A SIGNIFICANTLY LOW CO ABUNDANCE TOWARD THE TW Hya PROTOPLANETARY DISK: A PATH TO ACTIVE CARBON CHEMISTRY?

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Abstract

In this Letter we report the CO abundance relative to H2 derived toward the circumstellar disk of the T-Tauri star TW Hya from the HD (1–0) and Array C18O (2–1) emission lines. The HD (1–0) line was observed by the Herschel Space Observatory Photodetector Array Camera and Spectrometer whereas C18O (2–1) observations were carried out with the Submillimeter Array at a spatial resolution of 2″8 × 1″9 (corresponding to ~151 × 103 AU). In the disk’s warm molecular layer (T > 20 K) we measure a disk-averaged gas-phase CO abundance relative to H2 of χ(CO) = (0.1–3) × 10−5, substantially lower than the canonical value of χ(CO) = 10−4. We infer that the best explanation of this low χ(CO) is the chemical destruction of CO followed by rapid formation of carbon chains, or perhaps CO2, that can subsequently freeze-out, resulting in the bulk mass of carbon locked up in ice grain mantles and oxygen in water. As a consequence of this likely time-dependent carbon sink mechanism, CO may be an unreliable tracer of H2 gas mass.

Key words: astrochemistry – ISM: abundances – protoplanetary disks – stars: formation

Online-only material: color figures

1. INTRODUCTION

Molecular hydrogen is the main gas-phase constituent in star-forming gas. However, it does not appreciably emit for typical gas conditions. Consequently carbon monoxide is widely used as a proxy for H2 in the molecular interstellar medium (ISM; e.g., Dickman 1978) and protoplanetary disks (Koerner & Sargent 1995; Dutrey et al. 1996). With a suite of transitions at millimeter/submillimeter wavelengths, the optically thick and thermalized 13CO lines trace gas temperature while optically thin CO isotopologues (namely 13CO and C18O) probe the ISM; e.g., Dickman 1978) and protoplanetary disks (Koerner 2013).

2. OBSERVATIONS AND DATA REDUCTION

The observations of TW Hya were made on 2005 February 27 and April 10 using the Submillimeter Array (SMA; Ho et al. 2004) located atop Mauna Kea, Hawaii. The SMA receivers operated in a double-sideband mode with an intermediate frequency band of 4–6 GHz from the local oscillator frequency, sent over fiber optic transmission lines to 24 overlapping “chunks” of the digital correlator. The correlator was configured to include CO, 13CO and C18O, in one setting: the tuning was centered on the CO (2–1) line at 230.538 GHz in chunk S15, while the 13CO/C18O (2–1) transitions at 220.399/219.560 GHz were simultaneously observed in chunks 12 and 22, respectively. CO (2–1) data were reported in Qi et al. (2006). Combinations of two array configurations (compact and extended) were used to obtain projected baselines ranging from 6 to 180 m. The observing loops used J1037–295 as the gain calibrator, with bandpass calibration using observations of 3C279. Flux calibration was done using observations of Titan and Callisto. Routine calibration tasks were performed using the MIR software package,4 imaging and deconvolution were accomplished in the MIRIAD software package. The resulting synthesized beam sizes were 2″8 × 1″9 (P.A. = −13°) and 2″7 × 1″8 (P.A. = −3°) for C18O and 13CO, respectively. HD observations toward TW Hya were carried out with the Herschel Space Observatory Photodetector Array Camera and Spectrometer (Poglitsch et al. 2010; Pilbratt et al. 2010). Further informations concerning both reduction and line analysis are presented in B13.

In the present work we focus on the integrated line fluxes from HD, 13CO, and C18O. Spectroscopic parameters of these molecules and measured spectrally integrated fluxes within an

4 http://www.cfa.harvard.edu/~cqi/mircook.html
8" box (or 432 AU assuming a distance of 54 pc; van Leeuwen 2007) are given in Table 1. The spatially integrated spectra of C18O (2 − 1) and 13CO (2 − 1) are presented in Figure 1.

### 3. ANALYSIS

In the present study, we derive TW Hya’s disk-averaged gas-phase CO abundance from the observed C18O (2 − 1) and HD (1 − 0) lines. The conversion from integrated line intensity to physical column density is dependent on optical depth and temperature. In the following sections we explore a range of physically motivated parameter space assuming the emission is co-spatial and in LTE. Based upon these assumptions we calculate a range of χ(CO) in the warm (T > 20 K) disk using HD as our gas mass tracer. Caveats of this approach and their implications for our measurement will be discussed in Section 4.

#### 3.1. Line Opacity

The determination of the CO mass from the C18O emission relies on the assumption that C18O (2 − 1) is optically thin and an 16O/18O ratio. To estimate the disk-averaged opacity of C18O, we compare C18O (2 − 1) to 13CO (2 − 1) and find the disk-averaged 13CO/C18O flux ratio is ≈3.3 ± 0.9. This measurement is strongly affected by the opacity of 13CO (2 − 1), where τ(C13O) ∼ 2.9 assuming isotope ratios of 12C/13C = 70 and 16O/18O = 557 for the local ISM (Wilson 1999). This ratio suggests that the spatially integrated C18O emission is thin, τ(C18O) ∼ 0.36.

#### 3.2. Hints from Disk Models

The mismatch between the normal CO abundance and mass needed to match HD can be understood by computing the optically thin C18O emission predicted by the sophisticated Gorti et al. (2011) model. For this purpose we adopt the non-LTE code LIME (Brinch & Hogerheijde 2010) with the Gorti et al. (2011) physical structure employed in the original modeling effort of Bergin et al. (2013), which best matched the HD emission. In these calculations we include CO freeze-out assuming a binding energy of 855 K (Öberg et al. 2005). The disk model natively assumes χ(CO) = 2.5 × 10^{-4} and if one adopts 16O/18O = 500, over-predicts the C18O (2 − 1) flux by ∼10×. Furthermore, the C18O (2 − 1) emission is predicted to be optically thick and, to match the observed flux, χ(C18O) needs to be reduced to ∼7 × 10^{-9}, i.e., χ(CO) = 4 × 10^{-6}. We note that this abundance is dependent on the assumed binding energy, discussed further in Section 4.2.

#### 3.3. Mass and Model Independent χ(CO) Determination

Under the assumption of optically thin HD (1 − 0) and C18O (2 − 1) emission, we can define the observable R_{obs} as the ratio between the observed number (denoted N) of C18O and HD molecules in their respective upper states,

\[ R_{obs} = \frac{N(C18O, J_u = 2)}{N(HD, J_u = 1)} = \frac{F_{C18O}A_{HD}V_{HD}}{F_{HD}A_{C18O}V_{C18O}}. \]

where \( v_x, A_x \) and \( F_x \) are the frequency, Einstein A coefficient and total integrated flux of the measured transition, respectively (see Table 1). To determine the total CO abundance in LTE, we must calculate the fractional population in the upper state, \( f_u \), and assume isotopic ratios. We adopt the isotopic oxygen ratio described in Section 3.1 and an isotopic ratio of HD relative to H2 of χ(HD) = 3 × 10^{-5}, based on a D/H elemental abundance of (1.50 ± 0.10) × 10^{-5} (Linsky 1998). Assuming LTE and inserting the measured fluxes, the 12CO abundance relative to H2 can be written as:

\[ \chi(CO) = 1.76 \times 10^{-5} \left(\frac{16O/18O}{557}\right) \left(\frac{R_{obs}}{1.05 \times 10^{-3}}\right) \times \left(\frac{\chi(HD)}{3 \times 10^{-5}}\right) \frac{f_u(HD, J_u = 1)}{f_u(C18O, J_u = 2)}. \]

It is important to note that the above analysis hinges upon the assumption that HD (1−0) and C18O (2−1) are in LTE. Based on the Gorti et al. (2011) model, at radii between R ∼ 50−150 AU the typical H2 density at gas temperatures near T_g = 30 K ranges between ∼10^{10}−10^{15} cm^{-3}. Critical densities for the HD (1−0) and C18O (2−1) transitions are 2.7 × 10^3 cm^{-3} and 10^4 cm^{-3} at T_g ∼ 30 K, respectively, which assumes collision

| Table 1 | C18O, 13CO and HD Spectroscopic Line Parameters and Total Integrated Fluxes Observed Toward TW Hya |
|---------|--------------------------------------------------------------------------------------------------|
| Molecule | Frequency (GHz) | Transition | A (10^{-8} s^{-1}) | \( E_u \) (K) | \( F^b \) (10^{-18} W m^{-2}) |
|----------|-----------------|------------|-------------------|-------------|----------------|
| HD       | 2674.986        | 1−0        | 5.44              | 128.38      | (6.3 ± 0.7) × 10^{-3} |
| C18O     | 219.560         | 2−1        | 60.12             | 15.81       | (6.0 ± 1.2) × 10^{-3} |
| 13CO     | 220.399         | 2−1        | 60.74             | 15.87       | (20.0 ± 1.3) × 10^{-3} |

Notes.

\(^a\) All spectroscopic data from 13CO, C18O and HD are available from the CDMS molecular line catalog (Müller et al. 2005) through the Splatalogue portal (www.splatalogue.net, Remijan et al. 2007) and are based on laboratory measurements and model predictions by Goorvitch (1994), Klapper et al. (2000, 2001), Cazzoli et al. (2004), Pachucki & Komasa (2008), Drouin et al. (2011).

\(^b\) The total integrated fluxes are given with 1σ uncertainty, which includes the calibration uncertainty.

\(^c\) From B13.
rate coefficients with H₂ at 30 K of HD (2 × 10⁻¹¹ cm³ s⁻¹; Flower et al. 2000) and C₁⁸O (6 × 10⁻¹¹ cm³ s⁻¹; Yang et al. 2010). Under these conditions both lines are thermalized and the assumption of LTE is reasonable.

The measured gas-phase disk-averaged χ(CO), Equation (2), depends sensitively on the temperature of the emitting material, viz., the upper state fraction, fᵤ. Formally, gas temperatures vary by orders of magnitude throughout the disk. However, to first order, as a result of the abundance distribution and excitation of a given rotational transition, emission generally arises from a narrower range of temperatures. There are two ways temperatures can be estimated: (1) by observing optically thick lines originating from the same gas and measuring an average kinetic temperature of the emitting gas within the beam, or (2) by inferring temperatures from disk thermochemical models.

In the latter case we estimate a characteristic temperature of CO by dividing up the emissive mass of the Gorti et al. (2011) model into temperature bins for both C₁⁸O and HD, Figure 2.

To compute the emissive mass we: following the Gorti et al. (2011) TW Hya model, for each temperature bin integrate the mass in HD (J = 1) and in C₁⁸O (J = 2) in the upper state within the specified temperature range, and normalize this to the total mass throughout the disk in the corresponding upper state for each species, i.e., M_upper(HD) = 4π ∫ n_upper(J = 2)rdrdz, where n_upper(J = 1) is the upper state volume density calculated from the LIME excitation models (Brinch & Hogerheijde 2010) performed for HD in B13.

One notable feature of Figure 2 is that the two lines have slightly different peak maximally emissive temperatures, ~20 K for C₁⁸O and ~40–60 K HD. However, over the temperature range expected for HD, the difference in the ratio of fractional populations for HD and C₁⁸O is not enough to bring the CO abundance close to 10⁻⁴ using Equation (2).

Guided by this range of temperatures, we compute the χ(CO) from Equation (2) assuming a C₁⁸O gas temperature of Tₑ = 20 K and varying the HD emitting temperature Tₑ(HD) between 20 and 60 K, accounting for the possibility of HD emitting from warmer gas than the C₁⁸O. The obtained χ(CO) is provided in Figure 3. In all cases, χ(CO) in the gas is lower than the canonical value of χ(CO) ~ 10⁻⁵; ranging between (0.1–3) × 10⁻⁵.

From the modeled mass distribution shown in Figure 2, the center of the gas temperature distribution probed by HD is Tₑ ≈ 40 K, while C₁⁸O mostly emits from 20 K. With this value the resulting CO abundance is only χ(CO) = 7 × 10⁻⁶, over 10× less than the canonical value.

Therefore, to get χ(CO) up to the 10⁻⁴ range, significant corrections to the upper state fraction of each species is required. Concerning C₁⁸O, that requires the gas to be either significantly colder or hotter such that the J = 2 becomes depopulated. Both scenarios are unlikely (see Figure 2) and unsupported by C₁⁸O data (Qi et al. 2006).

Alternatively, C₁³O emission can constrain the temperature in the layers where its emission becomes optically thick. Using the resolved Band 6 TW Hya ALMA Science Verification (S.V.) observations of C₁³O(2–1), the peak beam temperature is 24.5 K within a 2′′83 × 2′′39 (P.A. = 44°) beam. This temperature represents the beam averaged kinetic temperature of the CO emitting gas within the inner R ~ 70 AU, in agreement with values reported by B13 for the Band 7 S.V. data of the CO (3 – 2) line and the observations of Qi et al. (2006) for
CO (6 – 5) ($T_R \sim 29.7$ K and $\sim 30.6$ K respectively). Under these conditions, the CO abundance is less than $3 \times 10^{-6}$. We conclude that it is difficult for excitation alone to reconcile the emission with a CO abundance of $10^{-5}$.

4. $\chi$(CO) MEASUREMENT CAVEATS

The analysis above assumes HD and CO emit from similar regions and therefore trace the gas-phase $\chi$(CO) directly. In the following section we relax this assumption and discuss various physical mechanisms that could modify the interpretation of the measured $\chi$(CO).

4.1. Different Emitting Regions

In Figure 4 we illustrate some of the key issues concerning the above discussion. First, while HD is spatially distributed broadly, gas-phase C$^{18}$O is not, freezing onto dust grains with $T_{\text{dust}} < 20$ K. Because of the strong temperature dependence in the Boltzmann factor for the $J = 1$ state, we would expect the HD emission to be sharply curtailed below $T_e \lesssim 20$ K. For a massive midplane, some HD emission could arise from dense gas directly behind the CO snow-line (shown as magenta) but the HD emissivity from this cold gas is lessened by the fact that adding more mass (or enriching the dust) would increase the dust optical depth at 112 $\mu$m, hiding some fraction of the HD emission. Furthermore, this emission cannot contribute significantly to the HD emission in the midplane. For example, if $\sim 20\%$ of the HD (1 – 0) emission arises from gas at 15 K, the H$_2$ mass at this temperature is $0.05 M_\odot$ in addition to the contribution from the rest of the disk. Therefore it is difficult for the 15 K mass to add appreciably to the emission without driving the disk to extremely high masses.

Another likely scenario is where the HD gas emits from primarily warm gas in the innermost disk, while CO and C$^{18}$O trace cooler emitting regions and thus larger physical radii. As a result, CO would trace more gas (full disk) than HD (warm inner disk). Consequently, HD (1 – 0) would miss H$_2$ mass in the outer disk, resulting in a lower limit to the disk mass estimation and in turn an overestimate of $\chi$(CO). The CO abundance could hence be lower. In addition, it is important to note that in B13 the authors find the outer disk does not emit appreciably, with only $\sim 10\%$ of the HD flux coming from outside of 100 AU (see their Figure 2(c)) based upon the model of Gorti et al. (2011).

4.2. Freeze-out

Previous studies have attributed measured low CO abundances to gas-phase depletion by adsorption onto grains (Aikawa et al. 1996; Dartois et al. 2003). Under normal conditions CO freezes-out at low temperatures present in the midplane, $T < 20$ K, where HD does not strongly emit, and therefore the reduced measured $\chi$(CO) in the gas-phase is unlikely to be the result of freeze-out.

In fact a number of studies find the measured CO antenna temperatures of $T < 17$ K (Piétu et al. 2007; Dartois et al. 2003; Hersant et al. 2009). If these estimates are correct, then the total volume of gas traced by the C$^{18}$O line exceeds that traced by the HD line, leading to an over-prediction of the true $\chi$(CO).

There is, however, uncertainty in the freeze-out temperatures, which depend formally on the binding energies assumed. The binding energies are a function of the binding-surface, often assumed to be CO ice. Alternatively, if the grain surface is water ice or bare dust, the binding energy can be significantly higher (Bergin et al. 1995; Fraser et al. 2004). If this is the case, CO can freeze-out at higher temperatures $T > 25$ K, and therefore the CO emitting region would be smaller than the HD emitting region. In this instance the measured CO abundance would be lower than the true CO abundance.

4.3. Opacity

Another caveat of our $\chi$(CO) estimates are the opacities of the HD (1 – 0) and C$^{18}$O (2 – 1) lines. In this study, we assume that emission of both species is optically thin. Although we show in Section 3.1 that the C$^{18}$O (2 – 1) emission is thin in the disk-averaged data, the possibility of optically thick HD emission still remains. However, if $\tau_{\text{HD}} \gtrsim 1$, the derived HD mass should be a lower limit and therefore the measured $\chi$(CO) is an upper limit on the true CO abundance.

4.4. Photodissociation and Self-shielding

Photodissociation by UV is a major CO destruction mechanism in disks that regulates the molecular abundance of species in the gas. Photodissociation models for HD and CO isotopologues have been investigated by Roueff & Node-Langlois (1999), Le Petit et al. (2002), and Visser et al. (2009). Roueff & Node-Langlois (1999) finds HD should self-shield at smaller $A_V$ than CO. Therefore, in the absence of dust shielding and selective isotopologue photodissociation, HD could emit from warm layers where C$^{18}$O is destroyed. If those surface layers are essential contributors to the HD emission, $\chi$(CO) would be underestimated. However, the modeling of B13 suggests that the high surface layers do not dominate the emissive mass of HD, and therefore, even if photodissociation cannot be ruled out, it only minimally affects the measured $\chi$(CO). Alternatively, if selective isotopologue photodissociation operates for C$^{18}$O from external UV irradiation, we may be missing CO mass from the outer disk edge. As discussed in Section 4.1, however, the outer disk does not significantly contribute to the HD emission.

5. IMPLICATIONS: WHERE IS THE CARBON?

Our study shows that the main reservoir of gas-phase carbon, CO, is reduced by at least an order of magnitude in the TW Hya disk compared to dense clouds. In both T-Tauri and Herbig
Ae disks similarly low CO abundances have been inferred and attributed to photodissociation and freeze-out (e.g., Dutrey et al. 2003; Chapillon et al. 2008; Qi et al. 2011). The difference between the previous studies and the results reported here is the use of HD to probe H₂ above 20 K and hence provide stronger constraints on χ(CO) in the warm molecular layer. It is important to state that both C¹⁸O and HD do not trace the midplane of the disk because of freeze-out (C¹⁸O) and low excitation (HD). Thus it is possible that the χ(CO) is “normal” in the midplane, which would be consistent with the similarity between interstellar ices and cometary volatiles (Mumma & Charnley 2011). We argue differences in photodissociation of C¹⁸O and HD are unlikely to account for the low χ(CO). This would argue against the possibility that the carbon is sequestered in atomic form either neutral or ionized. Bruderer et al. (2012) supports this assertion with observations of all primary forms of carbon in a Be star disk (HD 100547). They argue the total carbon abundance is depleted in the warm atmosphere, which is consistent with our conclusion.

This finding leads one to ask where the missing carbon might be found. One possibility is suggested by the modeling of kinetic chemistry in disks by Aikawa et al. (1997). The deep disk layers are exposed to X-rays from the central star (Glassgold et al. 1997), though likely not cosmic rays (Cleeves et al. 2013). In these layers CO can exist in the gas via thermal- or photo-desorption from grains. X-rays produce He⁺ and, with sufficient time, carbon can be extracted from CO via reactions with He⁺. CO reforms, but a portion of the carbon is placed into hydrocarbons (CₓHₓ) or CO₂. Many of these species have freeze-out temperatures higher than CO and trap the carbon in ices. In a sense the chemistry works toward the first carbon-bearing molecule that freezes-out, creating a carbon sink (Aikawa et al. 1997). Therefore we suggest that the low measured gas-phase CO abundance in the TW Hya disk is a result of this chemical mechanism, and the use of CO as a mass tracer has very significant, and likely time-dependent, uncertainty.

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Facilities: SMA, Herschel, ALMA

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