ETHYNYL (C$_2$H) IN MASSIVE STAR FORMATION: TRACING THE INITIAL CONDITIONS?

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ABSTRACT

APEX single-dish observations at submillimeter wavelengths toward a sample of massive star-forming regions reveal that C$_2$H is almost omnipresent toward all covered evolutionary stages from infrared dark clouds via high-mass protostellar objects to ultracompact H ii regions. High-resolution data from the Submillimeter Array toward one hot-core-like high-mass protostellar object show a shell-like distribution of C$_2$H with a radius of $\sim$9000 AU around the central submillimeter continuum peak position. These observed features are well reproduced by a 1D cloud model with power-law density and temperature distributions and a gas-grain chemical network. The reactive C$_2$H radical (ethyny1) is abundant from the onset of massive star formation, but later it is rapidly transformed to other molecules in the core center. In the outer cloud regions the abundance of C$_2$H remains high due to constant replenishment of elemental carbon from CO being dissociated by the interstellar UV photons. We suggest that C$_2$H may be a molecule well suited to study the initial conditions of massive star formation.

1. INTRODUCTION

Spectral line surveys have revealed that high-mass star-forming regions are rich reservoirs of molecules from simple diatomic species to complex and larger molecules (e.g., Schilke et al. 1997; Hatchell et al. 1998; Comito et al. 2005; Bisschop et al. 2007). However, there have rarely been studies undertaken to investigate chemical evolution during massive star formation from the earliest evolutionary stages, i.e., from high-mass starless cores (HMSCs) and high-mass cores with embedded low- to intermediate-mass protostars destined to become massive stars, via high-mass protostellar objects (HMPOs), to the final stars that are able to produce ultracompact H ii regions (UCHii; see Beuther et al. 2007 for a recent description of the evolutionary sequence). The first two evolutionary stages are found within so-called infrared dark clouds (IRDCs). While for low-mass stars the chemical evolution from early molecular freezeout to more evolved protostellar cores is well studied (e.g., Bergin & Langer 1997; Dutrey et al. 1997; Pavlyuchenkov et al. 2006; Jørgensen et al. 2007), it is far from clear whether similar evolutionary patterns are present during massive star formation.

To better understand the chemical evolution of high-mass star-forming regions we initiated a program to investigate the chemical properties from IRDCs to UCHii from an observational and theoretical perspective. We start with single-dish line surveys toward a large sample obtaining their basic characteristics, and then perform detailed studies of selected sources using interferometers on smaller scales. These observations are accompanied by theoretical modeling of the chemical processes. Long-term goals are the chemical characterization of the evolutionary sequence in massive star formation, the development of chemical clocks, and the identification of molecules as astrophysical tools to study the physical processes during different evolutionary stages. Here we present an initial study of the reactive radical ethynyl (C$_2$H) combining single-dish and interferometer observations with chemical modeling. Although C$_2$H was previously observed in low-mass cores and photon-dominated regions (e.g., Millar & Freeman 1984; Jansen et al. 1995), so far it has not been systematically investigated in the framework of high-mass star formation.

2. OBSERVATIONS

The 21 massive star-forming regions were observed with the Atacama Pathfinder Experiment (APEX) in the 875 m window in fall 2006. We observed 1 GHz from 338 to 339 GHz and 1 GHz in the image sideband from 349 to 350 GHz. The spectral resolution was 0.1 km s$^{-1}$, but we smoothed the data to $\sim$0.9 km s$^{-1}$. The average system temperatures were around 200 K; each source had on-source integration times between 5 and 16 minutes. The data were converted to main-beam temperatures with forward and beam efficiencies of 0.97 and 0.73, respectively (Belloche et al. 2006). The average 1σ rms was 0.4 K. The main spectral features of interest are the C$_2$H lines around 349.4 GHz with upper level excitation energies $E_u/k$ of 42 K [line blends of C$_2$H(4_5,4–3_4,3) and C$_2$H(4_4,4–3_3,3) at 349.338 GHz, and C$_2$H(4_4,4–3_3,3) and C$_2$H(4_3,3–3_2,2) at 349.399 GHz]. The beam size was $\sim$18".

The original Submillimeter Array (SMA) C$_2$H data toward the HMPO 18089–1732 were first presented in Beuther et al. (2005a). There we reworked these data using only the compact and extended configurations resulting in good images for all spectral lines except for C$_2$H. For this project, we reworked these data using only the compact configuration. Because the C$_2$H emission is distributed on larger scales (see § 3), we were now able to derive a C$_2$H image. The integration range was from 32 to 35 km s$^{-1}$, and the achieved 1σ rms of the C$_2$H image was 450 mJy beam$^{-1}$. For more details on these observations see Beuther et al. (2005a).

3. RESULTS

The sources were selected to cover all evolutionary stages from IRDCs via HMPOs to UCHii. We derived our target list from the samples of Klein et al. (2005), Fontani et al. (2005), Hill et al. (2005), and Beltrán et al. (2006). Table 1 lists the observed sources, their coordinates, distances, and luminosities, and a first-order classification into the evolutionary subgroups IRDCs, HMPOs, and UCHii based on the previously available data. Although this classification is only based on a limited set of data, here we are just interested in general evolutionary trends. Hence, the division into the three main classes is sufficient.

Figure 1 presents sample spectra toward one source of each
evolutionary group. While we see several CH$_2$OH lines as well as SO$_2$ and H$_2$CS toward some of the HMPOs and UCHts but not toward the IRDCs, the surprising result of this comparison is the presence of the C$_2$H lines around 349.4 GHz toward all source types from young IRDCs via the HMPOs to evolved sources. Table 1 lists the peak brightness temperatures, the integrated intensities, and the FWHM line widths of the C$_2$H line blend at 349.338 GHz; for all other sources it is the C$_2$H line at 349.399 GHz.

### Table 1: Source Parameters

| Name              | Type      | R.A. (J2000.0) | Decl. (J2000.0) | $d$ (kpc) | $L$ (log$L_{\odot}$) | $T_{mb}$ (K) | $I_{mb}$ (K km s$^{-1}$) | $\Delta v(C_2H)$ (km s$^{-1}$) | Ref. |
|-------------------|-----------|----------------|----------------|----------|---------------------|-------------|-------------------------|-------------------------------|------|
| IRAS 07029 ...... | IRDC ...... | 07 05 11.1     | −12 19 02      | 1.0      | 0.21                | 0.52        | 2.4 ± 0.3               | 1                             |      |
| IRAS 08477 ...... | IRDC ...... | 08 49 32.9     | −44 40 17      | 1.8      | 0.23                | 0.76        | 3.1 ± 0.5               | 2, 3                          |      |
| IRAS 09014 ...... | IRDC ...... | 09 03 09.8     | −47 48 28      | 1.3      | ...                 | ...         | ...                    | 2, 3                          |      |
| IRAS 13039 ...... | IRDC ...... | 13 07 07.0     | −61 24 47      | 2.4      | ...                 | ...         | ...                    | 2, 3                          |      |
| IRAS 14000 ...... | IRDC ...... | 14 03 36.6     | −61 18 28      | 5.6      | 0.38                | 1.13        | 2.8 ± 0.5               | 2, 3                          |      |
| IRAS 08211 ...... | HMPO ...... | 08 22 52.3     | −42 07 57      | 1.7      | 3.5                  | 0.85        | 2.1 ± 0.2               | 2, 3                          |      |
| IRAS 08470 ...... | HMPO ...... | 08 48 47.9     | −42 54 22      | 2.2      | 4.2                  | 1.85        | 3.5 ± 0.4               | 3                             |      |
| IRAS 08563 ...... | HMPO ...... | 08 58 12.5     | −42 37 34      | 1.7      | 3.2                  | 1.08        | 2.9 ± 0.1               | 2, 3                          |      |
| IRAS 09131 ...... | HMPO ...... | 09 14 55.5     | −37 36 36      | 1.7      | 3.4                  | 0.23        | 2.1 ± 0.3               | 2, 3                          |      |
| IRAS 09209 ...... | HMPO ...... | 09 22 34.6     | −41 56 26      | 6.4      | 4.1                  | ...         | ...                    | 2, 3                          |      |
| IRAS 09578 ...... | HMPO ...... | 09 59 31.0     | −57 03 45      | 1.7      | 3.9                  | 0.21        | 2.8 ± 0.4               | 3                             |      |
| IRAS 10123 ...... | HMPO ...... | 10 14 08.8     | −57 42 12      | 0.93/0.40 | 3.4/4.4            | 0.17        | 2.5 ± 0.4               | 2, 3                          |      |
| IRAS 10184 ...... | HMPO ...... | 10 20 14.7     | −58 03 38      | 5.4      | 5.5                  | 0.41        | 3.9 ± 0.3               | 3                             |      |
| IRAS 10276 ...... | HMPO ...... | 10 29 30.1     | −57 26 40      | 5.9      | 4.9                  | 0.24        | 2.6 ± 0.5               | 3                             |      |
| IRAS 10295 ...... | HMPO ...... | 10 31 28.3     | −58 02 07      | 5.0      | 5.8                  | 0.69        | 4.3 ± 0.7               | 3                             |      |
| IRAS 10320 ...... | HMPO ...... | 10 33 56.4     | −59 43 53      | 9.1      | 5.4                  | 0.85        | 3.8 ± 0.6               | 3                             |      |
| G294.97 ......... | UCHt ...... | 11 39 09.0     | −63 28 38      | 1.35/0.8 | 3.95/3.0           | 0.31        | 2.3 ± 0.4               | 4                             |      |
| G305.20 ......... | UCHt ...... | 11 13 12.3     | −62 44 37      | 3.06/6.8  | 5.16/1.6           | 0.44        | 11.1 ± 0.5              | 4                             |      |
| G305.37 ......... | UCHt ...... | 13 12 36.3     | −62 33 39      | 3.06/6.8  | 4                  | 1.24        | 6.28 ± 0.2              | 4                             |      |
| G305.561 .......... | UCHt ...... | 13 14 25.8     | −62 44 32      | 4.0      | 5.1                  | 0.94        | 4.71 ± 0.6              | 4, 5                          |      |
| IRAS 14416 ...... | UCHt ...... | 14 45 22.0     | −59 49 39      | 2.8      | 5.1                  | 1.24        | 6.19 ± 0.6              | 4, 5                          |      |

**Note.**—Units of right ascension are hours, minutes, and seconds, and units of declination are degrees, arcminutes, and arcseconds.

a Since the IRDCs are by default not detected at short wavelengths, they are not IRAS sources and we cannot derive a luminosity.

b Near and far distances and corresponding luminosities.

c For these sources we list the parameters of the C$_2$H line blend at 349.338 GHz; for all other sources it is the C$_2$H line at 349.399 GHz.

d No IRAS counterpart, hence no luminosity estimate.

**References.**—(1) Klein et al. 2005; (2) Fontani et al. 2005; (3) Beltrán et al. 2006; (4) Hill et al. 2005; (5) Faúndez et al. 2004; (6) Vig et al. 2007.

To understand the observations, we conducted a simple chemical modeling of massive star-forming regions. A 1D cloud model with a mass of 1200 $M_\odot$, an outer radius of 0.36 pc, and a power-law density profile ($\rho \propto r^{-\beta}$ with $\beta = -1.5$) is the initially assumed configuration. Three cases are studied: a cold isothermal cloud with (1) $T = 10$ K and (2) $T = 50$ K, and (3) a warm model with a temperature profile $T \propto r^\beta$ with $\beta = -0.4$ and a temperature at the outer radius of 44 K. The cloud is illuminated by the interstellar UV radiation field (IRSF; Draine 1978) and by cosmic ray particles (CRPs). The ISRF attenuation by single-sized 0.1 $\mu$m silicate grains at a given radius is calculated in a plane-parallel geometry following van Dishoeck (1988). The CRP ionization rate is assumed to be $1.3 \times 10^{-17}$ s$^{-1}$ (Spitzer & Tomasko 1968). The gas-grain chemical model by Vasyunin et al. (2008) with the desorption energies and surface reactions from Garrod et al. (2007) is used. Gas-phase reaction rates are taken from RATE 06 (Woodall et al. 2007); initial abundances were adopted from the “low metal” set of Lee et al. (1998).
Figure 1.—Sample spectra obtained with APEX in a double-sideband mode. The spectra cover 1 GHz of data around 349.5 GHz and 1 GHz around 338.5 GHz. All spectral lines are labeled; lines in the lower sideband are marked with “(L)”. The top panel shows an IRDC example, the middle panel a typical HMPO/hot core, and the bottom panel a UCHii region. The C2H line widths are indicated in each panel.

Figure 2.—Gray scale shows the integrated emission (from 32 to 35 km s\(^{-1}\)) of the line blend of C2H(45,5–34,4) and C2H(45,4–34,3) around 349.338 GHz obtained with the Submillimeter Array using only the compact configuration data (Beuther et al. 2005a). The resulting synthesized beam is shown at the lower left corner (2.9" × 1.4"). The C2H emission is presented in gray scale with thin contours (dashed contours indicate negative features), and the 860 μm continuum peak is shown in thick contours. The C2H emission starts at the 2 \(j\) level and continues in 1 \(j\) steps with the 1 \(j\) level of 450 mJy beam\(^{-1}\). The 860 μm emission is contoured from 10% to 90% (steps of 10%) of the peak emission of 1.4 Jy beam\(^{-1}\).

Figure 3 presents the C2H abundances for the three models at two different time steps: (1) 100 yr, and (2) in a more evolved stage after 5 \(×\) 10\(^4\) yr. The C2H abundance is high toward the core center right from the beginning of the evolution, similar to previous models (e.g., Millar & Nejad 1985; Herbst & Leung 1986; Turner et al. 1999). During the evolution, the C2H abundance stays approximately constant at the outer core edges, whereas it decreases by more than 3 orders of magnitude in the center, except for the cold T = 10 K model. The C2H abundance profiles for all three models show similar behavior.

The chemical evolution of ethynyl is determined by relative removal rates of carbon and oxygen atoms or ions into molecules such as CO, OH, and H2O. Light ionized hydrocarbons CH\(^+_n\) (\(n = 2–5\)) are quickly formed by radiative association of C\(^+\) with H\(_2\) and hydrogen addition reactions: C\(^+\) → CH\(^+_2\) → CH\(^+_3\) → CH\(^+_4\) → CH\(^+_5\) → CH\(^+_n\). The protonated methane reacts with electrons, CO, C, OH, and more complex species at later stages and forms methane. The CH\(_n\) molecules undergo reactive collisions with C\(^+\), producing C\(^+\)H\(_n\) and C\(^+\)H\(_n\). An alternative way to produce C\(^+\)H\(_n\) is the dissociative recombination of CH\(^+_n\) into CH\(_3\) followed by reactions with C\(^+\). Finally, CH\(_3\)H\(_3\) and CH\(_3\)H\(_3\) dissociatively recombine into CH, C2H, and C3H\(_2\). The major removal for C2H is either the direct neutral-neutral reaction with O that forms CO, or the same reaction but with heavier carbon chain ions that are formed from C2H by subsequent insertion of carbon. At later times, depletion and gas-phase reactions with more complex species may enter into this cycle. At the cloud edge the interstellar UV radiation instantaneously dissociates CO despite its self-shielding, reenriching the gas with elemental carbon.

The transformation of C2H into CO and other species proceeds efficiently in dense regions, in particular in the "warm" model where endothermic reactions result in rich molecular complexity of the gas (see Fig. 3). In contrast, in the "cold" 10 K model gas-grain interactions and surface reactions become important. As a result, a large fraction of oxygen is locked in water ice that is hard to desorb (\(E_{\text{des}} \sim 5500\) K), while half of the elemental carbon goes to volatile methane ice (\(E_{\text{des}} \sim 1300\) K). Upon CRP heating of dust grains, this leads to a much higher gas-phase abundance of C2H in the cloud core for the cold model compared to the warm model. The effect is not that strong for less dense regions at larger radii from the center. Since the C2H emission is anticorrelated with the dust continuum emission in the case of IRAS 18089–1732 (Fig. 2), we do not have the H\(_2\) column densities to quantitatively compare the abundance profiles of IRAS 18089–1732 with our model. However, data and model allow a qualitative comparison of the spatial structures. Estimating an exact evolutionary
time for IRAS 18089—1732 is hardly possible, but based on the strong molecular line emission, its high central gas temperatures, and the observed outflow-disk system (Beuther et al. 2004a, 2004b, 2005a), an approximate age of $5 \times 10^4$ yr appears reasonable. Although dynamical and chemical times are not necessarily exactly the same, in high-mass star formation they should not differ too much: following the models by McKee & Tan (2003) or Krumholz et al. (2007) the luminosity rises strongly right from the onset of collapse, which can be considered as a starting point for the chemical evolution. At the same time disks and outflows evolve, which should hence have similar timescales. The diameter of the shell-like C$_2$H structure in IRAS 18089—1732 is $\sim 5''$ (Fig. 2), or $\sim 9000$ AU in radius at the given distance of 3.6 kpc. This value is well matched by the modeled region with decreased C$_2$H abundance (Fig. 3). Although in principle optical depths and/or excitation effects could mimic the C$_2$H morphology, we consider this as unlikely because the other observed molecules with many different transitions all peak toward the central submillimeter continuum emission in IRAS 18089—1732 (Beuther et al. 2005a). Since C$_2$H is the only exception in that rich data set, chemical effects appear the more plausible explanation.

The fact that we see C$_2$H at the earliest and the later evolutionary stages can be explained by the reactive nature of C$_2$H: it is produced quickly early on and gets replenished at the core edges by the UV photodissociation of CO. The inner “chemical” hole observed toward IRAS 18089—1732 can be explained by C$_2$H being consumed in the chemical network, forming CO and more complex molecules such as larger carbon-hydrogen complexes, and/or depletion.

The data show that C$_2$H is not suited to investigate the central gas cores in more evolved sources; however, our analysis indicates that C$_2$H may be a suitable tracer of the earliest stages of (massive) star formation, like N$_2$H$^+$ or NH$_3$ (e.g., Bergin et al. 2002; Tafalla et al. 2004; Beuther et al. 2005b; Pillai et al. 2006). While a spatial analysis of the line emission will give insights into the kinematics of the gas and also the evolutionary stage from chemical models, multiple C$_2$H lines will even allow a temperature characterization. With its lowest transition at 87 GHz, C$_2$H has easily accessible spectral lines in several bands between 3 mm and 850 $\mu$m. Furthermore, even the 349 GHz lines presented here still have relatively low upper level excitation energies ($E_J/k \sim 42$ K), hence allowing the study of cold cores even at submillimeter wavelengths. This prediction can further be proved via high spectral and spatial resolution observations of different C$_2$H lines toward young IRDCs.

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