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A timeline for massive star-forming regions via deuterium chemistry

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Abstract Chemistry is an extremely powerful tool to estimate the duration of the prestellar phase; it can provide key tools to distinguish between a slow or a fast path towards the formation of stars. The most promising tracers of the quiescent phase are the light, depletion-resistant H_2D^+ and D_2H^+. Our observational effort has led to the first detections of both ortho- and para-H_2D^+ in massive clumps using APEX, ALMA and SOFIA.
We confirm that the anticorrelation among the abundance of o-H_2D^+ and N_2D^+, a species that can be relatively easily observed, is real and that their relative abundance strongly decreases with evolution in the very first stages of the star formation process. The behaviour of these species can be explained with simple considerations on the chemical formation paths, depletion of heavy elements, and evaporation from the dust grain mantles, and can be used as a powerful evolutionary indicator.
Our unique 3D MHD simulations, coupled with chemistry, take us one step further than a simple relative timeline, allowing to follow abundance variations with time. Combining these pieces of the puzzle with the first measurement of the ortho-to-para ratio of H_2D^+ in a massive clump, we will have the opportunity to investigate the duration of the quiescent phase in different mass regimes.

Key words. stars: formation – ISM: abundances – ISM: molecules

1. Introduction

High-mass stars (i.e., with masses in excess of 8 – 10 $M_\odot$) have a critical influence on the physical and chemical conditions of the interstellar medium. They create and disseminate the vast majority of heavy elements, they dominate the energy budget from their immediate surroundings to galactic scales, stir, heat and ionise the gas in their environment, determining how galaxies appear to us.

Although progress has been made recently in the study of the process through which high-mass stars form from cold and dense molecular clumps, many pivotal questions remain open in this research field, mainly due to the extremely short timescales of the first stages, that happen enshrouded in the parent molecular cloud. The initial conditions, how long this process takes, whether high-mass stars are formed first or last in a cluster, and which is their role in regulating the subsequent star-formation activity, are some of these questions. To investigate these issues, a detailed comparison between realistic models and observations is necessary. While this may seem easy, observationally speaking, it is very complex to separate different evolutionary stages and measure their duration.

The first step is to identify where the next generation of high-mass stars will form in the Milky Way. We have recently published a complete sample of high-mass clumps in the inner Galaxy (Urquhart et al. 2018), based on the ATLASGAL survey (Schuller et al. 2009), that offered an unprecedented sensitivity and angular resolution (19″). We classified all the clumps into four evolutionary classes, defined using the well-studied ATLASGAL TOP100 sample (e.g. Giannetti et al. 2014; König et al. 2017; Giannetti et al. 2017b), finding indications for a shortening of the quiescent phase for increasing masses.

The initial phases of the process of high-mass star formation are the critical ones to distinguish between competing theories that predict a fast or slow path towards the formation of stars (Mouschovias et al. 2006; Hartmann et al. 2012). In order to study these phases, we need to have reliable tracers for the cold and dense material that constitutes starless and prestellar cores.

The most common tracers, such as CO and its isotopologues, are not ideal for the task: their abundance is strongly reduced by depletion onto dust grains for temperatures below $\sim 20-25$ K and volume densities of H_2 above $\approx$ few $\times\ 10^4\ \mathrm{cm}^{-3}$, typical of the molecular cores that are the progenitors of stars. This problem is even more severe in the high-mass regime, where these physical conditions transcend the core scale, and characterise clumps, from which entire clusters form (Giannetti et al. 2014), as opposed to single stars or small multiple systems in the case of cores. Even above

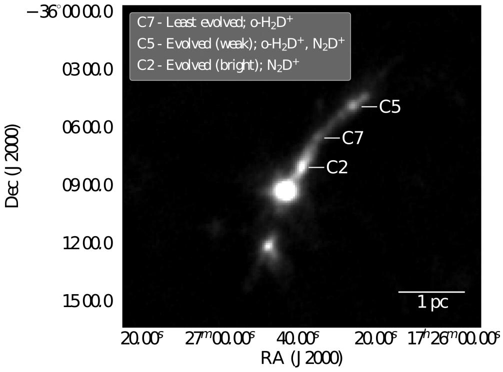

Figure 1. The complex G351.77–0.51, as it appears in ATLASGAL. The selected clumps are indicated.

that, significant depletion characterises entire filaments that host massive clumps (Hernandez et al. 2011; Sabatini et al. 2019; see also Sabatini et al. in this book).

The removal from the gas-phase of the second most abundant molecule in the Universe determines significant changes in the chemistry. Thanks to the exothermicity of the reaction:

$$H_3^+ + HD \leftrightarrows H_2D^+ + H_2 + \Delta E, \qquad (1)$$

the fraction of deuterated H_3^+ increases by orders of magnitude above the canonical value, pushed by the strongly-reduced efficiency of the destruction reactions of H_2D^+ and H_3^+, driven by CO.

It has indeed been observed in low-mass cores that N_2D^+ has a much better resistance to depletion than C-bearing molecules, and selectively traces cold gas. However, evidence has emerged that N_2D^+ and its parent species H_2D^+ appear to be anticorrelated in high-mass objects (Pillai et al. 2012). This anticorrelation has been observed in the Cygnus-X complex combining JCMT observations of the ground-state transition of o-H_2D^+ and interferometric images made with the Submillimeter Array (SMA) of N_2D^+(3-2). It could therefore be spuriously generated by interferometric filtering.

In this work we have set out to understand whether this anticorrelation is real, and if so, what generates it.

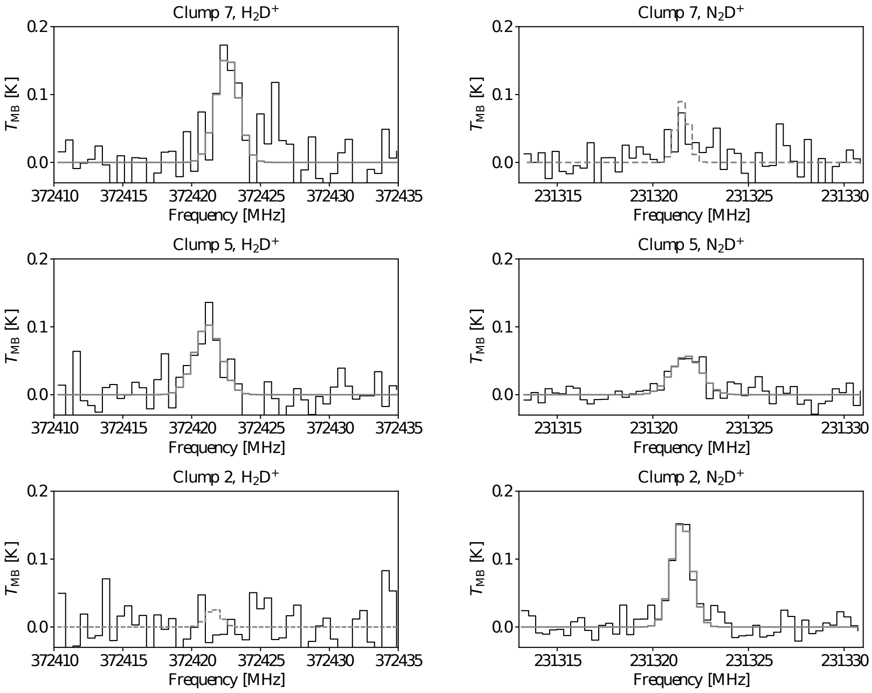

Figure 2. Spectra of the clumps in o-$H_2D^+(1_{1,0} - 1_{1,1})$ (left column) and N_2D^+(3–2) (right column). The best fit is indicated with a solid grey line, while for upper limits dashed lines are used. Adapted from Giannetti et al. (2019), reprinted with permission.

2. The experiment

We have carried out observations with the Atacama Pathfinder Experiment 12 meter submillimeter telescope (APEX) of three clumps in G351.77–0.51 (Fig. 1), the closest and most massive filament (D = 1 kpc, $M \sim 2000$ M$_\odot$; Leurini et al. 2019) identified in ATLASGAL. The clumps were selected in the same complex to minimise the effects of distance and chemical initial conditions, as well as to have similar masses and peak column densities to facilitate direct comparison; a summary of their properties is given in Table 1. The evolutionary stage of the clumps ranges from seemingly quiescent to likely hosting a zero-age main sequence star, based on their luminosity-to-mass ratio, and their continuum properties. Line-of-sight- and beam-averaged CO depletion also varies from high (only 25% of CO in gas-phase) to modest (~ 50% in gas-phase).

To obtain the maximum from the data obtained so far, we have initiated detailed chemical modelling of the pre-stellar phase (e.g. Körtgen et al. 2017, 2018), and we have set up a postprocessing pipeline for the simulations, to derive synthetic observations (Zamponi et al. 2018).

3. Results and discussion

Ortho-$H_2D^+(1_{1,0} - 1_{1,1})$ is detected towards Clumps 7 and 5, while Clumps 2 and 5 have a significant detection in N_2D^+(3–2). Figure 2 shows the observed spectra for all sources, readily indicating an opposite behaviour of the two species.

The column densities are obtained, under the assumption of local thermodynamic equilibrium (LTE), with MCWeeds (Giannetti et al. 2017b). For this calculation we assumed that gas and dust are coupled (i.e. the excitation temperature for the species and the dust tem-

Table 1. Properties of the clumps derived from dust continuum emission. Adapted from Giannetti et al. (2019), reprinted with permission.

Source	T_d	$N(H_2)$	$L_{bol}(R < 14'')^a$	$M(R < 14'')^a$	M^b	*Diameter*	$n(H_2)$
	K	10^{22} cm^{-2}	$L_\odot$	$M_\odot$	$M_\odot$	pc	10^5 cm^{-3}
Clump 7	13.0	7.3	23	31	120	0.18	1.3
Clump 5	15.5	8.7	111	35	100	0.10	2.9
Clump 2	20.0	10.5	331	44	200	0.19	1.8

[a]Within the central 28″. [b]Rescaled for the new dust temperatures from the values in Leurini et al. (2011).

peratures are equal), justified by the high average densities of the clumps.

We estimate the beam- and line-of-sight-averaged abundances taking the ratio of the molecular column density and the H_2 column density, as derived from a grey-body fit to the dust continuum emission, assuming a gas-to-dust mass ratio of 120, from the results of Giannetti et al. (2017a), using a galactocentric distance of 7.4 kpc. The results are shown in Fig. 3 (left), together with the relative abundance of the two species (right), source by source, ordered from the least to the most evolved. Our results strongly indicate that the anticorrelation found in Pillai et al. (2012) is real, and that the abundance of o-H_2D^+ progressively drops in the first stages of the star formation process, contrary to that of N_2D^+, with the former being a factor $\gtrsim$ 10 more abundant in the least evolved clumps (7 and 5).

In order to explain this behaviour, we turned to the chemical evolution in the cold and dense gas. H_2D^+ rapidly forms via reaction 1, which under these conditions proceeds exclusively in the forward direction. Only if there is a substantial fraction of o-H_2 the reaction can happen backwards in cold material (e.g. Gerlich et al. 2002), slowing down the deuteration process; observational evidence towards cold sources indicates that this is not dominant (e.g. Brünken et al. 2014). The increased fraction of D-bearing molecules is then passed on to those species, involved in the ion-neutral chemistry, that have a larger deuteron affinity compared to H_2D^+.

The calculated abundance of o-H_2D^+ is of the order of $\sim 3 \times 10^{-11}$, similar to the values reported for the o-H_2D^+ emission peaks by Pillai et al. (2012), and those in the outskirts of L1544 (Vastel et al. 2006). Such high abundances suggest the presence of extreme CO depletion in the clumps (Caselli et al. 2003). On the contrary, N_2D^+ is not detected in this source, which could be related to the time lag between the formation of H_2D^+ and that of N_2D^+. Recent models (Sipilä et al. 2015) show that reaching abundances close to our estimates could take $\sim 10^5$ yr, setting a qualitative upper limit to the age of Clump 7. The ortho-to-para conversion of H_2, if possible onto dust grain surfaces (Bovino et al. 2017), could push this number down even more. While this process could reproduce the abundances in Clump 7, after N_2D^+ had time to form, one would expect a correlation between the abundance of the two molecules, which is the opposite of what is observed.

Another limiting factor for $X(N_2D^+)$ could be the gas-phase abundance of N_2, which is formed via slow neutral-neutral reactions. Alternatively, N_2 may deplete onto dust grains, having a binding energy similar to CO, but sufficiently smaller to cause a significant difference in the evaporation timescales for the physical properties of our clumps (Giannetti et al. 2019). In both cases, the net effect is a rising N_2 abundance with evolution. To this, one has to add the progressive conversion of H_2D^+ into multiply-deuterated forms (D_2H^+, D_3^+) in cold, highly-depleted gas (Flower et al. 2004). These species are also more efficient in forming N_2D^+. The combination of these processes could explain the observed anticorrelation between o-H_2D^+ and N_2D^+, which acts as a much more efficient evolutionary indicator for the first stages of the star formation process, compared to their individual abundances.

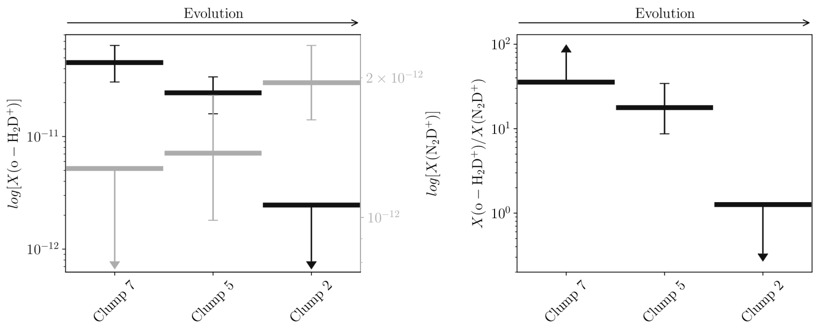

Figure 3. Left: Abundances of o-H_2D^+ (black) and N_2D^+ (grey). Right: Relative abundance of the two species. The clumps appear in order of evolution, from the least to the most evolved. The 95% credible interval is indicated for abundances and ratios; for non-detections, only the upper limit is shown. Adapted from Giannetti et al. (2019), reprinted with permission.

4. Outlook

Ortho-H_2D^+ was recently used, in combination with para-H_2D^+ observations performed with the Stratospheric Observatory for Infrared Astronomy (SOFIA), to estimate the age of a low-mass core ($\gtrsim 10^6$ years; Brünken et al. 2014). The same approach could be used to estimate the lifetime of more massive objects, and thus independently investigate the suggested shortening of the quiescent phase with increasing mass. We started an APEX survey of o-H_2D^+ in the massive clumps of the TOP100, obtaining more than 15 detections (Ordenes et al., in prep.). From these we selected the most promising candidates for SOFIA follow-ups with the upGREAT instrument (Risacher et al. 2018), obtaining the first tentative detection of p-H_2D^+ in a high-mass clump. We also have obtained time in the last cycle to secure this detection.

To infer the age of the clump from these data, we will make use of our unique set of numerical simulations coupled with chemistry, as outlined in Sect. 2. In a major advancement from existing one-zone models that assume constant density, that ignore dynamical evolution and inhomogeneities, we have recently performed for the first time a large set of three-dimensional magneto-hydrodynamical simulations including a complex non-equilibrium chemical network with spin isomers, aimed at following deuterium fractionation in fully depleted clumps and filaments (Körtgen et al. 2017, 2018).

We are also implementing a much more complex chemical network that includes CO and nitrogen chemistry, so that we can directly follow, in particular, the depletion of carbon monoxide, and the behaviour of the o-H_2D^+/N_2D^+ ratio (Bovino et al., in prep.). If this indicator can be calibrated against the ortho-to-para ratio of H_2D^+, it would provide a much more efficient (observationally speaking) way of estimating the age of molecular clumps and cores.

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