Spatial distribution of small hydrocarbons in the neighborhood of the ultra compact HII region Monoceros R2^{★,★★,★★★}

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ABSTRACT

Context. We study the chemistry of small hydrocarbons in the photon-dominated regions (PDRs) associated with the ultra-compact H II region (UCH II) Mon R2.

Aims. Our goal is to determine the variations in the abundance of small hydrocarbons in a high-UV irradiated PDR and investigate the chemistry of these species.

Methods. We present an observational study of the small hydrocarbons CH, CCH, and c-C₃H₂ in Mon R2 that combines spectral mapping data obtained with the IRAM-30 m telescope and the *Herschel* space observatory. We determine the column densities of these species, and compare their spatial distributions with that of polycyclic aromatic hydrocarbon (PAH), which trace the PDR. We compare the observational results with different chemical models to explore the relative importance of gas-phase, grain-surface, and time-dependent chemistry in these environments.

Results. The emission of the small hydrocarbons show different spatial patterns. The CCH emission is extended, while CH and c-C₃H₂ are concentrated towards the more illuminated layers of the PDR. The ratio of the column densities of c-C₃H₂ and CCH shows spatial variations up to a factor of a few, increasing from $N(\text{c-C}_3\text{H}_2)/N(\text{CCH}) \approx 0.004$ in the envelope to a maximum of $\approx 0.015\text{--}0.029$ towards the 8 μm emission peak. Comparing these results with other galactic PDRs, we find that the abundance of CCH is quite constant over a wide range of G_0 , whereas the abundance of c-C₃H₂ is higher in low-UV PDRs, with the $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio ranging $\approx 0.008\text{--}0.08$ from high to low UV PDRs. In Mon R2, the gas-phase steady-state chemistry can account relatively well for the abundances of CH and CCH in the most exposed layers of the PDR, but falls short by a factor of 10 of reproducing c-C₃H₂. In the low-density molecular envelope, time-dependent effects and grain surface chemistry play dominant roles in determining the hydrocarbon abundances.

Conclusions. Our study shows that the small hydrocarbons CCH and c-C₃H₂ present a complex chemistry in which UV photons, grain-surface chemistry, and time dependent effects contribute to determining their abundances. Each of these effects may be dominant depending on the local physical conditions, and the superposition of different regions along the line of sight leads to the variety of measured abundances.

Key words. ISM: abundances – ISM: individual objects: Monoceros R2 – photon-dominated region (PDR) – ISM: molecules – radio lines: ISM

1. Introduction

Ultracompact H II regions (UCH II) represent one of the earliest phases in the formation of a massive star. In these environments, the chemistry is strongly driven by the mutual interaction among the gas, the dust, and the UV photons from nearby stars. The H-ionizing photons are absorbed in a thin layer around the star, forming the H II region, while the UV radiation carrying energies below 13.6 eV penetrates the deeper layers of the molecular cloud and produces the so-called photon-dominated region

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*** Appendix B is available in electronic form at

<http://www.aanda.org>

(PDR). In these environments, the thermal balance, the chemistry, and ionization balance are driven by UV photons. PDRs associated with UCH II are characterized by extreme UV field intensities (expressed in units of the Habing field G_0 , see [Habing 1968](#)) and small physical scales ($\lesssim 0.1$ pc). These environments are therefore ideal for studying the effect of a strong UV field on the chemistry of gas-phase species.

The chemistry of small hydrocarbons in PDRs is still poorly constrained. The comparison of observations and gas-phase chemical models has shown that this type of chemistry alone cannot account for the abundance of small hydrocarbons, especially for those species containing more than two C atoms: in NGC 7023, the Orion Bar ([Fuente et al. 2003](#)), and the Horsehead nebula ([Teyssier et al. 2004](#)), the abundances of $c\text{-C}_3\text{H}_2$ and C_4H derived from the observations are at least an order of magnitude larger compared to model predictions. This discrepancy was confirmed by high spatial resolution observations and detailed modeling of the Horsehead nebula ([Pety 2005](#)), in which the emission of small hydrocarbons was compared to other PDR tracers, such as the mid-IR emission in the aromatic infrared bands (AIBs) due to polycyclic aromatic hydrocarbons (PAHs). The authors suggest that small hydrocarbons may form through non gas-phase processes, such as the photodestruction of the AIB carriers. In the Horsehead ([Pety 2005](#)) and in NGC 7023 ([Pilleri et al., in prep.](#)), the spatial distributions of CCH and $c\text{-C}_3\text{H}_2$ are strikingly similar. Similarly, a tight correlation between these two hydrocarbons has been observed by [Lucas & Liszt \(2000\)](#) and [Gerin et al. \(2011\)](#) on several lines of sight in the diffuse medium. The small radical CH also has a relatively constant abundance in these environments ([Sheffer et al. 2008](#)). In low- to mild-UV irradiated PDRs ($G_0 \sim 100$ for the Horsehead and ~ 2600 for NGC 7023), the tight correlation between CCH and $c\text{-C}_3\text{H}_2$ suggests a common origin of these two small hydrocarbons. However, this spatial correlation has not been explored yet in highly UV-illuminated PDRs ($G_0 \gtrsim 1 \times 10^4$).

In this paper, we present new observations of several lines of CH, CCH, and $c\text{-C}_3\text{H}_2$ in the PDRs associated with the UCH II region Mon R2 and investigate the relative variations of these species. In Sect. 2 we present the source and the observations, and the results are reported in Sect. 3. In Sect. 4 we calculate column densities and abundances, while in Sect. 5 we compare the spatial distributions to that of other PDR tracers and discuss the quantitative consistence with different chemical models. Finally, Sect. 6 presents the conclusions and perspectives.

2. Observations

2.1. Mon R2

Mon R2 is a close-by ultracompact H II region ($d = 830$ pc), which comprises several PDRs that can be spatially resolved in both the mm and IR domains. Thanks to its brightness and proximity, this source can be used as a reference for other PDRs illuminated by a strong UV field. The most intense UV source is called IRS1, and it is located at the center of the UCH II (see Fig. 1). A low-density molecular cloud surrounds this innermost region and extends for several arcminutes. The brightest PDR of Mon R2, which surrounds the UCH II and peaks at about $20''$ to the NW of IRS1, shows both very intense AIB emission and H_2 rotational lines ([Berné et al. 2009](#)) and is due to the illumination of the internal walls of the molecular cloud by IRS1. This PDR is very compact ($d \sim 5''$) and illuminated by a very strong

Fig. 1. Overview of the region. The color image displays the IRAC $8\,\mu\text{m}$ emission ([Ginard et al. 2012](#)), in which both the bright circular PDR and the extended northern PDR can be distinguished beneath the peaks due to the young stellar objects. The white contours represent the integrated intensity of the C^{18}O ($2\rightarrow 1$) line between 5 and $15\,\text{km s}^{-1}$ observed at the IRAM 30 m telescope ([Pilleri et al. 2012a](#)), with contour levels from 16 to $24\,\text{K km s}^{-1}$ in linear steps of $2\,\text{K km s}^{-1}$. The black squares represent the positions of the ionization front (IF) and the molecular peak (MP2), whereas the triangles and the white line indicate the positions observed with HIFI. The black stars indicate the position of the most intense infrared sources following the nomenclature of [Henning et al. \(1992\)](#). The yellow arrow indicates the direction of the NW molecular outflow ([Tafalla et al. 1994](#)).

radiation field ($G_0 \sim 5 \times 10^5$). A secondary PDR, detected north of the UCH II at a distance of about $1'$ from IRS1, is much fainter and more extended. The northern molecular peak position at $[0''; 40'']$ (hereafter MP2 following the nomenclature of [Ginard et al. 2012](#)) is clearly detected in the AIB emission at $8\,\mu\text{m}$, and its chemical properties seem to be similar to those of low- to mild-UV irradiated PDRs ([Ginard et al. 2012](#)). The origin of this PDR could be the outer envelope of the molecular cloud illuminated by an external UV field, or it could be due to UV photons that are escaping from IRS1 through a hole, illuminating its walls.

Although there are some asymmetries in the general shape of the cloud, such as the molecular hole to the NW, we can assume as a zero-order approximation that the dense core around the UCH II region is spherical and composed of concentric shells centered on IRS1, a simplified model that is close to reality in most outwards directions. Each of the shells has its own physical conditions (kinetic temperature, gas density, G_0), which vary with radius. In the following, we assume the physical parameters presented in [Pilleri et al. \(2012a\)](#) and schematized in Fig. 2: the region immediately surrounding the star is an H II region, which is expanding at a velocity of $\sim 10\,\text{km s}^{-1}$ ([Choi et al. 2000](#)) and which is free of any molecular gas. The diameter of the region is $\sim 40''$, corresponding to ~ 0.08 pc. This is followed by a thin (1 mag), high UV-irradiated PDR, which has a density of $n_{\text{H}_2} \sim 2 \times 10^5\,\text{cm}^{-3}$ and a gas kinetic temperature of ~ 100 K ([Berné et al. 2009](#)). Going farther from IRS1, there is a thicker (~ 8 mag), warm ($T_{\text{kin}} \sim 70$ K), and high density ($n_{\text{H}_2} \sim 3 \times 10^6\,\text{cm}^{-3}$, [Rizzo et al. 2003](#)) PDR, which is expanding at a velocity of $\lesssim 1\,\text{km s}^{-1}$ ([Fuente et al. 2010](#); [Pilleri et al. 2012a](#)). This high-density layer is surrounded by the parent molecular cloud, which is about 40 mag thick, has a relatively low density ($n_{\text{H}_2} \sim 5 \times 10^4\,\text{cm}^{-3}$) and temperature ($T_{\text{kin}} \sim 35$ K),

Fig. 2. 1D schematic of the geometry of MonR2 as a function of the radial distance to IRS1.

and is rather quiescent (Fuente et al. 2010; Pilleri et al. 2012a). The cloud is also illuminated from the outside with a UV field of $G_0 \sim 100$.

The presence of these different phases and its proximity make Mon R2 the best source to investigate the chemistry and physics of these extreme PDRs and their parent molecular clouds.

2.2. IRAM and Herschel observations

We observed several low-lying rotational transitions of CCH and c-C₃H₂ at mm wavelengths using the IRAM-30 m telescope. We completed this dataset with *Herschel* (Pilbratt et al. 2010) observations of a higher excitation line of CCH and two lines of CH. A summary of the spectroscopic parameters for all the observed lines are given in Table B.1. Throughout the paper, we use main beam temperature as intensity scale. Offset positions are given relative to the ionization front (IF: $\alpha_{J2000} = 06^{\text{h}}07^{\text{m}}46.2^{\text{s}}$, $\delta_{J2000} = -06^{\circ}23'08.3''$). For all the observations, the OFF position was chosen to be free of molecular emission ($[+10', 0']$ for *Herschel*; $[+400'', -400'']$ for IRAM). A summary of the observations is shown in Table 1.

The 3 mm and 2 mm observations were performed in July 2012 at the IRAM-30 m telescope in Pico Veleta (Spain). We observed the CCH multiplet at 87 GHz and the c-C₃H₂ line at 85 GHz using the EMIR receivers with the VESPA correlators, covering a $180'' \times 180''$ region centered toward the IF. The 1 mm observations were performed in two different sessions using the HERA 3 $\times$ 3 dual-polarization receiver and in a successive run with the EMIR receivers. During the first run (HERA) we obtained a $150'' \times 150''$ map of the CCH multiplet at 262 GHz and the c-C₃H₂ line at 217 GHz. The second observing run (January 2012) was part of a 2D spectral survey at 1 mm (Treviño-Morales et al., in prep.). The resulting c-C₃H₂ maps have a lower signal-to-noise ratio (S/N), and the field of view covered in this second run was smaller, $2' \times 2'$.

The *Herschel* observations were obtained with the Heterodyne Instrument for the Far Infrared (HIFI, de Graauw et al. 2010) in the context of the WADI guaranteed-time key program (Ossenkopf et al. 2011). The CH lines were observed with both the Wide Band Spectrometer (WBS) and the High-Resolution Spectrometer (HRS). They provide spectral resolutions (at 500 GHz) of $\Delta v = 1.2 \text{ km s}^{-1}$ and 0.3 km s^{-1} , respectively, allowing to resolve the line profiles. Cross-calibration between the two backends and between the two polarizations indicates an uncertainty of $\sim 20\%$. The CH ($J = 3/2-1/2$) and CCH ($N = 6-5$) observations were performed in on-the-fly (OTF) observing mode along the strip

indicated in Fig. 1, while the excited ($J = 5/2-3/2$) line of CH was observed in single-pointing observing mode towards the IF, with a double beam-switching pattern. In this paper we also compare the new observations with the [C II] strip already presented by Pilleri et al. (2012a).

2.3. Data reduction

The basic data reduction of *Herschel* observations was performed using the standard pipeline provided with the version 7.0 of HIPE¹ (Ott 2010), and Level 2 data were exported to the FITS format. The *Herschel* and IRAM-30 m data were then processed using the GILDAS/CLASS software² suite (Pety 2005). The spectra were first calibrated to the T_{A}^* scale using the chopper wheel method (Penzias & Burrus 1973), and finally converted to the main beam temperatures (T_{mb}) using the nominal forward (F_{eff}) and main beam (B_{eff}) efficiencies. Table 1 shows the value $\eta_l = B_{\text{eff}}/F_{\text{eff}}$. The HIFI efficiencies have been recently calculated by Roelfsema et al. (2012). The resulting amplitude accuracy is $\sim 10\%$ for both HIFI and IRAM observations.

Visual inspection of the IRAM data revealed for all the observed lines 1) more or less pronounced spikes at one quarter and three quarter of the correlator window; 2) platforming in the middle of the correlator window; 3) but otherwise clean baselines. Windows around the well-defined frequencies displaying spikes were set before baselining. The line windows were defined on the spectra averaged over the map, from $[-1, 24.5 \text{ km s}^{-1}]$ for the brightest lines to $[6, 16 \text{ km s}^{-1}]$ for the faintest ones. To correct for the platforming, a zero-order baseline was subtracted from each correlator sub-bands of each spectrum. A first-order baseline was needed for c-C₃H₂. The bad channels, which occurred in a line-free section of the HERA spectra, were replaced by Gaussian noise of the same rms. The resulting spectra were resampled and convolved with a Gaussian to a higher map resolution than the HPBW of the telescope. The map resolution is reported in Table 1. The spectral cubes were finally blanked where the spectra weights (resulting from the gridding) were too low, giving the fringed aspect of the map edges.

3. Results

In this section, we describe the spectral and spatial variations of the various molecular tracers. First, we present all the observations obtained towards the IF, which is one of the best-known positions (see, for instance, Fuente et al. 2010; Ginard et al. 2012; Pilleri et al. 2012a). We then describe the spatial/spectral variations along the *Herschel* strip (see Fig. 1), and finally, we present the full maps.

3.1. The ionization front

In Fig. 3 we show the spectra of several CH, CCH, and c-C₃H₂ transitions observed towards the IF with the IRAM-30 m and *Herschel*. The lower-lying transitions show a self-absorption feature at the ambient velocity of the cloud ($\sim 11 \text{ km s}^{-1}$). It is clearly detected in the main hyperfine components of CH, CCH, and c-C₃H₂ and coincides with the self-absorption detected in the [C II] strip observed with *Herschel* (Pilleri et al. 2012a). The

¹ HIPE is a joint development by the *Herschel* Science Ground Segment Consortium, consisting of ESA, the NASA *Herschel* Science Center, and the HIFI, PACS, and SPIRE consortia

² See <http://www.iram.fr/IRAMFR/GILDAS> for more information about the GILDAS softwares.

Table 1. Summary of the observations.

Line(s)	Frequency [GHz]	Instrument	<i>FWHM</i> [$''$]	η_l^a	Position	OM ^b	T_{rms}^c [K]
C ¹⁸ O $J = 2-1$	219.560	IRAM-HERA	10.0	0.67	Map	OTF	0.025
C ¹⁸ O $J = 5-4$	548.830	<i>Herschel</i> -HIFI	38.6	0.79	Strip	OTF	0.008
CH $J = 3/2-1/2$	536.761*	<i>Herschel</i> -HIFI	38	0.77	Strip	OTF	0.041
CH $J = 5/2-3/2$	1656.961*	<i>Herschel</i> -HIFI	12.8	0.74	IF	SP	0.284
CCH $N = 1-0$	87.317*	IRAM	29	0.85	Map	OTF	0.070
CCH $N = 3-2$	262.004*	IRAM-HERA	9	0.6	Map	OTF	0.380
CCH $N = 6-5$	523.972*	<i>Herschel</i> -HIFI	40.5	0.78	Strip	OTF	0.057
c-C ₃ H ₂ $J_{K_A,K_C} = 2_{1,2}-1_{0,1}$	85.33889	IRAM	29	0.85	Map	OTF	0.070
c-C ₃ H ₂ $J_{K_A,K_C} = 4_{0,4}-3_{1,3}$	150.82067	IRAM	16	0.64	Map	OTF	0.054
c-C ₃ H ₂ $J_{K_A,K_C} = 4_{1,4}-3_{0,3}$	150.85191	IRAM	16	0.64	Map	OTF	0.054
c-C ₃ H ₂ $J_{K_A,K_C} = 6_{1,6}-5_{0,5}$	217.82215*	IRAM-HERA	11	0.61	Map	OTF	0.016
c-C ₃ H ₂ $J_{K_A,K_C} = 5_{1,4}-4_{2,3}$	217.94005	IRAM	11	0.61	Map	OTF	0.150
c-C ₃ H ₂ $J_{K_A,K_C} = 4_{3,2}-4_{2,1}$	227.16913	IRAM	10	0.59	Map	OTF	0.150
c-C ₃ H ₂ $J_{K_A,K_C} = 7_{0,7}-6_{1,6}$	251.31434*	IRAM	9	0.55	Map	OTF	0.115
c-C ₃ H ₂ $J_{K_A,K_C} = 6_{2,5}-5_{1,6}$	251.52730	IRAM	9	0.55	Map	OTF	0.115

Notes. ^(a) $\eta_l = B_{\text{eff}}/F_{\text{eff}}$. ^(b) Observing modes: on the fly (OTF), single pointing (SP). ^(c) Calculated on a T_{mb} scale with $\Delta v = 0.5 \text{ km s}^{-1}$. ^(*) Frequency of the most intense transition of the hyperfine structure.

self-absorption is barely visible in the faintest hyperfine components of the CCH 1–0 line and is not detected in any of the higher energy transitions. The structure of the CCH 3–2 line is due to the superposition of two hyperfine transitions with very similar frequencies that are not self-absorbed³. The lower-lying transitions show some emission in the red and blue wings, which may trace either an expanding PDR (Pilleri et al. 2012a) or the molecular outflow (Tafalla et al. 1997).

3.2. The NE-SW strip

Both CH and C¹⁸O (5–4) have been observed only towards the NE-SW strip shown in Fig. 1. This strip, already studied in Pilleri et al. (2012a), passes through the IF and extend up to 1.5' in each direction, crossing the main PDRs of the region and extending to offsets where the emission is dominated by the molecular envelope. However, the large beam of *Herschel* at this frequency ($\sim 40''$) results in even the positions $[\pm 40'', \pm 40'']$ picking up some emission from the innermost PDR.

In Fig. 4 we show the position–velocity (PV) diagrams along the cut observed with *Herschel*, i.e. in the direction perpendicular to the molecular outflow (Tafalla et al. 1994, 1997), which extends in the NW-SE direction from the IF. For a comparison, we also display the PV diagram of the [C II] line along the same cut (Pilleri et al. 2012a). For each transition, we show the diagram of the component with the highest S/N. Although the data have very different angular resolutions, the spatial variation of CH is in some way similar to that of [C II]: for instance, in both tracers the emission is extended up to 60'' from the IF and the main component shows self-absorption through the whole cut. Both lines present a secondary peak at a distance of $\sim 10''$ at about 8 km s^{-1} . The line widths are also similar, indicating that the CH emission, like [C II], originates in the innermost layers of the expanding central PDR.

The PV diagram of CCH 1–0 is very similar to the C¹⁸O 2–1 line in terms of the spatial extension and line width.

³ This is suggested by the excellent quality of the fit of the observed lines using a Gaussian function for each of the hyperfine component, and assuming a standard intensity ratio and frequency shift, see Table B.1.

They are both detected along the entire strip, and their typical line width is about 2.5 km s^{-1} . However, the CCH line toward the IF displays self-absorption at central velocities and emission in the red wing. Similarly to the CCH 1–0 line, the c-C₃H₂ 2_{1,2}–1_{0,1} transition shows self-absorption at 11 km s^{-1} and emission in the red wing toward the IF. However, it is less spatially extended and therefore likely associated with the innermost layers of the PDR. The higher energy transitions of all species are less spatially extended compared to [C II] and CH and do not show self-absorption. Finally, there is a systematic shift of the peak velocity of about 2 km s^{-1} going from the SW towards the NE of the IF, which has been attributed to either an asymmetry in the expansion pattern or to a large-scale slow rotation of the entire cloud (Loren 1977; Pilleri et al. 2012a).

3.3. Maps

The maps carried out with the 30 m telescope allow us to investigate the spatial distribution of CCH and c-C₃H₂. Figure 5 shows the spatial distribution of the integrated line intensity of the CCH 3–2 and c-C₃H₂ 6–5 lines between 5 and 15 km s^{-1} observed with HERA⁴ at the spatial resolution of $10''$. The spatial pattern of CCH is very similar to that of C¹⁸O 2–1 (Fig. 1): the emission to the NE and SW extends up to 1' from the IF and peaks at a distance of $\sim 30''$. The emission is opened to the north and the NW, following the cometary shape of the molecular bar. The c-C₃H₂ emission is more compact, with the center at an offset $[-10'', +10'']$ relative to the IF. The emission extends less than $40''$ from the center and peaks at a distance of about $10''$ south of the IF. The line intensity also displays a peak toward the MP2 position, which does not have a correspondence in the CCH map. The emission to the north is more extended compared to CCH, following the IRAC $8 \mu\text{m}$ emission (Ginard et al. 2012).

4. Column densities and abundances

In this section, we derive the column densities and abundances of CH, CCH, and c-C₃H₂. First, we concentrate on the SW-NE

⁴ The EMIR maps of all the observed lines are shown in Fig. B.1.

Fig. 3. *Herschel* and IRAM observations of CCH and c-C₃H₂ towards the IF. 1 mm observations have been convolved to the spatial resolution of 39". Solid blue lines show the single-component Gaussian fits. The velocity scale in each panel is relative to the most intense line in the hyperfine groups (see also Tables 1 and B.1).

strip, where we use the *Herschel* observations to study CH and the excitation of C¹⁸O. We study in more detail the excitation of CCH using a two-phase LVG model towards the IF and study the emission in the line wings. Finally, we extrapolate these results to the analysis of the full maps to obtain more information on the spatial distribution of these tracers. The self-absorption features are discussed in Appendix A.

4.1. The SW-NE strip

C¹⁸O

To obtain an estimate of the excitation temperature and column density of C¹⁸O along the *Herschel* strip, we have combined our $J = 2-1$ observation with the $J = 5-4$ observations published in Pilleri et al. (2012a) and with the $J = 1-0$ observations of Ginard et al. (2012). We convolved the data to the lowest spatial

resolution (40" for the $J = 5-4$) and built rotational diagrams for the five positions along the strip. The $J = 1-0$ data cannot be convolved, since they were single-pointing observations, but the spatial resolutions are not very different (29" vs. 40"), and the C¹⁸O emission is very extended, so that the emission fills the beam at both spatial resolutions. The corresponding rotational diagrams are shown in Fig. B.2. The results are consistent with those of Ginard et al. (2012): the rotation temperature slightly decreases from ~ 37 K toward the IF to ~ 31 K at a distance of 50". We obtain a column density of $8.3 \times 10^{15} \text{ cm}^{-2}$ toward the IF, and slightly (20%) higher values at larger offsets. These values are consistent within a factor of 2 with the geometrical model presented by Pilleri et al. (2012a) to fit the high- J lines of CO, ¹³CO, and C¹⁸O. This model consists of a spherical cloud with an $A_V = 8$ PDR and an $A_V = 40$ low-density envelope. This geometrical model yields a factor of 2 higher column densities compared to the C¹⁸O values, assuming

Fig. 4. PV diagrams of the *Herschel* and IRAM observations along the SW-NE strip. The C II diagrams comes from Pilleri et al. (2012a). The double-peaked structure of the CCH lines is due to two hyperfine components of the same line, while the strong dip in both CH and [C II] are partially due to self-absorption. The white line in the top-right corner of each diagram represents the HPBW of the observation. The black dotted line indicates $v_{\text{LSR}} = 11.5 \text{ km s}^{-1}$.

an isotopic ratio $^{16}\text{O}/^{18}\text{O} = 500$ and a standard abundance of CO relative to H_2 of 1×10^{-4} . In the following, we assume therefore an uncertainty of a factor of 2 in the column density of H_2 and in the abundances of the hydrocarbons. However, the absolute value of the column densities, and consequently the relative abundances, are not affected by this uncertainty.

CH

As shown in Fig. 3, the main component of CH is self-absorbed at the ambient cloud velocity and the line wings of the different

components overlap. To obtain the integrated intensity of the CH line, we used the $P = 1^- - 0^+$ and the $P = 2^- - 1^+$ transitions for the velocity intervals $[5-12] \text{ km s}^{-1}$ and $[12-15] \text{ km s}^{-1}$, respectively. Using the first satellite to obtain the area in the blue interval we avoid the self-absorption that affects the main component. On the other hand, the red part of the $P = 1^- - 0^+$ line is contaminated by the overlap with the second satellite, so that we have to rely on the main component for this interval. The integrated areas for each interval are shown in Table 2.

Fig. 5. Maps of integrated intensity (in the range 5–15 km s⁻¹) for CCH (262.004 GHz) and c-C₃H₂ (217.822 GHz) obtained with the EMIR receivers. Black contours are the C¹⁸O line shown in Fig. 1. White triangles and squares represent the single positions studied in this paper. White contours in the left panel represent the c-C₃H₂ line integrated intensities (in the range 5–15 km s⁻¹) starting from 0.6 km s⁻¹ and in linear steps of 0.2 km s⁻¹.

Table 2. Integrated intensity (using T_{mb} scale) between 5 and 15 km s⁻¹, after smoothing the data to the larger HPBW (40'' for CCH and C¹⁸O, 28'' for c-C₃H₂).

	IF [0''; 0'']	[20''; 20'']	[40''; 40'']	[-20''; -20'']	[-40''; -40'']	MP2 [0''; 40'']
Transition	Area [K km s ⁻¹]	Area [K km s ⁻¹]	Area [K km s ⁻¹]	Area [K km s ⁻¹]	Area [K km s ⁻¹]	Area [K km s ⁻¹]
C ¹⁸ O 2–1	14.56	15.55	15.71	15.68	13.12	13.90
C ¹⁸ O 5–4	13.04	13.38	13.26	12.12	11.03	–
CH _{J=3/2-1/2, P=1-0⁺} [5–12] ^(a)	1.81	1.43	0.62	1.03	0.22	–
CH _{J=3/2-1/2, P=2-1⁺} [12–15] ^(a)	1.19	0.74	0.36	0.95	0.22	–
CH _{J=5/2-3/2}	≤0.84	–	–	–	–	–
CCH _{N=1-0, F=0-1}	0.98	1.35	1.39	1.61	1.87	1.29
CCH _{N=3-2, J_K=5/2, F=4-3 and F=3-2}	13.75	13.85	11.70	15.63	11.99	12.19
CCH _{N=6-5, J_K=13/2, F=7-6 and F=6-5}	4.97	4.97	4.05	5.02	3.73	–
c-C ₃ H ₂₂₁₂	0.73	1.55	1.71	1.73	1.32	1.71
c-C ₃ H ₂₄₀₄	0.45	0.44	0.44	0.45	0.19	0.67
c-C ₃ H ₂₄₁₄	1.42	1.71	1.34	1.52	0.80	2.0
c-C ₃ H ₂₄₃₂	0.63	0.46	0.37	0.49	0.32	0.53
c-C ₃ H ₂₅₁₄	0.76	0.56	0.33	0.46	0.20	0.87
c-C ₃ H _{2616 and 606}	0.99	1.00	0.52	0.85	0.42	1.01
c-C ₃ H ₂₆₂₅	0.57	<0.3	<0.3	<0.3	<0.3	0.41
c-C ₃ H _{2707 and 717}	0.69	0.61	<0.4	0.58	<0.3	0.78

Notes. Nondetections are given at a 3σ level assuming a line width of 1 km s⁻¹. See Table B.1 for the spectroscopic parameters. ^(a) The numbers in brackets indicate the velocity range over which the line has been integrated to avoid self-absorption or contamination from a satellite line.

When computing the CH column density, we faced the difficulty that there are no collisional rates available for CH, so that one can only assume a given rotational temperature T_{rot} per velocity interval. The nondetection of the CH triplet at 1656 GHz provides an upper limit to T_{rot} if we assume LTE conditions, so that both transitions share the same rotation temperature. This gives upper limits for T_{rot} of 25 K (blue) and 30 K (red) towards the IF. Considering the high dipole moment of CH and the physical conditions in Mon R2, we can estimate a lower limit to the rotational temperature to be about 7 K. Assuming that the emission

is optically thin and that it fills the beam, we derive a column density of $1.2^{+1.9}_{-0.6} \times 10^{14}$ cm⁻² towards the IF for $T_{\text{rot}} = 10$ K, with the uncertainties driven by upper and lower limits in T_{rot} . At the [-40''; -40''] position, the CH column density is a factor of 10 lower, $1.7^{+3.1}_{-1.1} \times 10^{13}$ cm⁻², assuming $T_{\text{rot}} = 10$ K. At this position, T_{rot} is likely lower compared to the IF, due to a decrease in kinetic temperature and local density, which yields an overestimate of the column density by a factor of 2 for $T_{\text{rot}} = 7$ K. At offsets greater than 60'', the ground state transition of CH is not detected, implying that the column density is even lower. Thus,

we consider the column density at $[-40'', -40'']$ as an upper limit of the CH abundance in the envelope.

Using the H column density derived through $C^{18}O$ ($N(H) = 9 \times 10^{22} \text{ cm}^{-2}$), we estimate a CH abundance relative to H nuclei of $\sim 1.5 \times 10^{-9}$ toward the IF decreasing to $\sim 3 \times 10^{-10}$ at an offset of $[-40'', -40'']$, for $T_{\text{rot}} = 10 \text{ K}$. This is consistent with most of the CH emission at central offsets arising from the central expanding PDR. However, if the bulk of CH emission arises indeed in the PDR layers, using $C^{18}O$ as a probe of H_2 most likely underestimates the abundance because *i*) the abundance of $C^{18}O$ is affected by photodissociation and *ii*) because $C^{18}O$ may not coexist with the CH present in the gas where $C^{18}O$ is partly photodissociated. If we consider that the emission stems only from the innermost 10 mag in each side of the spherical cloud ($N(H) = 4 \times 10^{22} \text{ cm}^{-2}$, cf. Sects. 4.2, 5.2 and Pilleri et al. 2012a), the mean abundance in the PDR would be of $3.3^{+6.0}_{-2.2} \times 10^{-9}$ relative to H nuclei, with the error bars driven by the uncertainty in T_{rot} .

CCH

The CCH line at 87 GHz is composed of six hyperfine components. The most intense line is self-absorbed at a velocity of $\sim 11 \text{ km s}^{-1}$. To estimate the molecular column density, we used the faintest observed component (87.407 GHz), which is less affected by self-absorption. We have observed four hyperfine components of the $J = 3-2$ and $6-5$ multiplets, which are blended in pairs of two. For each group, we derived the total integrated intensity of the lines and then scaled it according to the relative strengths to estimate the contribution of each blended lines separately.

Figure B.2 shows the rotational diagrams at several position along the *Herschel* cut. We have convolved the $J = 3-2$ line to the spatial resolution of the $J = 6-5$ observations ($39''$). For all the lines, we assumed a 30% uncertainty for the intensity, except for the $1-0$ line where we assumed an uncertainty of a factor of 2 due to a possible self-absorption. For the 3 mm transitions we used the hyperfine fit task inside CLASS, and found that the relative line intensities of the 3 mm transitions are consistent with optically thin emission. For the higher frequencies, the hyperfine lines overlap, and this method is not reliable. However, our LVG results (see below) show that the opacities of these lines are also lower than 0.1.

One single component cannot fit the rotational diagram at any of the positions. For this reason, we used a two-component rotational diagrams to fit the integrated intensities of all the lines along the strip. The warm component has a rotational temperature of $\sim 35 \text{ K}$, while the cold component is at about 10 K. These temperatures are consistent with the superposition of two phases along the line of sight: a dense and high-UV illuminated PDR and a low-UV irradiated envelope (Pilleri et al. 2012a).

The CCH column density is approximately constant ($\sim 7.5 \times 10^{14} \text{ cm}^{-2}$) along the entire strip, but the column density of the hot component decreases by about 25% at larger offsets, where the emission is dominated by the envelope. This supports the interpretation of the warm component being associated with the PDR around the H II region. Hereafter, we refer to this component as the PDR component. It is important to note that this gradient is a lower limit to the real one because these column densities have been determined at a low spatial resolution ($40''$), thus diluting higher gradients in their distribution that may be present in the beam. Using the H_2 column density derived from $C^{18}O$, we estimate a mean CCH abundance of 9×10^{-9} relative to H nuclei.

c-C₃H₂

The c-C₃H₂ $2_{1,2}-1_{0,1}$ transition is self-absorbed towards the IF implying that we can only establish a lower limit to the column density of c-C₃H₂ at this position. Elsewhere, the spectra are not self-absorbed, so we can derive accurate column densities.

We convolved the higher- J transition to the spatial resolution of the $2_{1,2}-1_{0,1}$ line, and used the rotational diagram technique to compute the corresponding column densities. The rotational diagrams show that the column density decreases at larger offsets, from $\sim 6.0 \times 10^{12} \text{ cm}^{-2}$ towards the IF to $\sim 4.3 \times 10^{12} \text{ cm}^{-2}$ at an offset of $[-40'', -40'']$ to the SW. Only one component is needed to fit the observed intensities reasonably well, with a rotational temperature in the range 8–16 K. The excitation temperature seems to decrease farther from the IF. The spatial distribution of this species suggests that its emission is dominated by the dense PDR around the H II region, similarly to the warm component of CCH. The difference between the rotation temperature of c-C₃H₂ and that of the hot component of CCH partially comes from the higher different dipole moment of c-C₃H₂, which makes it much more difficult to excite by collisions. This is also consistent with the results of the LVG modeling in Sect. 4.2.

Again, using $C^{18}O$ as a tracer of the H_2 column density yields an abundance relative to H of $X(\text{c-C}_3\text{H}_2) = 7.3 \times 10^{-11}$ towards the IF, decreasing by about 30% at the position $[-40'', -40'']$. As for CCH, more details can be obtained assuming a rotational temperature and using only the 1 mm observations, improving the spatial resolution by a factor of 2.5. This improvement is shown in Sect. 4.4.

4.2. Two-phase decomposition towards the IF

The CCH rotational diagrams indicate that there are two emission components towards the IF. This is also consistent with the source model proposed by Pilleri et al. (2012a), in which a very dense PDR ($n_{H_2} = 3 \times 10^6 \text{ cm}^{-3}$) is surrounded by a lower density envelope ($T_{\text{kin}} = 35 \text{ K}$, $n_{H_2} = 5 \times 10^4 \text{ cm}^{-3}$). In the previous section we interpreted the warm component of CCH and the emission of c-C₃H₂ as arising in the PDR, with the cold component arising from the envelope. To verify this assumption and quantify the excitation effects on CCH and c-C₃H₂, we used the MADEX large velocity gradient (LVG) code (Cernicharo 2012) to reproduce the CCH and c-C₃H₂ emission towards the IF using the collisional coefficients of Spielfiedel et al. (2012) and Chandra & Kegel (2000), respectively.

We only have a few transitions with different upper energy levels, and therefore we cannot accurately constrain all the physical parameters (n_{H_2} , T_{kin} , N). Therefore, we have to rely on previous knowledge of the source structure (Pilleri et al. 2012a) to fix the temperature and density in each of these two phases and fit the column densities. We assumed densities of $n_{H_2} = 3 \times 10^6 \text{ cm}^{-3}$ and $5 \times 10^4 \text{ cm}^{-3}$ and kinetic temperatures of 70 K and 35 K for the PDR and the envelope, respectively.

The line width for both components has been set to 2 km s^{-1} . By assuming these parameters and varying the column densities in each of the two phases, we obtain the best fit to the observations with the solutions shown in Table 3. The line opacities returned by MADEX are lower than 0.1 for all the transitions. For CCH, we reproduce all the observed intensities within a 10% uncertainty. For c-C₃H₂, we are able to reproduce within a 15% error the observations with the best S/N, while the other transitions are fitted within 30%. This approach gives the column densities and abundances reported in Table 3. The results of

Table 3. Results of the two-phase LVG modeling towards the IF.

	Combined	PDR	Envelope
$N(\text{CCH}) [\text{cm}^{-2}]$	1.0×10^{15}	5.0×10^{14}	5.0×10^{14}
$X(\text{CCH})$	5.7×10^{-9}	1.7×10^{-8}	3.5×10^{-9}
$N(\text{c-C}_3\text{H}_2) [\text{cm}^{-2}]$	6.0×10^{12}	4.0×10^{12}	2.0×10^{12}
$X(\text{c-C}_3\text{H}_2)$	3.5×10^{-11}	1.4×10^{-10}	1.4×10^{-11}
$N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$	0.006	0.008	0.004

Notes. Abundances are relative to H nuclei and are calculated assuming that the PDR has a thickness of $A_V = 8$ and the envelope of $A_V = 40$ on each side of the spherical cloud.

MADEX modeling for all the transitions observed toward the IF are shown on the rotational diagrams in Fig. B.2. The uncertainties in the abundances are dominated again by the uncertainty in the total H column density and can be estimated to be a factor of 2.

4.3. Emission in the high-velocity wings

The ground-state transitions of both CCH and c-C₃H₂ show a broad emission at red-shifted velocities, which is not clearly detected in the higher energy lines (see Fig. 3). Toward the IF, the integrated intensity in the interval $[15\text{--}25] \text{ km s}^{-1}$ is 0.64 K km s^{-1} for CCH and 0.44 K km s^{-1} for c-C₃H₂. This allows an upper limit to the gas density of the region emitting in the wings to be estimated from LVG models that fit the intensity of the 3 mm lines and stay below the detection limit for the other transitions. This yields an upper limit to the gas density of $n_{\text{H}_2} = 1 \times 10^5 \text{ cm}^{-3}$ for $T_{\text{kin}} = 70 \text{ K}$. Assuming this density, we derive column densities of $3.5 \times 10^{13} \text{ cm}^{-2}$ for CCH and $1.5 \times 10^{12} \text{ cm}^{-2}$ for c-C₃H₂.

We repeated the rotational diagram for the C¹⁸O lines in this velocity interval to estimate the column density of the gas in this region, finding $N(\text{C}^{18}\text{O}) = 1.9 \times 10^{14} \text{ cm}^{-2}$, which corresponds to $N(\text{H}) = 1.9 \times 10^{21} \text{ cm}^{-2}$, or about 1 mag. This can be used to obtain an estimate of the abundance of CCH and c-C₃H₂ in the region emitting in the wings, which gives 1.8×10^{-8} for CCH and 7.8×10^{-10} for c-C₃H₂. If the density was lower (e.g. $n_{\text{H}_2} = 1 \times 10^4 \text{ cm}^{-3}$), the column density required to reproduce the wing intensity would be 15% higher for CCH and a factor of 4 higher for c-C₃H₂, yielding a higher $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio.

4.4. Spatial distributions

In the previous paragraphs we studied the excitation of single positions for all the species and derived some patterns in both the column density and rotational temperature. Here, we generalize the study to the mapping observations. First, we convolved all the maps to the lowest spatial resolution in the mapping dataset ($29''$). For each pixel in the map, we constructed a rotational diagram for each molecule and derived an excitation temperature and a column density for both CCH and c-C₃H₂. For simplicity, we used only one slope also for CCH. The results are shown in Fig. 6.

For C¹⁸O, our analysis is limited by the fact that the $J = 5\text{--}4$ line was observed only in the NE-SW strip. We have therefore to assume a given T_{rot} in each pixel based on this dataset. We have interpolated the mean T_{rot} obtained along the strip to obtain the rotation temperature of C¹⁸O as a function of the distance from the IF. Then we derived the corresponding column

densities (Fig. 6) assuming LTE. Since the C¹⁸O emission is optically thin, this yields an estimate of the H₂ column density and allows normalizing the column densities obtained for CCH and c-C₃H₂ to derive their abundances. The corresponding maps are shown in Fig. 6.

For a deeper insight into the hydrocarbon chemistry, we produced a map of $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$, the ratio of the c-C₃H₂ to CCH column densities. The $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio shows variation up to a factor of 3 across the whole region, with the minimum in the bulk of the molecular cloud, then increasing towards the PDR around the HII region and with the maximum located $40''$ towards the north, i.e., at the position of the low-UV PDR identified by [Ginard et al. \(2012\)](#). In fact, the $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ seems to follow the emission of the hot dust (PAH and larger grains) traced by the $8 \mu\text{m}$ emission. We can improve the angular resolution of our $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ image by directly using the CCH 3–2 and c-C₃H₂ 6–5 images (both with an angular resolution of $\sim 10''$) to derive the $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ but assuming the CCH and c-C₃H₂ rotation temperatures shown in Fig. 6 although these rotation temperatures were derived with a lower ($\sim 29''$) angular resolution. The angular resolution of the IRAC $8 \mu\text{m}$ image is $2''$. This higher resolution $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ image confirms the correlation with the $8 \mu\text{m}$ image (see Fig. 7) corroborating the association of an enhanced $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ with the external part of the PDR. In Sect. 5.2.1 we discuss the chemical implications of this correlation.

5. Discussion

5.1. Comparison with other PDRs

In the previous section, we have derived the abundances of small hydrocarbons in the different environments of Mon R2. In the PDR, the abundances are $X(\text{CH}) = 3.3 \times 10^{-9}$, $X(\text{CCH}) = 1.7 \times 10^{-8}$ and $X(\text{c-C}_3\text{H}_2) = 1.4 \times 10^{-10}$.

Table 4 shows the comparison of the CCH and c-C₃H₂ abundances in different PDRs. With the exception of the Orion Bar, the CCH abundance is relatively constant in PDRs, in the range $(0.6\text{--}1.4) \times 10^{-8}$. The abundance in the PDR of Mon R2 is consistent with these results. However, the envelope matches with the values found in the Orion Bar better ([Fuente et al. 1996, 2003; Ungerechts et al. 1997](#)). The case of the Orion Bar is interesting because, similar to Mon R2, it is a high-UV PDR with an associated envelope, which is the background molecular cloud not directly affected by the UV photons from the Trapezium cluster. The abundances for the Orion Bar shown in Table 4 were estimated using low angular resolution observations ($29''$). The beam of these observations comprises both the high-UV irradiated PDR and the warm envelope that hinders from a reliable comparison with the values in other PDR; however, the CCH abundance in the Orion Bar is similar to the mean CCH abundance in Mon R2 (Table 6).

On the other hand, the c-C₃H₂ abundance shows a larger variation among the various PDRs. The sources with a relatively low G_0 show an abundance of $(0.6\text{--}1.1) \times 10^{-9}$, whereas NGC 7023 NW and Mon R2 show much lower values, $(0.4\text{--}2) \times 10^{-10}$. This is also seen as the trend in the $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio in the different PDRs. Again, the values in the Orion Bar are more similar to the mean value in Mon R2. The $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio obtained in the PDRs of Mon R2 is an order of magnitude lower compared to that found in “classical” PDRs (see, for instance, [Pety 2005](#)) and in the diffuse medium ([Gerin et al. 2011](#)), and more similar to the value found in the

Fig. 6. First two rows: maps of the integrated intensity of the CCH (262.004 GHz) and $c\text{-C}_3\text{H}_2$ (217.822 GHz) lines, and of the column density and rotation temperature derived by applying the rotational diagram technique to each pixel. Black contours indicate the CCH 3–2 integrated intensity, and go from 5 K km s^{-1} to 20 K km s^{-1} in linear steps of 2.5 K km s^{-1} . The position of the infrared sources IRS1/2/3/4 (Henning et al. 1992) and the MP2 position (Ginard et al. 2012) are shown as black triangles. All the maps have been convolved to a spatial resolution of $29''$. Bottom row: CCH and $c\text{-C}_3\text{H}_2$ abundance maps, obtained using C^{18}O as a reference and assuming $^{16}\text{O}/^{18}\text{O} = 500$ and a CO abundance of 5×10^{-5} relative to H nuclei. The $N(c\text{-C}_3\text{H}_2)/N(\text{CCH})$ ratio is also shown.

dense gas surrounding the UCH II region IRAS 20343+4129 (Fontani et al. 2012).

5.2. Comparison with chemical models

In this section, we compare the observational results with the results of different chemical models, in order to qualitatively distinguish which effects may be dominant in the different phases that coexist in this region. Fully modeling the chemistry of this complex is beyond the scope of this paper, where our goal is to explore the possible impact of different factors, such as the grain-surface chemistry or time dependency, on the carbon chemistry in these environments.

The PDR layers (hereafter, L_{PDR} and L_{HD} for the exposed PDR and the high-density PDR, see Fig. 2) have different characteristics, in terms of physical conditions and time scales compared to the cold envelope. We assumed the density structure described in Sect. 2 (see also the top panel in Fig. 8), in which the mainly atomic layer L_{PDR} ($A_V < 1$, $n_{\text{H}_2} = 2 \times 10^5 \text{ cm}^{-3}$, $G_0 = 5 \times 10^5$) is followed by the high-density layer L_{HD} ($1 < A_V < 10$,

$n_{\text{H}_2} = 3 \times 10^6 \text{ cm}^{-3}$), where many molecular species start to be abundant. These innermost layers are surrounded by the low-density envelope L_{env} ($10 < A_V < 50$, $n_{\text{H}_2} = 5 \times 10^4 \text{ cm}^{-3}$). The assumption of constant density has to be taken with caution: local variations in gas density (clumps) and smoother gradients are expected to be found in the PDR layers, and the density in the envelope most likely decreases with the distance from the IF. However, this zero-order approximation allows reducing the free parameters of the modeling to a few, which eases the comparison of models and observational data.

To model the L_{PDR} and L_{HD} layers, we used the Meudon PDR code (Le Petit et al. 2006; Goicoechea & Le Boulbot 2007; Gonzalez Garcia et al. 2008; Le Boulbot et al. 2012) version 1.4.3 using the density profile shown in Fig. 8. The Meudon Code computes the steady-state solution to the thermal balance and gas-phase chemical networks using accurate radiative transfer calculations and a plane-parallel geometry. The transition between L_{HD} and L_{PDR} is calculated self-consistently by the code. This yields stationary solution for the gas and dust temperature, as well as the abundance of each molecule in each of the

Table 4. Comparison of CCH and c-C₃H₂ abundances in different PDRs.

	G_0	n_{H_2} [cm ⁻³]	$X(\text{CCH})^*$	$X(\text{c-C}_3\text{H}_2)^*$	$N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$	References
MonR2						
MonR2 IF			5.7×10^{-9}	3.5×10^{-11}	0.006	(a), (b)
MonR2 MP2			$2.6 \times 10^{-9***}$	$7.6 \times 10^{-11**}$	0.029***	(a), (b)
MonR2 PDR	5×10^5	3×10^6	1.7×10^{-8}	1.4×10^{-10}	0.008	a
MonR2 env	1–100	5×10^4	3.5×10^{-9}	1.4×10^{-11}	0.004	(a)
MonR2 red wing			1.8×10^{-8}	7.8×10^{-10}	0.04	(a)
Other PDRs						
Horsehead	100	1×10^5	1.4×10^{-8}	1.1×10^{-9}	0.08	(c)
Oph-W	400	2×10^4	6.0×10^{-9}	6.0×10^{-10}	0.1	(d)
IC 63	1500	1×10^5	1.1×10^{-8}	9.0×10^{-10}	0.08	(d)
NGC 7023	2600	10^4 – 10^6	6.0×10^{-9}	2.0×10^{-10}	0.03	(e), (f), (g)
Orion Bar	2×10^4	1×10^5	2.0×10^{-9}	3.8×10^{-11}	0.01–0.03	(f), (h), (i)

Notes. (*) The uncertainty in the abundances is driven by the uncertainty in the H₂ gas column density, which is assumed to be a factor of 2. (**) Calculated using the C¹⁸O observations of [Ginard et al. \(2012\)](#) as reference for the H₂ gas column density: $N(\text{C}^{18}\text{O}) = 1.3 \times 10^{16}$ cm⁻². (***) In MP2, we have to rely only on the 3 mm and 1 mm transitions of CCH. Thus, we may underestimate the CCH column density (and consequently, overestimate $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$) by a factor of 2.

References. (a) this work; (b) [Ginard et al. \(2012\)](#); (c) [Pety et al. \(2005\)](#); (d) [Teyssier et al. \(2004\)](#); (e) [Fuente et al. \(1993\)](#); (f) [Fuente et al. \(2003\)](#); (g) [Pilleri et al. \(2012b\)](#); (h) [Ungerechts et al. \(1997\)](#); (i) [Fuente et al. \(1996\)](#).

Fig. 7. Color image shows the ratio of c-C₃H₂ to CCH column densities as derived from 1 mm observations, assuming the rotational temperature of Fig. 6. Pixels without a detection of both CCH and c-C₃H₂ have been masked. The black contours represent the integrated intensity of the 262.004 GHz CCH line (from 15 to 25 K km s⁻¹ in steps of 2.5 K km s⁻¹), and white contours represent the Spitzer IRAC 8 μm emission.

layers by assuming equilibrium conditions. Time-dependent effects and gas-grain interactions are not included in the model and therefore its use is justified for the region where chemical equilibrium has already been reached and where gas-grain interaction is not expected to play a major role. However, the Meudon PDR code has very extensive gas-phase chemical networks and is best-suited to studying the gas-phase chemistry of Mon R2.

To study the low-density, cold envelope we used the UCL_CHEM code ([Viti et al. 2004](#)). This code includes gas-grain interaction. For the purpose of this paper it is used as a two-phase model which consists of the collapse of a prestellar core (Phase I), followed by the subsequent warming and evaporation of grain mantles due to the enhanced (with respect to the ISRF) radiation field (Phase II). In phase I, a diffuse cloud of density 10² cm⁻³ undergoes free-fall collapse until it has reached a final

Table 5. Input parameters for the Meudon PDR code.

Parameter		Value
G_0	Radiation field intensity	5×10^5
G_0^{ext}	External radiation field intensity	100
A_V	Total cloud depth	50 mag
Extinction		Standard Galactic
R_V	A_V/E_{B-V}	3.1
ζ	Cosmic ray ionization rate	5×10^{-17} s ⁻¹
a_{min}	Dust minimum radius	3×10^{-7} cm
a_{max}	Dust maximum radius	3×10^{-5} cm
α	MRN dust size distribution index	3.5
He/H	Helium abundance	0.1
O/H	Oxygen abundance	3.2×10^{-4}
C/H	Carbon abundance	1.3×10^{-4}
N/H	Nitrogen abundance	7.5×10^{-5}
S/H	Sulfur abundance	1.8×10^{-5}

density (set by the user). This phase occurs at a temperature of 10 K. During the collapse, atoms and molecules collide with, and freeze onto, grain surfaces. The advantage of this approach is that the ice composition is not assumed, but it is derived by a time-dependent computation of the chemical evolution of the gas-dust interaction process which, in turns, depends on the density of the gas. Hydrogenation occurs rapidly on grain surfaces, so that, for example, some percentage of carbon atoms accreting will rapidly become frozen out as methane, CH₄.

For all the models we use the same initial elemental abundances (see Table 5). The codes employ the reaction rate data from the UMIST astrochemical database, augmented with grain-surface (hydrogenation) reactions as in [Viti et al. \(2004\)](#) and [Viti et al. \(2011\)](#) for the UCL_CHEM models. In both phases of this code, nonthermal desorption is also considered as in [Roberts et al. \(2007\)](#).

5.2.1. Abundances in the PDRs

The column densities and abundances in the PDR obtained from the observations refer to the innermost 10 mag of the PDR.

Therefore, we have to compare them with the mean values in the $L_{\text{PDR}} + L_{\text{HD}}$ layer. Another way to study the chemical difference between these species and minimize the uncertainties due to the assumed physical structure is to consider the column density ratios $N(\text{CH})/N(\text{CCH})$ and $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ instead of absolute abundances.

In the exposed PDR layer (L_{PDR}), the gas temperature and UV field are so high that gas-phase chemistry is expected to be dominant. We can safely assume that all hydrocarbons have evaporated from grain surfaces and that there are no ices, since the dust temperature (100–150 K, Pilleri et al. 2012a) is above the sublimation limit for all the molecules involved in reactions with hydrocarbons, especially methane (Tielens 2005).

The results of the Meudon code modeling are displayed in Fig. 8. The model shows that all the hydrocarbons are expected to have their abundance peak at $A_V \sim 1$. For CCH, the model predicts a peak abundance of $\sim 10^{-6}$, which rapidly decreases to 10^{-15} . Similarly, $\text{c-C}_3\text{H}_2$ has an abundance peak toward the PDR of $\sim 10^{-10}$ and a decrease to 10^{-15} . The abundance gradient is less abrupt for CH, which passes from a peak of 10^{-8} in the PDR to 10^{-12} in the more shielded layers of the molecular cloud.

The column densities (and abundances) of CH and CCH are reproduced relatively well by the Meudon PDR code, considering the integrated column density in the two layers L_{PDR} and L_{HD} (see Table 6). Concerning $\text{c-C}_3\text{H}_2$, the model predicts an $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio of 0.0003, while the observed value is on the order of 0.01 in the PDR, which shows that the $\text{c-C}_3\text{H}_2$ is overabundant compared to the model predictions. This is consistent with several previous studies showing that in PDRs the gas-phase model predictions cannot account for the observed abundances of small hydrocarbons (Fuente et al. 1993; Teyssier et al. 2004; Pety et al. 2005), especially $\text{c-C}_3\text{H}_2$.

A link with PAHs?

A possible way to reduce the discrepancy could be the injection of fresh hydrocarbons by the photodestruction of PAHs or larger grains (Fuente et al. 2003; Pety 2005). Indeed, laboratory experiments show that the photodissociation of small PAHs ($N_C \leq 24$) can lead to the production of small hydrocarbons C_nH_m ($n > m$) that can be injected into the gas phase (Useli Bacchitta & Joblin 2007). To understand whether PAHs can be linked to a chemical differentiation of CCH and $\text{c-C}_3\text{H}_2$, it is useful to compare the ratio between the column density of $\text{c-C}_3\text{H}_2$ and CCH with the spatial distribution of PAHs. In Fig. 7 we display the comparison of the $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ ratio with the IRAC $8\mu\text{m}$ map.

In low- to mild-UV irradiated PDR, the $8\mu\text{m}$ map is dominated by the emission of the AIB at $7.7\mu\text{m}$, but in high-UV excited environments, larger grains at thermal equilibrium can reach temperatures high enough to have continuum emission at these wavelengths. To check whether this is the case in Mon R2, we have compared the IRAC $8\mu\text{m}$ map with one obtained with the IRAC $3.5\mu\text{m}$ filter, which is expected to be dominated either by the PAH $3.3\mu\text{m}$ feature or by the stellar continuum. The two IRAC maps are very similar, except for very point-like features in correspondence with the infrared source IRS 2 and IRS 3. Therefore, we can assume that most of the IRAC $8\mu\text{m}$ emission is indeed due to AIB emission. Finally, visual inspection of the IRS spectra in the central region of Mon R2 shows that the PAH features dominate the emission at $8\mu\text{m}$, except towards the bright infrared sources. The comparison of the ratio of the $\text{c-C}_3\text{H}_2$ and CCH column densities with the spatial distribution of CCH suggests that i) $\text{c-C}_3\text{H}_2$ is overabundant in the innermost layers of the cloud; and ii) the $\text{c-C}_3\text{H}_2$ spatial distribution

Fig. 8. Model results using the gas-phase steady-state chemistry with the Meudon PDR code. The cloud is illuminated from the left side with a UV field of $G_0 = 5 \times 10^5$.

extends to the NW, following the northern IR ridge that is observed at $8\mu\text{m}$ (Ginard et al. 2012).

The correlation between the PAH emission and the $\text{c-C}_3\text{H}_2$ overabundance, although suggestive of a chemical link between these species, does not prove yet that these two tracers are chemically linked (i.e. by UV processing), since they are both good PDR tracers. For instance, it has been observed that PAH and [C II] emission are spatially correlated in PDRs (Joblin et al. 2010), since both tracers arise in the most exposed layers of the PDR. This could also mean that the chemical differentiation of CCH and $\text{c-C}_3\text{H}_2$ in PDRs can also be due to an increased abundance of C^+ in these environments. Furthermore, C II and PAHs also trace the electron density, which is mainly due to the ionization of C and photoelectric effect on PAHs. Since $\text{c-C}_3\text{H}_2$ is supposed to form by electron recombination of the C_3H_3^+ , a higher production efficiency of photoelectrons ejected from PAHs may be a cause of $\text{c-C}_3\text{H}_2$ enhancement. However, including these effects in PDR models is still very challenging and beyond the scope of this paper.

5.2.2. Low-density envelope

Our observations indicate that the abundances of small hydrocarbons in the envelope are about five to ten times lower compared to the PDR. The column densities of CH and $\text{c-C}_3\text{H}_2$ relative to CCH are also a factor of 3 and 2 lower compared to the PDR. Even though, the CCH and $\text{c-C}_3\text{H}_2$ abundances are larger by several orders of magnitude than those predicted by steady-stage gas chemical models. In our sketch of MonR2, we assume the envelope to be 40 mag thick on each side of the spherical

Table 6. Comparison between the abundances derived from observations and model predictions.

	A_V [mag]	$X(\text{CH})^a$	$X(\text{CCH})^a$	$X(\text{c-C}_3\text{H}_2)^a$	$N(\text{CH})/N(\text{CCH})$	$N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$
$X_{\text{obs}}^{\text{PDR}}$	1–10	$3.3^{+6.0}_{-2.2} \times 10^{-9}$	1.7×10^{-8}	1.4×10^{-10}	0.15	0.008
Meudon $L_{\text{PDR}} + L_{\text{HD}}$	1–10	1.1×10^{-8}	4.8×10^{-8}	1.3×10^{-11}	0.22	0.00025
$X_{\text{obs}}^{\text{env}}$	10–50	$1.9^{+3.3}_{-1.2} \times 10^{-10}$	3.5×10^{-9}	1.4×10^{-11}	0.054	0.004
UCL_CHEM $L_{\text{env}} f = 10^b$	41	5.1×10^{-10}	1.3×10^{-9}	4.8×10^{-13}	0.39	0.0004
UCL_CHEM $L_{\text{env}} f = 25^b$	41	9.5×10^{-10}	6.9×10^{-10}	3.5×10^{-11}	1.37	0.05
UCL_CHEM $L_{\text{env}} f = 45^b$	41	7.5×10^{-10}	3.5×10^{-10}	1.4×10^{-10}	2.1	0.40

Notes. For the UCL_CHEM code, we show the results at $t = 10^4$ years. For the observed abundances and the Meudon PDR results, we report mean values of the abundances, while for the UCL_CHEM results, we report the value at a given A_V , and assume that these values are relatively constant in the respective layers. ^(a) Except for CH, where the uncertainty is driven by the excitation temperature, the abundance uncertainty is driven by the H₂ gas reference, and is a factor of 2. ^(b) The f value indicates the percentage of CO on the icy mantles at the end of Phase I.

cloud, with a gas density of $n_{\text{H}_2} = 5 \times 10^4 \text{ cm}^{-3}$ and a gas kinetic temperature of 35 K. With these physical conditions, gas-grain chemistry and time-dependent effects may play a role.

To study these processes we used the UCL_CHEM models running Phase 1 from diffuse core up to a density of $n_{\text{H}_2} = 5 \times 10^4 \text{ cm}^{-3}$, while the temperature and radiation field were kept at 10 K and 1 Habing respectively. Once the final density was reached we increased the radiation field to $G_0 = 100$ and the kinetic temperature to 35 K (Phase 2). The model assumes a number of parameters, such as the freeze-out, photo- and thermal-desorption efficiencies. We use the standard values for the different nonthermal desorption efficiencies as in Roberts et al. (2007). In particular, the models are strongly dependent on the freeze-out efficiency during phase 1, which determines the initial abundances of CH, CCH, and c-C₃H₂ in Phase 2. We tested the impact of the kinetic temperature in the envelope in the final hydrocarbon abundances, and found no significant difference in the range [10–35] K. This is consistent with the fact that at $T_{\text{dust}} = 35 \text{ K}$, most of the species remain in the grain mantles (Viti et al. 2004) and the rates of main gas phase reactions involved in the formation and destruction of hydrocarbons do not present strong variations in this temperature range.

In Fig. 9 we report an example of the time evolution during Phase 2 for an $A_V = 41$, assuming a low (10%) CO freeze-out. The model predicts that all the hydrocarbon abundances are constant up to 10^4 years. At this time, each of the absolute abundances for CH and CCH are reproduced within a factor of 3 but their ratio is overpredicted by a factor of 7 (see Table 6). Considering the high uncertainties in the absolute column density of CH (driven by the unknown excitation temperature), it is difficult to further constrain the model based on this ratio. After 1×10^4 years, gas phase CH decreases by a factor of a few, whereas CCH and c-C₃H₂ decrease by the more than one order of magnitude: for $t \gtrsim 10^5$ years, the agreement of $N(\text{c-C}_3\text{H}_2)/N(\text{CCH})$ with observations improves, but the absolute abundances and the CH/CCH ratio do not agree as well as at 1×10^4 years.

By repeating the calculations for higher freeze-out fractions (25% and 45%, see Table 6), one can find a better agreement for one or the other molecule, but it is difficult to find a solution that fits all the abundances or column densities reasonably well.

In any case, the chemistry of Mon R2 seems to be dominated by grain-surface processes and time-dependent effects, since at the age of UCH II region ($\sim 0.1 \text{ Myr}$), the molecular chemistry is far from the steady state yet. In this scenario the current abundances of small hydrocarbons are dependent on the previous history of the cloud. This is consistent with recent results of

Fig. 9. Results of the UCL CHEM code to model the low-density envelope L_{HD} for a starting CO freeze-out of 10%. The results are given at A_V of 41 magnitudes and by setting the temperature fixed to 35 K. The bottom panel shows the ratio of gas-phase CH and c-C₃H₂ relative to CCH. The vertical dashed line marks the age of 10^4 years, which is used in Table 6.

Mookerjee et al. (2012), who studied these effects in the envelope associated with DR21. They investigated the impact of time-dependent effects for the carbon chemistry of this warm cloud, showing that PAH-related chemistry is not needed to explain the abundances of either CCH or c-C₃H₂ in this molecular envelope.

6. Conclusions

In this paper, we have presented new observations of small hydrocarbon molecules (CH, CCH, and c-C₃H₂) in MonR2, which were obtained with the IRAM-30 m telescope and the HIFI instrument onboard *Herschel*. In particular, the HIFI observations allowed the $N = 6-5$ rotational transitions of CCH to be accessed with good spatial and spectral resolution. This allowed the excitation conditions to be constrained and the different phases in which this species is abundant to be distinguished.

Profiting from a multi-transition and spatial study, we derived the spatial distribution of these molecules, determining their abundances in the different layers of Mon R2.

We compared the observational results with predictions of different PDR models to investigate which kind of chemistry can dominate in the different environments that coexist in Mon R2:

- In the high-UV illuminated PDR, grain mantles have already been evaporated, and we can safely assume that chemical equilibrium has been reached. In this case, the gas-phase chemistry can explain the abundances of CH and CCH quite well but fails to reproduce $c\text{-C}_3\text{H}_2$. The chemical differentiation of these two molecules happens in correspondence with PAH emission, suggesting once again a link between these species.
- In the cold (~ 35 K), low-density molecular cloud, time-dependent effects seem to be very important. Around 10^4 years, the abundances predicted by the models are relatively consistent with those derived from the observations. At this time all the absolute abundances are reproduced relatively well, although CH is overpredicted relative to both CCH and $c\text{-C}_3\text{H}_2$. These models are, however, strongly dependent on the initial abundances due to the freeze-out in the cloud collapse phase.

This study shows that several effects must be taken into account for understanding the chemistry of small hydrocarbons such as CCH and $c\text{-C}_3\text{H}_2$: the relative contribution of UV radiation, grain-surface chemistry and time-dependent effects may vary in different environments. Regarding PDRs, a more detailed analysis of the small hydrocarbon chemistry in these environments requires (i) a larger sample of PDRs spanning a wide range of physical conditions to minimize effects of a peculiar geometry of a particular source; (ii) to revise the possible chemical routes to the formation of small hydrocarbons, such as the photodestruction of PAHs and very small grains. *Herschel* data will allow the hydrocarbons chemical models to be constrained, including related species that are not observable from the ground (e.g., C^+ , CH^+). Finally (iii) higher resolution observations with the Plateau de Bure Interferometer, NOEMA, ALMA, and JCMT will allow observations of several key species with unprecedented spatial resolution. This will enable the small-scale chemical frontiers to be resolved in PDRs. This seems to be key for interpreting the link between small hydrocarbons and PAHs.

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Appendix A: Diffuse gas in the line of sight

The low-lying transitions of all the hydrocarbons show a clear self-absorption at about the velocity of $\sim 11 \text{ km s}^{-1}$ toward the IF (see Fig. 3). A similar, narrow self-absorption component has also been reported for the $[\text{C II}]$ $158 \mu\text{m}$ line (Pillari et al. 2012a; Ossenkopf et al. 2013). This feature suggests the presence of a relative diffuse phase in the line of sight. The velocity at which the absorption features appears is the same as for the emission of the quiescent molecular cloud. Thus, it is likely that this absorbing layer is a low-density gas associated with the most external layer of the molecular cloud.

To determine the column density of the absorbing gas, we need to estimate a reference for the spectral profile of the emission line. We assume that the widths of the lines belonging to a species are similar, and use a transition that is less affected by self-absorption to estimate the FWHM of a Gaussian profile. We obtain an FWHM of 5.5 km s^{-1} for CCH (using the $J = 87.407 \text{ GHz}$ line) and 3 km s^{-1} for $c\text{-C}_3\text{H}_2$ (using the 150.820 GHz line) and 6 km s^{-1} for CH. Using these line widths, we can adjust the blue-shifted wing of the self-absorbed line with a Gaussian and use it as reference to calculate the integrated opacity of the self-absorption. By assuming an excitation temperature $T_{\text{ex}} = 2.73 \text{ K}$, we derive column densities associated to the foreground of $N(\text{CH}) = 4.8 \times 10^{13} \text{ cm}^{-2}$, $N(\text{CCH}) = 5.0 \times 10^{13} \text{ cm}^{-2}$ and $N(c\text{-C}_3\text{H}_2) = 1.4 \times 10^{12} \text{ cm}^{-2}$.

From CH, we can derive the H_2 column density associated with the absorption, hence an estimate of the extinction. The standard abundance of CH relative to H_2 in diffuse gas is 3.5×10^{-8} (Sheffer et al. 2008), which leads to a molecular hydrogen column density of $N(\text{H}_2) \sim 1.3 \times 10^{21} \text{ cm}^{-2}$ or about 1.3 mag of extinction. This yields CCH and $c\text{-C}_3\text{H}_2$ abundances (relative to H_2) of 3.9×10^{-8} and 1.6×10^{-9} , respectively. These values are consistent with the typical values observed in diffuse gas (Liszt & Lucas 2002; Gerin et al. 2011). The results are similar when considering an offset of $[20'', 20'']$, where the self-absorption is still detected with a sufficient S/N to infer relatively accurate column densities.

These estimates suffer from the uncertainty due to the assumed line profile and on the observed continuum. Nevertheless, the detection of this foreground, $1A_V$ thick layer associated with the external layer of the envelope is interesting and moves toward a deeper understanding of this source.

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Appendix B: Spectroscopic parameters, maps, and rotational diagrams

Table B.1. Spectroscopic parameters of the observed transitions.

Transition	Frequency [GHz]	E_u [K]	A_{ul} [s ⁻¹]	g_u
CH $2\Pi_{1/2}$, $N = 1$, $J = 3/2-1/2$				
$P = 2^- - 1^+$	536.76115	0.00072	0.0638	5
$P = 1^- - 1^+$	536.78195	0.00072	0.0213	3
$P = 1^- - 0^+$	536.79568	0.0	0.0425	3
CH $2\Pi_{1/2}$, $N = 2$, $J = 5/2-3/2$				
$P = 3^+ - 2^-$	1656.961	25.727	0.03719	7
$P = 2^+ - 2^-$	1656.970	25.727	0.00372	5
$P = 2^+ - 1^-$	1656.972	25.727	0.03348	5
CCH $N = 1-0$				
$J = 3/2-1/2$, $F = 1-1$	87.28410	0.00216	2.5920×10^{-7}	3
$J = 3/2-1/2$, $F = 2-1$	87.31690	0.00216	1.5274×10^{-6}	5
$J = 3/2-1/2$, $F = 1-0$	87.32859	0.00000	1.2684×10^{-6}	3
$J = 1/2-1/2$, $F = 1-1$	87.40199	0.00216	1.2715×10^{-6}	3
$J = 1/2-1/2$, $F = 0-1$	87.40716	0.00216	1.5324×10^{-6}	1
CCH $N = 3-2$				
$J = 7/2-5/2$, $F = 4-3$	262.00426	12.57513	5.30542×10^{-5}	9
$J = 7/2-5/2$, $F = 3-2$	262.00648	12.57383	5.10470×10^{-5}	7
$J = 5/2-3/2$, $F = 3-2$	262.06499	12.58203	4.87506×10^{-5}	7
$J = 5/2-3/2$, $F = 2-1$	262.06747	12.58261	4.45975×10^{-5}	5
CCH $N = 6-5$				
$J = 13/2-11/2$, $F = 7-6$	523.97157	62.87103	4.5697×10^{-4}	15
$J = 13/2-11/2$, $F = 6-5$	523.97217	62.86987	4.5179×10^{-4}	13
$J = 11/2-9/2$, $F = 6-5$	524.03390	62.88685	4.4939×10^{-4}	13
$J = 11/2-9/2$, $F = 5-4$	524.03453	62.88757	4.4205×10^{-4}	11
c-C ₃ H ₂ $J_{K_A, K_C} = 2_{1,2}-1_{0,1}$	85.33889	4.1	2.55335×10^{-5}	15
c-C ₃ H ₂ $J_{K_A, K_C} = 4_{0,4}-3_{1,3}$	150.82067	19.3	1.79933×10^{-4}	9
c-C ₃ H ₂ $J_{K_A, K_C} = 4_{1,4}-3_{0,3}$	150.85191	17.0	1.80086×10^{-4}	27
c-C ₃ H ₂ $J = 6-5$				
$K_A, K_C = 1, 6-0, 5$	217.82215	36.3	5.93376×10^{-4}	39
$K_A, K_C = 0, 6-1, 5$	217.82215	38.6	5.93403×10^{-4}	13
c-C ₃ H ₂ $J_{K_A, K_C} = 5_{1,4}-4_{2,3}$	217.94005	33.1	4.42680×10^{-4}	33
c-C ₃ H ₂ $J_{K_A, K_C} = 4_{3,2}-3_{2,1}$	227.16913	26.7	3.42484×10^{-4}	27
c-C ₃ H ₂ $J = 7-6$				
$K_A, K_C = 0, 7-1, 6$	251.31434	48.3	9.34953×10^{-4}	45
$K_A, K_C = 1, 7-0, 6$	251.31434	50.7	9.34781×10^{-4}	15
c-C ₃ H ₂ $J = 6-5$				
$K_A, K_C = 2, 5-1, 4$	251.52730	45.1	7.42318×10^{-4}	39

References. CH: (McCarthy et al. 2006) and CDMS; CCH: (Padovani et al. 2009) and CDMS; c-C₃H₂: JPL.

Fig. B.1. Integrated intensity of all the observed c-C₃H₂ and CCH transitions. The upper state energy level and the principal quantum numbers are shown for each transition. The smaller scale maps have been convolved to the spatial resolution of 15'' to improve the S/N.

Fig. B.2. Rotational diagrams for CCH (top), c-C₃H₂ (middle), and C¹⁸O (bottom) along the *Herschel* strip. Data have been convolved to 40'' for CCH and C¹⁸O, and to 29'' for c-C₃H₂. Green diamonds represent the MADEX simulation towards the IF (cf. Sect. 4.2).