# Observing the $NH_3$ snowline in protoplanetary disks with ngVLA

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### Abstract

The snowline is the boundary where molecules freeze-out/sublimate in a protoplanetary disks. The elemental compositions of gas and solid (ice + dust) change significantly across the snowlines of major volatiles such as $H_2O$, $NH_3$, $CO$, etc., Then the detection of the snowlines and revealing the compositional changes across the snowlines are essential for understanding planetary composition. In this article, we discuss the observability of the $NH_3$ snowline in Class II protoplanetary disks with ngVLA. $NH_3$ is a key species to trace the chemical evolution of nitrogen during star- and planet formation and is also useful as a proxy to trace the $H_2O$ snowline. We find that the $NH_3$ snowline is detectable in a disk around a Herbig Ae/Be star with ngVLA, while the detection is challenging for a disk around a T-Tauri star.

**Key words:** protoplanetary disks — ISM: molecules — ISM: abundances

## 1. Introduction

Ammonia ($NH_3$) is one of the major reservoirs of nitrogen in star-forming regions, accounting for $\sim$10 % of overall nitrogen (e.g., Öberg et al. 2011). The significant fraction of remaining nitrogen is likely present as $N_2$ (e.g., Furuya et al. 2018), which is not directly observable. As $N_2$ is more volatile and chemically stable than $NH_3$, $NH_3$ could be a raw material of N-bearing complex organic molecules (Daranlot et al. 2012), including amino acids. Taken together, $NH_3$ is a key species to trace the chemical evolution of nitrogen during star- and planet formation.

The bulk of $NH_3$ in star-forming regions forms in molecular clouds and cores as ice. The $NH_3$ evolution in the later stages of star-formation, i.e., after protostellar formation, is still largely unknown due to the lack of high spatial resolution observations at cm wavelengths, where $NH_3$ has rotation-inversion transitions. Gas-phase $NH_3$ has been detected in the warm ($>$100 K) gas of a deeply embedded protostellar source with VLA (Choi et al. 2010), where $NH_3$ ices have sublimated. To the best of our knowledge, there is only one detection of $NH_3$ in class II protoplanetary disks in the literature (Salinas et al. 2016). The observed gas-phase $NH_3$ by the *Herschel Space Observatory* traces the cold outer regions of the disk, where only a fraction of $NH_3$ ice desorbes via photodesorption. In order to trace the bulk $NH_3$ in disks, the observations of gas-phase $NH_3$ inside the $NH_3$ snowline is necessary. It is known that $NH_3$ is poor in cometary ices with the abundance ratio of $NH_3/H_2O \lesssim 1$ % (Mumma & Charnley 2011 and references therein), which is much lower than that in interstellar ices, $\sim$5 % (e.g., Öberg et al. 2011). Recent detection of ammonium salts in comet 67P/Churyumov-Gerasimenko by the ROSINA instrument on Rosetta (Altwegg et al. 2020) implies that $NH_3$ is largely converted into ammonium salts during star- and planet-formation.

ngVLA is the unique instrument that allows us to detect $NH_3$ inside its snowline and thus to reveal the $NH_3$ evolution.
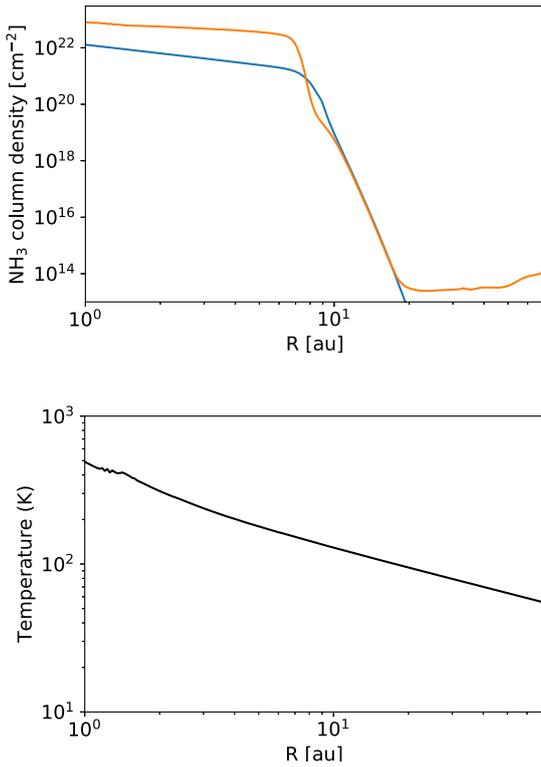
$NH_3$ would be also useful to locate the water snowline in protoplanetary disks. The detection of water snowline by observing water emission lines with ALMA would be challenging, if the inner disk regions, where water snowline locates, are optically thick for dust continuum at mm wavelengths (e.g., Banzatti et al. 2015). Even when dust continuum is optically thick at mm wavelengths, it is likely optically thin at cm wavelengths. In addition, laboratory experiments of the sublimation of interstellar/cometary ice analogs have shown that at least significant fraction of $NH_3$ ice sublimates together with $H_2O$ ice (Martín-Doménech et al. 2014). Then, $NH_3$ is suggested to be a good proxy to trace the water snowline (e.g., Zhang et al. 2018).
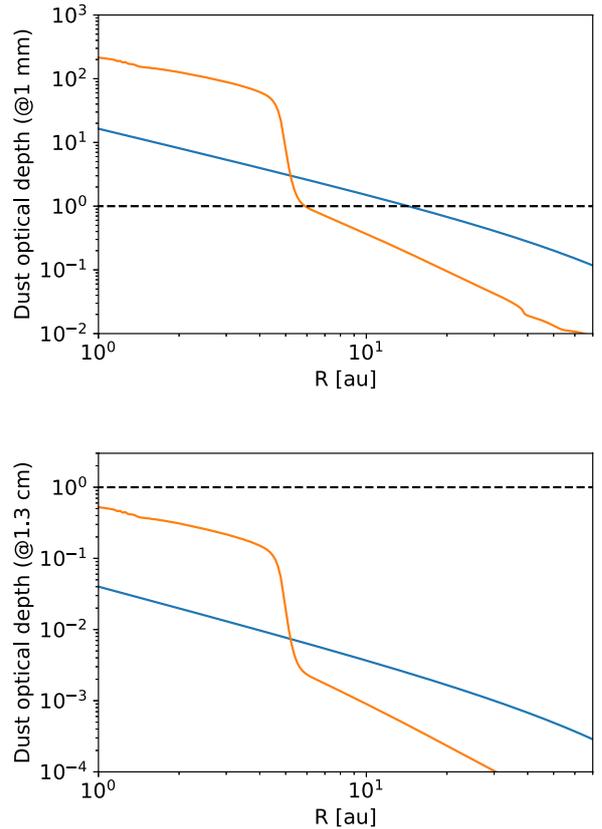
## 2. Sensitivity estimate

Here we discuss the observability of the $NH_3$ snowline in a Class II protoplanetary disk with ngVLA. For this sake, we conduct the line radiation transfer calculations, using a genetic disk model.

### 2.1. Numerical setup

For the physical and chemical structures of a disk, we consider a disk around a Herbig Ae/Be star with the mass of 2 $M_\odot$. We adopt the simulation results from Furuya et al. (in prep.), in which the viscous evolution of gas, the dust evolution (collisional growth and radial drift), and gas-phase and grain surface chemistry are considered in a time-dependent manner. In this 1D radial model, temperature is calculated from the balance between heating by stellar irradiation and viscous dissipation and radiative cooling, using initial disk conditions. The initial disk gas mass is 0.05 $M_\odot$ with the dust-to-gas mass ratio of $\sim$0.01. The binding energy of $NH_3$ is set to be the same as that

**Fig. 1.** Upper panel) Column density of gas-phase NH$_3$ as a function of the distance from the central star in the disk model at $t = 0$ yr (blue line) and $3 \times 10^5$ yr (orange line). Lower panel) Temperature distribution in the disk model.



**Fig. 2.** Dust optical depth at 1 mm (upper panel) and at 1.3 cm (lower panel) as a function of the distance from the central star in the disk model at $t = 0$ yr (blue line) and $3 \times 10^5$ yr (orange line).

of H$_2$O, so that the snowlines of NH$_3$ and H$_2$O are co-located in the disk model. It is assumed that the initial chemical composition of the disk is similar to that of dense molecular clouds for simplicity, with the total (gas+ice) initial NH$_3$ abundance of $\sim 10^{-5}$ with respect to hydrogen nuclei, corresponding to the NH$_3$/H$_2$O abundance ratio of $\sim 10$ %.

The upper panel of Figure 1 shows that the column density distribution of gas-phase NH$_3$ in the model at $t = 0$ yr and at $3 \times 10^5$ yr, while the lower panel shows the temperature distribution adopted in the simulations. We chose the two specific time to explore the impact of the NH$_3$ column density distribution on the NH$_3$ emission. The NH$_3$ column density sharply increases at $\sim 10$ au, corresponding to the snowline of NH$_3$. The NH$_3$ column density inside the snowline is higher at the later time, because of the radial drift of ice-coated dust grains and sublimation of NH$_3$ ice at the snowline. Outside the NH$_3$ snowline, the majority of NH$_3$ is present as ice coatings of dust grains, but some amount of NH$_3$ still exist in the gas-phase due to the gas-phase chemistry, which converts N$_2$ to NH$_3$, and photodesorption of NH$_3$ ice. The NH$_3$ column density outside the snowline also increases with time, because the total surface area of dust grains, which allows freeze-out of gas-phase NH$_3$, reduces with time due to the coagulation and radial drift of dust grains.

Figure 2 shows that the optical depth for dust continuum at 1 mm and at 1.3 cm in the disk model. The sharp increases of the dust optical depth is seen at $\lesssim 5$ au, corresponding to

the accumulation of dust grains there. This is caused by the assumption that the threshold fragmentation velocity of bare dust grains is lower than that of dust grains coated by more than one monolayer of water ice (e.g., Banzatti et al. 2015). The dust opacity is calculated with the `dsharp_Opac` package (Birnstiel et al. 2018), assuming the minimum and maximum dust sizes of 0.005 $\mu$m and 1 mm, respectively, with the power law of -3.5. The dust absorption coefficients are 2.7 cm$^2$/g at 1 mm and $6.6 \times 10^{-3}$ cm$^2$/g at 1.3 cm, respectively, in our models. Dust continuum at 1 mm wavelength (300 GHz) is optically thick at $\lesssim 10$ au, while at 1.3 cm wavelength (23 GHz), the dust continuum is optically thin in the whole region in the disk. This comparison demonstrates that ngVLA is suitable to observe molecular lines from the midplane of the inner disk regions.

As the adopted disk structure model is a 1D radial model, we have to assume the vertical disk structure. For simplicity, we assume that gas is vertically isothermal, the gas distribution is in the hydrostatic equilibrium, the dust-to-gas mass ratio is vertically uniform (but not uniform radially), and NH$_3$ gas is present only below one scale height of the gas. In reality, the distribution of NH$_3$ gas inside the snowline would depend on the vertical temperature structure and the strength of vertical mixing. Such details are beyond the scope of this article.

The line radiation transfer calculations of para-NH$_3$ inversion transitions are performed with LIME (Brinch &

Hogerheijde 2010), assuming local thermal equilibrium (LTE). Molecular data are taken from the Leiden Atomic and Molecular Database (LAMBDA; Schöier et al. 2005). The assumption of LTE is valid as we focus on inner disk midplane, where the gas density is very high ($>10^{10}$ cm$^{-3}$). For simplicity, we neglect hyper-fine structures of NH$_3$ transitions here, which should be explored in the future work. We assume that the distance of the disk from the Earth is 140 pc and the inclination angle of the disk is 30°.

## 2.2. *Results*

We performed the line transfer calculations to predict emission in (1,1)-(5,5) rotation-inversion transitions at 23-25 GHz for two snapshots ($t = 0$ yr and $3 \times 10^5$ yr) of the disk structure model. We found that the results for the two snapshots are similar, and thus we here only show the results at $t = 3 \times 10^5$ yr. The left panel of Figure 3 shows the moment 0 map of the NH$_3$(5, 5) emission model obtained by LIME with the spatial resolution of 0.004" per pixel, while the right panel shows the moment 0 map of the emission model convolved with the 0.1" Gaussian beam. As the intensity sharply drops at the snowline position, one can locate the snowline from the moment 0 map if the spatial resolution is high enough ($<<$10 au). Considering the sensitivity of ngVLA for line observations, the beam size of $\sim$0.1" ($\sim$14 au in our simulations) would be the minimum for the detection of NH$_3$ inversion transitions with reasonable observing time (see below). Then, the NH$_3$ snowline would be only marginally resolved.

Even when the snowline is not spatially resolved, one can constrain the snowline location from the spectrally resolved observations (e.g., Notsu et al. 2017). Figure 4 shows the spectral of the NH$_3$(5,5) emission extracted from inner $\sim$20 au. The peak brightness temperature is $\sim$50 K. Then, assuming a beam size of 0.1" and velocity resolution of 1 km/s, we can detect the emission with $\gtrsim$10 $\sigma$ ($\gtrsim$5 $\sigma$) for 10 hour (2.5 hour) integration time to locate the NH$_3$ snowline (cf. https://ngvla.nrao.edu/page/performance). We do not see significant deference between (5,5) and (1,1) transitions (Fig. 4), although the upper energy levels are very different (295 K versus 23 K). A higher transition would be better to avoid blending between the main components and the satellite components (note again that our calculations do not consider hyper-fine structures). As the NH$_3$ emission from inside the snowline is optically thick, it is hard to constrain the NH$_3$ column density. The observations of rarer isotopologoues, $^{15}$NH$_3$, spectrally resolving the hyperfine components, may be helpful to constrain the column density.

In our calculations, we consider a disk around a Herbig Ae/Be star. The detection of the NH$_3$ snowline in a T-Tauri disk would be challenging due to the smaller size of the NH$_3$ snowlines (at $\sim$1 au) (Zhang et al. 2018).

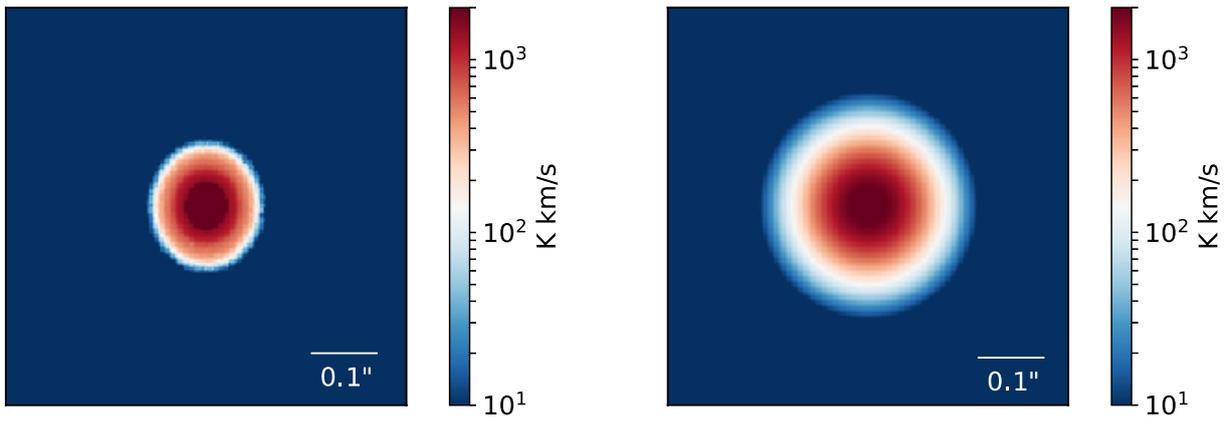## 3. Conclusion

In this article, we discussed the observability of the NH$_3$ snowline in a Class II protoplanetary disk. We performed the line radiation transfer of rotation-inversion transition of NH$_3$, using a genetic disk model of Furuya et al. (in prep.). W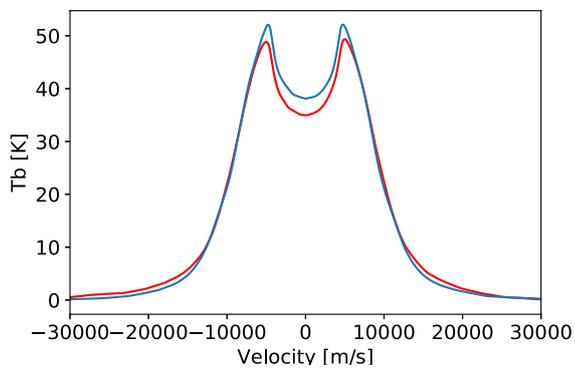e found that the NH$_3$ snowline can be detected in a disk around a Herbig Ae/Be star with ngVLA with reasonable integration time, while the detection is challenging for a disk around a T-Tauri star. The $^{14}$NH$_3$ emission lines are most likely optically thick. Then the observations of rarer isotopologoues, $^{15}$NH$_3$, would be required to constrain the amount of NH$_3$ inside its snowline. This article focuses on NH$_3$, while Furuya et al. disk model predicts that complex organic molecules (COMs), such as CH$_3$OH and CH$_3$OCH$_3$, are accumulated in inner disk regions inside water snowline. These COMs would also be interesting targets for ngVLA.

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**Fig. 3.** Left panel) Moment 0 map of the $NH_3(5, 5)$ emission model obtained by line radiative transfer code LIME. Right panel) The $NH_3(5, 5)$ emission model convolved with the 0.1" Gaussian beam.



**Fig. 4.** Spectra of the $NH_3(1, 1)$ emission (blue line) and the $NH_3(5, 5)$ emission (red line).