Compression and ablation of the photo-irradiated molecular cloud the Orion Bar

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The Orion Bar is the archetypal edge-on molecular cloud surface illuminated by strong ultraviolet radiation from nearby massive stars. Our relative closeness to the Orion nebula (about 1,350 light years away from Earth) means that we can study the effects of stellar feedback on the parental cloud in detail. Visible-light observations of the Orion Bar show that the transition between the hot ionized gas and the warm neutral atomic gas (the ionization front) is spatially well separated from the transition between atomic and molecular gas (the dissociation front), by about 15 arcseconds or 6,200 astronomical units (one astronomical unit is the Earth–Sun distance). Static equilibrium models used to interpret previous far-infrared and radio observations of the neutral gas in the Orion Bar (typically at 10–20 arcsecond resolution) predict an inhomogeneous cloud structure comprised of dense clumps embedded in a lower-density extended gas component. Here we report one-arcsecond-resolution millimetre-wave images that allow us to resolve the molecular cloud surface. In contrast to stationary model predictions, there is no appreciable offset between the peak of the $H_2$ vibrational emission (delineating the $H_2$/H$^+$ transition) and the edge of the observed CO and HCO$^+$ emission. This implies that the H/$H_2$ and C$^+$/C/CO transition zones are very close. We find a fragmented ridge of high-density substructures, photoablative gas flows and instabilities at the molecular cloud surface. The results suggest that the cloud edge has been compressed by a high-pressure wave that is moving into the molecular cloud, demonstrating that dynamical and non-equilibrium effects are important for the cloud evolution.

The Atacama Large Millimeter/submillimeter Array (ALMA) radio-telescope allows us to resolve the transition from atomic to molecular gases at the edge of the Orion molecular cloud, which is directly exposed to energetic radiation from the Trapezium stars (Fig. 1). The strong ultraviolet field drives a blister ‘H II region’ (hot ionized hydrogen gas or $H^+$) that is eating its way into the parental molecular cloud. At the same time, flows of ionized gas stream away from the cloud surface at about 10 km s$^{-1}$ (roughly the speed of sound at about $10^4$ K). The so-called photon-dominated or photodissociation region (PDR), see Extended Data Fig. 1, starts at the $H$ II region/cloud boundary where only far-ultraviolet radiation penetrates the ‘neutral’ cloud, that is, stellar photons with energies below 13.6 eV that cannot ionize H atoms but do dissociate molecules ($H_2 + photon \rightarrow H + H$), and ionize elements such as carbon ($C + photon \rightarrow C^+ + electron$). Inside the PDR, the far-ultraviolet photon flux gradually decreases due to dust grain extinction and $H_2$ line absorption, as do the gas and dust temperatures. These gradients produce a layered structure with different chemical compositions as one moves from the cloud edge to the interior. The ionized nebula (the H II region) can be traced by the visible light emission from atomic ions (such as the [S II] 6,731 Å electronic line). The ionization front is delineated by the [O I] 6,300 Å line of neutral atomic oxygen (Fig. 1). Both transitions are excited by high-temperature collisions with electrons. Therefore, their intensities sharply decline as the electron abundance decreases by a factor of 10 at the H II/H transition layer. In Fig. 1b, the dark cavity between the ionization front and the HCO$^+$-emitting zone is the neutral ‘atomic layer’ ($x$($H_2$) $> x$(H)$ \gg x$(H$^+$)), where $x$ is the species abundance with respect to $H$ nuclei. This layer is very bright in mid-infrared polycyclic aromatic hydrocarbon emission, and cools via the far-infrared O and C$^+$ emission lines. Although most of

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the electrons are provided by the ionization of C atoms (thus \(x(e^{-}) \approx x(C^{+}) \approx 10^{-4}\))\(^{14,16}\), the gas is mainly heated by collisions with energetic (about 1 eV) electrons photo-activated from small grains and polycyclic aromatic hydrocarbons\(^{2-14}\). For the strong far-ultraviolet radiation flux impinging the Orion Bar\(^{3,5}\), which is approximately \(4.4 \times 10^{4}\) the average flux in a local diffuse interstellar cloud\(^{16}\), a gas density \(n_{H} = n(H) + 2n(H_{2})\) of \((4-5) \times 10^{4}\) cm\(^{-3}\) in the atomic layer is consistent with the observed separation between the ionization and dissociation fronts\(^{3,4}\).

ALMA resolves the sharp edge where the HCO\(^{+}\) and CO emission becomes intense (Fig. 2). These layers spatially coincide with the brightest peaks of H\(_{2}\) vibrational emission (H\(_{2}\)) tracing the H\(_{2}\)/H\(_{2}\) transition (Extended Data Fig. 2). Therefore, the H\(_{2}\)/H\(_{2}\) and the C\(^{+}\)/C/CO transition zones occur very close to each other. Static equilibrium models of a PDR with \(n_{H} = (4-5) \times 10^{4}\) cm\(^{-3}\) predict\(^{4,9,14}\), however, that the C\(^{+}\)/CO transition should occur deeper inside the molecular cloud because of the lower ionization potential of C atoms (11.3 eV) and because CO may not self-shield from photodissociation as effectively as H\(_{2}\). The spatial coincidence of several H\(_{2}\) and HCO\(^{+}\) emission peaks shows that the formation of carbon molecules starts at the surface of the cloud (initiated by reactions of C\(^{+}\) with H\(_{2}\)). This shifts the C\(^{+}\)/CO transition closer to the ionization front and suggests that dynamical effects are important\(^{17,18}\).

To zero order, the CO \(J = 3\rightarrow 2\) (where \(J\) is the rotational quantum number) line intensity peak (\(T_{\text{peak}}^{\text{CO}}\) in K) is a measure of the gas temperature \(T\) in the molecular cloud (\(\delta x > 15''\) in Fig. 2c, where \(\delta x\) is the distance to the ionization front). The HCO\(^{+}\) \(J = 4\rightarrow 3\) integrated line intensity (\(W_{\text{CO}}^{\text{HCO}}\) in K km s\(^{-1}\)), however, scales with the gas density \(n_{H}\) (see Methods and Extended Data Fig. 3). Although the \(T_{\text{peak}}^{\text{CO}}\) image shows a relatively homogenous temperature distribution, the \(W_{\text{CO}}^{\text{HCO}}\) image shows small-scale structure (Fig. 2a, b). In particular, ALMA resolves several bright HCO\(^{+}\) emission peaks (filamentary substructures, some akin to globules) surrounding the dissociation front and roughly parallel to it. These substructures are surrounded by a lower-density gas component, with \(n_{H} \approx (0.5-1.0) \times 10^{3}\) cm\(^{-3}\), producing an extended (ambient) emission\(^{4,5}\). The HCO\(^{+}\) substructures (with a typical width of about \(2'' \approx 4 \times 10^{-3}\) pc) are located at the molecular cloud edge, and are different to the bigger (5''-10'') condensations previously seen deeper inside the molecular cloud\(^{6,19}\).

To investigate the stratification of molecular emission inside the cloud, we constructed averaged emission cuts perpendicular to the Orion Bar. Three emission maxima are resolved in the \(W_{\text{CO}}^{\text{HCO}}\) crossections at roughly periodic separations of about 5'' (approximately 0.01 pc; Fig. 2c). Excitation models show that the average physical conditions that reproduce the mean CO and HCO\(^{+}\) intensities towards the dissociation front (at \(\delta x \approx 15''\)) are \(T \approx 200-300\) K and \(n_{H} \approx (0.5-1.5) \times 10^{6}\) cm\(^{-3}\) (see Methods and Extended Data Fig. 3). Hence, the over-dense substructures have compression factors of about 5-30 with respect to the ambient gas component and are submitted to high thermal pressures (\(P/k = n_{H}T \approx 2 \times 10^{8}\) K cm\(^{-3}\)). The three periodic maxima suggest that a high-pressure compression wave exists, and is moving into the molecular cloud. This wave may be associated with an enhanced magnetic field (several hundred microgauss; see Methods).

In the very early stages of an expansion of the H\(_{II}\) region into molecular clouds, theory predicts that the ionization and dissociation fronts are co-spatial (an R-type front\(^{15,20}\)). Soon after (\(t < 1,000\) yr), the expansion slows down and the dissociation front propagates ahead of the ionization front and into the molecular cloud\(^{16,17}\). The ionization front changes to a D-type front (a compressive wave travels ahead of the ionization front\(^{16,20}\) and the neutral gas becomes denser than the ionized gas). For a front advancing at a speed\(^{17,18}\) of 0.5-1.0 km s\(^{-1}\), the observed separation between the ionization and dissociation fronts in the Orion Bar implies a crossing time of 25,000-50,000 yr. Later in the expansion phase, when \(t\) is several times greater than the dynamical time \(t_{\text{dyn}}\) of the expanding H\(_{II} \) region (the ratio of the initial radius of the H\(_{II}\) region, the so-called Strömgren radius, and \(R_{\text{HII}}\)), the compressive wave slowly enters into the molecular cloud\(^{21,22}\) (\(t_{\text{dyn}} \approx 0.2\) pc per 10 km s\(^{-1}\) \approx 20,000yr for the Orion Bar). Observational evidence of such dynamical effects is scarce.

In the compressed layers suggested by ALMA (where \(\delta x\) is between 7'' and 30'' in Fig. 2a), the distribution of the gas densities follows a relatively narrow log-normal distribution (Fig. 2d). This is consistent
with magnetohydrodynamic simulations of non-gravitating turbulent clouds\textsuperscript{23,24}. When the entire observed field is analysed, the shape of the distribution is closer to a double-peaked log-normal distribution. This resembles specific simulations in which the cloud compression is induced by the expansion of the ionized gas\textsuperscript{24,25} (and not by a strong turbulence). Searching for further support for this scenario, we investigated the degree of turbulence and compared the different contributions of the gas pressure in the PDR (Extended Data Table 1). The inferred non-thermal (turbulent) velocity dispersion, about 1 km s\textsuperscript{-1}, results in a moderate Mach number of \( \lesssim 1 \) (the ratio of the turbulent velocity dispersion to the local speed of sound)—that is, only a gentle level of turbulence. The thermal pressure exerted by the H II region at the H\textsuperscript{+}/H interface\textsuperscript{1} is several times higher than the turbulent and thermal pressures in the ambient molecular cloud. These pressure differences, together with the detection of over-dense substructures close to the cloud edge, agree with the ultraviolet radiation-driven compression scenario\textsuperscript{25,26}. Whether these substructures could be the seeds of future star-forming clumps (for example, by merging into massive clumps) is uncertain\textsuperscript{22,27}. Gravitational collapse is not apparent from their density distribution (no high-density power-law tail\textsuperscript{24,25}). Indeed, their estimated masses (less than about 0.005\(M_\odot\), where \(M_\odot\) is the mass of the Sun) are much lower than the mass needed to make them gravitationally unstable. Even so, the increased ultraviolet shielding produced by the ridge of high-density substructures probably contributes to protecting the molecular cloud from photodestruction for longer periods.

The ALMA images also show CO emission ripples\textsuperscript{28} along the surface of the molecular cloud (undulations separated by less than about 5\(''\) \(\approx 0.01\) pc in Fig. 2b), which are indicative of instabilities at the dissociation front. Such small-scale corrugations resemble the ‘shell’ instability produced by the force imbalance between thermal (isotropic) and ram (parallel to the flow) pressures\textsuperscript{29}. Characterizing these interface instabilities in detail would require new magnetohydrodynamic models that include mesh-resolutions that are well below the 0.1–0.01 pc scales achieved in current simulations\textsuperscript{30} and include neutral gas thermochemistry.

Finally, ALMA reveals fainter HCO\textsuperscript{+} and CO emission in the atomic layer (HCO\textsuperscript{+} globulettes and plume-like CO features at \( l < 15''\), Fig. 2a, b). The dense gas HCO\textsuperscript{+} emission structures must have survived the passage of the dissociation front\textsuperscript{30}, whereas the CO plumes (isotropic) and ram (parallel to the flow) pressures\textsuperscript{29}. Characterizing these interface instabilities in detail would require new magnetohydrodynamic models that include mesh-resolutions that are well below the 0.1–0.01 pc scales achieved in current simulations\textsuperscript{30} and include neutral gas thermochemistry.

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Author Information We used the ALMA data ADS/JAO.ALMA#2012.1.00352.S available at https://almascience.eso.org/ao/#/project_code=2012.1.00352.S. Reprints and permissions information is available at www.nature.com/reprints. The authors declare no competing financial interests. Readers are welcome to comment on the online version of the paper. Correspondence and requests for materials should be addressed to J.R.G. (jrgoicoechea@icmm.csic.es).

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METHODS
ALMA interferometric and IRAM 30-m single-dish observations. ALMA Cycle-1 observations of the Orion Bar were carried out using 27 12 m antennas in band 7 at 345.796 GHz (CO J = 3–2) and 356.734 GHz (HCO⁻ J = 4–3). The observations consisted of a 2-pointing (the array points to 27 different positions to cover the field) mosaic centred at right ascension α(2000) = 5h 35 min 20.6 s; declination δ(2000) = −05° 25′ 20″. The total field-of-view is 58° × 52°. Baseline configurations from about 12 m to about 444 m were used (C23-23 non-antenna configurations). The data were observed with correlators providing a resolution of approximately 500 kHz (ν×≈0.4 km s⁻¹) over a 937.5 MHz bandwidth. The total observation time on the ALMA 12 m array was around 2h. ALMA executing blocks were first calibrated in the CASA software (version 4.2.0) and then exported to GILDAS. To recover the large-scale extended emission filtered out by the interferometer, we used fully sampled single-dish maps as ‘zero-’ and ‘short-spacings’. Maps were obtained with the IRAM 30 m telescope (Pico Veleta, Spain) using the EMIR330 receiver under excellent winter conditions (<1 mm of precipitable water vapour). On-the-fly scans of a 170° × 170° region were obtained both along and perpendicular to the Orion Bar. The beam full-width at half-maximum power (FWHM) at 350 GHz is about 7″. The GILDAS/MAPPING software was used to create the short-spacing visibilities¹¹ not sampled by ALMA. These visibilities were merged with the interferometric observations. Each mosaic field was imaged and a dirty mosaic was built. The dirty image was deconvolved using the standard Hög bomb CLEAN algorithm and the resulting cubes were scaled from Jansky per beam to a brightness temperature scale using the synthesized beam size of about 1″. This resolution is a factor of approximately 9 higher than previous interferometric observations of the HCO⁻ J = 1–0 line towards the Orion Bar²⁰. The achieved root mean squared noise is about 0.4 K per 0.4 km s⁻¹. In the early phase, the achieved root mean squared noise is about 0.4 K per 0.4 km s⁻¹. Compared with most PDR models, the columns of H2 are treated on a grid of nonlocal, non-local thermodynamic equilibrium excitation and radiative transfer models for CO and HCO⁻. Therefore, minor morphological differences between the near-infrared and millimetre wave images could reflect a small-scale or patchy extinction differences in the region¹. Extinction and radiative transfer models for CO and HCO⁻. To estimate the physical conditions of the HCO⁻–emitting gas near the dissociation front we run a grid of nonlocal, non-local thermodynamic equilibrium excitation and radiative transfer (Monte Carlo) models. This approach allows us to explore different column densities, gas temperatures and densities. Compared with most PDR models (using local escape probability approximations) our models take radiative pumping, line trapping and opacity broadening into account. This allows for the treatment of optically thick lines (see the appendix in ref. 36 for code details and benchmarking tests). Our models use the most recent inelastic collisional rates of HCO⁻ with H₂ and with electrons, and of CO with both H₂ and H. The electron density, nₑ, is an important factor in the collisional excitation of molecular cations in a far-ultraviolet-illuminated gas. For HCO⁻, collisions with electrons start to contribute above nₑ > 10⁻³ cm⁻³ (or nₑ > 10⁵ cm⁻³ if most of the electrons are provided by carbon atom ionization). In PDRs, collisions of molecules with H atoms can also contribute because the molecular gas fraction, f = 2n(H)/[n(H) + 2n(H₂)], is not 1 (a fully molecular gas). We adopted f = 0.8 and varied xₑ between 0 and 10⁻⁴. The H₂ ortho-to-para ratio was computed for each gas temperature T. Radiative excitation by the cosmic microwave background (T_CMB = 2.7 K) and by the far-infrared dust continuum in the Orion Bar (simulated by optically thin thermal emission at T_dust = 55 K) were also included. Column densities of (HCO⁻) (5–1) × 10¹³ cm⁻² and (HCO⁻) (1.0–0.5) × 10¹⁸ cm⁻² were estimated using information from our IRAM 30-m telescope line-survey towards the dissociation front. Several HCO⁻, H₂CO⁺, H²CO⁺ and C²O rotational lines were included in the estimation (the quoted dispersions in the column densities reflect the uncertainty obtained from least square fits to rotational population diagrams). They are consistent with previous observations in the region²⁶. Radiative transfer models were run for (HCO⁻) = 5 × 10¹⁶ cm⁻², N(CO) = 1.0 × 10¹⁸ cm⁻², and N(H) = (2 + n(H₂)/2) × 10¹⁰ cm⁻³ (equivalent to A_T ≃ 27 mag for the dust properties in Orion). This results in x(HCO⁻) ≃ (2–3) × 10⁻⁵ and x(CO) ≃ (2.5–7.5) × 10⁻⁵ abundances. In addition, the HCO⁻/H₂CO⁺ column density ratios derived from single-dish observations are similar to the 12C/13C = 67 isotopic ratio in Orion²⁸. Therefore, the HCO⁻/H₂CO⁺ line intensity ratios would be considerably smaller. A non-thermal (turbulent) velocity dispersion (δv_turb) of about 1 km s⁻¹ reproduces the observed line widths. A similar value, 1–1.5 km s⁻¹, is inferred directly from the observed line profiles (δv_turb = σ_v/(x(12C/13C) = 1.0–1.7 km s⁻¹, where m is the mean mass per particle and kB is the Boltzmann constant) this results in moderate Mach numbers M = δv_turb/crit ≤ 1. Extended Data Fig. 3 shows model predictions for the CO J = 3–2 line intensity peak, W_CO³²–⁴₃ (upper left panel), and HCO⁻ J = 4–3 line integrated intensity, W_HCO⁻₄₃–⁵₄ (where Tₖ is the line brightness temperature) (K km s⁻¹), for different T and n_H₂ values. For optically thick lines (τ_lines ≫ 1), W_CO³²–⁴₃ provides a good measure of the excitation temperature, with T_lines ≃ k_B T_k/σ_B × [exp (k_B T_k/σ_B) − 1]⁻¹ (where T_k is the excitation temperature of the transition and σ_B is the upper level energy). In addition, for low-critical-density (n_H₂) transitions such as the low-J CO transitions, the lines are close to thermalization at densities above about 10¹⁰ cm⁻³, thus T_lines ≃ T (with n_H₂ ≃ A_v/T_k, where A_v is the Einstein coefficient for spontaneous emission and T_k is the coefficient of the collisional de-excitation rate). In this case, T_lines = k_B T_k/σ_B is a good thermometer of the the CO/T₂→₃ emitting layers. The HCO⁻ J = 4–3 line, however, has much higher critical densities (n_H₂_th > 5 × 10¹⁰ cm⁻³ and n_H₂ ∝ 10 cm⁻³). For n_H₂ ≤ 2 × 10¹⁰ cm⁻³, T_lines (sub-thermal excitation), the integrated line intensity W_HCO⁻₄₃–⁵₄ is approximately linearly proportional to (T lines) = x(HCO⁻)/n_H₂ (where l is the cloud length along the line of sight) even if the line is moderately thick. PDR models²⁷ and CO observations strongly suggest that x(HCO⁻) and T_lines do not change substantially in the PDR layers around the H₂ emission peaks (cloud depths between A_v ≃ 1 and 2 mag). In a nearly edge-on PDR, the spatial length along the line of sight does not change greatly either. We compute that for the inferred T and (HCO⁻) values in the region, the integrated line intensity W_HCO⁻₄₃–⁵₄ is proportional to the density in the n_H₂ = 10¹⁰–10¹⁺ cm⁻³ range (the correlation coefficient is r = 0.98 for models with xₑ = 0 and xₑ = 10⁻⁴). Moreover, W_HCO⁻₄₃–⁵₄ still increases with a density of up to several 10¹⁰ cm⁻³ (r = 0.94). This reasoning justifies the use of W_HCO⁻₄₃–⁵₄ as a proxy for n_H₂ in the region. Average physical conditions in the compressed structures. The physical conditions that reproduce the mean CO J = 3–2 line peak and HCO⁻ J = 4–3 integrated line intensity towards the compressed structures at l = 15° (peak_w_CO³²–⁴₃ = 164 ± 10 K and W_CO³₂–⁴₃ = 69 ± 18 K km s⁻¹) are T = 200–300 K and n_H₂ = (1.0 ± 0.5) × 10¹³ cm⁻² (Extended Data Fig. 3). This implies high thermal pressures, P_COMP = k_B T_l(1.0–4.5) × 10⁷ K cm⁻³ (where P_COMP is the pressure in the compressed gas component). The brightest HCO⁻ emission peaks (with W_HCO⁻₄₃–⁵₄ ≃ 100 K km s⁻¹, Fig. 2a) probably correspond to specific gas density enhancements. For the range of column densities and physical conditions at l = 15°, the gas temperature uncertainty is determined by the lack of higher-J CO lines, observed at high angular resolution, to better constrain T from excitation models. The range of estimated gas densities is dominated by the dispersion (about 25%) of the mean W_HCO⁻₄₃–⁵₄ value. The above physical conditions suggest that the cloud edge contains substructures that are denser than the atomic layer (l = (4–5) × 10⁻³ cm⁻¹) and denser than the ambient molecular cloud (n_H₂ = (0.5–1.0) × 10¹⁳ cm⁻³). The equivalent
Gas pressures, magnetic field and compression. In the ambient molecular cloud (Extended Data Table 1). As we find similar contributions from the thermal and non-thermal (turbulent) pressures in both the ambient cloud and the over-dense substructures (\(\sigma = P_{\text{th, amb}}/P_{\text{amb, comp}} = P_{\text{th, amb}}/P_{\text{amb, comp}} \approx 1\)), it is reasonable to assume equipartition of thermal, turbulent and magnetic energies to quantify the magnetic pressure in the PDR (\(P_{B} = B^{2}/8\pi\)). In particular, for \(\beta = P_{B}/P_{\text{th}} = 1\) we estimate the magnetic field strengths \(B\) to be 200 \(\mu\)G and 800 \(\mu\)G in the ambient and in the high-density substructures, respectively. Such strong magnetic fields at small scales need to be confirmed observationally (both the strength and the orientation) but seem consistent with the high values (approximately 100 \(\mu\)G) measured in the low-density foreground material\(^{38}\) (the Orion Veil) confirming that \(B\) is particularly strong in the Orion complex. On much smaller spatial scales, low-angular-resolution observations do suggest that \(B\) increases with density at \(H\)\(\upalpha\)/cloud boundaries (\(B \propto n_{H}^{-1/2}\)) (ref. 46).

A strong magnetic field would be associated with large magnetosonic speeds (\(v_{\text{ms}}\)) in the PDR. If an ultraviolet radiation-driven shockwave is responsible for the molecular gas compression, its velocity is predicted to slow down to \(v_{\text{ms}} \approx 3 \text{ km s}^{-1}\) once it enters the molecular cloud\(^{43}\). Such a slow, magnetized shock wave could travel ahead of the shock front\(^{42}\). Thus, a high magnetic field strength may be related to the \(H\)\(\upalpha\)/cloud undulations seen perpendicular to the Orion Bar (Fig. 2c). The inferred compression factor in the observed substructures (\(f = n_{\text{comps}}/n_{\text{amb}} = 5–30\)) is consistent with slow shock velocities\(^{46}\), \(v_{\text{ms}} \approx 0.5 \times 10^{-3} \text{ km s}^{-1}\) where \(v_{\text{ms}}\) is the initial sound speed of the unperturbed molecular gas. The necessarily small \(v_{\text{ms}}\) agrees with the relatively narrow molecular line-profiles (\(\Delta v_{\text{FWHM}} \leq 4 \text{ km s}^{-1}\)) seen in PDRs\(^{14}\) (including observations of face-on sources in which the shock would propagate in the line of sight). Owing to the high thermal pressure in the compressed structures, we also find that a pressure gradient, with \(P_{\text{th, comp}} > P_{\text{th, amb}}\), exists. This subtle effect is seen in simulations of an advancing shockwave around an H\(\upalpha\) region\(^{24,48}\). Molecular gas between the ionization and dissociation fronts. ALMA reveals fainter HCO\(^{+}\) and CO emission in the atomic layer (HCO\(^{+}\) globules and plume-like CO features at \(v_{\text{loc}} < 15\) km s\(^{-1}\), Fig. 2). Previous low-angular-resolution observations and models had suggested the presence of dense spherical clumps with sizes of \(5–10 \text{ km}^{-1}\) deeper inside the molecular cloud\(^{38}\) (at \(v_{\text{loc}} \approx 20\) km s\(^{-1}\)) (from the ionization front\(^{38,39}\). The dense substructures resolved by ALMA are smaller (\(\lesssim 2 \times 4\) ) and are detected at \(v_{\text{loc}} \approx 7\) km s\(^{-1}\) (even before the peak of the \(H\)\(\upbeta\) line emission). The molecular line profiles towards the plumes typically show two velocity emission components (Fig. 3) at one centred at \(v_{\text{loc}} \approx 8.5 \text{ km s}^{-1}\), (where \(v_{\text{loc}}\) refer to the emission velocity with respect to the local standard of rest), the velocity of the background molecular cloud in the back-side of M 42 (ref. 11; not directly associated with the Orion Bar), and at \(v_{\text{loc}} \approx 11\) km s\(^{-1}\), the velocity component of the molecular gas in the Orion Bar. In addition, despite the small size of the observed region, the crosscuts of the HCO\(^{+}\) line (at \(v_{\text{loc}} \approx 20\) km s\(^{-1}\)) (at \(v_{\text{loc}} \approx 20\) km s\(^{-1}\)) are detected at \(v_{\text{loc}} \approx 7\) km s\(^{-1}\) (even before the peak of the \(H\)\(\upbeta\) line emission). Molecular line profiles towards the plumes typically show two velocity emission components (Extended Data Fig. 4), one centred at \(v_{\text{loc}} \approx 8.5 \text{ km s}^{-1}\), (where \(v_{\text{loc}}\) refer to the emission velocity with respect to the local standard of rest), and the velocity of the background molecular cloud in the back-side of M 42 (ref. 11; not directly associated with the Orion Bar), and at \(v_{\text{loc}} \approx 11\) km s\(^{-1}\), the velocity component of the molecular gas in the Orion Bar. 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HF + C⁺ → CF⁺ + H reactions and is quickly destroyed by recombination with electrons\textsuperscript{31,33}. Hence, the (lower-than-predicted) observed CF⁺ abundances probably reflect a dynamical PDR behaviour as well.

Stationary PDR models of strongly irradiated dense gas (with \(N_\text{H}\) values of a few \(10^5\) cm\(^{-2}\)) have been presented in the literature\textsuperscript{3,4,5}. The above densities are similar to those inferred in the compressed substructures at the Orion Bar edge. Thus they can be used to gain insight into the chemistry that leads to the formation of HCO⁺ and CO in ultraviolet-irradiated dense gas. Owing to the higher densities and enhanced H\(_2\) collisional de-excitation heating, the gas attains higher temperatures. This triggers a warm chemistry in which endothermic reactions and reactions with energy barriers become faster. As a result, higher HCO⁺ abundances are predicted close to the dissociation front (x(HCO⁺) > several \(10^5\)) of several \(10^5\) cm, or an angular-scale of about 0.5 arcseconds with gas densities of a few \(10^6\) cm\(^{-3}\).

In the Orion Bar, the intensity of the H\(_2\) line is approximately proportional to the gas density\textsuperscript{42}. Therefore, the HCO⁺ formation route from CH\(_3\)⁺ can dominate over the formation of HCO⁺ from CO\(^+\) (after the \(O + H_2 \rightarrow OH + H\) reaction, followed by C\(^+\) + OH \rightarrow CO\(^+\) + H, and finally CO\(^+\) + H \rightarrow HCO⁺ + H\(^+\))\textsuperscript{31,33}. Both OH and CO\(^+\) have been detected in the Orion Bar\textsuperscript{36,37}, but high-angular-resolution maps do not exist. Recombination of HCO⁺ with electrons then drives CO production near the dissociation front\textsuperscript{31,33}.

Extrapolating the above chemical scenario, the brightest HCO⁺ \(J = 4 \rightarrow 3\) emission peaks in the Orion Bar should be close to H\(_2\) emission peaks. Extended Data Fig. 2a shows a remarkable spatial agreement between the H\(_2\) \(v = 1 \rightarrow 0\) (S(1)) emission peaks and several HCO⁺ emission peaks. Detailed H\(_2\) excitation models (including both far-ultraviolet-pumping and collisions) show that for the conditions prevailing in the Orion Bar, the intensity of the H\(_2\) \(v = 1 \rightarrow 0\) S(1) line is approximately proportional to the gas density\textsuperscript{22}. Therefore, the HCO⁺ peaks that match the position of the H\(_2\) \(v = 1 \rightarrow 0\) S(1) line peaks probably correspond to gas density enhancements as well. This agrees with the higher H\(_2\) \(v = 1 \rightarrow 0\) S(1)/\(v = 2 \rightarrow 1\) S(1) \(\equiv S\) line intensity ratios observed at the dissociation front and consistent with efficient H\(_2\) collisional excitation\textsuperscript{22}. The ALMA images thus confirm that in addition, or as a consequence of dynamical effects, reactions of H\(_2\) with abundant atoms and ions contribute to the molecular gas production towards the cloud edge. Even higher-angular-resolution observations of additional tracers will be needed to fully understand this, and to spatially resolve the chemical stratification expected in the over-dense substructures themselves. We note that if most of the carbon becomes CO at \(A_V \approx 2\) (\(N_\text{CO}\) of several \(10^{12}\) cm\(^{-2}\)) in substructures with gas densities of a few \(10^5\) cm\(^{-3}\), this depth is equivalent to a spatial length of several \(10^5\) cm, or an angular-scale of about 0.5 arcsec at the distance to Orion.

Deeper inside into the molecular cloud (\(b \approx 30^\circ\)), the CO\(^+\), CH\(_3\)⁺, and CH\(_2\)⁺ abundances sharply decrease. The far-ultraviolet flux greatly diminishes, and the gas and dust grain temperatures accordingly decrease. The HCO⁺ abundance also decreases until the CO + H\(_2\) \rightarrow HCO⁺ + H reaction starts to drive the HCO⁺ formation at low temperatures. Gas-phase atoms and molecules gradually deplete and dust grains become coated by ices as the far-ultraviolet photon flux is attenuated at even larger cloud depths (see Extended Data Fig. 1).

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**Extended Data Figure 1 | Structure of a strongly ultraviolet-irradiated molecular cloud edge.** The incident stellar ultraviolet radiation comes from the left. The velocity of the advancing ionization and dissociation fronts are represented by $v_{IF}$ and $v_{DF}$ respectively. In the Orion Bar, the dissociation front is at about 15″ (about 0.03 pc) from the ionization front. UV, ultraviolet; PAH, polycyclic aromatic hydrocarbons. The snow line refers to the inner cloud layers where molecular gases start to freeze and dust grains become coated by ices.
Extended Data Figure 2 | Comparison with other tracers. a, ALMA HCO$^+$ $J = 4–3$ line integrated intensity. b, ALMA CO $J = 3–2$ line peak (Orion Bar velocity component). The red contours represent the H$^{13}$CN $J = 1–0$ emission (from 0.08 to 0.026 in steps of 0.02 Jy beam$^{-1}$ km s$^{-1}$) of dense condensations inside the Orion Bar$^{19}$. The black contours show the brightest regions of H$_2$ $v = 1–0$ S(1) emission (from 1.5 to 4.5 in steps of 0.5·10$^{-4}$ erg s$^{-1}$ cm$^{-2}$ sr$^{-1}$). The H$_2$ image is saturated between $\delta x = 19''$ and 23'' (that is, no data are shown). Figures have been rotated 127.5° anticlockwise to bring the incident ultraviolet radiation from the left.
Extended Data Figure 3 | Excitation models for different gas temperatures and densities. a, CO $J = 3–2$ line peak (for $N(\text{CO}) = 10^{18}$ cm$^{-2}$). b–d, HCO$^+$ $J = 4–3$ integrated line intensity at 100 K (b), 200 K (c) and 300 K (d). Each curve represents a different electron abundance model: $x_e = 0$ (blue) and $x_e = 10^{-4}$ (red).

Continuous curves are for $N(\text{HCO}^+) = 5 \times 10^{13}$ cm$^{-2}$ and dotted lines for $N(\text{HCO}^+) = 2 \times 10^{14}$ cm$^{-2}$ (appropriate for deeper inside the Orion Bar, $\delta x > 30''$). The horizontal green dashed line represents the average $T_{\text{peak}}^{\text{CO} 3-2}$ (a) and $W(\text{HCO}^+)$ (b–d) with their standard deviation (grey shaded) towards the dissociation front (at $\delta x \approx 15''$).
Extended Data Figure 4 | Line velocity centroid, dispersion and profiles. 

**a**. Vertically averaged cuts perpendicular to the Orion Bar in the HCO$^+$ $J = 4–3$ line velocity centroid (magenta curve) and FWHM velocity dispersion (grey curve).

**b**. CO and HCO$^+$ spectra at representative positions. The top and middle plots show positions between the ionization and dissociation fronts, the bottom plot is inside the molecular Orion Bar. Offsets are given with respect to the rotated images in Extended Data Fig. 2. The velocity of the background cloud is $v_{\text{LSR}} \approx 8.5 \text{ km s}^{-1}$ (black dashed line), whereas the velocity of the Orion Bar is $v_{\text{LSR}} \approx 11 \text{ km s}^{-1}$ (green line).
### Extended Data Table 1 | Gas pressures and estimated magnetic field strengths

|                  | Ionisation front | Atomic layer | Compressed structures | Ambient PDR component |
|------------------|------------------|--------------|-----------------------|-----------------------|
| **Thermal pressure (K cm⁻²)** | $P_{\text{th,eff}}/k = 6 \times 10^7$ | $P_{\text{th,eff}}/k = 5 \times 10^7$ | $P_{\text{th,env}}/k = 2 \times 10^9$ | $P_{\text{th,env}}/k = 10^7$ |
| Non-thermal pressure\(^\dagger\) (K cm⁻²) | $P_{\text{th,env}}/k = 2 \times 10^9$ | $P_{\text{th,env}}/k = 10^7$ |
| Magnetic field $B$ (for $I=I_0/P_0=1$) | $\approx 800$ μGauss | $\approx 200$ μGauss |

All values are for a non-thermal velocity dispersion of $\sigma_{\text{nth}} \approx 1$ km s⁻¹.