

SUPPLEMENTARY INFORMATION

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1. Herschel Observations

TW Hya ($\alpha(2000) = 11^h01^m51.91^s$; $\delta(2000) = -34^\circ43'17.0''$) was observed as part of an open time Herschel Program (OT1_obergin_4) using the PACS¹⁸ instrument on November 20, 2011. The PACS Range scan chop-nod mode was used. The background emission from the the telescope and sky was subtracted using two nod positions 1.5' distant from the source in each direction. The data cover a small spectral range (111.2-114.2 μm and 55.6-57.1 μm), with high sampling density (for a total of 81 steps). The first range includes HD $J = 1 \rightarrow 0$ and the second was designed to detect HD $J = 2 \rightarrow 1$. We used 12 repetitions to increase sensitivity for a deep scan, for a total integration time of 25124 seconds (36 repetitions) on TW Hya. The predicted line RMS was $0.62 \times 10^{-18} \text{ W m}^{-2}$ and $2.65 \times 10^{-18} \text{ W m}^{-2}$ at 112 and 56 μm , respectively.

The data were reduced using the Herschel Interactive Processing Environment (HIPE)³¹ v8.1 pipeline (calibration set 32). PACS is a 5×5 integral field unit spectrometer with a pixel size of $9.4'' \times 9.4''$; the source showed no sign of extended emission beyond the point spread function and was centered within 0.2 pixels (within $2''$) of the centerpoint in each case. We used the standard ‘‘calibration block’’ script to reduce the data for optimal signal-to-noise utilizing only the central pixel of the array, and then scaled this value to the spectra extracted from the central 3×3 pixels. We compared this to the PSF-corrected output from the pipeline, and the flux levels matched to within 10%. The PSF-corrected flux was 10% *higher* than the 3×3 extraction, which indicates an overcorrection and no sign of extended emission. Thus, we increased the flux measured from the central-spaxel-only spectrum by 10% to match that of the 3×3 extraction, yielding line fluxes, $F_l = (4.4 \pm 0.7) \times 10^{-18} \text{ W m}^{-2}$ for CO $J = 23 \rightarrow 22$ (centered at 113.509 μm indicating a possible blend between CO at 113.46 μm and H₂O at 113.53 μm), and $F_l = (6.3 \pm 0.7) \times 10^{-18} \text{ W m}^{-2}$ for HD $J = 1 \rightarrow 0$ (centered at 112.086 μm). The line flux was obtained using a Gaussian fit. The continuum was determined by a first-order polynomial simultaneous fit in a fairly tight region around the line, avoiding the CO transition. The HD $J = 2 \rightarrow 1$ transition was not detected with a 3σ upper limit of $F_l < 8.0 \times 10^{-18} \text{ W m}^{-2}$. The lines are not resolved with $\lambda/\Delta\lambda \sim 1000$ at 112 μm and ~ 1500 at 56 μm . The absolute uncertainty on flux calibration is potentially larger, with an important factor being the overall pointing and presence/absence of extended flux. Because TW Hya is a point source, the observations are well centered, and we included a PSF correction, the uncertainty in F_l is limited to 10-20%, negligible compared to other uncertainties.

From the CDMS database³², the $J = 1 \rightarrow 0$ line at 2674.986 GHz has $E_{J=1} = 128.5 \text{ K}$ with $A_{10} = 5.44 \times 10^{-8} \text{ s}^{-1}$. The $J = 2 \rightarrow 1$ line at 5331.561 GHz has $E_{J=2} = 384.58 \text{ K}$ with $A_{21} = 5.16 \times 10^{-7} \text{ s}^{-1}$. The A-coefficients have been calculated using the dipole moment of $8.56 \times 10^{-4} \text{ D}^{33}$.

2. Simple Estimate of the Gas Mass

The mass implied by a line flux of optically thin emission from an unresolved source can be derived in two steps. The total number of HD molecules (\mathcal{N}_{HD}) is related to the line flux by this relation, assuming that the beam encompasses the source:

$$F_l = \frac{\mathcal{N}_{\text{HD}} A_{10} h \nu f_u}{4\pi D^2}. \quad (1)$$

In this expression $f_u = 3.0 * \exp(-128.5 \text{ K}/T)/Q(T)$ is the fractional of HD molecules in $J = 1$, D is the distance, and ν is the frequency. Converting to mass, and assuming all is in H₂, $M_{\text{gas disk}} =$

$2.37 * m_H \mathcal{N}_{HD} / x_{HD}$, where x_{HD} is the abundance of HD relative to H_2 , m_H is the mass of a hydrogen atom, and 2.37 is the mean molecular weight per particle, including helium and heavy elements³⁴. This gives

$$M_{gas\ disk} = \frac{2.37 m_H 4\pi D^2 F_l}{A_{10} h\nu x_{HD} f_u}. \quad (2)$$

The partition function, $Q(T)$, is near unity below ~ 50 K³². Inserting values of physical constants yields:

$$M_{gas\ disk} > 5.21 \times 10^{-5} \left(\frac{F_l}{6.3 \times 10^{-18} \text{ W m}^{-2}} \right) \left(\frac{3 \times 10^{-5}}{x_{HD}} \right) \left(\frac{D}{55 \text{ pc}} \right)^2 \exp \left(\frac{128.5 \text{ K}}{T_{gas}} \right) M_{\odot}. \quad (3)$$

This estimate represents a lower limit because the HD emission may not trace all the mass in the disk.

3. CO Emission and T_{gas} from TW Hya

In the main text we used the resolved ALMA Science Verification CO $J = 3 \rightarrow 2$ data to set a limit on the gas temperature. In Supplementary Figure 1 we show the integrated emission map with a beam size $1.7'' \times 1.5''$, which corresponds to a radius of 47×41 AU. The map demonstrates that the CO emission is resolved, so we assume unity filling factor. Based on the central spectrum the observed peak radiation temperature is $T_R = 22.2 \pm 0.1$ K (we note that this data has a calibration uncertainty of 10%). T_R is linearly related to the intensity, so a correction for the difference between the Planck function and the Rayleigh-Jeans approximation results in an average gas kinetic temperature of $T_{gas} = 29.7$ K in the beam, assuming optically thick and thermalized emission. Observations of CO $J = 6 \rightarrow 5$ confirm this value. The observed CO $J = 6 \rightarrow 5$ peak intensity is $T_R = 16.9 \pm 3.2$ K³⁵, which corresponds to a gas temperature of 30.6 K.

Assuming $T_{gas} = 30$ K yields a minimum disk mass of $3.9 \times 10^{-3} M_{\odot}$.

4. HD Emission Line Models

For more detailed models we use two predicted physical structures (Gorti et al.¹⁴ and the Thi et al.¹³ TW Hya models) derived from thermochemical calculations that match a range of gas phase emission lines. The Gorti et al. TW Hya model has a disk gas mass of $0.06 M_{\odot}$, and we used direct output from the model. For the Thi et al. TW Hya model we use a reproduction. Specifically, to reproduce this model we adopt the physical parameters for the dust structure as given in their¹³ Table 2. The dust optical constants are as prescribed³⁶ with a dust grain size distribution from $3 \times 10^{-2} \mu\text{m}$ to 1 mm and a power law index of 3.4. These inputs were placed into RADMC³⁷ where we verified that the model reproduced the observed spectral energy distribution and the dust thermal structure given in their Fig. A.2. For this calculation the total disk gas mass is $0.003 M_{\odot}$ and we verified that our gas density distribution matched that provided in their Figure A.1. We do not model the H- H_2 transition; this is appropriate for HD which will emit below this transition region. Finally we used the gas temperature distribution given in their Fig. A.3 as input to our LIME calculations for HD. As a final check we computed the predicted emission of this reproduction for CO and $^{13}\text{CO } J = 3 \rightarrow 2$ to observed values³⁸ and found them to be in agreement to within a factor of two.

To predict the HD line emission from the physical models we calculate the solution of the equations of statistical equilibrium including the effects of line and dust opacity using the LIME code³⁰. Although the HD line emission is fairly close to LTE, we adopt the collision rate coefficients of HD with H_2 ³⁹. The collision rates are insensitive to the rotational state of the H_2 collision partner⁴⁰. The disk dust optical depth

is determined by the dust opacity coefficient κ_λ and the dust mass distribution within the disk. Typical dust mixtures^{36,41} suggest $\kappa_{112\ \mu\text{m}} \sim 30\ \text{cm}^2\ \text{g}^{-1}$. The excitation model explicitly explores pumping by continuum radiation, which is found to be negligible when compared to the effects of the dust optical depth.

Table S1 provides the predictions from the specific thermochemical model including an emission calculation with dust opacity at $112\ \mu\text{m}$ (the realistic case) and without dust opacity. The Thi et al. TW Hya model with the lowest mass predicts an HD emission line that is too weak. To match observations within the framework of the Thi et al. TW Hya model we require an increase in mass by a factor of 20. We stress that this is approximate as scaling the mass will change the thermal solution (gas temperature, chemistry). Thus, this factor only illustrates the mass dependency and is not definitive. The thermochemical model that comes closest to the observed flux is the Gorti et al. TW Hya $0.06\ M_\odot$ model – which is still about a factor of two smaller than the observed HD emission.

References

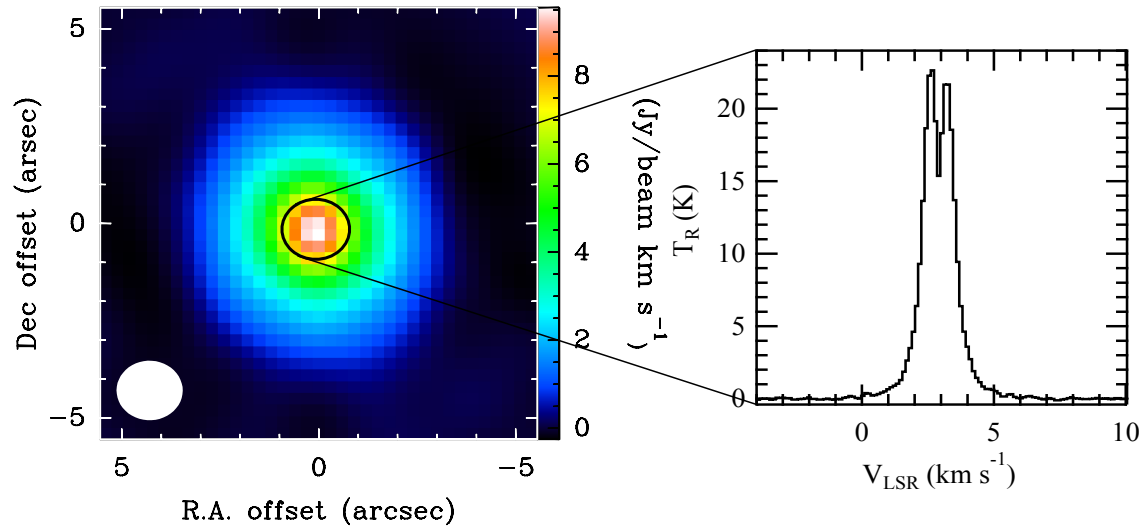
31. Ott, S. The Herschel Data Processing System – HIPE and Pipelines – Up and Running Since the Start of the Mission. In Mizumoto, Y., Morita, K.-I. & Ohishi, M. (eds.) *Astronomical Data Analysis Software and Systems XIX*, vol. 434 of *Astronomical Society of the Pacific Conference Series*, 139–142 (2010).
32. Müller, H. S. P., Schlöder, F., Stutzki, J. & Winnewisser, G. The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists. *Journal of Molecular Structure* **742**, 215–227 (2005).
33. Pachucki, K. & Komasa, J. Electric dipole rovibrational transitions in the HD molecule. *Phys. Rev. A* **78**, 052503 (2008).
34. Kauffmann, J., Bertoldi, F., Bourke, T. L., Evans, N. J., II & Lee, C. W. MAMBO mapping of Spitzer c2d small clouds and cores. *Astron. & Astrophys.* **487**, 993–1017 (2008).
35. Qi, C. *et al.* CO J = 6-5 Observations of TW Hydrae with the Submillimeter Array. *Astrophys. J. Letters* **636**, L157–L160 (2006).
36. Dorschner, J., Begemann, B., Henning, T., Jaeger, C. & Mutschke, H. Steps toward interstellar silicate mineralogy. II. Study of Mg-Fe-silicate glasses of variable composition. *Astron. & Astrophys.* **300**, 503–520 (1995).
37. Dullemond, C. P. & Dominik, C. The effect of dust settling on the appearance of protoplanetary disks. *Astron. & Astrophys.* **421**, 1075–1086 (2004).
38. van Zadelhoff, G.-J., van Dishoeck, E. F., Thi, W.-F. & Blake, G. A. Submillimeter lines from circumstellar disks around pre-main sequence stars. *Astron. & Astrophys.* **377**, 566–580 (2001).
39. Flower, D. R., Le Bourlot, J., Pineau des Forêts, G. & Roueff, E. The cooling of astrophysical media by HD. *MNRAS* **314**, 753–758 (2000).

40. Flower, D. R. A quantum mechanical study of the rotational excitation of HD by ? *Journal of Physics B Atomic Molecular Physics* **32**, 1755–1767 (1999).
41. Pollack, J. B. *et al.* Composition and radiative properties of grains in molecular clouds and accretion disks. *Astrophys. J.* **421**, 615–639 (1994).

Supplementary Table S1: Specific Model Predictions

Disk Model	Gas Mass (M_{\odot})	HD $J = 1 \rightarrow 0^a$ (W m^{-2})	HD $J = 2 \rightarrow 1$ (W m^{-2})
Thi et al. TW Hya	0.003	3.8×10^{-19}	1.4×10^{-19}
Gorti et al. TW Hya	0.06	3.1×10^{-18}	3.3×10^{-18}
Observations		$6.3 \pm 0.7 \times 10^{-18}$	$< 8.0 \times 10^{-18}$

^aFluxes without dust optical depth are $7.4 \times 10^{-19} \text{ W m}^{-2}$ (Thi et al. $0.003 M_{\odot}$), $4.2 \times 10^{-18} \text{ W m}^{-2}$ (Gorti et al. $0.06 M_{\odot}$)



Supplementary Figure 1: ALMA Science Verification Observations of CO $J = 3 \rightarrow 2$ in TW Hydra. (Left) Map of CO $J = 3 \rightarrow 2$ integrated emission with intensity scale given on the left. The beam size of this observation is $1.7'' \times 1.5''$ and is shown in the figure. (Right) Blow-up of the central spectrum.