Supporting Online Material for

Organic Molecules and Water in the Planet Formation Region of Young Circumstellar Disks

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Materials and Methods

**Data and Reduction.** The high S/N and quality of the IRS spectrum of AA Tauri (Fig. 1) are made possible by both the observations and the data processing procedures. AA Tauri was observed in standard staring mode in both the Short-high and Long-high IRS modules. The integration times of 720 sec and 960 sec, respectively, were sufficiently long to provide high S/N in the absence of systematic effects. Observations were also obtained for a nearby, empty off-source position in order to subtract background emission and remove hot pixels. One-half as much time was spent integrating on the off-source position as on the target.

The data reduction procedures are critical for obtaining the maximum S/N possible. We started with the non-flat-fielded “droop” images. With the large number of observed co-adds, we were able to perform statistics on each pixel of the array to identify unstable pixels and cosmic rays. The mean off-source image was subtracted from each of the two mean on-slit images. The pipeline flat-fields were divided by low-order polynomials in order to remove large-scale spectral and spatial structure. This preserves the noise statistics and avoids artificial increases in the noise near the ends of the slit that result from division with the pipeline flat-field. After division by the flat-field, pixels identified as unstable and permanently bad pixels were replaced by interpolation in the spectral direction. The spectra were then extracted using optimal weighting. The wavelength scale for the extracted spectra was obtained by fitting a polynomial function to the
pipeline wavelength calibration table. The extracted spectra were then divided by the spectrum of an archival standard star (ξ Dra) to provide flux calibration and fringe removal. The standard spectrum was processed in the same way as the target but divided by a model template spectrum. Residual fringing in the Short-high spectrum was removed using IRSFRINGE (S7). Finally, the individual spectral orders were combined with appropriate weighting in the wavelength overlap regions.

**Modeling.** Parameters for the molecular gas were determined by modeling the disk emission as a slab of gas with an independent temperature, column density, and area for each molecular species. The slab is viewed at AA Tauri’s inclination angle of 75 degrees (S2) at a distance of 150 parsec. The column density (Table 1) is the observed slant column density. We assume that the rotational and vibrational levels are thermally populated in LTE. The local line broadening is taken as equal to the thermal broadening. The molecular line lists are from the HITRAN database (S3).

For H2O, we carried out a curve of growth analysis of using measured line fluxes for features identified as single H2O transitions or ortho-para pairs of transitions. This analysis yields the best combination of temperature and column density. Synthetic spectra were then calculated to confirm the solution and to determine the emitting area required to produce the absolute H2O flux. We find that nearly all of the measurable H2O lines are optically thick, with best-fit parameters of temperature T = 575 K and water column density N(H2O) = 6.5 x 10^{17} cm^{-2}. Because the emission is optically thick, the emitting surface area is well constrained, equivalent to a circular area with radius R = 2.1
Applying the same analysis to the OH emission features, we find $T = 525$ K, $N(\text{OH}) = 8.7 \times 10^{16}$ cm$^{-2}$, and $R = 2.2$ AU.

Parameters for HCN, C$_2$H$_2$, and CO$_2$ were derived from fitting synthetic spectra to the observed bands. Because H$_2$O contributes to each of these unresolved bands, the previously calculated H$_2$O spectrum was added. In addition, the HCN and C$_2$H$_2$ bands were synthesized together since each molecule contributes some lines to the Q-branch of the other. In general, the shape of these bands depends on the combination of temperature and column density, and over some range these two parameters can vary simultaneously to yield similarly acceptable fits to the observations. The limits for acceptable fits are the uncertainties given in Table 1. This is illustrated for the HCN band in Fig. S2, which compares the best synthesis with two syntheses considered unacceptable that use temperatures ± two times the temperature uncertainty. The radius (R) of the equivalent emitting area only affects the absolute flux of the emission bands.

Optically thick emission lines provide the best fits for all these molecules. Fitting the shape of the HCN band places good constraints on the HCN parameters, with $T = 650$ K, $N(\text{HCN}) = 6.5 \times 10^{16}$ cm$^{-2}$ and $R = 0.60$ AU. The best fit for the C$_2$H$_2$ Q-branch also gives $T = 650$ K but is less sensitive to the column density. Because the temperature is the same as that for HCN, we adopt the same area, which yields $N(\text{C}_2\text{H}_2) = 8.1 \times 10^{15}$ cm$^{-2}$. CO$_2$ requires a much lower temperature than HCN and C$_2$H$_2$, $T = 350$ K with $R = 1.2$ AU; however, modest changes in temperature require large changes in column density to fit the band, giving a range in $N(\text{CO}_2)$ from $2.1 \times 10^{15}$ to $1.3 \times 10^{17}$ cm$^{-2}$. The
combined best-fit synthetic spectrum in the 15 µm spectral region is shown in Figure 2 where it is compared to the observed continuum subtracted spectrum.

Modeling of the CO fundamental emission spectrum off AA Tauri followed similar procedures as for the IRS data, but we fit the models to an excitation plot (column density in the upper level for each transition versus the energy of the upper level) for the CO emission. The best parameters are $T = 900$ K, $N(\text{CO}) = 4.9 \times 10^{17}$ cm$^{-2}$, and $R = 0.7$ AU. Table 1 summarizes the results for each molecular species and gives their abundances with respect to CO.

References

S1. F. Lahuis et al., C2d Spectroscopy Explanatory Suppl. (Spitzer Science Center: Pasadena, 2006).
Fig. S1. Comparison of abundances relative to H$_2$O. The abundances for each molecule relative to H$_2$O derived for AA Tauri (squares) is compared to the abundances for sublimated ices in comets ($S4$, $S5$) (diamonds), for ices observed towards star-forming regions ($S6$) (triangles), and to disk chemical models ($S7$) at radii of 1 and 5 AU (open circles with radius labeled).
Fig. S2. Synthesis of the HCN band for AA Tauri. The black histogram is the observed spectrum, and the red histogram is the best synthetic spectrum shown in Fig. 2 using the parameters in Table 1. The other colored histograms show unacceptable models with $T = 450$ K (blue) and $T = 850$ K (green), which correspond to twice the temperature uncertainty in Table 1. For each temperature, the column density is varied to provide the best possible fit to the observations.