Role of NH₃ binding energy in the early evolution of protostellar cores

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ABSTRACT

Context. $NH₃(ammonia)$ plays a critical role in the chemistry of star and planet formation, yet uncertainties in its binding energy (BE) values complicate accurate estimates of its abundances. Recent research suggests a multi-binding energy approach, challenging the previous single-value notion.

Aims. In this work, we use different values of NH₃ binding energy to examine its effects on the NH₃ abundances and, consequently, in the early evolution of protostellar cores.

Methods. Using a gas-grain chemical network, we systematically vary the values of NH₃ binding energies in a model Class 0 protostellar core and study the effects of these binding energies on the NH₃ abundances.

Results. Our simulations indicate that abundance profiles of $NH₃$ are highly sensitive to the binding energy used, particularly in the warmer inner regions of the core. Higher binding energies lead to lower gas-phase NH₃ abundances, while lower values of binding energy have the opposite effect. Furthermore, this BE-dependent abundance variation of NH_3 significantly affects the formation pathways and abundances of key species such as HNC, HCN, and CN. Our tests also reveal that the size variation of the emitting region due to binding energy becomes discernible only with beam sizes of 10 arcsec or less.

Conclusions. These findings underscore the importance of considering a range of binding energies in astrochemical models and highlight the need for higher resolution observations to better understand the subtleties of molecular cloud chemistry and star formation processes.

Key words. Astrochemistry – ISM: molecules – Radiative transfer – ISM: abundances – Stars: protostars

1. Introduction

Since its detection [\(Cheung et al.](#page-6-0) [1968\)](#page-6-0), NH₃ has been ubiquitously observed in a variety of environments like molecular clouds [\(Irvine et al.](#page-6-1) [1987\)](#page-6-1), prestellar cores [\(Crapsi et al.](#page-6-2) [2007\)](#page-6-2), the galactic centre [\(Winnewisser et al.](#page-6-3) [1979\)](#page-6-3), diffuse clouds [\(Liszt et al.](#page-6-4) [2006\)](#page-6-4), galaxies [\(Sandqvist et al.](#page-6-5) [2017;](#page-6-5) [Gorski et al.](#page-6-6) [2018\)](#page-6-6), star-forming regions [\(Fehér et al.](#page-6-7) [2022\)](#page-6-7), comets [\(Poch](#page-6-8) [et al.](#page-6-8) [2020\)](#page-6-8), and planet-forming disks [\(Salinas et al.](#page-6-9) [2016\)](#page-6-9). It is one of the six major molecules found in interstellar ices in the solid form [\(Boogert et al.](#page-6-10) [2015a\)](#page-6-10). It serves as an important tracer in the interiors of dense, starless cores where common tracers like CO and CS are depleted from the gas phase onto dust grains [\(Caselli et al.](#page-6-11) [1999;](#page-6-11) [Tafalla et al.](#page-6-12) [2002\)](#page-6-12) due to temperatures as low as ∼ 6K [\(Crapsi et al.](#page-6-2) [2007;](#page-6-2) [Pagani et al.](#page-6-13) [2007\)](#page-6-13) and number densities between 10^4 and 10^6 cm⁻³ [\(Keto & Caselli](#page-6-14) [2010\)](#page-6-14). Although NH₃ is affected by freeze-out [\(Caselli et al.](#page-6-15) [2022\)](#page-6-15), $NH₃$ is selectively tracing dense material, as it is not abundant in the molecular cloud surrounding dense cores (unlike CO and CS).

An important parameter that influences the grain surface abundance of $NH₃$ (and other species) is the binding energy. It serves as a measure of the strength of the interaction between the species and an adsorbate or grain surface. Additionally, once the species is adsorbed onto dust grains, the binding energy plays a crucial role in governing both its diffusion across and residence

time on the grain surface. These factors, in turn, significantly influence the physical and chemical conditions governing the evolution of star-forming regions. For example, in the vicinity of a low-mass protostar, the binding energy determines the distance from the central protostar at which sublimation fronts emerge due to the desorption of volatile species from ice grain surfaces. Furthermore, the location of these sublimation fronts, also known as "snowlines" in protoplanetary disks, directly shapes the composition of the planets forming within protoplanetary disks. Hence, precise knowledge of the binding energies is critical for an accurate interpretation of observational data and reliable prediction of abundances through simulations.

Earlier studies, such as [Hama & Watanabe](#page-6-16) [\(2013\)](#page-6-16), [Penteado](#page-6-17) [et al.](#page-6-17) [\(2017\)](#page-6-17) and [Wakelam et al.](#page-6-18) [\(2017\)](#page-6-18), provided a singular binding energy value for $NH₃$ on different types of water ice. However, recent research has challenged this notion, suggesting that NH₃ exhibits a distribution of binding energies. Experiments conducted by [He et al.](#page-6-19) [\(2016\)](#page-6-19) revealed a surface coverage-dependent distribution of binding energies for NH³ at sub-monolayer coverages. Additionally, [Kakkenpara Suresh](#page-6-20) [et al.](#page-6-20) [\(2024\)](#page-6-20) observed a distribution of binding energies on crystalline ice (3780K – 4080K) and compact amorphous solid water ice (3630K – 5280K) at monolayer coverages. Theoretical calculations by [Ferrero et al.](#page-6-21) [\(2020\)](#page-6-21), [Tinacci et al.](#page-6-22) [\(2022\)](#page-6-22), and [Germain et al.](#page-6-23) [\(2022\)](#page-6-23) have also supported this conclusion. The notion of a binding energy distribution is logical given that the

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structure of ice on dust grains is amorphous, resulting in the formation of diverse and unique adsorption sites. This idea is further substantiated by [Bovolenta et al.](#page-6-24) [\(2020\)](#page-6-24), who obtained a Gaussian-like distribution of binding energies for hydrogen fluoride on amorphous solid water (ASW).

In their numerical study, [Grassi et al.](#page-6-25) [\(2020\)](#page-6-25) have illustrated that employing a binding energy distribution allows molecules to occupy higher energy binding sites, thereby increasing their residence time on the grain surface. This prolonged residence time enhances their availability to react with other molecules, even at dust temperatures that conventionally exhibit limited or no reactivity. Building upon their findings and our previous work in [Kakkenpara Suresh et al.](#page-6-20) [\(2024\)](#page-6-20), the present study evaluates the influence of incorporating a range of binding energy values for NH_3 in astrochemical models, in particular the impact of binding energy on the abundance distribution of $NH₃$. We also investigate the possible effect that $NH₃$ abundance variations may have on the distributions of other molecules chemically linked to NH3. We do not expect the measured values of binding energy to have an impact on the chemistry in prestellar cores due to their low temperatures. Hence, in the present work, we focus our attention on protostellar cores. We focus on the very early stages of the evolution of a protostellar core, and use a model of the well-studied class 0 protostellar core, IRAS 16293-2422, as a template for our simulations.

This work is organised in the following way. In Section 2, we outline the physical and chemical model of the protostellar core used. Section 3 presents our results, and Section 4 delves into the implications of these findings along with potential avenues for future research. A concise summary of our work is provided in Section 5.

2. Model

2.1. Physical Model

The core is characterized using the model by [Crimier et al.](#page-6-26) [\(2010\)](#page-6-26) (Fig. [1\)](#page-1-0) where the radial density profile follows as $n(H_2) \propto r^{-1.8}$ within 6900 AU from the centre, where $n(H_2)$ is the H_2 number density. The source exhibits a pronounced temperature and density gradient. In this model, the temperature of the gas rises significantly towards the interior due to both gas compression during collapse and radiation emitted by the protostar. We assume that the dust temperature and the gas kinetic temperature are equivalent. The analytical approach involves dividing the core into concentric shells, and the final results are combined radially. A two-phase (gas + ice) chemical model with a dust grain radius = $0.1 \mu m$ is employed, where the entire ice layer covering the grain is available for desorption.

The abundance profiles are obtained in two steps. First, the initial conditions corresponding to the parent cloud are obtained by running a single-point simulation with $T_{dust} = T_{gas}$ = 10K, $n(H_2) = 10^4$ cm⁻³, grain radius = 0.1 μ m, cosmic-ray ionization rate $\zeta = 1.3 \times e^{-17}$ s⁻¹ and visual extinction A_V ionization rate, $\zeta = 1.3 \times e^{-77}$ s⁻¹, and visual extinction A_V
= 10 mag Adsorption desorption and photodesorption are = 10 mag. Adsorption, desorption, and photodesorption are also considered, and the simulation is allowed to proceed until a time, $t = 10^6$ years, consistent with the previous work of [Brünken et al.](#page-6-27) [\(2014\)](#page-6-27) and [Harju et al.](#page-6-28) [\(2017\)](#page-6-28) on the source. At this stage, the abundances of all the species are extracted. These are then used as the initial abundances to trace the evolution of the protostellar core. Finally, the abundances of this core

Fig. 1: (Top) The H_2 number density and (bottom) the temperature distribution assumed to model IRAS 16293-2422.

are extracted after an evolutionary time of $t = 10^4$ years. The choice of time is arbitrary; sub-structure (e.g., a protostellar disk) is expected to form within the inner regions in a timescale of 10^4 - 10^5 years which is not taken into account by the present static physical model. Hence, we chose an early time step $(10⁴$ years) to obtain the abundances, giving an estimate of the initial chemical conditions of the forming small-scale structures.

2.2. Chemical Model

The chemical evolution of the core is monitored by the gas-grain chemical code, *pyRate*, discussed in [Sipilä](#page-6-29) [\(2012\)](#page-6-29); [Sipilä et al.](#page-6-30) [\(2010\)](#page-6-30). The model is pseudo-time dependent, i.e., we track the chemical evolution assuming a static core. *pyRate* employs the rate equation method for computing the molecular abundances. The gas-phase network is constructed based on the kida.uva.20[1](#page-1-1)4¹ network [\(Wakelam et al.](#page-6-31) [2015\)](#page-6-31) with modifications to incorporate deuterated species and spin state chemistry [\(Sipilä et al.](#page-6-32) [2015a](#page-6-32)[,b\)](#page-6-33). Here we employ a large chemical network that contains a combined total of over 75,000 reactions in the gas phase and on grain surfaces, with which we simulate the chemistry of $NH₃$ and its deuterated forms. In addition, the KIDA network is also used to study the effect of proton transfer reactions on the abundances of $NH₃$ (Section [4.2\)](#page-5-0).

Initially, the species are assumed to be atomic, except for H₂ and HD, and the initial ortho/para H₂ ratio is set to 10^{-3} consistent with a spin temperature, $T_{spin} \sim 20$ K [\(Brünken et al.](#page-6-27) [2014;](#page-6-27) [Crabtree et al.](#page-6-34) [2011\)](#page-6-34). Choosing this specific value for the ratio of ortho/para H_2 corresponds to the assumption that the spin-state ratio has had the time to undergo thermalization prior to the formation of the core. The initial abundances of the species are provided in Table [1.](#page-2-0) The binding energies for $NH₃$ on water ice surfaces are sourced from [Kakkenpara Suresh et al.](#page-6-20) [\(2024\)](#page-6-20). Binding energies of various other species on water ice are obtained from [Garrod & Herbst](#page-6-35) [\(2006\)](#page-6-35) and [Sipilä](#page-6-29) [\(2012\)](#page-6-29). The simulated abundances of $NH₃$ represent the combined

¹ https://kida.astrochem-tools.org/networks.html

Species	Abundance
H ₂	5.00×10^{-1}
He	9.00×10^{-2}
HD	1.60×10^{-5}
C^+	1.20×10^{-4}
N	7.60×10^{-5}
O	2.56×10^{-4}
S^+	8.00×10^{-8}
$Si+$	8.00×10^{-9}
$Na+$	2.00×10^{-9}
$Mg+$	7.00×10^{-9}
$Fe+$	3.00×10^{-9}
P^+	2.00×10^{-10}
$\rm C1^+$	1.00×10^{-9}

abundances of the ortho and para forms of the molecule.

3. Results

3.1. Abundance Profiles

Motivated by the experimental results of [Kakkenpara Suresh](#page-6-20) [et al.](#page-6-20) (2024) , we investigated how variations in NH₃ binding energy impact the chemical composition of a protostellar core. For this purpose, we conducted a series of simulations where we systematically varied only the binding energy of $NH₃$ in each model and traced the resulting chemical evolution with time within the core. We extracted the abundances of NH₃ at $t = 10^4$ years representing the protostar at its early stages of formation.

Figure [2](#page-2-1) presents the abundances of $NH₃$ at this time in the gas-phase (solid lines) and on grain surfaces (dashed lines) with respect to the radial distance from the centre to the outer edges of the core. The gas-phase abundance of NH_3 decreases moving radially inwards toward the centre of the core before increasing rapidly by several orders of magnitude. The abundance profile shows clear differentiation based on the value of binding energy employed. The region of high NH₃ gas-phase abundance appears closer to the centre with the radius of the desorption zone varying between 150 and 300 AU with increasing binding energy value used. Investigation of the reaction rates at this time step revealed that the primary contributor influencing NH₃ gas-phase abundances is thermal desorption from dust grains. As the binding energy increases, $NH₃$ remains on the grains until a higher temperature is reached at which point it acquires sufficient thermal energy for desorption.

Notable related effects are only seen in species like HNC, CN, HCN etc (Fig. [3\)](#page-3-0). We find that their abundance profiles vary within the same spatial zone where $NH₃$ abundances vary. The effects are directly tied via chemical reactions to the variations in the $NH₃$ abundances. This effect is further discussed in section [4.1.](#page-4-0) Furthermore, we analyzed the relative abundances of key volatile compounds found in ices, namely NH_3 , CO, CO₂, CH₄, and CH₃OH with respect to H₂O. We compared our predictions with the reported values in [Boogert](#page-6-36) [et al.](#page-6-36) [\(2015b\)](#page-6-36), but direct comparisons are challenging due to

Fig. 2: Radial abundances of NH₃ in gas phase *(solid lines)* and on grain surfaces *(dashed lines)* at 10⁴ years. The binding energies of NH₃ used in each model (colours) are displayed in the lower right corner.

differences in the sources and uncertainties related to the parameters employed for calculating ice abundances in the cited study. Further details of these comparisons are available in appendix [A.](#page-7-0)

3.2. Column Density maps of p -NH₃

To assess the potential observational impact of the $NH₃$ abundance variations, we have simulated $NH₃$ column density maps individually for each BE value. Here we consider p-NH₃ only so that we can compare the column density maps against the simulated emission of the (1,1) transition of this molecule (see Sect. [3.3\)](#page-2-2). To generate the column density maps, we employ the radial abundances of p-NH₃ obtained in the previous section as input, which are then interpolated to create a two-dimensional map of the cloud core. The abundances are convolved to a beam size of 2" for the object situated at 120 pc to simulate interferometric observations (the distance to IRAS 16293-2422, although this can be applied to other similar sources by simply changing the distance value). The radial distribution of column density, denoted as *N*, is calculated using the formula:

$$
N = \sum_i p \times X_i \times n(H_2)
$$

Here, *Σ* represents the summation across *i* elements of the core model, p is the path length through an element i in cm, X_i is the abundance of the species (here, $p-NH_3$) in *i* with respect to H₂, and $n(H_2)$ is the volume density of *i* in mol cm⁻³. Figure [4](#page-3-1) shows the 2D maps of column densities of p-NH³ within a 300 AU radius where the binding energy-dependent variations are apparent. The radius of the desorption zone decreases as the binding energy increases. The column density as displayed in Fig. [4](#page-3-1) traces the part of the distribution that could only be observed with specific $NH₃$ lines, for example, the $(1,1)$ inversion line. The column density maps also indicate the extent of desorbed NH_3 that will be available in the gas phase.

3.3. Radiative transfer studies of $NH₃$ (1,1) transition

Subsequently, one-dimensional radiative transfer modelling of the 23 GHz $(1,1)$ rotational-inversion transition of p-NH₃ is carried out to verify the observability of the binding energydependent variation in the radius of the desorption zone using

Fig. 3: Variation in the (a) gas-phase and (b) grain abundances of NH_3 , HNC, HCN and CN with binding energy. The colour scheme for the lines follows the same as in Fig. [2](#page-2-1)

the non-LTE radiative transfer code LOC [\(Juvela](#page-6-37) [2020\)](#page-6-37). The first step in this analysis is to simulate the cloud that contains the protostellar core and its envelope. Given that our source is a Class 0 object, the core represents a deeply embedded source surrounded by an envelope. The methodology employed to determine NH₃ abundances within the envelope closely follows the two-step approach outlined for the core in Section 2.1. First, we obtain the abundances corresponding to the parent cloud by running a single-point simulation for $t = 10^6$ years under the same conditions as the parent cloud, similar to that described in Section 2.1. After extracting the $NH₃$ abundances at this stage, we run a second single-point simulation, this time using the specific physical conditions for the envelope. These conditions include an envelope thickness set to 0.1 pc $(5 \times 10^{17} \text{ cm})$ assuming a visual extinction, A_V , = 5 mag, $n(H_2)$ = 10⁴ m⁻³ and $T = 10$ K. The modelling is done taking into consideration the 18 hyperfine components of p-NH3. The velocity resolution is set to ∼ 0.835 km/s such that it is high enough to distinguish the hyperfine components. The spectra are obtained for 1000 lines of sight across the radius of the whole object. Each spectrum is then convolved to a synthesized beam of 2". The intensity of the transition from these spectra is integrated and interpolated to create a two-dimensional intensity map (Fig. [5\)](#page-4-1) assuming

Fig. 4: Column density map of p-NH³ without the envelope (see text) for binding energy (a) 3870K (b) 4080K and (c) 5280K. The angular size simulated by each pixel for each map is given in the top left corner of Fig. [4c.](#page-3-1)

spherical symmetry.

The collisional and radiative rate coefficients for the p- $NH₃$ line simulations were taken from the LAMDA database [\(Schöier et al.](#page-6-38) [2005\)](#page-6-38). The provided coefficients (collisional

Fig. 5: Integrated intensity map of $p-NH_3(1,1)$ in the core for binding energy (a) 3870K (b) 4080K and (c) 5280K with envelope

data from [Danby et al.](#page-6-39) [\(1988\)](#page-6-39)) do not resolve the hyperfine

structure, and hence we assumed that the coefficients for the individual hyperfine components were distributed according to LTE. To investigate the potential effect of hyperfine-resolved collisional rate coefficients on our results, we ran another series of line simulations adopting instead the set of collisional rate coefficients presented recently by [Loreau et al.](#page-6-40) [\(2023\)](#page-6-40). The hyperfine-resolved radiative transition frequencies and Einstein A coefficients were derived from data in the CDMS [\(Endres](#page-6-41) [et al.](#page-6-41) [2016\)](#page-6-41). These two approaches led only to small differences in simulated lines, and in what follows we present the results of simulations carried out using the data originating in LAMDA.

In each model, we observe that the peak intensity is centrally concentrated and declines going outwards. The location and size of this zone are in good agreement with the simulations of the column densities (Fig. [4\)](#page-3-1), despite optical thickness effects that were missed by calculating the column density directly from the simulated abundances. Predominantly, the intensity originates from the inner zone due to elevated NH_3 gas-phase abundance, as indicated by the abundance profiles (Fig. [2\)](#page-2-1). Moreover, the size of the emitting region diminishes with higher binding energy, attributed to a reduction in gas-phase NH₃ concentrations associated with increasing binding energy. Similar results are obtained for radiative transfer models using the (2,2) and (3,3) lines.

Convolutions of the spectra for the $(1,1)$ transitions at larger beam sizes are also conducted to evaluate the observability of this variation in the size of the emitting region. However, these effects become discernible only with beam sizes of 10 arcsec or smaller. This highlights the need for higher-resolution observations to detect such subtleties in the star-formation process. When convolved with a 6 arcsec beam, similar to in the observations by [Mundy et al.](#page-6-42) [\(1990\)](#page-6-42), we obtain brightness temperatures lower than but within a factor of two compared to their reported value of 16.5 K for the NH₃ $(1,1)$ emission towards the brightest regions of their source - IRAS 16293- 2422. They report NH_3 emissions arising from a ring-like region of 3000-4000 AU with a resolution of 6 arcsec (960 AU). In contrast, the BE-related effects in the model used in the present work originate from a region smaller than 300 AU, indicating that higher resolution observations will be necessary to draw important conclusions regarding effects due to NH³ binding energy towards this source. Additionally, we ran radiative transfer models assuming higher velocity resolution (0.15 km/s) for the lines based on observations by [Crapsi](#page-6-2) [et al.](#page-6-2) [\(2007\)](#page-6-2) using the Very Large Array (VLA) and found no difference in our results. Using the higher resolution requires more computational time but does not impact the results, so we decided to retain the lower velocity resolution for our models.

4. Discussion

4.1. Influence of $NH₃$ binding energy on abundance profiles of chemically related species

Interestingly, notable effects are observed on other species and their abundance profiles within the same zone where $NH₃$ abundances vary. A few examples are demonstrated in Fig. [3.](#page-3-0) The abundance profiles of these species vary depending on the chosen binding energy of NH3. To understand this, let us consider the example of HNC (Fig. [6\)](#page-5-1). In the inner regions of the model with binding energy = 3780K, HNC is efficiently pro-

duced through the reaction between HCNH⁺ and NH₃, yielding HCN and HNC. HCNH⁺ originates from HCN through the interaction with H_3^+ and can revert to HCN via reactions between $HCNH⁺$ and H_2CO (and $HCNH⁺ + NH_3$). Hence, the connection between HCN and HNC follows the sequence $HCN \rightarrow HCNH^+$ \rightarrow HNC, where the first step involves H_3^+ , and the second step involves NH₃.

 $NH₃$ binding energy = 3780 K

 $NH₃$ binding energy = 5280 K

In the lower figure ($BE = 5280$ K), the dashed arrow represents an alternative pathway for the formation of HNC through H-abstraction from $H₂CN$. This pathway becomes prominent when the gas-phase abundance of $NH₃$ is low, thereby inhibiting the formation via the reaction Fig. 6: Main formation and destruction pathways of HNC as predicted by the chemical model for the two extreme binding energy (BE) values. between $NH₃$ and $HCNH⁺$.

In contrast, in the model with binding energy $= 5280K$, the gas phase abundance of $NH₃$ is low, which effectively closes off the HCNH⁺ + NH₃ route. HNC is being created instead via H-abstraction from H_2CN (dashed arrow in Fig. [6\)](#page-5-1), but at approximately ~10% of the rate of the NH₃ route of the previous model; HNC formation is severely inhibited by the lack of available NH_3 NH_3 . This can be seen in Fig. 3 where the shape of the HNC abundance profile follows that of $NH₃$. Simultaneously, the rate of the reaction HCNH⁺ + H₂CO \rightarrow $HCN + H_2COH⁺$ increases (as the HCNH⁺ destruction channel with $NH₃$ is absent). These findings support the importance of further investigations into the role of $NH₃$ binding energy in the abundances of various species in the protostellar core.

4.2. Effect of Proton Transfer reactions on $NH₃$ abundances

[Taquet et al.](#page-6-43) [\(2016\)](#page-6-43) demonstrated that methanol abundances are significantly enhanced through proton transfer reactions involving NH_3 , as compared to simulations lacking NH_3 .

Subsequently, we introduced the following reaction

$$
CH_3OH_2^+ + NH_3 \longrightarrow CH_3OH_{gas}
$$

derived from the network outlined in their research, which contributes to the synthesis of dimethyl ether or methyl formate. We then ran a new chemical simulation with this reaction included, wherein only NH₃ binding energies were varied to investigate potential effects on methanol abundances. For this test, we used the KIDA network [\(Wakelam et al.](#page-6-31) [2015\)](#page-6-31) in place of our full deuterium and spin-state containing networks, for two main reasons: 1) to check if our overall conclusions on the binding energy-dependent NH³ desorption region remain unaffected regardless of the chemical network used (i.e., that the presence of deuterium and spin states does not affect the conclusions to a significant degree); and 2) to search for potential effects on some complex organic molecules (COMs) that are not included in our fiducial chemical network (for example, $CH₃OCH₃$, $CH₃CH₂OH$, etc). The grain-surface network used in this test is the same as our fiducial one, but with deuterium and spin states removed.

In the investigation of [Taquet et al.](#page-6-43) [\(2016\)](#page-6-43), protonation by $NH₃$ extended the survival time of methanol from $10⁴$ years to 10^5 years. In our study, methanol remained for up to 10^6 years even without their reaction integrated into the KIDA network. Upon inclusion of their reaction, our simulations validated their results, showing an increase in methanol abundances of up to two orders of magnitude for a specific binding energy value. However, this enhancement became noticeable only beyond 10⁶ years. Analysis of abundances for different binding energy values at a specific time step revealed marginal variations in methanol abundances, even at 10⁶ years, where the most substantial difference emerged between simulations with and without the proton-transfer reaction. The discrepancy in the evolutionary time in our model versus that of [Taquet](#page-6-43) [et al.](#page-6-43) (2016) regarding when the effect on $CH₃OH$ becomes apparent is very likely due to different simulation parameters. We have not attempted to duplicate their results. Nevertheless, the comparison indicates that proton-transfer reactions can be very important and should be explored in more detail in later simulations.

5. Conclusions

NH₃ is an important molecule widely observed in various astronomical sources and on dust grain surfaces. However, uncertainties pertaining to its binding energy values prevent an accurate determination of its abundance and role in the chemistry of star and planet formation. The binding energy is a key parameter determining the abundance and chemistry of a species in the ISM. Recent studies have challenged previous notions of a unique binding energy value for $NH₃$ proposing instead a multi-binding energy approach.

Drawing on previously established experimental work by [Kakkenpara Suresh et al.](#page-6-20) [\(2024\)](#page-6-20), we incorporated multiple NH₃ binding energy values derived from these studies into gas-grain chemical networks to examine their impact on $NH₃$ abundance within a protostellar core. We conducted multiple simulations, systematically varying only the NH₃ binding energy, to discern its influence on the abundance profiles of $NH₃$ and other species. Our findings reveal a distinct dependence of $NH₃$ abundance

profiles on the binding energy employed, particularly in the inner warm regions of the model. This variability extends its influence on other key species, including HCN, HNC, CN, wherein the NH₃ abundance dictates the preferred pathway for their formation. On the contrary, in proton transfer reactions involving NH3, expected to enhance methanol formation, the abundance variation of $NH₃$ due to binding energy does not appear to be a significant contributing factor.

Simulation of column density maps for p-NH₃ reveals that the size of the desorption region diminishes as the binding energy increases. These findings align with radiative transfer studies on the $(1,1)$ inversion line of NH₃, where we added an envelope to our physical model to examine absorption and emission effects. In these studies, we observed that the peak intensity is centrally concentrated and decreases outward. Additionally, the intensity diminishes with higher binding energy due to a reduction in gas-phase $NH₃$. Our results highlight the importance of considering diverse binding energies in astrochemical models, providing a refined understanding of molecular cloud chemistry and star formation processes.

For future work, it is crucial to refine our understanding by further exploring the impact of varied binding energies on complex organic molecules (COMs) within astrochemical models. Additionally, investigations into the spatial distribution and temporal evolution of species influenced by multi-binding energy approaches would contribute valuable insights. The present results apply at very early times in the core evolution when the substructure is still absent and, hence, probe the very early stages of forming protostellar systems. Consequently, there is a critical need to enhance the physical model, incorporating more precise representations of observed substructures within protostellar cores. This improvement is essential for providing a more accurate and detailed description of the underlying phenomena in such sources.

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References

- Boogert, A. A., Gerakines, P. A., & Whittet, D. C. 2015a, Annual Review of Astronomy and Astrophysics, 53, 541
- Boogert, A. A., Gerakines, P. A., & Whittet, D. C. 2015b, Annual Review of Astronomy and Astrophysics, 53, 541
- Bovolenta, G., Bovino, S., Vöhringer-Martinez, E., et al. 2020, Molecular Astrophysics, 21, 100095
- Brünken, S., Sipilä, O., Chambers, E. T., et al. 2014, Nature, 516, 219
- Caselli, P., Pineda, J. E., Sipilä, O., et al. 2022, The Astrophysical Journal, 929, 13
- Caselli, P., Walmsley, C., Tafalla, M., Dore, L., & Myers, P. 1999, The Astrophysical Journal, 523, L165
- Cheung, A. C., Rank, D. M., Townes, C. H., Thornton, D. D., & Welch, W. J. 1968, Phys. Rev. Lett., 21, 1701
- Crabtree, K. N., Indriolo, N., Kreckel, H., Tom, B. A., & McCall, B. J. 2011, The Astrophysical Journal, 729, 15
- Crapsi, A., Caselli, P., Walmsley, M. C., & Tafalla, M. 2007, Astronomy & Astrophysics, 470, 221
- Crimier, N., Ceccarelli, C., Maret, S., et al. 2010, Astronomy & Astrophysics, 519, A65
- Danby, G., Flower, D. R., Valiron, P., Schilke, P., & Walmsley, C. M. 1988, MNRAS, 235, 229
- Endres, C. P., Schlemmer, S., Schilke, P., Stutzki, J., & Müller, H. S. P. 2016, Journal of Molecular Spectroscopy, 327, 95
- Fehér, O., Tóth, L. V., Kraus, A., et al. 2022, The Astrophysical Journal Supplement Series, 258, 17
- Ferrero, S., Zamirri, L., Ceccarelli, C., et al. 2020, The Astrophysical Journal, 904, 11
- Garrod, R. & Herbst, E. 2006, Astronomy & Astrophysics, 457, 927
- Germain, A., Tinacci, L., Pantaleone, S., Ceccarelli, C., & Ugliengo, P. 2022, ACS Earth and Space Chemistry
- Gorski, M., Ott, J., Rand, R., et al. 2018, The Astrophysical Journal, 856, 134 Grassi, T., Bovino, S., Caselli, P., et al. 2020, Astronomy & Astrophysics, 643, A155
- Hama, T. & Watanabe, N. 2013, Chemical reviews, 113, 8783
- Harju, J., Sipilä, O., Brünken, S., et al. 2017, The Astrophysical Journal, 840, 63
- He, J., Acharyya, K., & Vidali, G. 2016, The Astrophysical Journal, 825, 89
- Irvine, W., Goldsmith, P., Hjalmarson, Å., Hollenbach, D., & Thronson, H. 1987, Reidel Dordrecht, 561
- Juvela, M. 2020, Astronomy & Astrophysics, 644, A151
- Kakkenpara Suresh, S., Dulieu, F., Vitorino, J., & Caselli, P. 2024, Astronomy & Astrophysics, 682, A163
- Keto, E. & Caselli, P. 2010, Monthly Notices of the Royal Astronomical Society, 402, 1625
- Liszt, H., Lucas, R., & Pety, J. 2006, Astronomy & Astrophysics, 448, 253
- Loreau, J., Faure, A., Lique, F., Demes, S., & Dagdigian, P. J. 2023, MNRAS, 526, 3213
- Mundy, L. G., Wootten, H., & Wilking, B. A. 1990, Astrophysical Journal, Part 1 (ISSN 0004-637X), vol. 352, March 20, 1990, p. 159-166., 352, 159
- Pagani, L., Bacmann, A., Cabrit, S., & Vastel, C. 2007, A&A, 467, 179
- Penteado, E., Walsh, C., & Cuppen, H. 2017, The Astrophysical Journal, 844, 71 Poch, O., Istiqomah, I., Quirico, E., et al. 2020, Science, 367, eaaw7462

Salinas, V. N., Hogerheijde, M. R., Bergin, E. A., et al. 2016, Astronomy &

- Astrophysics, 591, A122 Sandqvist, A., Hjalmarson, Å., Frisk, U., et al. 2017, Astronomy & Astrophysics,
- 599, A135
- Schöier, F. L., van der Tak, F. F. S., van Dishoeck, E. F., & Black, J. H. 2005, A&A, 432, 369
- Sipilä, O. 2012, Astronomy & Astrophysics, 543, A38
- Sipilä, O., Caselli, P., & Harju, J. 2015a, Astronomy & Astrophysics, 578, A55
- Sipilä, O., Harju, J., Caselli, P., & Schlemmer, S. 2015b, Astronomy & Astrophysics, 581, A122
- Sipilä, O., Hugo, E., Harju, J., et al. 2010, Astronomy & Astrophysics, 509, A98 Tafalla, M., Myers, P., Caselli, P., Walmsley, C., & Comito, C. 2002, The Astrophysical Journal, 569, 815
- Taquet, V., Wirström, E. S., & Charnley, S. B. 2016, The Astrophysical Journal, 821, 46
- Tinacci, L., Germain, A., Pantaleone, S., et al. 2022, ACS Earth and Space Chemistry, 6, 1514
- Wakelam, V., Loison, J.-C., Herbst, E., et al. 2015, The Astrophysical Journal Supplement Series, 217, 20
- Wakelam, V., Loison, J.-C., Mereau, R., & Ruaud, M. 2017, Molecular Astrophysics, 6, 22
- Winnewisser, G., Churchwell, E., & Walmsley, C. 1979, Astronomy and Astrophysics, vol. 72, no. 1-2, Feb. 1979, p. 215-223., 72, 215

Appendix A: Relative Ice Abundances of Key Volatiles

In our model, low ice abundances in the central regions of the source, attributed to the high temperatures (approximately 200K), render these ice abundance values less meaningful. As a result, in Fig. [A.1,](#page-7-1) we present simulated abundance ratios beyond 2000 AU only, where ice abundances are higher due to temperatures dropping to around 10-20 K. Our findings for CO and CH3OH align well with the range observed in low-mass young stellar objects (LYSOs) as described in [Boogert et al.](#page-6-36) [\(2015b\)](#page-6-36). Although our estimates for CH⁴ abundances are slightly elevated, they remain reasonably close to the values reported in the [Boogert et al.](#page-6-36) [\(2015b\)](#page-6-36). In our model, $CO₂$ exhibits levels lower by two orders of magnitude, while NH₃ is overestimated by a factor of three. These discrepancies may stem from a variety of factors, such as the elemental abundances used in our model, the impact of background emissions on the observed line intensities, or missing grain-surface chemistry (in the case of $CO₂$). A comprehensive discussion of the cause of these variations exceeds the scope of our current study and is therefore omitted.

Fig. A.1: Relative ice abundances of key volatiles with respect to water ice. The solid lines represent values obtained in this work and the shaded zones of the same colour represent the range of observed values reported in [Boogert et al.](#page-6-36) [\(2015b\)](#page-6-36)