

NH₂D in Orion KL: Results from ALMA, EVLA, and IRAM

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We present results from interferometric image cubes of five deuterated ammonia (NH₂D) transitions in the Kleinmann-Low Nebula (Orion KL), a nearby (~450 parsecs) star-forming region at the high-powered heart of the Orion Nebula. Our multi-interferometer sample spatially and kinematically resolves NH₂D into distinct emitting regions, and features diverse upper excitation levels from ~20 to 150 K above ground, a range sensitive to the source temperature in Orion KL. **In these data, we find unambiguous evidence that NH₂D is not currently being produced in the gas phase, supporting the hypothesis that the NH₂D population may have been preserved on dust grains, desorbing into the gas as the nebula's temperature increased.**

NH₂D Emission Lines Observed

Frequency (GHz)	Upper Excitation Level (Kelvin)	Observatory	Year
239.848	120.1 (ortho)	ALMA (SV)	2012
216.562	119.5 (para)	ALMA (SV)	2012
110.153	21.2 (para)	IRAM	2009
43.042	94.5 (para)	EVLA	2010
25.023	152.3 (para)	EVLA	2009

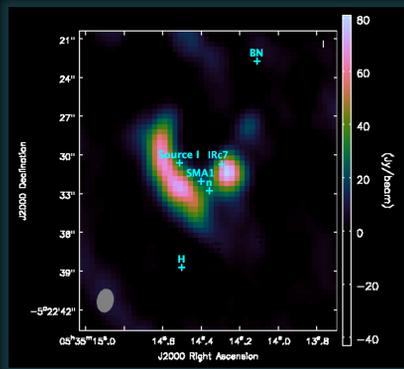


Fig. 1: (top) Moment 0 (integrated spectrum) map of the seemingly uncontaminated 239 GHz NH₂D line. Synthesized beam (resolution) is demarcated in the lower left of each map. The locations of various IR and radio continuum sources (Source I, BN, IRc7, n, SMA1, H), some of them young stellar objects, are marked. The fainter 43 and 25 GHz lines (not shown) are likewise uncontaminated and have similar morphologies.

Fig. 1: (bottom) A preliminary velocity field map (intensity weighted LSRK velocity) of the 239 GHz line is consistent with explosion models (e.g., Zapata et al. 2009, Peng et al. 2013), wherein Source I, BN, and n are emerging from a dynamical event ~500 years ago at the marked explosion center. A possible outflow from Source I is also seen here along the NE-SW filament.

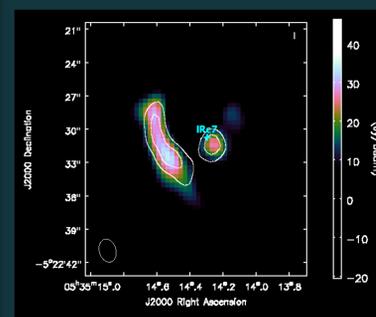
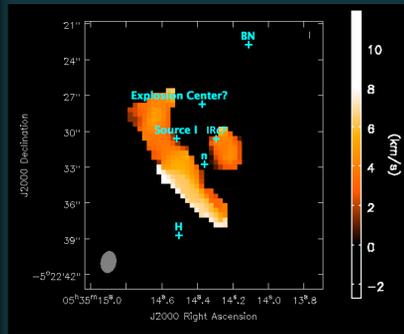


Fig. 2 (left): Moment 0 map of the 216 GHz NH₂D line, overlaid with contours of the 239 GHz line. Though the moment 0 morphology is similar, channel maps show 216 GHz is heavily contaminated by formaldehyde (H₂CO).

Fortunately, examination of an ortho-H₂CO line near 226 GHz, which is much stronger than the H₂CO line near 216 GHz, shows that the NH₂D peak near IRc7 is clear of contamination above ~2 km/s. Thus, while there is some hope of deconvolving the lines' contributions in the NE-SW filament, we focus for now on the peak near IRc7.

Fig. 3 (below): Moment 0 map of the 110 GHz NH₂D line, which is contaminated by methyl formate (HCOOCH₃) in the NE-SW filament and in the southern MF1 peak. There is strong evidence to suggest, however, that the IRc7 NH₂D peak is relatively clear of contamination below ~6 km/s. Point spectra near IRc7 and at MF1 are extracted below; the HCOOCH₃ line at MF1 is very narrow, and the synthesized beam near IRc7 is likely catching this line, adding an emission peak above ~6 km/s. Together with Fig. 6, this helps us conclude that the HCOOCH₃ emission is very well contained.

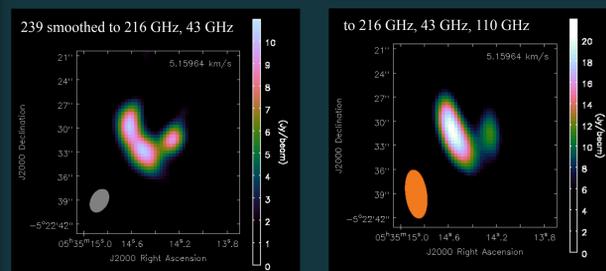
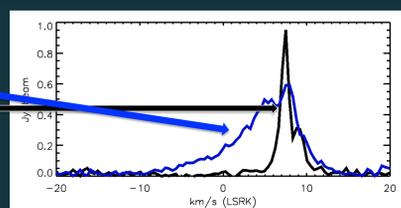
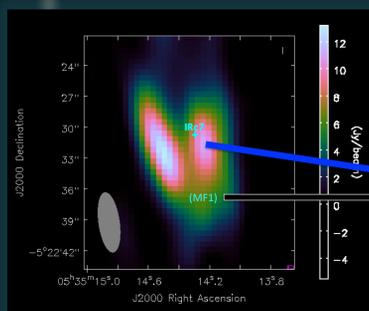


Fig. 4 (left): Smoothed data for analysis; 239 GHz moment 0 is shown as an example. Our different data have very different synthesized beams, with comparatively low resolution at 110 and 25 GHz. We smoothed the images to a beam that encompasses all these differing resolutions (lower-right panel). But to regain some spatial information, we carry out our analyses with fewer lines at three higher resolutions as shown in the other panels.

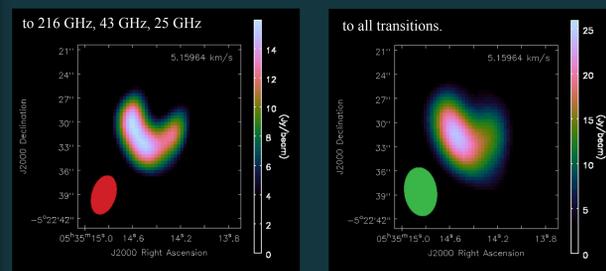


Fig. 5 (below): Normalized spectral extractions from synthesized beam-sized regions centered on the IRc7 peak at different frequencies and resolutions, color-coded to match the beam colors from Fig. 4, to investigate the effect of smoothing on extracted line shape. 239 GHz and 25 GHz line shapes showed no resolution dependence and are not shown.

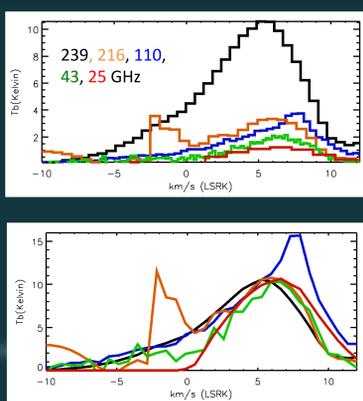
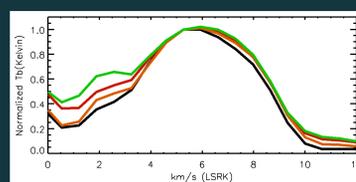


Fig. 6 (above): Spectral extractions, at the lowest resolution smooth, from near IRc7: raw data (top) and re-interpolated + scaled by eye for comparison (bottom). Except for areas of previously noted contamination, and perhaps slight effects from hyperfine structure at 43 GHz, the line profiles have very similar shapes, suggesting that the ~2 to 6 km/s range is uncontaminated in all lines.

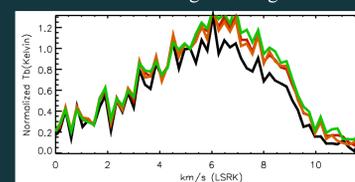
The 216 GHz line is scaled up by x3 to roughly match the 239 GHz line; since their S_{μ^2} line strengths are the same, this implies an ortho to para abundance ratio of 3, expected from spin statistical weights suggesting they are optically thin. However, the ratio does seem to vary slightly across the profile.

The 43 GHz line, which has the second-strongest S_{μ^2} after the 25 GHz line, might be expected to have more prominent structure or breadth from its three central components (separated by ~0.5 and ~1.35 km/s) if it were optically thick, which we do not observe.

216 GHz: picking up low-velocity H₂CO, mostly from the NE-SW filament, at low resolutions.



43 GHz: hyperfine structure letting the emission position (which varies slightly with velocity) fall out of the extraction region at high resolutions?



110 GHz: picking up extra methyl formate from the NE-SW filament at low horizontal resolutions.

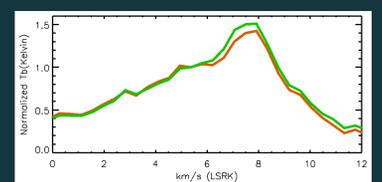
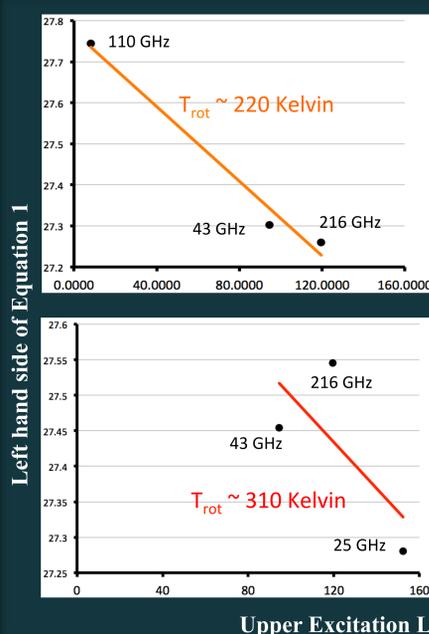


Fig. 7 (left): Rotation diagrams for para NH₂D at three resolution smooths (color-coded as before), using integrated brightness temperature from ~2.5 to 6 km/s and the equation below (assumes LTE, optically thin). Rotational temperatures are labeled.



Discussion: Gas Temperatures and Deuteration Chemistry
The gas temperatures we obtain are consistently high, and in each case we obtain a para column density of ~2E15, implying a total ortho+para NH₂D column density near ~8E15 [cm⁻²]. The 43 GHz line always lies below the trend, which might be due to its subtle hyperfine structure. The 216 GHz line always lies above the trend, which might be due to slight H₂CO contamination; indeed, the situation improves somewhat when the horizontal resolution is better (upper-left panel).

Deuteration of ammonia requires H₂D⁺ (which permits NH₃ → NH₃D⁺ → NH₂D, or more prominently, NH₂ → NH₂⁺ → NH₃D⁺ → NH₂D), created by H₃⁺ + HD → H₂D⁺ + H₂. At temperatures above ~10 K, the reverse (endothermic) reaction suppresses the formation of H₂D⁺, which is also depopulated by reactions with CO-like molecules that exist at low densities and high temperatures. (e.g., Parise et al. 2009, Roueff et al. 2007).

Thus, the observed temperature is too high to have allowed the development of an NH₂D population in the gas. One plausible scenario is that NH₂D condensed onto dust grains when the gas was colder, and evaporated into the gas phase (starting at ~80 K) as temperatures rose.

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