THE STUDY OF INTERSTELLAR CHEMISTRY THROUGH MID-INFRARED SPECTROSCOPY

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RESUMEN

Se presentan espectros en el infrarrojo de varios hidrocarburos en la dirección del núcleo caliente asociado con la protoestrella masiva NGC 7538 IRS 1. Debido a que una gran abundancia de moléculas totalmente hidrogenadas y de moléculas saturadas es característica de los núcleos calientes, estos constituyen laboratorios para estudiar la química interestelar. Estudiando las moléculas de C_2H_2 , HCN, NH₃, CH₄, y CH₃, podemos restringir los modelos químicos. Derivamos abundancias para C_2H_2 y HCN y las comparamos con las predicciones de los modelos. Las observaciones se realizaron con el "Texas Echelon Cross Echelle Spectrograph" (TEXES)

ABSTRACT

We present mid-infrared spectra of various hydrocarbons toward the hot core associated with the massive protostar NGC 7538 IRS 1. Because high abundances of fully hydrogenated molecules and saturated molecules are characteristic of hot cores, they provide laboratories in which to study interstellar chemistry. Through the study of C_2H_2 , HCN, NH₃, CH₄, and CH₃, we can constrain chemical models. We derive abundances for C_2H_2 and HCN and compare to model predictions. The observations were taken with the Texas Echelon Cross Echelle Spectrograph (TEXES).

Key Words: ISM: MOLECULES — ISM: ABUNDANCES — ISM: CLOUDS — ISM: MOLECULES

1. INTRODUCTION

The chemistry in star forming regions can be a useful tool in determining a sequence of massive star formation (e.g. van Dishoeck & van der Tak 2000). While there is a formation sequence for lowmass stars (Adams et al. 1987), such a sequence has not vet been determined for high-mass stars because massive stars can reach the main sequence while still embedded in dense molecular gas. Icy grain mantles are formed when molecules freeze out during the prestellar and collapse phases. Ices then evaporate when the protostar heats its surroundings. These newly evaporated molecules drive a rich chemistry in compact, optically thick hot cores. Hot cores have temperatures > 100 K, densities > 10^7 cm^{-3} , and diameters < 0.1 pc (Kurtz et al. 2000). Hot cores contain high abundances of fully hydrogenated molecules such as H₂O, NH₃, H₂S, as well as complex organics such as CH₃OH, CH₃CN, and CH₃OCH₃.

Because of the large extinction toward regions of massive star formation, most studies are done with millimeter or radio (hereafter simply radio) spectroscopy. Along with radio spectroscopy, midinfrared absorption spectroscopy is a powerful probe of physical conditions and chemical abundances in molecular clouds. In infrared absorption spectroscopy, the spatial resolution is set by the size of the background source, whereas, in radio spectroscopy, the spatial resolution is set by the size of the beam. In our study, the massive protostar provides a background source and we can study the material close to the star. Moreover, mid-infrared spectroscopy allows for the study of molecules without a dipole moment such as acetylene, C_2H_2 , and methane, CH_4 (Lacy et al. 1989b, Evans et al. 1991, Carr et al. 1995), which do not have rotational transitions. Previous mid-infrared studies have had low to moderate spectral resolution. For example,

the Short Wavelength Spectrometer (SWS) on board the Infrared Space Observatory (ISO) had resolving power, R, ~ 2000 and Irshell, a previous groundbased spectrograph (see Lacy et al. 1989a), had $R \sim 10^4$. Now, a new instrument, the Texas Echelon Cross Echelle Spectrograph (TEXES) (Lacy et al. 2002), is available with resolving power $R \approx 80000$, or $\delta v \sim 4 \text{ km s}^{-1}$ at $13\mu \text{m}$. TEXES allows for a new class of observations and addresses long-standing questions such as velocity structure.

NGC 7538 IRS 1, the brightest mid-infrared source (L = $1.3 \times 10^5 L_{\odot}$) in the NGC 7538 region, is a massive protostar with an ultra-compact HII region and possibly a hot core. Using *ISO-SWS*, Lahuis & van Dishoeck (2000) observed the Qbranches of HCN and C₂H₂ toward NGC 7538 IRS 1. The derived excitation temperatures are 500 K for C₂H₂ and 600 K for HCN. In this paper, we derive abundances for C₂H₂ and HCN and compare to chemical model predictions.

2. OBSERVATIONS

We have observed rovibrational lines for the following molecules toward NGC 7538 IRS 1: HCN, C_2H_2 , CH_4 , NH_3 , and CH_3 . Observations were made with TEXES (Lacy et al. 2002) at the NASA Infrared Telescope Facility in 2001 June, 2001 November, and 2002 September. The typical line width is $\sim 5 \text{ km s}^{-1}$ for both C_2H_2 and HCN lines. The paper with the complete data set is in preparation. Only the C_2H_2 and HCN results are presented here.

3. ABUNDANCES OF HCN AND C_2H_2

In order to determine the abundances of the various molecules, we first find the populations of the rotational level (N_J) from the equivalent widths, assuming optically thin lines. We can then solve for the temperature and column density. For HCN, we find that the data are best fitted by two temperature components, $T_{cool}=110$ K and $T_{hot}=685 \,\mathrm{K}$, with corresponding column densities, $N_{cool} = 10^{16} \text{cm}^{-2}$ and $N_{hot} = 10^{16} \text{cm}^{-2}$. For C_2H_2 , we also find two temperature components, $T_{cool}=110$ K and $T_{hot}=800$ K. The corresponding column densities are $N_{cool} = 4 \times 10^{15} \text{ cm}^{-2}$ and $N_{hot} = 6 \times 10^{15} \text{ cm}^{-2}$. In order to derive the abundance, we take the column density of H₂ from absorption measurements of ¹³CO from Mitchell et al. (1990), assuming ${}^{12}CO/{}^{13}CO=85$ (Wilson & Rood 1994) and 12 CO/H₂ = 2×10⁻⁴ (Lacy et al. 1994). Mitchell et al. also report two temperature components for 13 CO, T_{cold}=25 K and T_{cool}=176 K. (Mitchell et al. (1990) call the higher temperature T_{hot} but



Fig. 1. Predicted abundances from assuming NH_3 evaporating from grain mantles (model 1). The horizontal lines indicate the upper and lower limits from our observations for HCN (solid) and C_2H_2 (dotted). The vertical lines indicate the range of time in which the model fits the observations. For complete model results see Rodgers & Charnley (2001).

for comparison we will call it T_{cool}). We use the column densities of HCN, C_2H_2 , and CO associated with the cool temperature (T~100 K) as they most likely come from the same region. The abundances are $X(\text{HCN}_{cool}) = (1.7\pm0.4) \times 10^{-7}$ and $X((C_2H_2)_{cool}) = (6.7\pm0.8) \times 10^{-8}$. We do not derive abundances for the hot component because we do not have an estimate of the H₂ column density in that component.

4. CONSTRAINING CHEMICAL MODELS

With our derived abundances, we can help constrain the chemical models simulating the chemical evolution during star formation. Molecules, like HCN and C_2H_2 , are good probes for the chemical models since they can be produced by grain surface chemistry and by gas-phase interactions. We compare our results with the predicted abundances from low temperature models by Rodgers & Charnley (2001) (see figures 1 and 2). The models investigate the effects of NH₃ on CH₃OH chemistry. Ice evaporation from grain mantles is included in the models for the following molecules: CO, N_2, CH_4 , $H_2CO, C_2H_5OH, H_2S, C_2H_6, H_2O, and CH_3OH.$ Destruction of CH_4 produces C_2H_2 . In the two models presented here, one includes NH₃ ice evaporation while the other had no NH_3 (hereafter models 1 and 2, respectively). The core temperature is 100 K and the density is 10^7 cm^{-3} .



Fig. 2. Same as figure 1 but for model 2. For complete model results see Rodgers & Charnley (2001).

In figure 1, model 1 shows two different time intervals for HCN and one for C_2H_2 in which the predicted abundance is within the observed upper and lower limits of HCN (solid lines) and C₂H₂ (dashed lines) in NGC 7538 IRS 1. In addition, none of the time intervals overlap. In order for the model to fit our observations better, C₂H₂ should reach higher abundances at an earlier time in order for the time intervals for HCN and C₂H₂ to coincide. In figure 2, model 2 underpredicts the abundance of HCN we observe. This suggests that NH₃ ice did evaporate from grain mantles in NGC 7538 IRS 1. This model also shows two time intervals in which the predicted abundance of C_2H_2 is within our observed limits. Since the abundance of C_2H_2 depends on the initial abundance of CH_4 , varying the amount of CH_4 should change the C_2H_2 abundance. Boogert et al. (1998) report the CH₄ ice abundance in NGC 7538 IRS 9 (a neighboring source to IRS 1) to be 8.1×10^{-7} , which is about twice the assumed value of the models (3.8×10^{-7}) . Doubling the initial CH₄ abundance should increase the abundance of C₂H₂

but there may still be no overlap between HCN and C_2H_2 . Other possible ways to increase the abundance of C_2H_2 at earlier times are for C_2H_2 to form on grains and evaporate directly from icy mantles and for C_2H_2 to be a product of evaporation (not just CH₄ destruction). In order to constrain the chemical models further, observations of more molecules are needed. We will be able to constrain the abundance of gas-phase CH₄, CH₃ and NH₃ toward NGC 7538 IRS 1 with mid-infrared observations similar to the HCN and C_2H_2 observations.

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