

# Deuterium Fractionation in Disks

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## Introduction

Disks around pre-main sequence stars are the sites of the formation of planetary systems. As analogs to the Solar Nebular, circumstellar disks offer a unique opportunity to study the early stages of planet formation, especially the complex chemical evolution that must occur (see review by Bergin et al. 2007). In the outer disk that can be resolved by submillimeter interferometry, observations of deuterated species are particularly important because they provide constraints on the origin of primitive solar system bodies such as comets and other icy planetesimals (Irvine et al. 2000).

Deuterated molecule chemistry is sensitive to the temperature history of circumstellar gas. Roueff et al. (2007) have used a gas-phase steady-state chemical model to calculate the extent of deuterium fractionation at temperatures up to 70 K over a wide range of densities. In all conditions, high deuteration is associated with low temperature. Figure 1 shows deuterium fractionation ratios of DCO<sup>+</sup>/HCO<sup>+</sup> predicted in warm-core conditions.

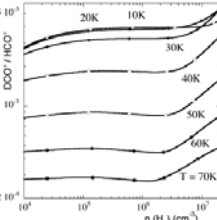


Fig. 1 Deuterium fractionation ratios, adopted from Figure 1 of Roueff et al. (2007)

## Purpose

Determine the distribution of deuterated molecules in disks and compare the deuterium chemistry in the Herbig Ae stars with that in their lower mass counterparts, the T Tauri stars.

## Observations

All of the observations were made between 2005 February and 2008 May using the SMA 8 antenna interferometer located atop Mauna Kea, Hawaii.

### Sources

- **TW Hya**: nearest T Tauri star (K7) at 51 pc, age 5-10 Myr,  $M_{\text{star}}=0.6 M_{\text{Sun}}$
- **HD 163296**: Herbig Ae star (A1) at 122 pc, age 3-5 Myr,  $M_{\text{star}}=2.3 M_{\text{Sun}}$

### Lines

- **HCO<sup>+</sup> 3-2**: 266.55762 GHz
- **DCO<sup>+</sup> 3-2**: 216.11260 GHz

## Methods

### Disk Structure

The kinetic temperature and density structure of the disk is determined by modeling the spectral energy distribution (SED) assuming well mixed gas and dust, with the results confirmed by the resolved (sub)mm continuum images.

### Molecular Distribution

- **Radial distribution**: the column densities are assumed to vary as a power law as a function of radius  $\Sigma_i(r) = \Sigma_i(10\text{AU}) \left(\frac{r}{10\text{AU}}\right)^{p_i}$
- **Vertical distribution**: fractional abundances at different radii are assumed as a function of the hydrogen column density measured from the disk surface (see details in Qi et al. 2008)

### $\chi^2$ Fitting

A grid of models with a range of disk parameters including the molecular distribution parameters (described above), outer radius  $R_{\text{out}}$ , the disk inclination  $i$ , position angle P.A. and the turbulent line width  $v_{\text{turb}}$  are produced and a 2D accelerated Monte Carlo model (Hogerheijde & van der Tak 2000) is used to calculate the radiative transfer and molecular excitation. The best fit model is obtained by minimizing the  $\chi^2$  measured at the selected points of the  $(u, v)$  plane.

## Results: TW Hya

### SED and Disk Structure

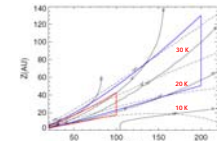
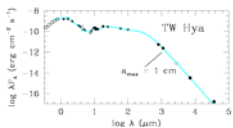


Fig 2. SED of TW Hya and disk models with gas and dust well mixed for  $a_{\text{min}}=1$  cm. The model requires both significant dust-size evolution and a partially evacuated inner disk region (Calvet et al. 2002).

Fig 3. The solid and dotted contours show the temperature and density profiles from the TW Hya model of Calvet et al. (2002). The blue and red lines confine the locations of HCO<sup>+</sup> and HCN in the fitted models (Qi et al. 2008)

## Results: HD 163296

### SED and Disk Structure

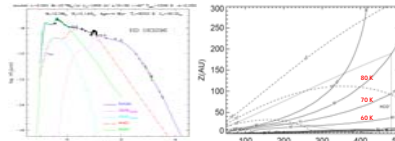


Fig 5. **Left**: SED of HD 163296 and best-fit disk model. **Right**: the solid and dotted contours show the temperature and density profiles from the HD 163296 model. The dotted lines confine the location of HCO<sup>+</sup> in the fitted model. Note that the temperature scale is much larger than that of TW Hya.

### DCO<sup>+</sup> 3-2: Data vs Models

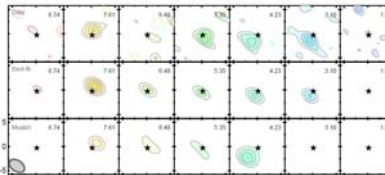


Fig 6. **Top**: Velocity channel map of the DCO<sup>+</sup> 3-2 emission toward HD 163296; **Middle**: best-fit model for DCO<sup>+</sup> with  $R_{\text{out}}=260$  AU; **Bottom**: simulated model with  $R_{\text{out}}=480$  AU, the same as that of HCO<sup>+</sup> (see below).

### Fitting results

- HCO<sup>+</sup>:  $R_{\text{out}}=480\pm 10$  AU; P (radial power index)  $-1.3\pm 0.1$
- DCO<sup>+</sup>:  $R_{\text{out}}=260\pm 40$  AU; P (radial power index)  $-1.3\pm 0.6$
- DCO<sup>+</sup>/HCO<sup>+</sup> = 0.42 at radii < 260 AU

## Discussion

- We find enhanced molecular D/H ratios in both TW Hya and HD 163296 disks.
- In the cold disk of TW Hya (see Fig 3), the distribution of DCO<sup>+</sup> differs markedly from that of HCO<sup>+</sup> (Fig 4). The D/H ratios inferred change by at least one order of magnitude [0.01 to 0.1] for radii < 30 AU to  $\geq 70$  AU due to low temperatures far from the star, as expected from low-temperature gas-phase deuterium fractionation processes.
- In the warm disk of HD 163296 (see Fig 5), the radial power index of DCO<sup>+</sup> is similar to that of HCO<sup>+</sup> (around -1.3) but the outer radius is significantly smaller than that of HCO<sup>+</sup>. It is very puzzling to find such a high D/H ratio in the order of 0.1 because in the outer disk with such warm temperatures ( $T > 60$  K), the gas-phase deuterium fractionation processes should be prohibited. Grain sublimation could contribute to the observed high deuteration but the detailed process leading to such high abundance of DCO<sup>+</sup> is still unknown.

## References

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### DCO<sup>+</sup> 3-2: Data vs Models

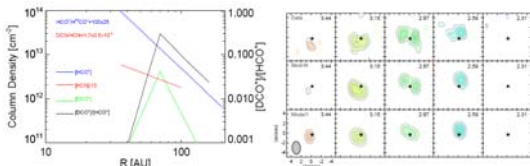


Fig 4. **Left**: Radial distribution of molecular column density of the best-fit models for TW Hya. The DCO<sup>+</sup>/HCO<sup>+</sup> abundance ratio increases with disk radius to around 70 AU. **Right top**: SMA channel maps of DCO<sup>+</sup> 3-2 toward TW Hya; **Right middle**: best-fit model for DCO<sup>+</sup> 3-2; **Right bottom**: simulated model for DCO<sup>+</sup> which follows the distribution of HCO<sup>+</sup>, which clearly provides a poor match to the data compared to the best-fit model. See details in Qi et al. (2008).