



# Onsala Proposal

**Trapman**

**0108.F-9314**

## Testing the robustness of N<sub>2</sub>H<sup>+</sup> as CO iceline tracer in protoplanetary disks using N<sub>2</sub>H<sup>+</sup> J=7-6

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Science Cat.: ISM and star formation

### Abstract

The molecule N<sub>2</sub>H<sup>+</sup>, a chemical tracer of CO-poor gas, is frequently used to locate the CO iceline in planet-forming disks, thought to play a crucial role in planet formation.

However, astrochemical models predict the existence of second N<sub>2</sub>H<sup>+</sup>-rich surface layer, whose origins are unrelated to CO freeze-out. We used APEX to detect N<sub>2</sub>H<sup>+</sup> 7-6 in the nearby planet-forming disk TW Hya, confirming the existence of this N<sub>2</sub>H<sup>+</sup>-rich surface layer. If this layer proves common, we may need to re-evaluate N<sub>2</sub>H<sup>+</sup> as a CO iceline tracer.

We propose to observe N<sub>2</sub>H<sup>+</sup> 7-6 with APEX-SEPIA660 in two planet-forming disks, LkCa 15 and V4046 Sgr. We will show if their distinctive differences in N<sub>2</sub>H<sup>+</sup> 3-2 emission morphology observed with ALMA are indicative of the presence/absence of a N<sub>2</sub>H<sup>+</sup>-rich surface layer and we will establish how well N<sub>2</sub>H<sup>+</sup> really traces the CO iceline.

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*Is this a long term proposal: No*

*No overall scheduling requirements*

### *Observing runs*

run	telescope	instrument	time request (minimal)	frequency (GHz)	weather (pwv)	LST range	comments/constraints
A	APEX	SEPIA660 (581-727 GHz)	10h (10h)	652	< 0.5mm		The target for this proposal is the N <sub>2</sub> H <sup>+</sup> J=7-6 line at 652.0956 GHz

### *Targets*

Source	RA	Dec	Epoch	Vlsr (km/s)	Duration (min)	Runs	Comments
LkCa 15	04:39:17.79	+22:21:03.3	J2000	6.2	71	A	integration time is without overheads
V4046 Sgr	18:14:10.47	-32:47:34.4	J2000	2.9	71	A	integration time is without overheads

## Testing the robustness of $\text{N}_2\text{H}^+$ as CO iceline tracer in protoplanetary disks using $\text{N}_2\text{H}^+ J = 7 - 6$

### 1 Scientific justification: is $\text{N}_2\text{H}^+$ a good CO iceline tracer?

Ice lines are defining locations inside planet-forming disks, where dominant volatiles (e.g.,  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{N}_2$ ) freeze out onto dust grains. These ice lines are thought to play crucial roles in planet formation by enhancing the sticking probability of grains, significantly increasing the solid surface density, and influencing the planetary bulk volatile compositions (e.g., Blum & Wurm 2008; Öberg et al. 2011; Ros & Johansen 2013). **Direct detection of ice lines is difficult:** the mid-plane location of the CO ice line is ‘hidden’ by gas-phase CO present at higher layers in the disk where temperatures are higher.

Using ALMA, the  $\text{N}_2\text{H}^+$  molecule has been successfully used to locate the CO ice line (Qi et al., 2013, 2015, 2019; Huang & Öberg, 2015).  $\text{N}_2\text{H}^+$  is formed through proton transfer from  $\text{H}_3^+$  to  $\text{N}_2$ . If CO is present in the gas it competes  $\text{N}_2$  for the available  $\text{H}_3^+$ , thus impeding the formation of  $\text{N}_2\text{H}^+$ . In addition,  $\text{N}_2\text{H}^+$  is rapidly destroyed by gas-phase CO. As a result,  **$\text{N}_2\text{H}^+$  is therefore expected to be abundant between the CO iceline and the  $\text{N}_2$  iceline** (see Figure 1). The ring-shaped  $\text{N}_2\text{H}^+$  emission that is detected should signal CO freeze-out at the inner radius of the ring.

However, there is increasing evidence for a **second  $\text{N}_2\text{H}^+$ -rich layer, situated higher up in the disk, that is unrelated to CO freeze-out**. This layer is the result of  $\text{N}_2$  having a slightly lower photo-dissociation rate compared with CO.  $\text{N}_2$  is thus able to self-shield higher up in the disk than CO, creating a layer of  $\text{N}_2$ -rich, CO-poor gas where  $\text{N}_2\text{H}^+$  can easily form, similar to the layer found between the two icelines (see Figure 1). This layer is seen clearly in physical-chemical models and can contribute significantly to the emission of low- $J$   $\text{N}_2\text{H}^+$  lines (van ’t Hoff et al., 2017). However, existence of this second layer of  $\text{N}_2\text{H}^+$  higher up in the disk has not yet been conclusively proven with observations of low- $J$   $\text{N}_2\text{H}^+$  lines (see Schwarz et al. 2019; Nomura et al. 2016).

Recently, **we detected  $\text{N}_2\text{H}^+ J = 7 - 6$  with the APEX telescope in the nearby TW Hya disk (see Figure 2)**. Due to its upper level energy of 125 K,  $\text{N}_2\text{H}^+ (7-6)$  only significantly emits at the high temperatures found higher up in the disk. This makes it an excellent probe of the  $\text{N}_2\text{H}^+$ -rich surface layer: **detecting  $\text{N}_2\text{H}^+ (7-6)$  is equivalent to detecting the  $\text{N}_2\text{H}^+$ -rich surface layer**. Moreover, the first detection of  $\text{N}_2\text{H}^+ (7-6)$  in TW Hya shows that line is  $3\times$  brighter than current models predict, suggesting that the  $\text{N}_2\text{H}^+$ -rich surface layer is an integral part of the  $\text{N}_2\text{H}^+$  abundance structure in disks. If the  $\text{N}_2\text{H}^+$ -rich surface layer is a common occurrence in protoplanetary disks, we might need to re-evaluate the use of  $\text{N}_2\text{H}^+$  as a CO iceline tracer.

Recent ALMA observations of  $\text{N}_2\text{H}^+ (3-2)$  show that protoplanetary disks can be divided into two categories based on their  $\text{N}_2\text{H}^+ (3-2)$  emission morphology (see Qi et al. 2019). Half of the disks show a bright ring of  $\text{N}_2\text{H}^+ (3-2)$ , surrounded by more tenuous emission. The other half instead show a more extended  $\text{N}_2\text{H}^+ (3-2)$  emission ring. Qi et al. (2019) attribute this difference to the vertical thickness of the  $\text{N}_2\text{H}^+$  layer between the CO and  $\text{N}_2$  icelines (see Figure 4): A thick layer results in a bright, narrow ring of  $\text{N}_2\text{H}^+ (3-2)$ , whereas a thin layer results in a broad  $\text{N}_2\text{H}^+ (3-2)$  emission ring.

However, **another explanation is that the thick vertical layer between the two icelines is the result of a  $\text{N}_2\text{H}^+$ -rich surface layer**. The high  $\text{N}_2\text{H}^+$  column density inferred from the bright, narrow ring would be the sum of the  $\text{N}_2\text{H}^+$ -rich surface layer and the  $\text{N}_2\text{H}^+$  layer between the two icelines. If this is the case, then the inner edge of the  $\text{N}_2\text{H}^+$  emission will be confused by the surface layer and would no longer trace the CO iceline (see Figure 4). The  $\text{N}_2\text{H}^+ (4-3)$  emission morphology and  $\text{N}_2\text{H}^+ (7-6)$  detection in TW Hya support this explanation.

Conversely, **the thin  $\text{N}_2\text{H}^+$  vertical layer inferred from the broad emission ring could indicate that there is no  $\text{N}_2\text{H}^+$ -rich vertical layer**, or at least that it contributes only minimally to the total  $\text{N}_2\text{H}^+$  column density. In that case, the broad emission ring would instead just trace the  $\text{N}_2\text{H}^+$  between the CO and  $\text{N}_2$  icelines, and can be used to determine the location of the CO iceline.

**After our first successful detection of  $\text{N}_2\text{H}^+ (7-6)$  with APEX, we propose to observe  $\text{N}_2\text{H}^+ (7-6)$  in two protoplanetary disks, LkCa 15 and V4046 Sgr, to prove the existence, or absence of the  $\text{N}_2\text{H}^+$ -rich layer higher up the disk between the CO and  $\text{N}_2$  photo-dissociation fronts (see Figure 4).**

## 2 Description of Observations

The goal of this proposal is to detect the N<sub>2</sub>H<sup>+</sup>  $J = 7 - 6$  in two protoplanetary disks, LkCa 15 and V4046 Sgr. To detect this line we will use the new APEX-SEPIA660 heterodyne receiver (analogue to ALMA Band 9). This instrument has already been successfully used to detect N<sub>2</sub>H<sup>+</sup>  $J = 7 - 6$  in the nearby TW Hya protoplanetary disk (see Figure 2).

**Detection experiment:** Due to the high temperature required to excite the N<sub>2</sub>H<sup>+</sup>  $J = 7$  level ( $T_{\text{ex}} = 125.2$  K) only the upper regions of the disk are expected to be warm enough to produce significant N<sub>2</sub>H<sup>+</sup> (7-6) emission (see Fig. 1). With our observations we aim to carry out a direct experiment: **detecting the N<sub>2</sub>H<sup>+</sup> (7-6) line is equivalent to detecting the N<sub>2</sub>H<sup>+</sup>-rich layer higher up in the disk.** A non-detection of N<sub>2</sub>H<sup>+</sup> (7-6) indicates that the N<sub>2</sub>H<sup>+</sup>-rich layer is absent.

**Selected sources:** We select two sources, LkCa 15 and V4046 Sgr, that have similarly bright N<sub>2</sub>H<sup>+</sup> (3-2) emission, but very different morphology. As shown at the top of Figure 4, LkCa 15 is a clear example of the bright, narrow ring of N<sub>2</sub>H<sup>+</sup> emission, and V4046 Sgr is an example of the broad ring N<sub>2</sub>H<sup>+</sup> emission morphology. These two disks are similar in both disk mass and size, as inferred from existing ALMA continuum and line observations (e.g., Loomis et al. 2020; Kastner et al. 2018).

**Required sensitivity:** Using the thermochemical code DALI (Bruderer et al., 2012) combined with the N<sub>2</sub>H<sup>+</sup> chemical network presented in van 't Hoff et al. (2017), we compute N<sub>2</sub>H<sup>+</sup> abundances and N<sub>2</sub>H<sup>+</sup> (3-2) and (7-6) integrated intensities for a suite of disk models with different vertical structures and CO and N<sub>2</sub> abundances (see Figure 3). Comparing these models to the observed N<sub>2</sub>H<sup>+</sup> (3-2) fluxes of our two sources **we find a minimal N<sub>2</sub>H<sup>+</sup> (7-6) total intensity of 47 mK km/s if the N<sub>2</sub>H<sup>+</sup>-rich surface layer is present** (See Figure 3)

In agreement with the official APEX time estimator and similar to our previous observations of TW Hya, for ON/OFF observations, using SEPIA660, and assuming PWV = 0.5 mm, a source elevation of 45 degrees, and a spectral resolution for the XFFTS backends of 1.5 km/s, a total observing time of 4.98 hours per source (including overheads) yields a final rms of 7 mK, which is sufficient to detect the N<sub>2</sub>H<sup>+</sup> (7-6) line at a S/N > 3 in our two disks. APEX observations with similar sensitivity were able to detect N<sub>2</sub>H<sup>+</sup> (7-6) at 10 $\sigma$  in the TW Hya disk (see Figure 2). **We therefore request a total of 10 hours of APEX observing time (including tunings and overheads) with SEPIA660 in order to detect the N<sub>2</sub>H<sup>+</sup> J=7-6 line in LkCa 15 and V4046 Sgr.**

**Immediate objective: Calibrating N<sub>2</sub>H<sup>+</sup> as CO iceline tracer:** The usage of N<sub>2</sub>H<sup>+</sup> as a tracer of the CO iceline is linked to the assumption that N<sub>2</sub>H<sup>+</sup> is only abundant between the CO and N<sub>2</sub> icelines. We will analyze our N<sub>2</sub>H<sup>+</sup> (7-6) observations together with existing N<sub>2</sub>H<sup>+</sup> (3-2) observations using DALI models to constrain the full N<sub>2</sub>H<sup>+</sup> abundance structure in LkCa 15 and V4046 Sgr. Based on our N<sub>2</sub>H<sup>+</sup> (7-6) observations we will determine if the existence of a N<sub>2</sub>H<sup>+</sup>-rich surface layer can explain the difference in N<sub>2</sub>H<sup>+</sup> (3-2) emission morphology. Furthermore we will constrain whether the N<sub>2</sub>H<sup>+</sup> (3-2) emission originates from the N<sub>2</sub>H<sup>+</sup>-layer between the CO and N<sub>2</sub> ice surfaces or from the N<sub>2</sub>H<sup>+</sup> surface layer and therefore calibrate the usage of N<sub>2</sub>H<sup>+</sup> emission as a CO iceline tracer.

**Secondary goal: CO underabundance in disk surface layer:** van 't Hoff et al. (2017) showed that presence and thickness of the N<sub>2</sub>H<sup>+</sup>-rich surface layer is directly linked to the CO/N<sub>2</sub> abundance ratio higher up in the disk. Using the characteristics of the N<sub>2</sub>H<sup>+</sup> surface layer obtained from our N<sub>2</sub>H<sup>+</sup> (7-6) observations we will constrain the CO/N<sub>2</sub> ratio in the surface layer of the disk. Coupled with the underabundance of CO inferred low- $J$  CO isotopologue lines deeper in the disk, this will provide valuable information about the processes responsible for this underabundance (e.g., the importance of vertical mixing; Kama et al. 2016; Krijt et al. 2020).

**References** Blum & Wurm 2008, ARA&A, 46, 21 • Bruderer et al. 2012, A&A, 541, A91 • Huang & Öberg 2015, ApJL, 809, L26 • Kama et al. 2016, A&A, 592, A83 • Kastner et al. 2018, ApJ, 863, 106 • Krijt et al. 2020, ApJ, 899, 134 • Loomis et al. 2020, ApJ, 893, 101 • Nomura et al. 2016, ApJL, 819, L7 • Öberg et al. 2011, ApJL, 743, L16 • Qi et al. 2015, ApJ, 813, 128 • Qi et al. 2013, Science, 341, 630 • Qi et al. 2019, ApJ, 882, 160 • Ros & Johansen 2013, A&A, 552, A137 • Schwarz et al. 2019, ApJ, 877, 131 • van 't Hoff et al. 2017, A&A, 599, A101

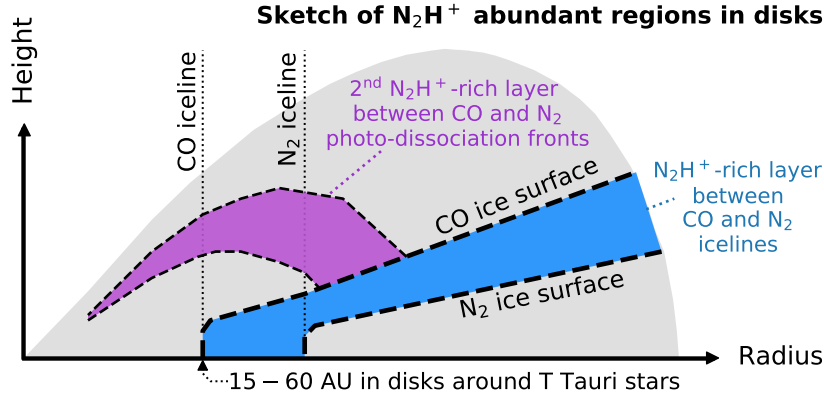


Figure 1: Sketch of the two  $N_2H^+$ -rich layers expected in protoplanetary disk (e.g. van 't Hoff et al. 2017). The  $N_2H^+$ -rich layer between the CO and  $N_2$  ice surface is shown in blue. Shown in purple is the second  $N_2H^+$ -rich layer close to the disk surface, between the  $N_2$  and CO photo-dissociation fronts.

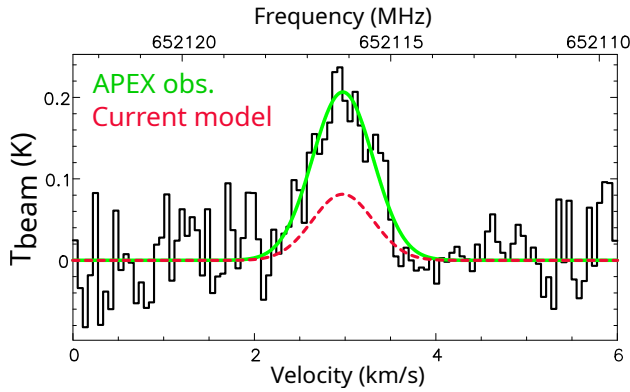


Figure 2: First APEX detection of  $N_2H^+$  (7-6) in the nearby disk TW Hya (project 0106.C-0669(A), PI: Trapman). Green line shows a Gaussian fit to the observations, which is  $3\times$  brighter than the expected  $N_2H^+$  (7-6) flux from existing models (van 't Hoff et al., 2017)

Table 1: Source information

Source	Dist (pc)	$M_*$ ( $M_\odot$ )	$T_{\text{eff}}$ (K)	$L_*$ ( $L_\odot$ )	$N_2H^+$ (3-2) flux (Jy km/s)	$N_2H^+$ (3-2) morphology
LkCa 15	158	1.2	4365	1.0	1.82	narrow ring
V4046 Sgr	72	1.75	4370	0.49	3.76	broad ring

Notes: Stellar properties are adopted from Gaia DR2.  $N_2H^+$  (3-2) emission properties from Qi et al. (2019)

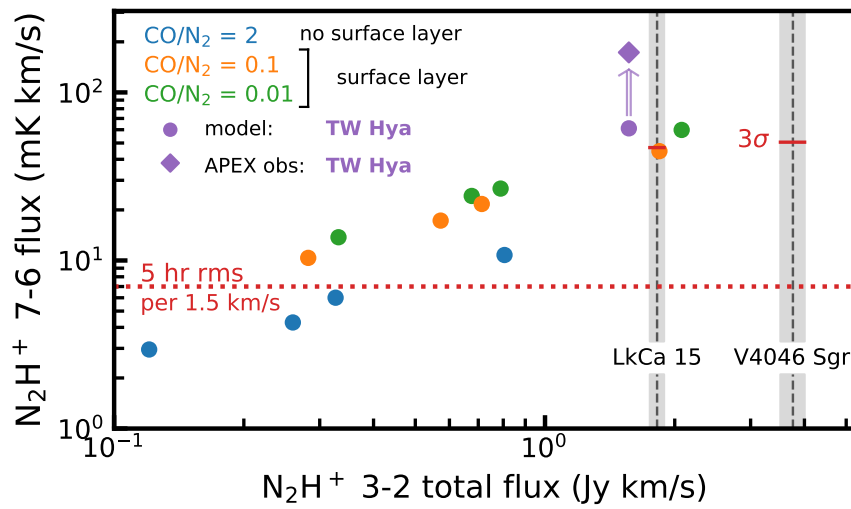


Figure 3:  $N_2H^+$  (7-6) and  $N_2H^+$  (3-2) integrated intensities for a suite of disk models of similar size and with similar mass to LkCa 15 and V4046 Sgr, but with different vertical structures (scale height, flaring angle and gas-to-dust mass ratio in the surface layer). Note that  $N_2H^+$  76 integrated intensity was calculated using the APEX beam at 652 GHz. Colors show different  $CO/N_2$  ratios, where  $CO/N_2 \leq 1$  results in a  $N_2H^+$ -rich surface layer. Integrated  $N_2H^+$  (3-2) line fluxes for LkCa 15 and V4046 Sgr are shown in gray (Qi et al., 2019). The purple markers show  $N_2H^+$  fluxes for TW Hya, where the APEX detection of  $N_2H^+$  7-6 (diamond; see Figure 2) is  $3\times$  brighter than what current models predict (circle; van 't Hoff et al. 2017). The red dotted lines shows the requested rms. The red lines show the  $3\sigma$  level for our two sources, based on the requested rms and the expected  $N_2H^+$  (7-6) line width ( $\sim 4 - 5$  km/s).

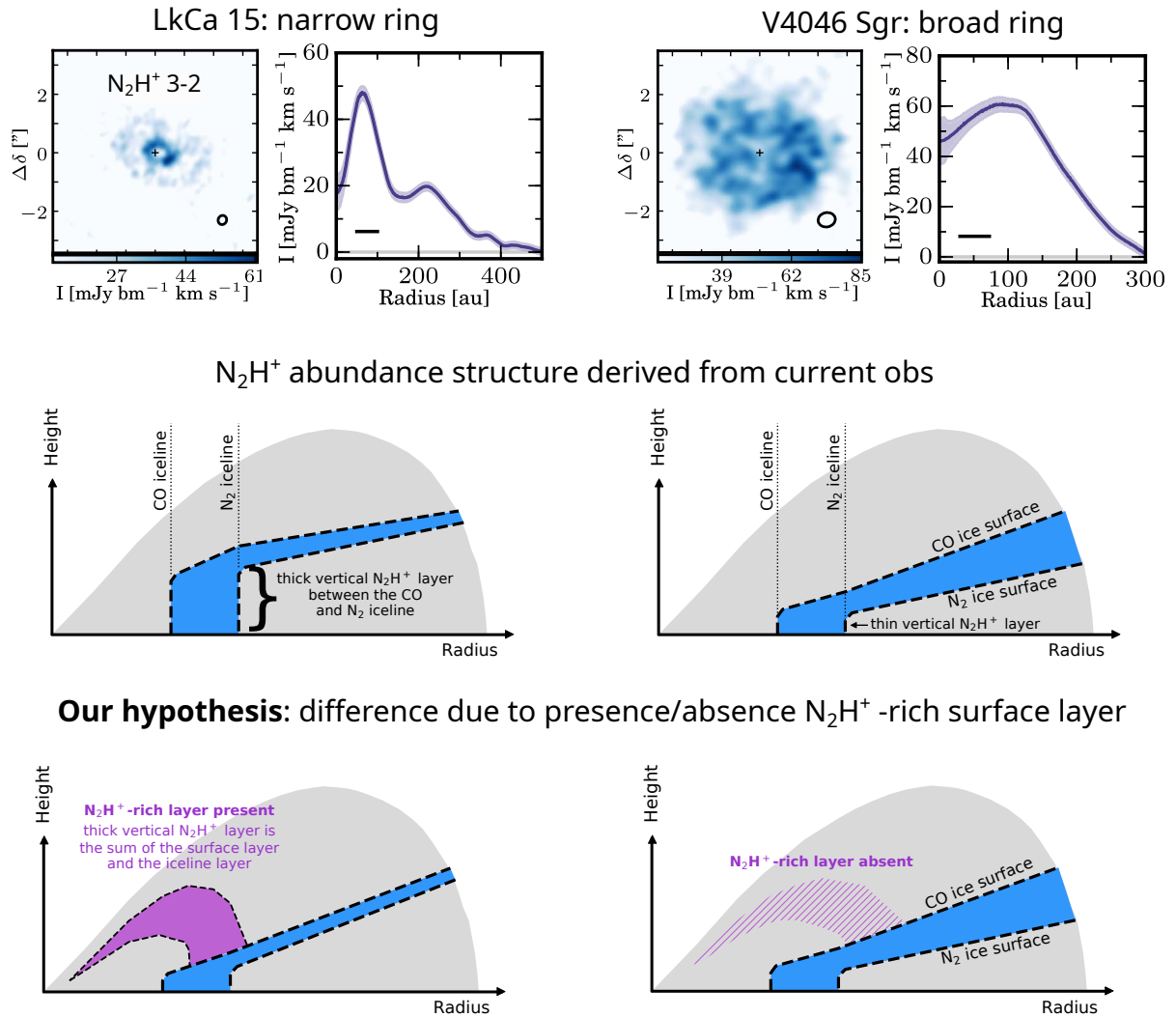


Figure 4: **Top panels:** N<sub>2</sub>H<sup>+</sup> (3-2) moment zero maps and radial intensity profiles of LkCa 15 (left), showing a narrow ring, and V4046 Sgr (right), showing a broad ring (Qi et al., 2019). **Middle panels:** sketches of the two types of N<sub>2</sub>H<sup>+</sup> abundance structures inferred from these observations, assuming N<sub>2</sub>H<sup>+</sup> is only abundant between the CO and N<sub>2</sub> icelines (adapted from Qi et al. 2019). **Bottom panels:** Our hypothesis for the inferred N<sub>2</sub>H<sup>+</sup> abundance structure, where the thick vertical N<sub>2</sub>H<sup>+</sup> layer on the left is the sum of a N<sub>2</sub>H<sup>+</sup>-rich surface layer and the N<sub>2</sub>H<sup>+</sup>-rich layer between the two iceline.

*No PhD Students involved*

*Linked proposal submitted to this TAC: No*

*Linked proposal submitted to other TACs: No*

*Relevant previous Allocations: Yes*

We used APEX SEPIA660 to detect N<sub>2</sub>H<sup>+</sup> 7-6 (S/N=10) in the nearby protoplanetary disk TW Hya (project 0106.C-0669(A)). This detection was obtained with 5 hours of observing time, including overheads.

*Additional remarks*

ESO=Itrapman

*Observing run info :*