Synthetic observations of H$_2$D$^+$ towards high-mass starless cores

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Abstract / Young massive stars are usually found embedded in dense and massive molecular clumps and are known for being highly obscured and distant. During their formation process, deuteration is regarded as a potentially good indicator of the formation stage. Therefore, proper observations of such deuterated molecules are crucial, but still, hard to perform. In this work, we test the observability of the transition o-H$_2$D$^+$(1$_{10}$-1$_{11}$), using a synthetic source, to understand how the physical characteristics are reflected in observations through interferometers and single-dish telescopes. In order to perform such tests, we post-processed a magneto-hydrodynamic simulation of a collapsing magnetized core using the radiative transfer code POLARIS. Using the resulting intensity distributions as input, we performed single-dish (APEX) and interferometric (ALMA) synthetic observations at different evolutionary times, always mimicking realistic configurations. Finally, column densities were derived to compare our simulations with real observations previously performed. Our derivations for o-H$_2$D$^+$ are in agreement with values reported in the literature, in the range of $10^{20-21}$ cm$^{-2}$ and $10^{22-23}$ cm$^{-2}$ for single-dish and interferometric measurements, respectively.

Keywords / ISM: molecules — stars: massive — stars: formation — radio lines: ISM

1. Introduction / ISM: molecules — stars: massive — stars: formation — radio lines: ISM

Massive star formation takes place in the the densest part of molecular clouds, which are characterized by low gas temperatures ($T_g < 20$K), high column densities ($N_g \sim 10^{23-25}$ cm$^{-2}$) and a large degree of CO-depletion. In the earlier stages, due to the latter process, further chemical reactions become much more efficient, such as the formation of deuterated molecules. This process is called deuterium fractionation ($D_{\text{frac}}$) and explains the increased ratio of a deuterated isotopologue column density and its hydrogenated version. The reactions that lead to deuteration are the following:

- $\text{H}_2^+ + \text{HD} \leftrightarrow \text{H}_2\text{D}^+ + \text{H}_2 + 230$ K,
- $\text{H}_2\text{D}^+ + \text{HD} \leftrightarrow \text{D}_2\text{H}^+ + \text{H}_2 + 180$ K,
- $\text{D}_2\text{H}^+ + \text{HD} \leftrightarrow \text{D}_3^+ + \text{H}_2 + 230$ K,

where $\text{H}_2\text{D}^+$ and $\text{D}_2\text{H}^+$ are the first two deuterated ions created. $\text{H}_2\text{D}^+$, in particular, has been suggested to be a reliable chemical clock for star forming regions, due to its sensitivity to environmental conditions (e.g., Caselli et al. [2003]; Brünken et al. [2014]).

Observations of several high-mass clumps have shown that deuteration increases over time as the collapse of the molecular clump proceeds, reaching a maximum point right before the formation of a protostellar object (Fontani et al. [2011]). At this stage, the radiation from the stellar object will lead to an increase of temperatures, with subsequent evaporation of CO, and an eventual decrease of the deuteration fraction.

In this work we traced the abundance of o-H$_2$D$^+$, by performing synthetic observations towards simulated massive starless cores, and compare the results with available observations.
Synthetic observations of high-mass starless cores

Figure 1: Flowchart of the pipeline workflow.

Table 1: Initial parameters of the core selected. The collapse is isothermal, at T=15 K.

| Run       | Radius (pc) | Mass (M☉) | tgf (kyr) | αvlu | M  |
|-----------|-------------|-----------|-----------|------|----|
| Hmu10M2   | 0.1         | 60        | 67        | 0.48 | 2  |

Fig. 1 shows a schematic view of the workflow followed here, since the acquisition of the source, until the final derived observatory-dependent column densities.

2. Synthetic sources

As synthetic sources we used a simulated collapsing molecular cloud core from Kortgen et al. (2017).

The core is turbulent and magnetized (B~70μG), 60 M☉ in mass, and 0.1 pc in radius. The main parameters of the core are listed in Table 1. A snapshot of its gas surface density distribution after 32.1 kyr of evolution is shown in the left panel of Fig. 2.

3. Radiative Transfer

We employed the POLARIS radiative transfer code (Reissl et al. 2016) to simulate the resulting intensity distributions of several quantities included in the cloud simulation, such as, temperature, dust, gas and magnetic field distribution. POLARIS makes use of a Monte Carlo approach to trace the path of light rays before reaching the synthetic detector. This method significantly reduces the numerical noise as well as the runtime compared to previous methods (Haworth et al. 2018).

To map the deuterated molecule distributions, the Line Radiative Transfer (LRT) simulation mode of POLARIS was used for the o-H₂D⁺ transition (1_{10}-1_{11}), assuming Local Thermodynamical Equilibrium (LTE) conditions. We analyzed 11 snapshots of the core at different evolutionary stages up to 1 tgf, placing it at a distance of 1.4 kpc. The resulting intensity distribution of a POLARIS simulation is shown in the second panel of Fig. 2.

4. Synthetic observations

To make observations as realistic as possible, we post-processed the ideal synthetic maps from POLARIS, in order to take into account instrument related effects.

4.1. Single-dish observations

For the single-dish case, new tasks were written to solve each step involved in the creation of realistic cubes. Here, we modeled an APEX-like observation. As we do not attempt to make statements of the APEX real throughput and performance, therefore, they are referred to as APEX-like observations. We developed an analysis tool to perform tasks on cubes and single images, such as the convolution with a Point Spread Function (PSF), conversion between observable quantities and addition of noise. We first convolved the ideal images with the beam of the telescope, represented by the PSF, here assumed to be Gaussian. The beam resolution was 16.8” at 372.4 GHz (∆ν=0.03 km s⁻¹). Then we added normally distributed noise to the images. In order to increase the peak signal-to-noise ratio (SNR), we binned the spectra up to 0.5 km s⁻¹, resulting in a noise level (T_{rms}) of 0.02 K. Such a setup returns detections at a 5σ confidence level, for an integration of 1.8 hr. The values were computed using the APEX Observing Time Calculator. See the rightmost panel in Fig. 2 for a 16.8” single-pointing synthetic observation.

4.2. Interferometric observations

For the interferometric observations, the Common Astronomy Software Applications (CASA) tool was used. CASA has been designed for ALMA and VLA data analysis, and provides also a simulation mode. As for a single-dish, we used the POLARIS outcome as the input model and generated the measurement set by calling the simobserve task with a synthesized beam of 0.55”, reached by the Cycle 6 C43-3 array configuration in band 7. ALMA spectral resolutions are one order of magnitude wider than APEX at this frequency (∆ν=0.23 km s⁻¹), improving in sensitivity. The noise level was set at 6 mJy for an integration time of 40 min, obtained by the ALMA Sensitivity Calculator. After the observation, we imaged the data by deconvolving the visibilities using the CLEAN algorithm. The cleaning step was performed by the simanalyze task. The outcome of an ALMA simulation is shown in the third panel of Fig. 2.

5. Results

5.1. Column densities

Column densities of o-H₂D⁺ were obtained as in Vastel et al. (2006), via

\[
N(X) = \frac{8\pi v^3 Q(T_{ex})}{c^3} \frac{e^{E_u/T_c} - 1}{\epsilon_{\nu} A_{\nu} \epsilon_{\nu}/kT_{ex} - 1} \int \tau dv,
\]

where u and l refer to the upper and lower energy level of each transition, respectively. All of the parameters required here are retrieved from the upper and lower level energy of each transition, respectively. All of the parameters required here are retrieved from the Leiden Atomic and Molecular Database (LAMDA) (Schoier et al. 2005), and summarized in Table 2. The partition function (Q) was recreated by a cubic spine interpolation of the available values in the Cologne Database for Molecular Spec-
Figure 2: *Left to right:* Gas surface density distribution of the clump used as synthetic source at 32.1 kyr; o-H$_2$D$^+$ emission taken as the output of the POLARIS radiative transfer simulation; ALMA synthetic observation of the clump at 0.5" resolution and APEX synthetic observation at 16.8" resolution.

Table 2: LAMDA parameters for the o-H$_2$D$^+$($1_{10-11}$) transition. The statistical weight $g_{ul}$ is 9 and $T_{ex}$ 15 K.

| Transition  | $\nu$ (GHz) | $A_{ul}$ (s$^{-1}$) | $E_{ul}$ (K) | $Q(T_{ex})$ |
|------------|-------------|---------------------|-------------|-------------|
| o-H$_2$D$^+$($1_{10-11}$) | 372.4 | 1.08 $\times$ 10$^{-4}$ | 17.87 | 1.122 |

Figure 3: *Top to bottom:* Column densities derived from the model (solid line) along with interferometric (green pentagons) and single-dish (blue hexagons) observations. Colored areas and horizontal dashed lines represent ranges of values observed onto similar sources.

6. Discussions

In this work we performed synthetic observations of a collapsing molecular magnetized core at different angular resolutions, attempting to understand the main differences that arise when observing either with an interferometer or a single-dish. In the upper panel of Fig. 3 we show the column densities derived from the model, along with ALMA and APEX, at 235 AU (highest resolution element in the simulation), 0.55" and 16.8", respectively, to explore the loss of information while reducing the resolution. Column densities at each time were calculated as the average inside a circular region defined by the highest resolution element. Based on this, as real column densities decay from their peak as a function of the impact parameter (Caselli et al., 2003), we can state that lower resolutions (wider beams) return lower values due to the inclusion of low column densities from external regions. Therefore, we expect APEX estimations to be lower than those retrieved by ALMA. Colored regions as well as semi-dashed and pointed lines represent observed column densities reported in the literature. All these values have been obtained via single-dish observations (APEX, JCMT and CSO). Even though some of the reported column densities are higher than what we obtained, our results match those from massive sources, such as Pillai et al. (2012) and G351 observations, where brightness temperatures are lower than toward high-mass sources ($T_{mb} < 1$ K), same as our case. Middle and bottom panels of Fig 3 show differences between both resolutions and the model average in a region corresponding to each beam. Quantities returned by both facilities show a similar reduction of the inferred column density by less than an order of magnitude, evidencing similar responses.

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