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PROBING PROTOPLANETARY DISK UPPER ATMOSPHERES FOR HEATING AND DUST SETTLING USING SYNTHETIC CO SPECTRA

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ABSTRACT

CO emission is a useful probe of the warm gas distribution in the planet forming regions of disks around Herbig Ae/Be (HAeBe) stars. We model UV fluoresced and thermally excited CO in the circumstellar disks of several HAeBes. We find indications of dust settling in the upper atmospheres of HD 141569 and HD 97048 and a correlation between PAH luminosity and gas heating in these two systems.

Subject headings: circumstellar matter—line: profiles—planetary systems: protoplanetary disks—stars: individual (HD 100546, HD 1415469, HD 97048)

1. INTRODUCTION

HAeBe stars are pre–main sequence stars of ∼2-10 $M_\odot$, distinguishing them from T Tauri stars, which are $<2M_\odot$. HAeBe stars are of spectral type A or B, luminosity class III to V, and exhibit H, Ca, O, and N emission lines, as well as excess NIR emission indicative of a circumstellar dust disk (Waters & Waelkens 1998; van den Ancker 1997; Thé et al. 1994). These disks are assumed to be in nearly Keplerian orbit. Accretion proceeds as material from the outer disk loses energy and moves radially inwards to lower potential. Extensive studies of the disk including those by Dullemond et al. (2002) have produced a detailed model of disk dynamics. All three of the systems studied in this work have optically thick outer disks with optically thin inner disks. Known as transitional disks, these may be in the late stages of disk evolution and indicative of planet formation.

Pre–main sequence stars with accretion disks are an area of intense study in order to develop a model of planet formation. Observations of various HAeBe and T Tauri stars have given rise to tentative models.

In the core accretion model of planet formation, dust grains agglomerate for a period of $\sim10^6$ years until they have formed planetesimals of $\sim10M_\oplus$, massive enough to accrete gas gravitationally. Over the next $\sim10^7$ years, these cores become gas giants.

In the gas instability model, gravitational instabilities cause a region of gas and dust to collapse simultaneously, forming a planet in only a few hundred years (Mayer et al. 2002). The gravitational instability model predicts that gas and dust will be removed from the inner disk contemporaneously, whereas the core accretion model predicts that the protoplanet will accumulate only dust grains and planetesimals for 10^6 years. The current understanding of gas evolution in typical HAeBe disks predicts the gas will dissipate long before the additional 10^7 years expected to pass during the formation of gas-giants by the core-accretion method (Zuckerman 1995). Determining the abundances and distribution of gas and dust in the inner "planet forming" region and disk upper atmosphere may provide observational constraints on these models.

A forming protoplanet would sweep out a clearing or inner gap in the disk. Such gaps have been detected through study of the spectral energy distribution (SED), which primarily traces dust. There are, however, other scenarios, such as photoevaporation and planetesimal formation, which could account for such clearings (Clarke et al. 2001, Dullemond & Dominik 2005). Analysis of spectral emission from the gas may be used to better understand and differentiate between the different possible causes of inner gaps in transitional disks by indicating the extent, composition, and dynamics of the gas.

At the edge of the disk atmosphere all gas and material is dissociated and ionized by stellar radiation, achieving gas temperatures of ∼5000 K and dust temperatures of ∼1000 K at 1 AU from the star (Glassgold et al. 2004). Moving along a column into the disk, the temperature decreases as the cloud is partially shielded by the layer above it. Once the temperature in the disk is low enough for molecules to form, emission following recombination rapidly cools the disk. Thus, column densities and mass estimates for the optically thick disk must be calculated as lower limits since they are based only on the "skin" of the disk. The total energy dissipated from the disk through radiation is given by the flux. The rovibrational emissions of CO are of primary importance to this work, and the flux for each rovibrational state is expressed as

$$F_{ij} = \frac{hc\tilde{\nu}_{ij}A_{ij}N_i}{4\pi d^2} \quad (1)$$

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where $N_i = \frac{Ng_i}{Q} e^{-E_i/kT}$ and Q is the rotational partition function. Therefore the flux detected is the total flux of that emission times the fraction of the spherical Gaussian surface subtended by the detection device. Taking the natural log of this equation gives a linear relation between $\ln(F_{ij}/(\nu A_{ij} g_i))$ and $-E_i/k$, where the temperature T is the negative inverse of the slope (Brittain et al. 2009).

CO has emerged as a viable molecule with which to probe circumstellar disks, particularly at small radii. As discussed by Brittain et al. (2007), CO is easily excited at many different wavelengths, and it demonstrates high Einstein A-values, making it a good emitter in the IR through rovibrational transitions. Despite being dramatically less abundant than molecular hydrogen, the former properties make CO relatively easy to detect. CO also has a high dissociation temperature of 5000 K, making it a good probe of higher temperature regions like the inner disk. Finally, UV fluoresced cool gas can be distinguished from thermally excited hot gas by its high vibrational temperature and low rotational temperature. UV radiation from the central star cannot penetrate deep into an optically thick disk, but the IR emissions by which CO re–radiates UV–absorbed energy can easily escape. Thus, emissions caused by stellar UV fluorescence will always originate near the surface of the disk directly exposed to the star. UV fluoresced CO, then, can trace the inner edge of optically thick disks, as well as indicating whether or not CO exists in optically thin inner holes.

In order to better understand the dynamics of circumstellar disks, we analyze and fit previously reduced spectral data for HD 141569 and HD 97048 to a synthetic model for CO excitation and emission, and compare our fits with that of HD 100546 by Brittain et al. (2009). All three of these stars appear to be transitional HAeBes, transitional disk-possessing stars, which are about to enter the main–sequence. The model is introduced and the parameters outlined in §2. In §3 we discuss the spectral data used and the process by which we optimized the synthetic spectra, and present the fitted synthetic data. We discuss and interpret our findings in §4. Finally, §5 summarizes the implications of the work.

2. MODELING THE CO EMISSION SPECTRA

Spectral synthesis has been used previously to measure the distribution of gas in circumstellar disks (e.g. Najita et al. 1996). The model applied in this work is built upon current understanding of circumstellar disks, HAeBe stars, and the CO molecule, as discussed in the introduction.

Circumstellar disks appear flared, with increasing scale height from inner to outer radii, such that the disk subtends an increasing solid angle relative as a function of radius relative to the central star. The optical thickness of the CO gas in the disk is dependent on dust density and grain size, as well as self-shielding and the turbulent velocity of the gas. UV radiation populates the first electronic excited state of CO, and the gas subsequently transitions rovibrationally, emitting in the IR. The relative strength of the rovibrational CO emission lines indicate which states were excited. This implies the temperature of the gas, which, in turn, is suggestive of the distance from the star and the optical thickness of the gas.

The model utilized in this work was used previously by Brittain et al. (2007, 2009). Code parameters are listed and identified in Table 1. In this model, the CO emission is assumed to originate in a thin vertically isothermal slab whose temperature and density are described by the power laws $T(R) = T(R_{in})(R/R_{in})^{-\alpha}$ and $n(R) = n(R_{in})(R/R_{in})^{-\beta}$. The UV luminosity of each star is taken from International Ultraviolet Explorer (IUE) data from about 1600 Å . τ is the line center optical depth of the strongest transition in the ground vibrational state (Brittain et al. 2009). The fraction of the inner disk face not obscured by the opposite side of the disk is estimated for given inclination and scale heights, and must be hard-coded for each star. This value was not strongly constrained by prior research or the model, so our approximations were broad. Finally, as will be discussed in the next paragraph, slit loss for each data set must be hard-coded into the program.

The model builds a disk as a series of annuli of width 1 AU, simulates the stellar object as a point source blackbody, and models UV fluorescence of the columns along the atmosphere of the disk (only one side is considered since one disk surface is always hidden) as well as the front face of the disk. Inner and outer scale height, which determine the angle of incidence of UV radiation, is not varied as parameters, but rather is hard-coded from theory and remained the same for the three subject systems. The UV fluorescence is calculated in steps of 0.2 τ into the atmosphere. The annuli are split into 1km s^{-1} segments of the disk, allowing relative velocities of emitted photons to be calculated. Those "bins" which are outside of the slit's resolution are discarded, based upon the distance, inclination, and radius of the disk and the instrumental seeing. Emission is modeled according to our knowledge of CO rovibrational transitions. The synthetic emission spectrum of CO is then compared to reduced spectral data.

It must be noted that the fit search was not exhaustive. Not only were initial parameter values and constraints culled from the literature, narrowing the space from which the fit was extracted, but the order of the fitting and the expectations of the researcher influenced the fit process. While some degeneracies were discovered and reported, it is possible that other optimizations of the parameters exist. The claim of the authors is that the current fits are local minima within uncertainty and S/N which generally concur with constraining data and theory.

3. PRESENTATION OF FITS

The stars investigated were HD 141569, HD 97048, and HD 100546. Properties and data sources for the former two are listed in Table 2. Original data sources include the Keck spectrograph,with a resolution of 12 km s^{-1}, and the Gemini PHOENIX spectrograph,with a resolution of 6 km s^{-1}. Reduced spectral data in the IR, the area for rovibrational CO v=0 and higher transitions, was fit with the synthetic spectra. HD 100546 was not fit in this work, rather, results were taken from Brittain et al. (2009). Best-fit parameter values are presented in Table 1.

3.1. *HD 100546*

As studied and discussed in detail by Brittain et al. 2009, HD 100546 is a B9 star which possesses a transi-

TABLE 1
Model Parameters

Parameter	HD 100546[a]	HD 141569	HD 97048	Units	Description
$M_\star$	2.4	2	2.5	$M_\odot$	Stellar mass
i	50	60	42.8	°	Inclination
d	103	108	180	pc	Distance to star
ΔR	6	6/12	6	km s^{-1}	Resolution of instrument
R_{in}	13	9	10	AU	Inner edge of disk
R_{out}	100	100	100	AU	Outer edge of disk
$v_{turbulent}$	2.0	4.5	1	km s^{-1}	Turbulent broadening
T_{col}	1400	200	550	K	Fiducial collisional temperature of CO at R_{in}
α_{col}	0.30	0.25	0.25		Power law of collisional rotational temperature
T_{fluor}	1400	200	500	K	Fiducial fluorescent temperature of CO at R_{in}
α_{fluor}	0.30	0.25	0.3		Power law of fluorescent rotational temperature
n_0	10^{11}	1.5×10^{9}	4×10^{11}	cm^{-3}	Fiducial density at 1 AU
β	1.35	1	1		Power law of density
X	4/1	1/1	1/1		CO/^{13}CO ratio
Y	34/1	10/1	1/1		CO/C^{18}O ratio

References. — Adapted from Brittain et al. (2009)

Note. — The first section of the table are parameters for which values were taken from the literature, and which were varied only minimally for a best fit.

[a] Brittain et al. (2009)

TABLE 2
Data and Sources

Object	Spectral grasp (cm^{-1})	Spectral type	Distance (pc)	Inclination (°)
Keck (12 km s^{-1})				
HD 141569	1963-1991, 1992-2024, 2061-2090, 2160-2190, 2093-2124, 2124-2128,[a]	A0	108	50
Gemini PHOENIX (6 km s^{-1})				
—	2138-2150[b]	—	—	—
HD 97048	2028-2038, 2104-2113, 2141-2150	B9.5V	180	42.8[c]
—	2141-2150	—	—	—

References. — All data not otherwise noted are from M. Troutman et al. (in preparation).

[a] Brittain et al. (2007)

[b] Troutman et al. (in preparation)

[c] van der Plas et al. (2008)

tional disk with an inner gap in the dust and CO gas inwards of 13 AU – likely swept out by a protoplanetary companion. HD 100546 demonstrates evidence of hot, UV fluoresced gas which is well-mixed with the dust below the optical depth of ^{13}CO. See Fig. 1 for the fit spectral data.

3.2. *HD 141569*

Because of the existing body of knowledge concerning HD 141569, this system served as a test for our model. Data from both Keck and Gemini were fit for HD 141569. One overall best fit was made for the 7 Keck spectral orders and 1 Gemini order. Best fits for the individual segments differed so slightly from the best overall fit as to be clearly within the uncertainties produced by noise. See Fig. 2 for a segment of the data fit with the synthetic spectrum.

Our ratio of CO to ^{13}CO was 1/1, surprising considering the ISM ratio of ∼65-80 (see Langer & Penzias 1990). This is indicative of a dust free disk skin, and is discussed in detail in §4. Perhaps even more interesting is that the ratio CO to C^{18}O was ∼10/1 rather than 1/1, although relatively close considering its ISM value of ∼550/1. This suggests that while the very skin of the disk is dust free, the dust becomes optically thick to UV before the radiation penetrates to the optical depth of CO.

We concur with previous studies that there is a gas-poor inner clearing in this system beginning, according to our best fit, at ∼9 AU. Our temperatures concur closely with those stated by Brittain et al. 2007.

3.3. *HD 97048*

Significant extinction was detected along the line of sight to this system at 0.15 microns. To correct for this we multiplied the luminosity approximated from IUE observations by 9.

We fit our model to two Gemini data sets for this star (Table 2). While the first contained a broader range of the spectrum, the second had higher signal to noise. Also the observations were separated by one year allowing us to investigate variability in this star. We fit each of the two data sets separately, and checked to see if the fit parameters were consistent (Fig. 3). We found no evidence

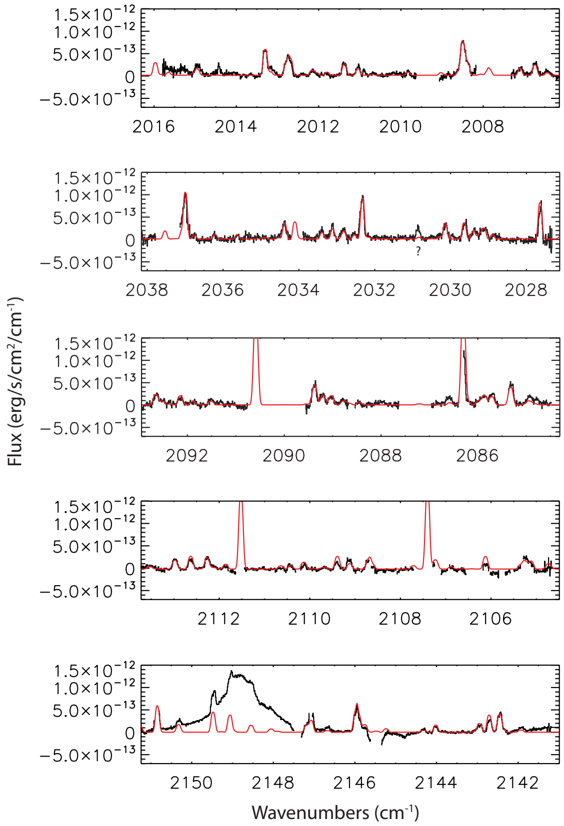

FIG. 1.— Synthetic spectra in red plotted over Keck data for HD 100546 in black. Figure from Brittain et al. (2009).

for variability in this data.

This disk is another instance of CO/^{13}CO = 1. In this case CO/C^{18}O is weakly constrained to be 1/1, the ISM value. As with HD 141569 we interpret this as suggestive of negligible dust to the optical depth of the isotopologue in question, in this case C^{18}O. Uncertainty for the density in this system was high. Polycyclic Aromatic Hydrocarbon (PAH) luminosity for this star is significantly higher than HD 141569, suggesting that PAHs are a primary source of heating. See §4 for a more detailed discussion of both dust settling and PAH heating.

4. DISCUSSION

Low CO isotopologue ratios in all three subject systems can be explained by a lack of dust in the upper disk atmosphere. These ratios allow us to put limits on the optical depth of the dust. In addition, PAH levels correlate with the temperature of each system.

4.1. *Interpretation of isotopologue ratios*

If the dust settles preferentially toward the disk midplane, dust extinction of stellar radiation will cease to be a significant factor in the relative luminosity of the CO and ^{13}CO lines. Without another significant source of continuum extinction in the UV, absorption for all CO isotopologues continues until the radiation reaches the depth at which CO becomes optically thick. This depth varies according the column density of the isotopologues, effectively cancelling the effect of the unequal abundances when viewed from the perspective of the absorption, and, subsequently, emission lines. The result is that for a disk with upper layers free of dust we expect a ratio of 1/1 for the various isotopologues. It must be noted however that all column densities and depths referred to here are along the radial direction from the star, not necessarily parallel to, and certainly not perpendicular to the disk midplane.

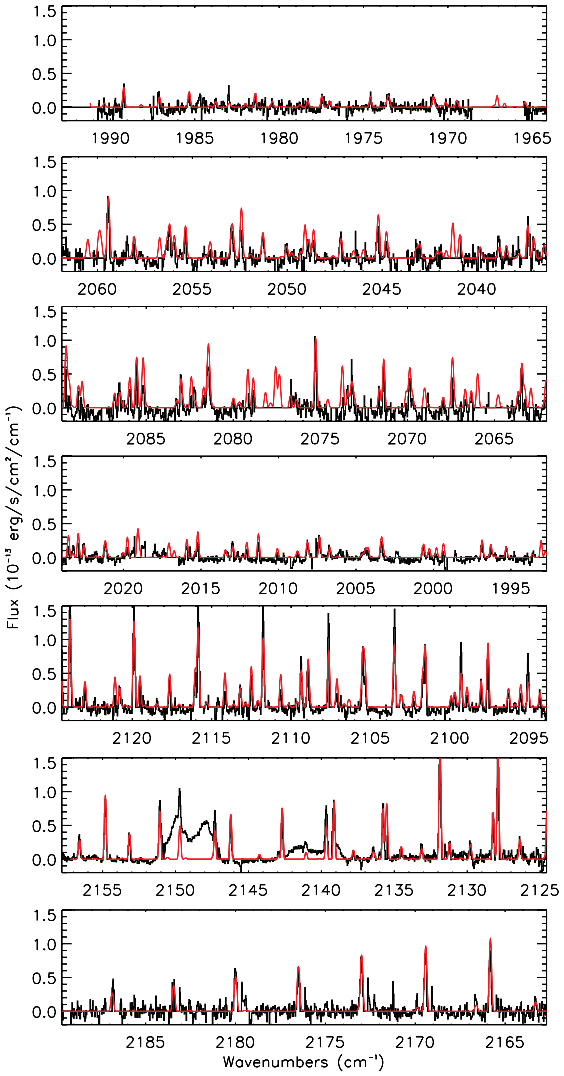

FIG. 2.— Synthetic spectra in red plotted over the Keck data in black for HD 141569. In this and later figures area represents flux. The two notable features over 2140 and 2150 cm^{-1} are atomic hydrogen recombination lines (the signature from roughly 2148-2150 is Pfβ).

4.2. *Interpretation of temperatures*

In addition to changing the isotopologue ratios we observe, dust settling should lower the temperature of the upper atmosphere, as dust is the primary source of photoelectric heating in the disk. Other notable sources of heating include X-rays (insignificant for typical HAeBe stars), accretion (typically significant only within 2 AU of the star), and PAH heating (a particular instance of dust photoelectric heating).

Thus a reduction in photoelectric heating should significantly lower the overall temperature of the disk. Dust settling, therefore, could be a major part of the explanation for the relatively low temperature of HD 141569 compared to similar HAeBe stars.

TABLE 3
PAH EMISSION

Object	Flux (10^{-15} W m^2)						Average T_{CO}
	6.2 μm	7.7-8.2 μm	8.6 μm	11.3 μm	12.0 μm	12.7 μm	
HD 100546	···	···	···	132 ±6	5 ±6	12 ±2	1000 K
HD 141569	8.7±0.4	19.2±0.4	1.1±0.1	0.7±0.1	<0.1	0.33±0.44	∼150 K
HD 97048	58 ±1	196 ±8	19 ±1	45 ±1	0.6±0.1	11.5 ±0.2	∼450 K

REFERENCES. — Adapted from Keller et al. 2008

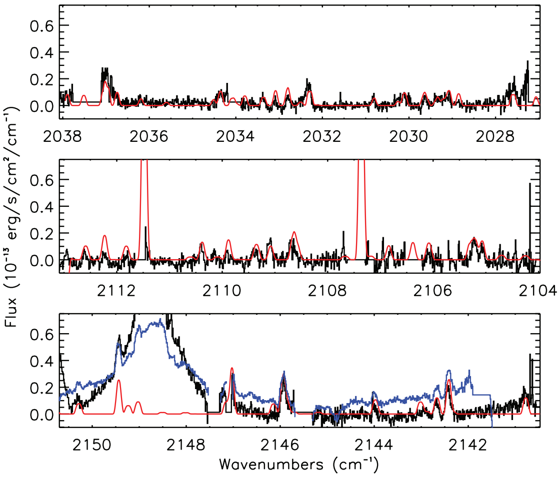

FIG. 3.— Gemini data for HD 97048 from March 22, 2008 in black and April 7, 2009 in blue, and the synthetic spectrum in red. While there is significant noise and background information, inspection of the last order will reveal a generally good fit of the CO lines to both data sets.

4.3. *PAH luminosity*

Even in a dust-poor scenario, however, photoelectric heating of the gas via PAHs may dominate so that the PAH luminsoity correlates with the temperature of the gas. Keller et al. (2008) writes on the possible reasons for low or non-detections of PAH in flared disks, suggesting four scenarios: 1) there is intrinsically low PAH in the disk atmosphere, 2) UV flux has destroyed the PAHs in the region of emitting gas, 3) our perspective of these systems is edge-on, 4) a puffed-up inner disk is shadowing the outer disk. However, Keller et al. cast doubt on case 2, none of the subject stars are inclined edge on as in case 3, and case 4 is only applicable under highly constrained circumstances, so we interpret low PAH luminosity as indicative of low PAH abundance in the CO emission region of the disk atmosphere since the radiation field of the stars in our sample are similar.

We therefore compare the PAH luminosity from HD 141569 and HD 97048. If both have dust-poor regions from which the CO emission originates, then we expect much higher PAH in HD 97048 in order to account for higher temperature.

See Table 3 for pertinent data from Keller et al. (2008). All three systems have strong PAH emission. Compared to each other, however, HD 141569 demonstrates ∼5-50 times less PAH luminosity than HD 97048 and, according to Brittain et al. (2009), 20 times less than that of HD 100546. This corresponds to a significantly lower temperature in HD 141569. The partial Keller data for HD 100546 shows a similar pattern as in HD 97048, agreeing with Brittain et al. 2009. Our isotopologue and temperature parameters for these three stars, then, fit well with our understanding of disk heating.

5. IMPLICATIONS FOR PROTOPLANETARY STUDIES

For HD 97048, we find unity CO/^{13}CO and CO/C^{18}O ratios, and so conclude that there is negligible dust to the optical depth of C^{18}O. We conclude that high PAH levels, indicated by high PAH luminosity, serve as an explanation for the relatively high temperature in spite of dust settling. High uncertainty on the CO/C^{18}O ratio indicates that the dust may be growing optically thick as it reaches the optical depth of C^{18}O.

Therefore we conclude that HD 97048 is similar to HD 100546 in gas/dust dynamics and PAH heating in the upper disk atmosphere, with the exception that it has lower PAH luminosity with a correspondingly lower temperature. In the case of HD 141569, we see evidence that the dust is optically thin to a depth between the optical depths of ^{13}CO and C^{18}O. The relatively low temperature at these depths supports this conclusion. HD 141569 is optically thin and we would expect a planet at the inner rim to have significant gas/dust mixing as a result. Due to the absence of gas in the inner gap, the overall tenuousness of the disk as reported by Brittain et al. (2007), and the lack of gas/dust mixing at the upper atmosphere, we find it likely that the inner gap is caused by photoevaporation, not a forming planet.

This work indicates that further study of CO isotopologue ratios and PAH luminosities in circumstellar disks may confirm and increase our understanding of dust settling and disk heating. Isotopologue ratios may place strong constraints on the optical depth of dust in the disk, and PAH luminosity may correspond to disk temperature in dust-poor situations.

This work also indicates the need for a faster, quantifiable optimization process to be applied to the model. The time spent tuning the parameters for the subject stars was a significant portion of the study. If an optimization routine, such as a χ^2 minimization, was applied, and the model was seeded to a cluster, significant time could be saved, and precise error bars could be applied to all fit values. The code is being converted to MATLAB for this purpose by M. Kronberg et al. (2009, in preparation), and, when completed, this process has the potential to greatly aid future study.

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