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Possibility to locate the position of the H_2O snowline in protoplanetary disks through spectroscopic observations

Shota Notsu[1,2], Hideko Nomura[3], Catherine Walsh[4], Mitsuhiko Honda[5], Tomoya Hirota[6], Eiji Akiyama[6] and T. J. Millar[7]

[1]Department of Astronomy, Graduate School of Science, Kyoto University, Kitashirakawa-Oiwake-cho, Sakyo-ku, Kyoto 606-8502, Japan
e-mail: snotsu@kusastro.kyoto-u.ac.jp
[2]Research Fellow of Japan Society for the Promotion of Science (DC1)
[3]Department of Earth and Planetary Science, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan
[4]School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK
[5]Department of Physics, School of Medicine, Kurume University, 67 Asahi-machi, Kurume, Fukuoka 830-0011, Japan
[6]National Astronomical Observatory of Japan, 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan
[7]Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, University Road, Belfast, BT7 1NN, UK

Abstract. Observationally measuring the location of the H_2O snowline is crucial for understanding the planetesimal and planet formation processes, and the origin of water on Earth. The velocity profiles of emission lines from protoplanetary disks are usually affected by Doppler shift due to Keplerian rotation and thermal broadening. Therefore, the velocity profiles are sensitive to the radial distribution of the line-emitting regions. In our work (Notsu *et al.* 2016, 2017), we found candidate water lines to locate the position of the H_2O snowline through future high-dispersion spectroscopic observations. First, we calculated the chemical composition of the disks around a T Tauri star and a Herbig Ae star using chemical kinetics. We confirmed that the abundance of H_2O gas is high not only in the hot midplane region inside the H_2O snowline but also in the hot surface layer and the photodesorption region of the outer disk. The position of the H_2O snowline in the Herbig Ae disk exists at a larger radius from the central star than that in the T Tauri disk. Second, we calculated the H_2O line profiles and identified that H_2O emission lines with small Einstein A coefficients ($\sim 10^{-6} - 10^{-3}$ s^{-1}) and relatively high upper state energies ($\sim$ 1000K) are dominated by emission from the hot midplane region inside the H_2O snowline, and therefore their profiles potentially contain information which can be used to locate the position of the H_2O snowline. The wavelengths of the H_2O lines which are the best candidates to locate the position of the H_2O snowline range from mid-infrared to sub-millimeter, and the total line fluxes tend to increase with decreasing wavelengths. We investigated the possibility of future observations using the ALMA and mid-infrared high-dispersion spectrographs (e.g., SPICA/SMI-HRS). Since the fluxes of those identified lines from a Herbig Ae disk are stronger than those of a T Tauri disk, the possibility of a successful detection is expected to increase for a Herbig Ae disk.

1. Introduction

Observationally locating the position of the H_2O snowline (Hayashi 1981; Hayashi *et al.* 1985) in a protoplanetary disk is important. It will provide information on the physical and chemical conditions in disks, such as the temperature structure, the dust-grain size distribution, and the water vapor distribution in the disk midplane (e.g., Oka *et al.*

2011; Piso *et al.* 2015), and will give constraints on the current formation theories of planetesimals and planets (e.g., Öberg *et al.* 2011; Okuzumi *et al.* 2012; Ros & Johansen 2013). It will help clarify the origin of water on rocky planets including the Earth (e.g., Morbidelli *et al.* 2000, 2012, 2016; Sato *et al.* 2016). Through recent space and ground infrared spectroscopic observations for protoplanetary disks, some infrared H_2O lines, which mainly trace the disk surface and the photodesorption region of the outer disk, have been detected (for more details, see e.g., Pontoppidan *et al.* 2010a,b; Hogerheijde *et al.* 2011; van Dishoeck *et al.* 2014; Blevins *et al.* 2016; Banzatti *et al.* 2017; Notsu *et al.* 2016, 2017).

The velocity profiles of emission lines from protoplanetary disks are usually affected by Doppler shift due to Keplerian rotation and thermal broadening. Therefore, the velocity profiles are sensitive to the radial distribution of the line-emitting regions. In our work (e.g., Notsu *et al.* 2016, 2017), we calculated the chemical composition and the H_2O line profiles in a T Tauri disk† and a Herbig Ae disk. We investigated the line properties in detail for candidate water lines to locate the position of the H_2O snowline over a wide wavelength range from mid-infrared to sub-millimeter, and discuss the possibility of detecting such lines with future observations. In this proceeding paper, we introduce the outline and key results of our recent work (Notsu *et al.* 2016, 2017).

2. Method & Result

2.1. *The physical models of the protoplanetary disks*

The physical structures of the protoplanetary disk models used here are calculated using the methods in Nomura & Millar (2005) including X-ray heating (Nomura *et al.* 2007). A more detailed description of the background theory and computation of this physical model is described in the original papers (Nomura & Millar 2005; Nomura *et al.* 2007) and our works (e.g., Notsu *et al.* 2015, 2016, 2017). Walsh *et al.* (2010, 2012, 2014, 2015), Heinzeller *et al.* (2011), Furuya *et al.* (2013) used the same physical models for a T Tauri disk and a Herbig Ae disk to study various chemical and physical effects, and they also describe the calculation of the physical structures in detail.

We adopted the physical models of a steady, axisymmetric Keplerian disks surrounding a T Tauri star with mass $M_* = 0.5 M_\odot$, radius $R_* = 2.0 R_\odot$, and effective temperature $T_* = 4000$K, and a Herbig Ae star with $M_* = 2.5 M_\odot$, $R_* = 2.0 R_\odot$, and $T_* = 10{,}000$K. We adopt the same compact and spherical dust-grain model of Nomura & Millar (2005). In Figure 1, we display the gas number density and the gas temperature of a Herbig Ae disk (Notsu *et al.* 2017).

2.2. *Chemical structures of the protoplanetary disks*

To investigate the chemical structure of disks, we use a large chemical network which includes gas-phase reactions and gas-grain interactions (freeze-out of gas molecules on dust grains, and thermal and non-thermal desorption from dust grains). The initial fractional abundances (relative to total hydrogen nuclei density) we use are atomic and oxygen-rich low-metallicity from Graedel *et al.* (1982), listed in Table 8 of Woodall *et al.* (2007).

Figure 2 shows the fractional abundances (relative to total gas hydrogen nuclei density, $n_{\rm H}$) of H_2O gas and ice in a Herbig Ae disk (Notsu *et al.* 2017). The H_2O snowline of the Herbig Ae disk exists at a radius of $r \sim 14$ au in the midplane (~ 120K), which is significantly larger than that for the T Tauri disk model ($r \sim 1.6$ au, see Figure 2 of

† In the remainder of this paper, we define the protoplanetary disks around T Tauri/Herbig Ae stars as "T Tauri/Herbig Ae disks".

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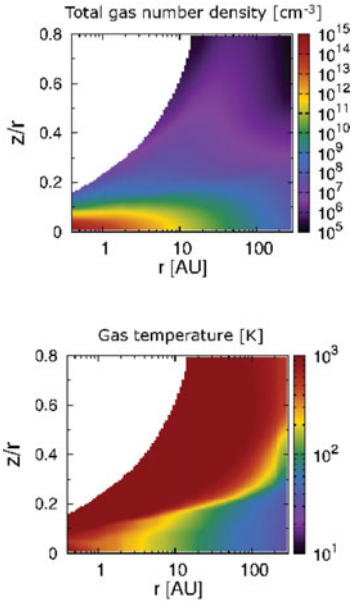

Figure 1. The total gas number density in cm^{-3} (top), the gas temperature in Kelvin (bottom) of a Herbig Ae disk as a function of the disk radius in au and height (scaled by the radius, z/r) up to maximum radius of r =300 au (Notsu *et al.* 2017).

Notsu *et al.* 2016). This is because the gas and dust temperatures, which are coupled in the midplane, are higher in the Herbig Ae disk than in T Tauri disk. We found that the abundance of H_2O is high (up to 10^{-4}) in the inner region with higher temperature ($\gtrsim$ 170K) within $\sim 7-8$ au, relatively high ($\sim 10^{-8}$) between $7-8$ au and 14 au (= the position of the H_2O snowline, ∼120K) near the equatorial plane. In addition, it is relatively high ($\sim 10^{-8}-10^{-7}$) in the hot surface layer and the photodesorbed region of the outer disk, compared to its value ($\sim 10^{-12}$) in the regions outside the H_2O snowline near the equatorial plane (for more details, see Notsu *et al.* 2017).

There is the radial difference between the exact H_2O snowline location (r ∼14 au) and the outer edge of the hot water vapor area ($r \sim 8$ au) in a Herbig Ae disk, although there is no significant difference between them in a T Tauri disk with the radial steeper temperature profile in the disk midplane. It is because the water formation rate by gas-phase reactions strongly depends on the gas temperature. Such water vapor distribution in the Herbig Ae disk midplane was discussed in Woitke *et al.* (2009).

2.3. *Calculations of* H_2O *emission lines from protoplanetary disks*

Using the H_2O gas abundance distribution obtained from our chemical calculation described in the previous paragraph, we calculate the H_2O emission line profiles ranging from near-infrared to sub-millimeter wavelengths from a T Tauri and a Herbig Ae disk assuming Keplerian rotation, and identify the lines which are the best candidates for probing emission from the inner thermally desorbed water reservoir, i.e., within the H_2O snowline. In our work (e.g., Notsu *et al.* 2016, 2017), we adopted the same calculation method to determine the H_2O emission line profiles from a T Tauri disk (based on Rybicki & Lightman 1986, Hogerheijde & van der Tak 2000, Nomura & Millar 2005, and Schöier *et al.* 2005), with the detailed model explained in Section 2.3 of Notsu *et al.* (2016). The code which we have built for calculating emission line profiles is a modification of

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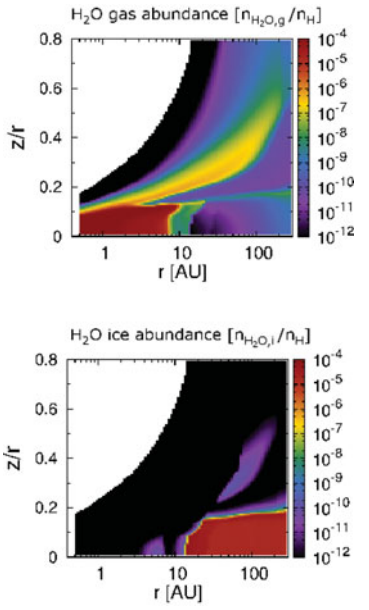

Figure 2. The fractional abundance (relative to total hydrogen nuclei density) distributions of H_2O gas (top) and H_2O ice (bottom) of a Herbig Ae disk as a function of disk radius and height (scaled by the radius, z/r) up to maximum radius of r =300au (Notsu *et al.* 2017).

the original 1D code called RATRAN‡ (Hogerheijde & van der Tak 2000). We adopt the data of line parameters in the Leiden Atomic and Molecular Database LAMDA¶ (Schöier *et al.* 2005). Here we note that in our method, we adopt the assumption of local thermal equilibrium (LTE) to obtain the level populations of the water molecule (n_u and n_l). In addition, we set the ortho to para ratio (OPR) of water to its high-temperature value of 3 throughout the disk.

According to our calculations (e.g., Notsu *et al.* 2016, 2017), we showed that H_2O emission lines with small Einstein A coefficients ($A_{ul} \sim 10^{-3} - 10^{-6}$ s^{-1}) and relatively high upper state energies ($E_{up} \sim 1000$K) are dominated by emission from the region inside the H_2O snowline, and therefore their profiles potentially contain information which can be used to locate the position of the snowline. This is because the water gas column density of the region inside the H_2O snowline is high enough that all lines are optically thick as long as $A_{ul} > 10^{-6}$ s^{-1}. On the other hand, the region outside the H_2O snowline has lower water gas column densities and lines with larger Einstein A coefficients have a more significant contribution to their fluxes since the lines are optically thin. In addition, we calculated the profiles of lines which have been detected by previous spectroscopic observations using *Herschel* (e.g., the ortho-H_2O 63.32μm and 538.29μm lines). These lines are less suited to locate the position of the H_2O snowline, because they are not dominated in flux by the region inside the H_2O snowline.

Figure 3 shows the emission profiles of ortho-H_2O lines at 682.66μm ($A_{ul} = 2.82\times10^{-5}$ s^{-1}, $E_u = 1088.7$K), 63.32μm ($A_{ul} = 1.77$ s^{-1}, $E_u = 1070.6$K) and 538.29μm ($A_{ul} = 3.50\times10^{-3}$ s^{-1}, $E_u = 61.0$K), for the Herbig Ae disk (Notsu *et al.* 2017). Figure 4 shows the line-of-sight emissivity (emissivity times extinction, $\eta_{ul}e^{-\tau_{ul}}$; see Equation (14) of Notsu *et al.* 2016) along the line-of sight direction (from $z = \infty$ to $-\infty$) of the

‡ http://home.strw.leidenuniv.nl/ michiel/ratran/
¶ http://home.strw.leidenuniv.nl/ moldata/

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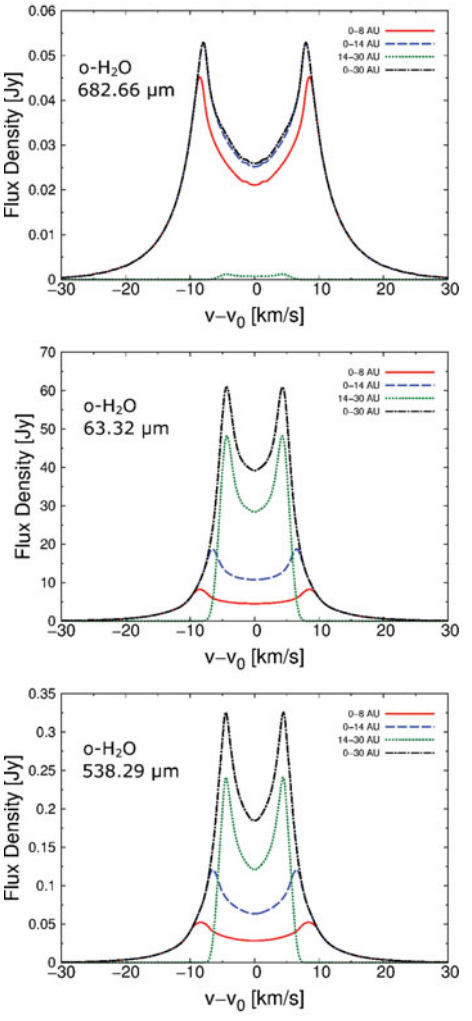

Figure 3. The emission profiles of ortho-H_2O lines at 682.66μm (top), 63.32μm (middle) and 538.29μm (bottom), for the Herbig Ae disk. We assume that the distance to the object d is 140pc ($\sim$ the distance of Taurus molecular cloud), and the inclination angle of the disk, i, is 30 degree (Notsu *et al.* 2017).

same three water lines for the Herbig Ae disk (Notsu *et al.* 2017). According to Figure 4, in the candidate 682.66μm line, the values of emissivity at $r \lesssim 14$ au (= the position of the H_2O snowline), $T_g \gtrsim$120K, and $z/r \sim 0.05 - 0.12$ are larger than those of the optically thin hot surface layer and the photodesorbed layer of the outer disk, and in particular those in the region with a higher H_2O gas abundance ($\sim 10^{-4}$, $r < 7 - 8$ au, and $T_g \gtrsim$170K) and $z/r \sim 0.05 - 0.12$ are much larger.

Figure 5 shows the total fluxes of the various ortho-H_2O lines which are the candidates for tracing emission from hot water vapor within the H_2O snowline for a Herbig Ae disk (top panel) and a T Tauri disk (bottom panel) (Notsu *et al.* 2017). Since the fluxes of these lines from Herbig Ae disks are larger than those from T Tauri disks, the possibility of a successful detection is expected to increase for a Herbig Ae disk. The wavelengths of those lines which are the best candidates to locate the position of the H_2O snowline range from mid-infrared to sub-millimeter. The values of total fluxes tend to be larger as

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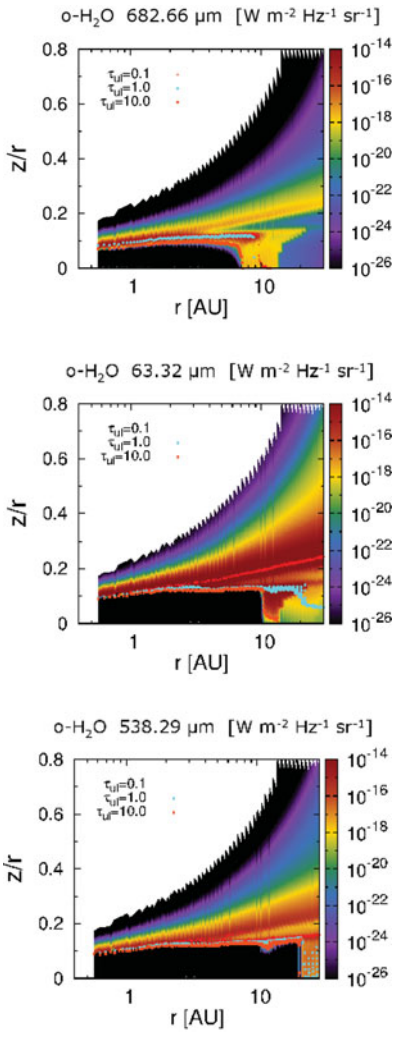

Figure 4. The line-of-sight emissivity of ortho-H_2O lines at 682.66μm (top), 63.32μm (middle) and 538.29μm (bottom), for the Herbig Ae disk. In these panels, we overplot the total optical depth contours $(\tau_{ul} = 0.1$ (red cross points), 1 (cyan circle points), and 10 (orange square points)) on top of these line emissivity panels (Notsu *et al.* 2017).

the wavelengths of the H_2O lines become shorter. This is because the peak wavelength of the Planck function at the gas temperature around the H_2O snowline ($T_g \sim 100 - 200$ K) is in the mid-infrared region.

3. Discussion and Conclusion

In this work, we calculated the disk water vapor distribution and corresponding H_2O line profiles for a T Tauri disk and a Herbig Ae disk, and identified candidate water lines which can locate the position of the H_2O snowline across a wide wavelength range from mid-infrared to sub-millimeter.

The wavelengths of such candidate lines which trace emission from the hot water vapor within H_2O snowline overlap with the capabilities of ALMA and future mid-infrared high-

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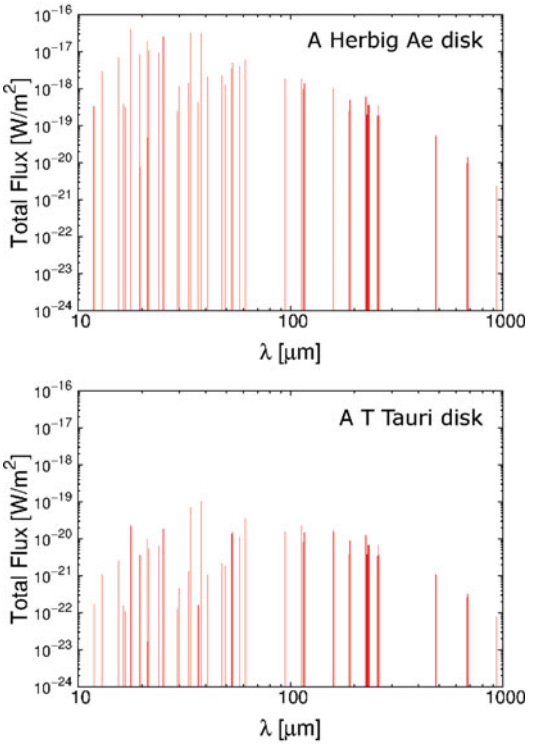

Figure 5. The total fluxes of the ortho-H_2O lines which are best candidates to trace the emission from the water vapor within the H_2O snowline, for a Herbig Ae disk (top panel) and a T Tauri disk (bottom panel) (Notsu *et al.* 2017).

dispersion spectrographs (e.g., SPICA/SMI-HRS). The successful detection in a Herbig Ae disk could be achieved with current ALMA capabilities using several lines. Mid-infrared instruments such as HRS on SPICA/SMI would have a high sensitivity in the Q band (e.g., $\sim$ 16-18μm).

4. Acknowledgements

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