratio of column densities between $H_2CO$ and $^{13}$CO may also not be equal everywhere. These variations could introduce uncertainty in the $H_2CO$ column density, which may vary by about an order of magnitude (Gong et al. 2023; Tang et al. 2018). For some representative values of $T_L$, $T_c$ and $\Delta V$, we can describe how $T_{\rm ex}$ and $\tau$ vary with changing $N_u$, as shown in Figure 2. Figure 2(a) illustrates that when $N_u$ ranges from $10^{12}$ to $10^{13}$ cm$^{-2}$, $T_{\rm ex}$ varies from 1.7 to 2.5 K. This indicates that the uncertainty in $T_{\rm ex}$ is about 0.8 K when $N_u$ changes by an order of magnitude, which is acceptable. Figure 2(b) shows that when $N_u$ ranges from $10^{12}$ to $10^{13}$ cm$^{-2}$, $\tau$ varies from 0.33 to 0.66. Thus, the uncertainty in $\tau$ is also acceptable.

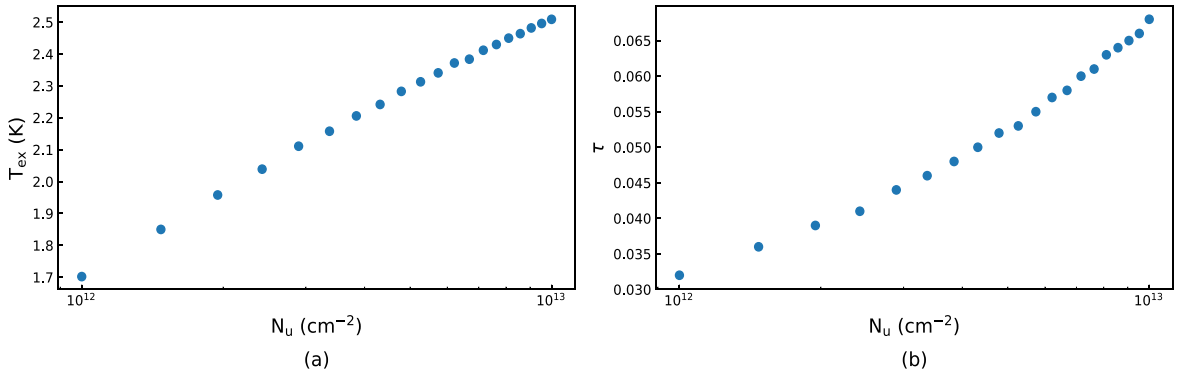


**Figure 2.** The variation of $T_{\rm ex}$ and $\tau$ with respect to $N_u$.

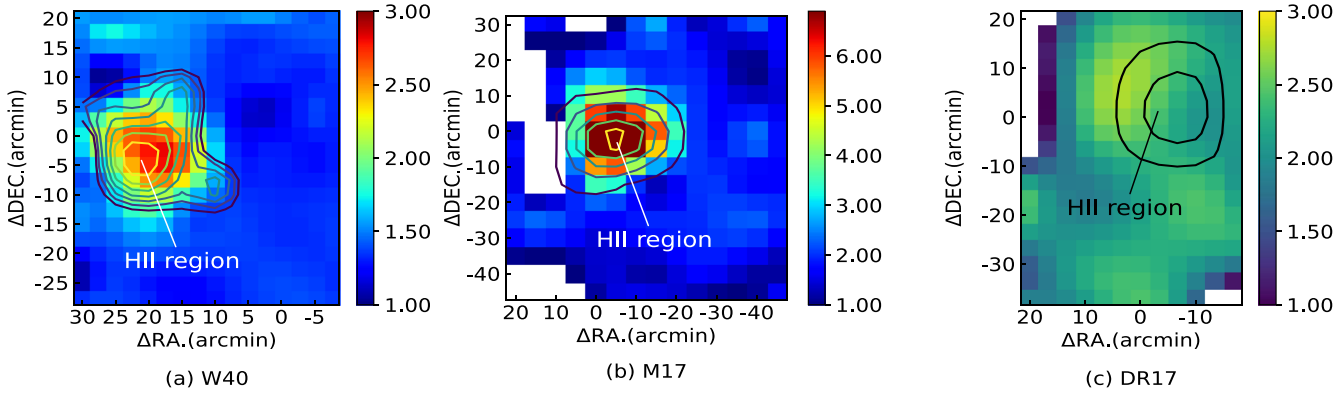


**Figure 3.** The distribution of $T_{\rm ex}$ for the $H_2CO$ ($1_{10}-1_{11}$) absorption line overlaid on H110$\alpha$ emission contours toward (b) M17 and (c) DR17, and on the $H_2CO$ ($1_{10}-1_{11}$) absorption contour toward (a) W40. The $T_{\rm ex}$ color bars are given in unit of K. Panel (a): the contour levels of $H_2CO$ ($1_{10}-1_{11}$) absorption fluxes are from $-0.5$ to $-1.1$ in steps of $-0.1$ K km s$^{-1}$. Panel (b): contour levels of H110$\alpha$ emission fluxes are from 1.17 to 14.4 in steps of 3 K km s$^{-1}$. Panel (c): contour levels of H110$\alpha$ emission fluxes are from 0.7 to 2.04 in steps of 1 K km s$^{-1}$.

The continuum observations sometimes do not distinguish foreground and background emissions. In our calculations, the continuum emissions are assumed to be mainly from behind the targeted molecular clouds, and such an assumption can bias the results. We have used Monte Carlo simulations to estimate the uncertainties in $T_{\rm ex}$ due to the variation of the continuum $T_c$, for example, with uncertainties of 10%, 50% and 80% for $T_c$. We conclude that larger uncertainties in $T_c$ may cause larger uncertainties in $T_{\rm ex}$. When $T_{\rm ex}$ is less than 3 K, the uncertainty in $T_{\rm ex}$ caused by $T_c$ is less than 1 K.

Although the above approximations are not perfect, they will likely result in representative values for both $T_{\rm ex}$ and $\tau$.

## 3. The Feasibility of the Method

In this section we will test the above method in three activity regions in the sources W40, M17, and DR17 using observational data from the literature. In Equations (1) and (2) there are four independent variable parameters: $T_L$, $T_c$, $\Delta V$, and $N_u$. For regions M17 and DR17, the observational data for parameters $\Delta V$, $T_L$ and $T_c$ are adopted from Tang et al. (2013), and the values of $N_u$ are estimated from N($^{13}$CO) and N($H_2$), respectively. For the region W40, the observational data for parameters $\Delta V$, $T_L$ and $T_c$ are adopted from Komesh et al. (2019), and the values of $N_u$ are estimated from N($^{13}$CO). The data for N($H_2$) are acquired from Marsh et al. (2017) and the data for N($^{13}$CO) are acquired from Tang et al. (2013).

In order to evaluate the results, the contours of the H110$\alpha$ emission for M17 and DR17 from Tang et al. (2013) and the $H_2CO$ ($1_{10}-1_{11}$) absorption data for W40 from Komesh et al. (2019) will be used for reference. The H110$\alpha$ recombination line is thought to be strongly associated with H II regions, so it would be a good probe of the extent of the H II region. Recent studies also show a positive correlation between the fluxes of the $H_2CO$ ($1_{10}-1_{11}$) absorption line and the presence of H II regions (Tang et al. 2013; Komesh et al. 2019).

In Figure 3, we show the distribution of the excitation temperature $T_{\rm ex}$ of the $H_2CO$ ($1_{10}-1_{11}$) absorption line superposed on the H110$\alpha$ emission contours toward (b) M17 and (c) DR17 and on the $H_2CO$ ($1_{10}-1_{11}$) absorption contours toward (a) W40. In panel (a), the contour levels of $H_2CO$ ($1_{10}-1_{11}$) absorption fluxes are from $-0.5$ to $-1.1$ in steps of $-0.1$ K km s$^{-1}$. In panel (b), the contour levels of H110$\alpha$

emission fluxes are from 1.17 to 14.4 in steps of 3 K km s$^{-1}$. In panel (c), the contour levels of H110$\alpha$ emission fluxes are from 0.7 to 2.04 in steps of 1 K km s$^{-1}$. In Figure 3, the $T_{\rm ex}$ ranges from 1 to 3 K both in W40 and DR17 and from 1 to 6 K in M17.

As mentioned earlier, the excitation temperature $T_{\rm ex}$ of the $H_2CO$ ($1_{10}-1_{11}$) absorption line at the location of H II regions may be much higher than that of the surroundings. An explanation is that the kinetic temperatures $T_k$ in H II regions are higher than those of the surrounding environment, and our calculations indicate that the excitation temperatures $T_{\rm ex}$ in H II regions are generally greater than 2 K. The RADEX calculations in Figure 1 show that when $T_{\rm ex}$ is greater than 2 K, the higher $T_k$ corresponds to the higher $T_{\rm ex}$. Therefore, the excitation temperatures are higher toward H II regions than those of the surroundings. As can be seen from the three subgraphs of Figure 3, the positions of the H II regions are in good agreement with the distribution of the peaks of $T_{\rm ex}$ for the $H_2CO$ ($1_{10}-1_{11}$) absorption line.

## 4. Summary and Discussion

The excitation temperature is an important parameter for interpreting $H_2CO$ absorption lines in molecular clouds and active star formation and H II regions. The excitation temperature determines whether the line is in emission or absorption. In observations of star formation regions using only a single transition, a fixed value of the excitation temperature is often adopted for interpreting the data, even though it is known that this value may not be constant across the region.

Two equations with two unknowns may be used to solve for the values of the excitation temperature $T_{\rm ex}$ and the optical depth $\tau$. Taking the 4.83 GHz ($\lambda = 6$ cm) $H_2CO$ ($1_{10}-1_{11}$) absorption line as an example for the three sources W40, M17 and DR17, the three independent variable parameters: $T_L$, $T_c$, and $\Delta V$ may result from observational data. The actual formaldehyde column density $N_{\rm tot}$ may be adopted from the $H_2$ or the $^{13}CO$ column densities as $N_{\rm tot} = 3 \times 10^{-9} N(H_2)$ or $N_{\rm tot} = 1.25 \times 10^{-3} N(^{13}CO)$. After solving for $T_{\rm ex}$ in the three sources, the distribution of $T_{\rm ex}$ appears in good agreement with the appearance of the H II regions. Because the H110$\alpha$ recombination line is a good probe of H II regions in M17 and DR17 and there is a positive correlation between the fluxes of the $H_2CO$ ($1_{10}-1_{11}$) absorption line and H II regions in W40, their contours are used for comparison with the distribution of $T_{\rm ex}$.

These results are consistent with the consensus that due to the stronger radio background radiation and higher kinetic temperatures at H II regions, the excitation temperature of the $H_2CO$ ($1_{10}-1_{11}$) absorption line at H II regions needs to be much higher than that of the surroundings.

Although assumptions are made about the abundance of $H_2CO$ relative to $^{13}CO$ or $H_2$, which may vary across the source, this method can obtain more reasonable values of the excitation temperature. It effectively overcomes the drawback that the excitation temperature in H II regions may be very different from the pre-assumed constant value. In future work, better approaches of estimating $N_u$ are necessary to obtain more precise values of $T_{\rm ex}$.

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*Software*: GILDAS/CLASS, Matplotlib, astropy.

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