Chemical stratification in the Orion Bar: JCMT Spectral Legacy Survey observations

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ABSTRACT

Context. Photon-dominated regions (PDRs) are expected to show a layered structure in molecular abundances and emerging line emission, which is sensitive to the physical structure of the region as well as the UV radiation illuminating it. Aims. We aim to study this layering in the Orion Bar, a prototypical nearby PDR with a favorable edge-on geometry. Methods. We present new maps of 2×2′ fields at 14″–23″ resolution toward the Orion Bar in the SO 8–9, H2CO 5–4, 13CO 3–2, C2H 4–3, and 4–3, C18O 2–1 and HCN 3–2 transitions. Results. The data reveal a clear chemical stratification pattern. The C2H emission peaks close to the ionization front, followed by H2CO and SO, while CO and HCN present a sequence of different chemical transitions. Conclusions. The discrepancies between the models and observations indicate that more sophisticated models, including production of H2CO through grain surface chemistry, are needed to quantitatively match the observations of this region.

Key words. ISM: molecules – ISM: structure – ISM: individual: Orion Bar – stars: formation

1. Introduction

In photon-dominated regions (PDRs), UV radiation between a few and 13.6 eV drives the thermal and chemical balance of interstellar gas (Hollenbach & Tielens 1999 and references therein). PDRs are ubiquitous in the universe: surfaces of molecular clouds adjacent to H ii regions, planetary nebulae, protoplanetary disks, and also the nuclei of distant active galaxies. As such, PDRs are signposts of radiative feedback processes driven by star formation. Heating proceeds through photo-electric emission from dust grains and cooling is mostly due to fine-structure emissions of [C ii] and [O i], and CO rotational lines (e.g., Sternberg & Dulsarno 1995; Kaufman et al. 1999; Meijerink & Spaans 2003; Röllig et al. 2007). Shielding of the UV radiation by dust and gas creates a layering structure where a sequence of different chemical transitions is produced by the gradual attenuation of the UV field (Ossenkopf et al. 2007).

The Orion Bar is a prototypical PDR located between the Orion molecular cloud and the H ii region surrounding the Trapezium stars, at a distance of 414 pc (Menten et al. 2007). Multi-wavelength observations (Tielens et al. 1993; Van der Werf et al. 1996; Hogerheijde et al. 1995; Young Owl et al. 2000; Walmsley et al. 2000) indicate a geometry for the Bar where the PDR is wrapped around the H ii region created by the Trapezium stars and changes from a face-on to an edge-on geometry where the molecular emissions peak. The mean density of the Bar is about 103 cm−3, the mean molecular gas temperature 85 K, and the impinging radiation field is \((1 - 4) \times 10^4 \chi_0\) (Hogerheijde et al. 1995), where the Draine field \(\chi_0 = 2.7 \times 10^{-3}\) erg s−1 cm−2.

The clumpiness of the PDR inferred by Hogerheijde et al. (1995) was confirmed by interferometric data (Young Owl et al. 2000; Lis & Schilke 2003). Clump densities up to \(10^4\) cm−3 were derived by Lis & Schilke (2003), while the density of the interclump medium should fall between a few \(10^3\) cm−3 (Young Owl et al. 2000) and 2 \(10^3\) cm−3 (Simon et al. 1997). The physical stratification of the PDR is well established (Tielens et al. 1993; Van der Werf et al. 1996; Simon et al. 1997; Lis & Schilke 2003). Vibrationally excited H2 emission is located 15″ from the ionization front, while HCO+ 1–0 peaks as well, while the CO peak resides at 20″ and CS slightly further in.

This paper presents emission maps of various molecular species, allowing us to probe and understand the chemical stratification in the Orion Bar in greater detail.

2. Observations

This work is based on data obtained as part of the Spectral Legacy Survey (SLS, Plume et al. 2007), being conducted at the James Clerk Maxwell Telescope on Mauna Kea, Hawai’i. The James Clerk Maxwell Telescope is operated by The Joint Astronomy Centre on behalf of the Science and Technology Facilities Council of the United Kingdom, the Netherlands Organisation for Scientific Research, and the National Research Council of Canada.
SLS is performing spectral imaging of 2′×2′ fields in the direction of the Orion Bar and four other targets. Once completed, the spectral range covered by the SLS will be 330–362 GHz. This Letter presents the first results from a selection of molecular lines in the already acquired data: two C2H lines and one transition each of SO, H2CO and 13CO between 330 and 350 GHz, and two lines in auxiliary data in the 230 GHz window: C18O 2–1 and HCN 3–2 (Table 1).

The SLS uses the 16-pixel HARP receiver (325–375 GHz) and the ACSIS correlator. The angular resolution of the JCMT at the observed frequencies is 14–15″ (~30 mpc at the distance of the Orion Bar); the harp4 mc jiggle position switch mode produces 2′×2′ maps sampled every 7′.5. The spectra are calibrated by observations at an off-position 10′ to the southeast. At an exposure time of 4 minutes per map pixel, the rms noise level in the current SLS data is 0.07–0.08 K in velocity bins of 0.83–0.89 km s–1. Single sideband system temperatures for these observations are ~700 K.

The HCN 3–2 and C18O 2–1 lines were observed in 2005 with the A-band (215–275 GHz) receiver and the DAS spectrometer. The same 2′×2′ field as with HARP was mapped at half-beamwidth spacing, using the raster mapping mode. The JCMT beam size at 220–266 GHz is 19–23″ (~40 mpc). The off-position for the A-band observations was at 20′ southeast of the map center. The HCN and C18O observations reach a noise level of 0.5–0.6 K at a spectral resolution of 0.18 and 0.21 km s–1, respectively. System temperature values are ~350 K (DSB); the integration time is 19 seconds per map pixel. The pointing accuracy was checked every hour and was generally better than 2″ during all observing runs.

The data were manually reduced using standard Starlink procedures. The SLS observations were handled in blocks of 1.6 GHz effective bandwidth and the other data as one set per emission line. The time series were converted to data cubes and first-order polynomial baselines were subtracted. Line intensities quoted here are given in terms of the main-beam temperature Tmb, i.e., they have been corrected for the JCMT main-beam efficiency of 63% in the 345 GHz window and 69% in the 230 GHz window. Single-channel signal-to-noise ratios at the peak in the northeast slice are ~16 for C18O and SO, ~40 for HCN, H2CO and C2H, and 900 for 13CO.

3. Results

Figure 1 presents images of the observed molecular emission, overlaid on an 8 μm image of the Orion Bar taken with the Spitzer Space Telescope (Megeath et al., in prep.). The mid-infrared emission traces warm dust at the surface layer between the H2 region and the molecular cloud. The molecular emission is seen to peak to the southeast of this layer, and the JCMT data reveal a clear stratification. The C2H emission peaks close to the surface layer, followed by SO and H2CO, whereas CO and HCN peak deep into the molecular cloud.

The stratification is more easily visible in Fig. 2 which shows slices through the images in Fig. 1 taken along the arrows in Fig. 1 perpendicular to the ionization front to produce these intensity profiles, all maps are regridded to 3′75 pixels, roughly half the pixel size of the original maps. Fitted peak positions and peaks fluxes for the seven profiles are listed in Table 1 along with the spectroscopic parameters of the observed lines; the position uncertainties include Gaussian fitting errors (< 1″ ≈ 2 mpc).

In addition to the stratification, the molecular emission shows a two-peak structure. The northeast peak is brighter in HCN and H2CO, while the southwest peak is brighter in SO and the peak brightness is roughly equal for CO and C2H. These variations are probably caused by variations in the filling factor of dense gas, as seen, e.g., in the high-resolution data by Lis & Schilke (2003). The measured line widths of 5–8 km s–1 will be useful for future detailed modeling, however, this paper focuses on integrated intensities.

We use the observed line intensities and the radiative transfer program RADEX (Van der Tak et al. 2007) to estimate beam-averaged molecular column densities. Although temperatures are known to range from 50 K in dense clumps up to 150 K in the interclump medium (Batrla & Wilson 2003, Lis & Schilke 2003), we assume a kinetic temperature of 85 K and a volume density of 103 cm–3, as applicable to the extended molecular gas (Hoogerheijde et al. 1995). Since some of the line emission may
Profiles of molecular emission along slices perpendicular to the ionization front at position angle 225° (see arrows in Fig. 1): (top panel) through the northeast core; (bottom panel) through the southwest core. The zero point of the distance scale is placed at the C$_{18}$O peak position: (RA=$5^h35^m25^s.4$, δ=$-5^\circ24'37''$) for the northeast slice and (RA=$5^h35^m21^s.6$, δ=$-5^\circ25'19''$) for the southwest slice.

To convert the observed C$^{18}$O line intensity to a total H$_2$ column density, we assume an isotopic ratio $^{16}$O/$^{18}$O=500 (Wilson & Rood 1994) and a CO abundance of $1.1\times10^{-3}$ as applicable for the Orion Bar PDR (Johnstone et al. 2003). The result is $N(H_2) = 1.0\times10^{23}$ cm$^{-2}$, which implies the following molecular abundances at the peak locations: $x$(C$_2$H) = $2\times10^{-9}$; $x$(H$_2$CO) = $4\times10^{-10}$; $x$(SO) = $7\times10^{-10}$; $x$(HCN) > $5\times10^{-10}$. Here we have assumed that the emission from all molecules except CO originates in the high-density gas. Based on Jansen et al. (1995), who propose the clumps to encompass 10% of the material along every line of sight, we estimate the clumps to provide for roughly half of the total column density for those molecules that exist in both phases. Hence, the resulting uncertainty in the derived abundances would not exceed a factor 2. Since C$_2$H and CO are hardly coexistent, the C$_2$H abundance is probably underestimated by a factor of 3–10.

4. Discussion
To interpret our observations we compare them to the predictions from a PDR model. Previous models of the Orion Bar do not present abundances for all six species in our data, so we use the global conditions of the Bar ($\chi=3\times10^4$, $n_H=10^5$ cm$^{-3}$, see Sect. 1) to construct a simple model using the KOSMA-τ PDR code (Röllig et al. 2006). We refer...
Table 1. Observed molecular lines.

| Molecule | Transition | Frequency (MHz) | $E_{\text{up}}$ (K) | Peak position (mpc) | $T_{\text{mb}}$ (K km s$^{-1}$) | $N_{\text{mb}}$ (cm$^{-2}$) | LTE |
|----------|------------|----------------|-----------------|-------------------|-----------------|-----------------|-----|
| C$_2$H | $N_2$ $\rightarrow 3_{1,2}$ | 349400.5$^{(a)}$ | 42 | -14 ± 1.8 | -23 ± 1.0 | -16 | 8.6 ± 1.6 | 4.4×10$^{14}$ | 2.3×10$^{14}$ |
| C$_2$H | $N_2$ $\rightarrow 3_{1,2}$ | 49337.3$^{(b)}$ | 42 | -14 ± 1.5 | -23 ± 1.6 | -16 | 11.3 ± 2.0 | 4.9×10$^{14}$ | 2.4×10$^{14}$ |
| C$_2$H | $N_2$ $\rightarrow 3_{1,2}$ | 50351.9$^{(c)}$ | 42 | -14 ± 1.5 | -23 ± 1.6 | -16 | 11.3 ± 2.0 | 4.9×10$^{14}$ | 2.4×10$^{14}$ |
| SO | $N_2$ $\rightarrow 3_{1,2}$ | 351768.2 | 62 | -3 ± 1.3 | -7 ± 1.9 | -12 | 9.3 ± 1.6 | 7.7×10$^{14}$ | 3.8×10$^{15}$ |
| $^{13}$CO | $J = 3$ $\rightarrow 2$ | 238858.0 | 32 | 4 ± 1.9 | -1 ± 3.0 | 2 | 186 ± 32 | >2.1×10$^{16}$ | >2.5×10$^{16}$ |

(a): Blend of $F=3-3$ and $F=3-2$ hyperfine components (separation 1.4 MHz). (b): Blend of $F=3-3$, $F=3-2$ and $F=2-1$ hyperfine components (total separation 1.5 MHz). (c): Fitted peak positions in the observed profiles for each species. (d): Column density uncertain due to high optical depth; values listed here are lower limits. (e): Beam-averaged abundance discrepancy might be explained by the evaporation of the cold material (at 8 mpc), following the distribution of the C$_2$H abundance derived in the LTE limit. (f): Fitted value of integrated intensity at peak position along the northeast slice (see Fig. 1); uncertainties include fitting uncertainty and 15% absolute calibration uncertainty. (g): Column density uncertain due to high optical depth; values listed here are lower limits. (h): Beam-averaged column densities for n=10$^{15}$ cm$^{-3}$ and in LTE, both at $T=85$ K.

SO abundance orders of magnitude larger than the observed value.

The underestimate of the C$_2$H abundance predicted by our pure gas-phase model might be explained by C$_2$H being formed via photo-destruction of PAH molecules, as proposed by Pety et al. (2005). This explains a detectable C$_2$H abundance in the outer layers where the PAH emission peaks (van der Werf et al. 1999).

Our modeled SO abundance is a factor 1.4×10$^3$ larger than observed. This is explained by the too high gas phase sulfur abundance of 2.8×10$^{-5}$ used in the KOSMA-τ model, which represents diffuse clouds and no depletion (Federman et al. 1993). Recent estimates of cosmic sulfur abundance provide values as low as 1.4×10$^{-5}$ (Asplund et al. 2005) and sulfur depletion factors in dense clouds may range from 4 (Gioioccoea et al. 2006) to 1000 (Tieftrunk et al. 1994). Depletion factors of several 10$^3$ would be required to match the Orion Bar observations with the current model. The low depletion seems not to apply to the entire Orion region, but to be specific for the Horsehead, which has a particularly low density.

The abundance of H$_2$CO derived in the LTE limit is slightly higher than the modeled abundance; the discrepancy increases sharply as soon as the H$_2$CO gas is not completely in LTE. This abundance discrepancy might be explained by the evaporation of molecules from warm (∼30 K) dust grains. Based on reaction rates from Woodall et al. (2007), the photo-dissociation lifetime for H$_2$CO at $A_V = 5$ mag is only ∼10 yr, which introduces the need for a continuous supply of H$_2$CO, e.g., from grain surfaces (Herbst 2000). This is consistent with the suggestion by Leurini et al. (2006) that H$_2$CO may originate primarily from the warm interclump medium.

Finally, the observed broad spatial profiles for HCN and $^{13}$CO (Fig. 2) may be explained by optical depth effects, since the optical depth inferred by RADEX is 5–10 for these molecules and <1 for the others. The different spatial distributions of the two CO isotopologs result mainly from the different beam sizes.

Future observations will test our hypothesis that grain surface chemistry plays a key role in PDRs. One such test will be JCMT-SLS observations of CH$_2$OH in the Orion Bar; while Leurini et al. (2006) suggest that CH$_2$OH traces the clumps and H$_2$CO traces the interclump medium, both molecules are thought to be the products of CO hydrogenation on ice (Watanabe et al. 2004), so their spatial coincidence would mark a critical validation step. Other analysis will explore sulfur chemistry using sulfur-bearing species covered by the SLS, such as CS and SO$_2$. 

There are also significant discrepancies between the model and the observations. (i) The model predicts that SO peaks deep in the cold material (at 8 mpc), following the distribution of HCN, not at the location where H$_2$CO peaks (in front of CO) as is observed. (ii) Conversely, the H$_2$CO peak in both slices is observed closer to the peaks of the CO isotopes than to the C$_2$H peak, while the model predicts H$_2$CO to peak significantly closer to C$_2$H. (iii) For HCN the model peaks 5–9 mpc deeper than is observed and (iv) the observations show an HCN emission wing toward the PDR surface which is weaker in the model. (v) We find that the absolute abundance of H$_2$CO and the lower limit to the absolute abundance of HCN at the model peak are consistent with the observations, while the model abundance of C$_2$H is ~2 times smaller than observed. (vi) In addition, our modeled
Once completed, the SLS data set will enable studies of multiple transitions of various molecules, so that the excitation of molecules (as well as their velocity structure) can also be compared to models. In the longer term, (sub)millimeter-wave imaging spectroscopy of other Galactic PDRs is needed to establish how common grain chemistry is and how it depends on environment. Important tests will be spectral surveys with the HIFI instrument on board ESA’s Herschel Space Observatory, which will target hundreds of molecular lines in many Galactic PDRs and allow a detailed picture of their chemistry to emerge.

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