Investigating the impact of X-rays on the molecular abundances of inner envelopes and disks around low-mass protostars with ngVLA

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Abstract

Water destruction by X-rays has been proposed to explain the low water gas fractional abundances ($< 10^{-6}$) in the inner warm envelopes and disks around several low-mass protostars, but the detailed chemistry, including the nature of alternative oxygen carriers, is not yet understood. Recently, we computed the chemical composition of low-mass protostellar envelopes using a gas-grain chemical reaction network, with various X-ray luminosities of the central protostars. We aimed to understand the impact of X-rays on the composition of low-mass protostellar envelopes, focusing specifically on water and related oxygen bearing species. According to our calculations, X-ray induced chemistry strongly affects the abundances of water and related species such as O, O_2. In addition, the fractional abundances of HCO^+ and CH_3OH, which have been considered to be tracers of the water snowline, significantly increase/decrease within the water snowline, respectively, as the X-ray fluxes become larger. Moreover, the fractional abundance of NH_3, one of the dominant Nitrogen carriers, is also affected by strong X-ray fields, especially within its snowline. Future molecular line observations with ngVLA will clarify the impact of X-rays, which enable us to make a more detailed picture of chemistry in the inner envelopes and disks around protostars.

Key words: Astrochemistry – ISM: molecules – Stars: formation – Stars: protostars – Protoplanetary disks –

1. Introduction

Water is a key molecule in star and planet forming regions. Recent water line observations toward several low-mass Class 0 and I protostars suggested low water gas fractional abundances ($< 10^{-6}$) in the inner warm envelopes and disks ($r < 10^2$ au, e.g., Persson et al. 2016; Jensen et al. 2019; Harsono et al. 2020; van Dishoeck et al. 2021). Water destruction by X-rays has been proposed to influence the water abundances in these inner regions (Stäuber et al. 2005; Stäuber et al. 2006), but the nature of alternative oxygen carriers is not yet understood. In addition, the chemical model that Stäuber et al. (2005) and Stäuber et al. (2006) adopted was limited. Most notably, they did not include detailed gas-grain interactions and grain-surface chemistry.

In our recent study (Notsu et al. 2021), we revisited the chemistry of water and related molecules in low-mass Class 0 protostellar envelopes, under various X-ray field strengths. We computed the chemical composition of the protostellar envelopes using a 1D gas-grain chemical reaction network (mostly based on Walsh et al. (2015) and Bosman et al. (2018)) with adding X-ray induced chemical processes. We aimed to understand the impact of X-rays on the composition of low-mass protostellar envelopes, focusing specifically on water and related oxygen bearing species.

On the basis of our calculations (Notsu et al. 2021), the X-rays from central protostars have strong effects on the water gas abundances. The behavior of the water abundances in the gas phase changes inside and outside the water snowline ($T_{\rm gas} \sim 10^2$ K, $r \sim 10^2$ au). Outside the water snowline, the water gas abundance increases with X-ray luminosities. Inside the water snowline, water maintains a high gas abundance of $\sim 10^{-4}$ for low X-ray luminosities, with water and CO being the dominant oxygen carriers. For high X-ray luminosities, the water gas abundances significantly decrease just inside the water snowline (down to $< 10^{-7}$) and in the innermost regions with $T_{\rm gas} \gtrsim 250$ K (down to $\sim 10^{-6}$). For these cases, the fractional abundances of gas-phase O_2 and O reach $\sim 10^{-4}$ within the water snowline, and they become the dominant oxygen carriers. However, observationally investigating the inner warm O_2 and O abundances for many objects is difficult (Yıldız et al. 2013; Taquet et al. 2018). This is partly because O_2 does not have electric dipole-allowed transitions.

2. Molecular line observations with ngVLA

According to our model calculations (see Section 1 and Notsu et al. 2021), the HCO^+ and CH_3OH gas abundances, which have been considered to be tracers of the water snowline (e.g., van 't Hoff et al. 2018a; van 't Hoff et al. 2018b; Leemker et al. 2021), significantly increase/decrease within the water snowline, respectively, as the X-ray fluxes become larger. Moreover, the fractional abundances of NH_3 are also affected by strong X-ray fields, especially within its own snowlines. Future high-spatial molecular line observations with ngVLA will be expected to constrain the inner gas abundances of these

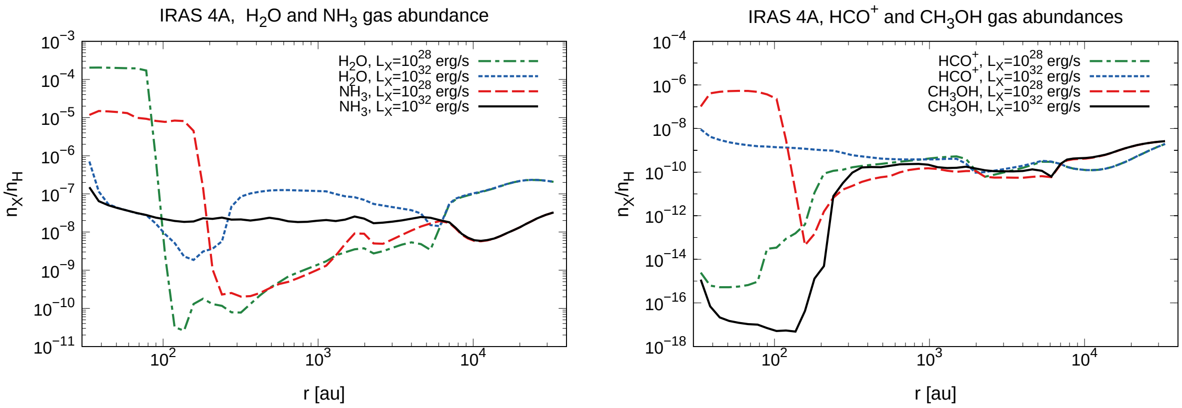

Fig. 1. [Left panels]: The green dashed dotted line and the blue dotted line show radial profiles of H_2O gas fractional abundances with respect to total hydrogen densities (n_{H_2O}/n_H) for values of central star X-ray luminosities L_X=10^{28} and 10^{32} erg s^{-1}, respectively. The red dashed line and the black solid line show radial profiles of NH_3 gas fractional abundances (n_{NH_3}/n_H). [Right panel]: The green dashed dotted line and the blue dotted line show radial profiles of HCO^+ gas fractional abundances with respect to total hydrogen densities (n_{HCO^+}/n_H). The red dashed line and the black solid line show radial profiles of CH_3OH gas fractional abundances (n_{CH_3OH}/n_H). In this Figure, these profiles are based on calculations of NGC 1333-IRAS 4A envelope models in Notsu et al. (2021).

molecules. By combining molecular line observations with ALMA (such as H_2O lines) and ngVLA, a more detailed picture of the X-ray effects on the oxygen chemistry will be obtained. In addition, they will also open a window into the independent nitrogen chemistry. Here, we briefly summarize the impact of X-rays on the abundances of CH_3OH, HCO^+, and NH_3, and consider the possible observations with ngVLA.

2.1. NH_3

Left panel of Figure 1 shows the radial profiles of the water and NH_3 gas fractional abundances for values of central star X-ray luminosities L_X=10^{28} and 10^{32} erg s^{-1}, respectively. As we explained in Section 1 and Notsu et al. (2021), the behavior of the water gas abundances changes outside and inside its snowline ($T_{gas} \sim 10^2$ K, $r \sim 10^2$ au).

NH_3 is a dominant nitrogen-bearing molecule in molecular cloud and pre-stellar cores (especially in the later stage of their evolutions), in which NH_3 ice abundances are as high as 10^{-5} (Mumma & Charnley 2011; Furuya & Persson 2018). Considering the differences in binding energies, the NH_3 snowline position locates outside the water snowline ($\gtrsim 2\times10^2$ au). Zhang et al. (2018) discussed the possibility to observe the NH_3 line emission (the 23GHz 1,1 and 2,2 lines) with ngVLA as a proxy of the water snowline in disks.

According to our calculations, the NH_3 gas abundances increase with X-ray luminosities outside its snowline. Inside the NH_3 snowline, as the X-ray fluxes increase, the NH_3 gas abundances also decrease from 10^{-5} to $\lesssim 10^{-7}$, as in the case of H_2O. Thus, with strong X-ray field, the NH_3 abundance is no longer dominant nitrogen carrier. In addition, it cannot be used as the tracer of the water snowline position, since gas-phase NH_3 abundances are similar inside and outside the NH_3 snowline. We note that by the destruction of NH_3, free nitrogen atoms are released into the gas phase, which will drive additional nitrogen chemistry there.

The NH_3 line emission (e.g., the 23GHz (1,1), (2,2), and (3,3) lines) have been observed toward protostellar disks and envelopes using VLA (e.g., Choi et al. 2007; Choi et al. 2010). However, the spatial resolutions of such VLA observations (∼ 1.0”) were not sufficient to resolve the inner structures around the protostars nearby (∼ a few hundreds pc). In addition, especially in the inner envelopes and disks around low-mass protostars, sensitivities of such VLA observations were insufficient to detect higher J and K transitions, which can potentially trace regions close to the protostars. Future ngVLA observations of these NH_3 lines with much higher resolutions ($\lesssim$ 0.3” at around 23 GHz) and much higher sensitivities will resolve the NH_3 gas emission within its snowline towards many protostars, and can also constrain the impact of X-rays on NH_3 gas abundances. Moreover, such observations will be important to trace the chemical history of nitrogen bearing molecules, since NH_3 is also one of key molecules in considering formation of nitrogen-bearing complex organic molecules.

2.2. HCO^+ and CH_3OH

Right panel of Figure 1 shows the radial profiles of the HCO^+ and CH_3OH fractional abundances in the gas phase for L_X=10^{28} and 10^{32} erg s^{-1}, respectively. The fractional abundances of HCO^+ and CH_3OH, which have been considered to be tracers of the water snowline, significantly increase/decrease within the water snowline, respectively, as the X-ray fluxes become larger (see also Notsu et al. 2021).

The HCO^+ and CH_3OH lines have been observed toward several protostars with ALMA (e.g., van ’t Hoff et al. 2018a; van ’t Hoff et al. 2018b; Hsieh et al. 2019). The HCO^+ (1-0) 89 GHz and $H^{13}CO^+$ (1-0) 87 GHz lines, and many CH_3OH lines are within the ngVLA frequency coverage. Since the dust opacities in the frequencies of ngVLA are smaller than those of ALMA, these observations will be useful to trace the inner gas abundances more precisely. Series of CH_3OH lines in 25 GHz band have been detected toward NGC1333 IRAS 4A1, where almost all of the molecular line emissions were absent in the ALMA bands (De Simone et al. 2020).

3. Summary

According to our calculations (Notsu et al. 2021), X-ray induced chemistry strongly affects the abundances of water and related species, such as O_2, HCO^+, CH_3OH, and NH_3, especially in the inner regions, and can explain the observed low water abundances in the inner protostellar envelopes. Future molecular line observations with ngVLA will constrain the inner gas abundances of such molecules, creating a more detailed picture of the oxygen and nitrogen chemistry. We note that the material in the protostellar envelopes accretes into disks, thus the molecular abundances in protostellar envelopes determine the initial abundances of chemical evolution in disks, where planet formation occurs (see e.g., Öberg & Bergin 2020). It will be important to discuss how the X-ray induced chemistry at protostar phases affect the initial abundances and chemical evolution in planet forming disks.

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