



Water Formation and Heritage Across Cosmic Time

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Objectives:

1. Investigate excitation and radiative transfer in the HD molecule, in order to understand its utility as tracer of disk mass.
2. Study how water and complex organic molecules (COMs) form in ices in molecular clouds and disks.
3. Study how water is distributed and how it migrates in protoplanetary disks to understand how water ends up in the planets, small bodies (comets, asteroids) and dust in planetary systems by carrying out state-of-the-art chemical and dynamical modeling.
4. Determine how the current value of the deuterium-to-hydrogen (D/H) ratio of Uranus and Neptune is reproduced by solid accretion taking place during the process of forming, using both analytical and numerical approaches.
5. Determine if polarization can be used to differentiate water clouds from sulfuric acid clouds, and if acid concentration is low enough to support life as we know it on an exo-Venus to be discovered using a future 6-m space telescope with a starshade.

Results:

1. We found that the inner portions of disks can easily have sufficient HD density to have optically thick $J = 1-0$ ($\lambda = 112 \mu\text{m}$) line perpendicular to the disk plane. This seriously compromises the accuracy of HD to trace disk mass (Figure 1).

2. We investigated the formation of complex organic molecules (COMs) in water ice in molecular cloud cores. We found that the type of COMs produced depends on the age of the cloud with nitrogen-bearing molecules forming early, and oxygen-bearing COMs and large hydrocarbons forming later (Figure 2).

3. We carried out 3,000 ProDiMo hydrostatic disk model calculations. We found that the D/H ratio in water vapor and ice do not correlate well (Fig. 3). Most of the water in the disk is in solid form, while it is easier to detect emissions from water vapor.

4. We investigated three solid accretion modes (pebble accretion vs drag-enhanced three-body accretion vs canonical planetesimal accretion). We find that if the minimum-mass solar nebula model is adopted, solids with a radius of ~ 1 m to ~ 10 km should be the main contributors to deuterium enrichment (Figure 4).

5. We calculated polarization models for an exo-Venus using the MIE and VLIDORT codes. At a noise level of 1% or better (of the planetary flux), differentiation of water and acid, and retrieval of acid concentration becomes possible. Estimated integration times for a 6-m space telescope with starshade are shown in Fig. 5.

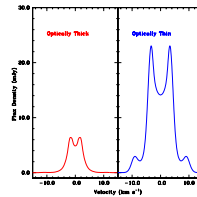


Figure 1. Calculation of HD emission from optically thick and thin Disks (Task 1)

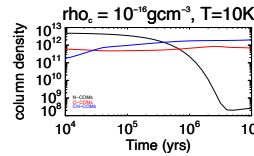


Figure 2. Complex molecules form in ices in molecular clouds, from the reaction of smaller molecules. Initially, N-bearing molecules such as CH3NH2 are produced. These are later broken down by cosmic rays, leading to an increase in simpler molecules such as ammonia, and the formation of other COMs from the reaction of CH3, such as CH3OH, C2H6 and CH3C2H. (Task 2)

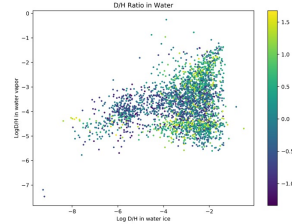


Figure 3. Correlation of HDO/H2O in water vapor and water ice. Colors denote the central star luminosity in the unit of Solar luminosity (Task 3)

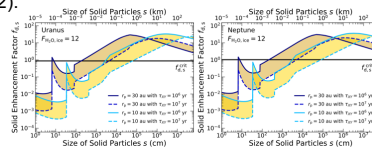


Figure 4. The enhancement factor of the solid surface density required to reproduce the estimated values of the solid mass in a planetary atmosphere as a function of the size of accreted solids for Uranus and Neptune on the left and right panels, respectively. Plausible values of the enhancement factor are shown by the shaded region. (Task 4)

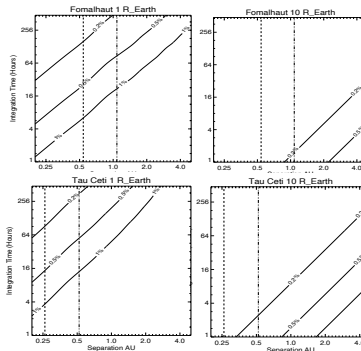


Figure 5. These four panels show contours of exo-Venus polarization uncertainty σ for a single passband ($0.1 \mu\text{m}$, centered on $0.7 \mu\text{m}$) for four cases (two example targets and two planet radii as indicated) as functions of star/planet distance in Astronomical Units and integration time. Contours are shown for three cases (as per Table 1), $\sigma = 1\%$, 0.5% , and 0.2% of the flux from the planet for a measurement consisting of two images in orthogonal polarizers. (Task 5)

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Publications:

Yasuhiro Hasegawa, "Solid Accretion onto Neptune-mass Planets. I. In Situ Accretion and Constraints from the Metallicity of Uranus and Neptune," The Astrophysical Journal, 935, 101 (21pp), 2022

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