UNDERSTANDING AMMONIA (NH_3) CHEMISTRY IN PROTO-PLANETARY DISKS

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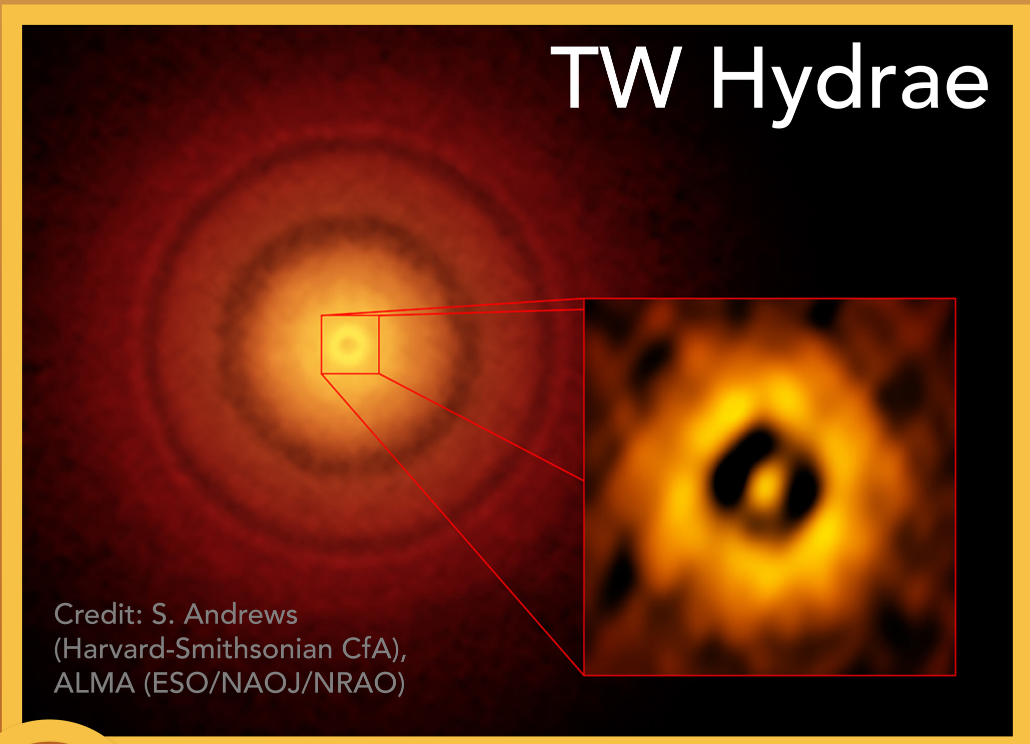
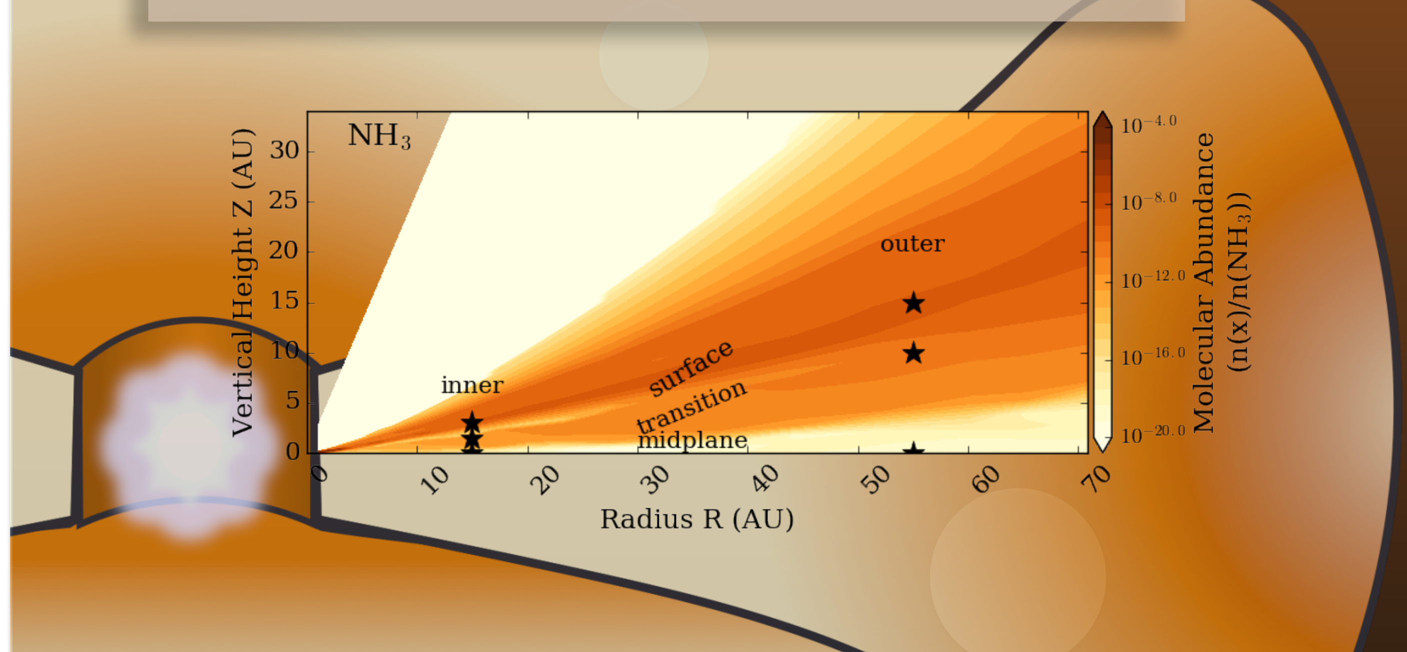
GOAL: Use numerical astrochemical modeling to investigate a theoretical discrepancy in the gas- and ice-phase ammonia-to-water ratio in proto-planetary disks, the earliest phases of planet formation around young stars.



PROTO–PLANETARY DISKS

Proto-planetary disks are dynamic regions of **gas and dust around young stars**, the remnants of star formation, that evolve and coagulate over millions of years in order to ultimately **form planets**. The chemical composition of proto-planetary disks is affected by both the chemical and physical conditions in which they develop, including the **initial molecular abundances** in the birth cloud, the **spectrum and intensity of radiation** from the host star and nearby systems.



Model representation of ammonia distribution in a TW Hydra-like system. Black stars represent the six locations examined in this work.

ICE–PHASE

NH_3 / H_2O

The ice-phase ammonia-to-water ratio of proto-planetary disks has been most accurately determined by observations of **comets**. Formed in the icy regions of our Solar System during its own disk phase, comets have retained the ice chemistry of the disk.

$NH_3/H_2O \sim$ **1%**

GAS–PHASE

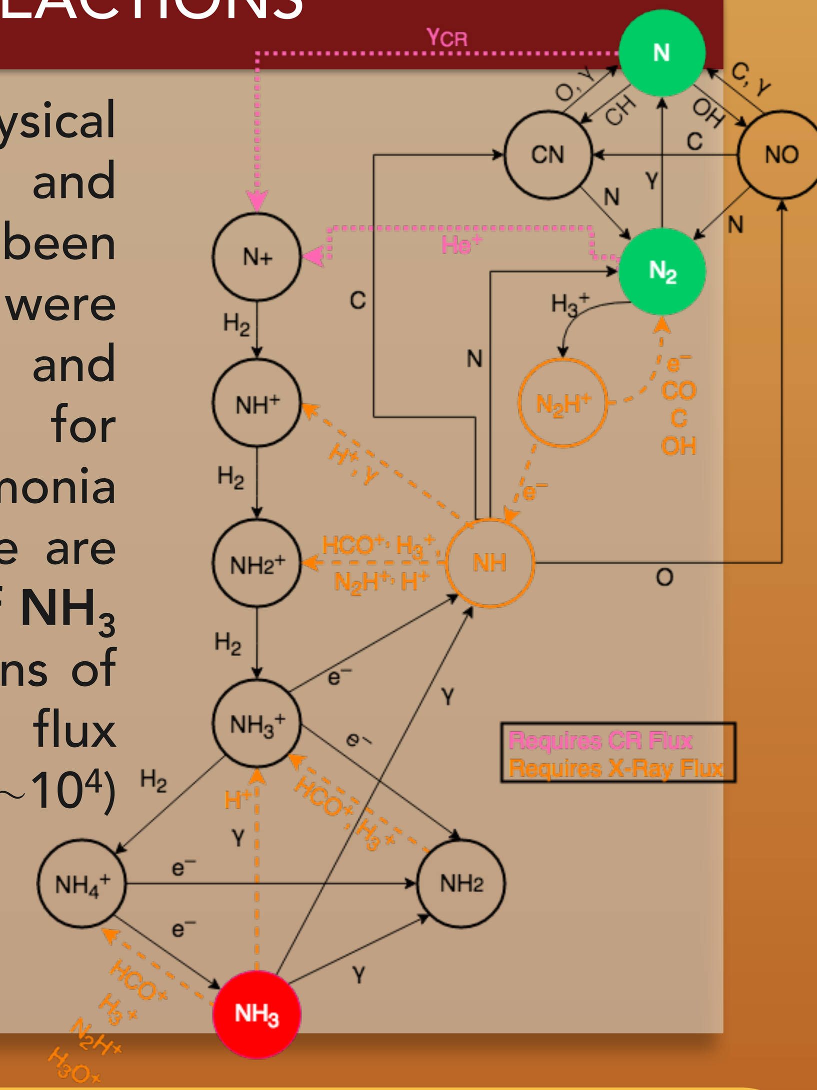
Just this year, **Salinas et al. 2016** published the very **first gas-phase detection of ammonia in a proto-planetary disk**, around TW Hydrae. Interestingly, the gas-phase ammonia-to-water ratio was greater than the ice-phase ratio from comet data.

$NH_3/H_2O \sim$ **7-84%**

This apparent discrepancy in the ice- and gas-phase ratios reveals a gap in our understanding of disk systems, possibly due to new chemistry or incorrectly characterized physical properties.

ILLUMINATING REACTIONS

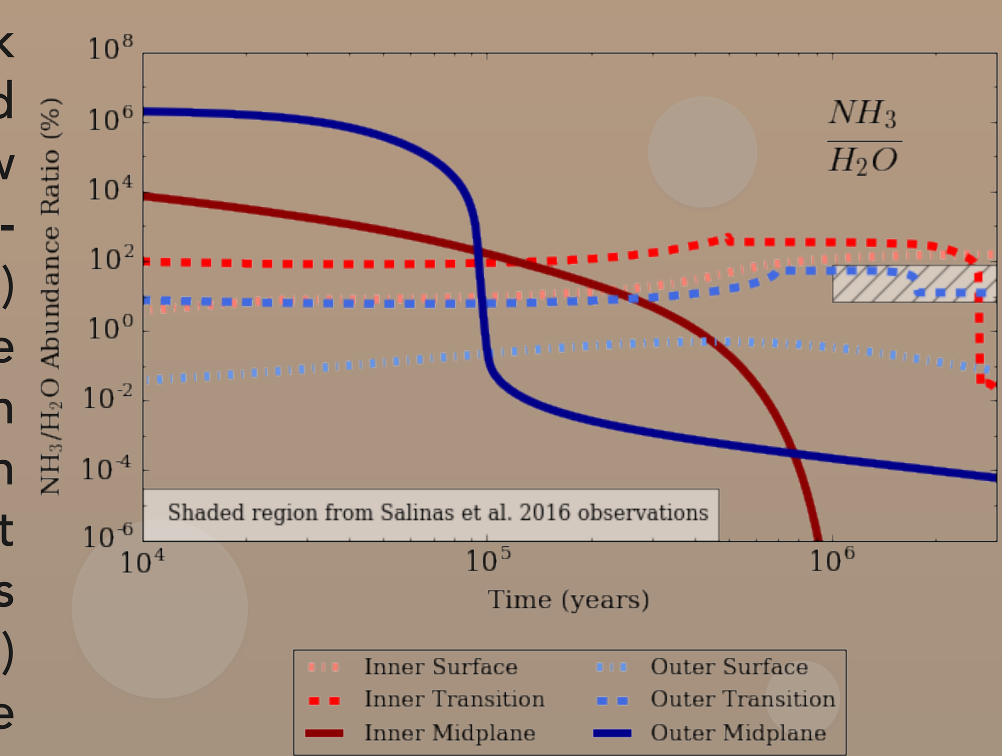
Both chemical and physical influences upon ammonia and water chemistry have been explored. These findings were included in the production and destruction pathway map for NH_3, shown at right. (1) Ammonia abundances in the midplane are coupled to the **formation of NH_3 on dust grains.** (2) Variations of the X-ray and cosmic ray flux supported a strong ($\sim 10^4$) dependency of gas-phase NH_3 on **ionizing radiation** throughout the disk.



CONCLUSION: Due to both spatial variations of physical parameters and chemical evolution, high gas-phase and low ice-phase NH_3/H_2O ratios can and do exist simultaneously within disk systems.

MODELING CHEMICAL EVOLUTION

Computational simulations of the TW Hydra system using a network with 6284 chemical reactions and over 500 molecular species show dramatic ($\sim 10^{10}$) **variance in gas-phase NH_3/H_2O** (shown at right) at **different locations** within the disk (black stars at left). An **elevated ratio**, in accordance with Salinas et al. 2016, is observed at 3 Myr at greater vertical heights (surface and transition regions) and at inner radii. Models of the ice ratio (not shown) agree with comet data ($\sim$1%).



FUTURE WORK

In future work, we will incorporate the answers to these qualitative questions and others into quantitative global models in an attempt to create **synthetic observations** to compare to the Salinas et al. 2016 detection and verify our new theories. This work also motivates **further observations of ammonia** with the newest molecular observatories, or NH_2D with ALMA.

REFERENCES:

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