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THE SEARCH FOR LIFE'S ORIGINS USING HIGH-RESOLUTION MID-IR SPECTROSCOPY AT A GIANT GROUNDBASED TELESCOPE

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1. Pre-biotic Molecules in Protoplanetary Disks

Determining the origin of life is arguably the most compelling quest in modern science. The study of extraterrestrial "pre-biotic" molecules is a fundamental part of that odyssey. Pre-biotic molecules are the large precursors to molecules of biological importance. They are essential building blocks of proteins, carbohydrates, nucleic acids, and lipids—key ingredients of life as we know it. They include amino acids, nucleobases, and sugar-related compounds, all of which have been identified in some members of the class of meteorites called carbonaceous chondrites (Botta & Bada 2002, review). Pre-biotic molecules as complex as ethylene glycol (antifreeze; $HOCH_2CH_2OH$) have also been identified in comets (Crovisier 2004, review). These parent bodies, if they impacted the Earth under the right conditions, may have seeded it with the chemical ingredients necessary for the development of life (Botta 2004). The relative importance of this pathway compared to *in situ* terrestrial evolution for life's precursors is unknown.

Complex hydrocarbons such as alcohols, acids, nitriles, and aldehydes have also been detected in dense interstellar clouds. The extent to which these and other interstellar organic material are destroyed or modified as it is accreted into, and processed within, protoplanetary disks is an open question (Ehrenfreund & Charnley 2000). Furthermore, as seems to be the case for simpler organic molecules (Carr & Najita 2008), complex organic molecules could have been synthesized in the protoplanetary disks themselves (e.g., Markwick et al.2002). Determining the abundances and distributions of pre-biotic molecules in protoplanetary disks will permit an assessment of the availability of ingredients necessary for the origin of life within planet-forming systems, and it will provide a basis for appraising whether, and at what rate, such pre-biotic molecules can be delivered to planets by bombardment of minor bodies. The exploration of pre-biotic molecules in protoplanetary disks with high-spectral-resolution mid-IR spectroscopy at a giant telescope is the focus of this White Paper.

2. High-Spectral-Resolution Mid-IR Spectroscopy

The speed of mid-IR (7-25 μm) observations, where sensitivities are background-noise limited, increases rapidly with telescope aperture D. The time to achieve a given signal-to-noise ratio is proportional to $1/D^4$, so that a 30-m telescope will be two orders of magnitude more efficient in the mid-IR than are the current 8-10-m telescopes. In conjunction with the factor of three-to-four better angular resolution, this huge gain in current capability will open up a large, exciting discovery space. At a 30-m-class telescope, high-spectral-resolution ($R \equiv \lambda/\Delta\lambda \approx 10^5$) mid-IR spectroscopy, in particular, will be able to move to the forefront as a unique, enormously incisive and valuable probe of astrophysical phenomena. This regime, which is virtually unexplored, will complement strongly those accessible with JWST's smaller aperture and much smaller (R=2000) spectral resolution, and with ALMA, which will probe primarily cooler astrophysical regions.

High-spectral-resolution mid-IR spectroscopy in combination with a giant telescope is an essential tool for exploring the organic-molecular content of protoplanetary disks. Most simple and complex hydrocarbon compounds have strong mid-IR transitions, many of which are accessible to ground-based observations. Disk temperatures at 1-10 AU from solar-type stars and out to several tens of AU in more massive stars—regions particularly germane to planet formation and evolution—provide excitation conditions conducive to the production of these

Table 1. *Some hydrocarbon compounds with ground-accessible mid-IR transitions.*

*ci	HCN	hydrogen cyanide	*	CH_2CCH_2	propadiene
*ci	C_2H_2	acetylene	*c	C_2H_6	ethane
* i	CH_3	methyl radical	r	CH_3COOH	acetic acid
cr	H_2CO	formaldehyde	cr	$HCOOCH_3$	methyl formate
* r	HNCO	isocyanic acid	r	CH_2OHCHO	glycolaldehyde
*ci	CH_4	methane	r	C_2H_5OH	ethanol
cr	HCOOH	formic acid	r	$(CH_3)_2CO$	acetone
*	C_2H_4	ethylene	cr	$HOCH_2CH_2OH$	ethylene glycol
cr	CH_3OH	methanol	?	NH_2CH_2COOH	glycine
r	NH_2CHO	formamide	*	C_3H_8	propane
cr	CH_3CHO	acetaldehyde	r	C_6H_6	benzene

* = observed in MIR in astronomical object with TEXES; c = observed in comets;
i/r = observed in the ISM in infrared (i) or radio (r)

lines. Table 1 indicates some of the hydrocarbons with mid-IR transitions accessible from the ground. Most of these have been detected in comets and the interstellar medium, and several have been detected in other astronomical sources, such as star-forming regions, with the mid-IR echelle spectrograph TEXES at the 3-m IRTF or the 8-m Gemini telescopes. While many of these have only been detected in the radio (r) and may be difficult to detect in the mid-IR even with a giant telescope, many (e.g., CH_3, CH_4, C_2H_2, and C_2H_4) are not detectable in the radio, leaving the mid-IR as the primary or sole probe in obscured regions like protoplanetary disks. The richness and potential of this spectral region for exploring pre-biotic molecules is evident.

Spectral resolution as high as 10^5 is critically important for several reasons. First, it substantially increases the chances of detecting rare species, because the mid-IR region is crowded with lines of astrophysical interest, as illustrated by the 10-34 μm Spitzer spectrum (Fig. 1) of the circumstellar disk around the young star AA Tau (Carr & Najita 2008). The best

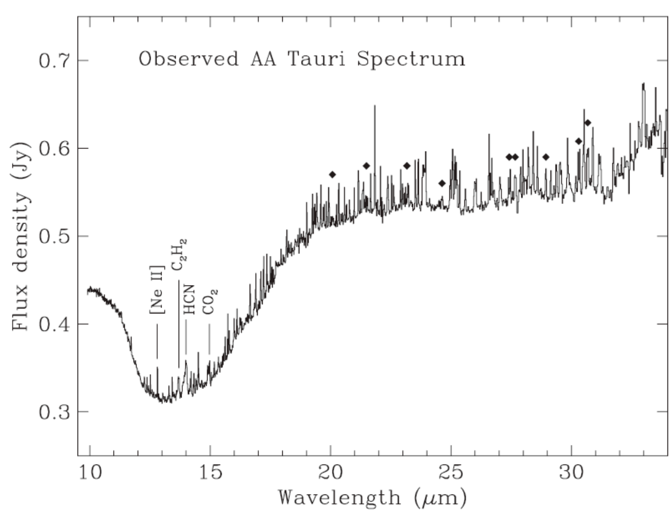

Figure 1. *Spitzer spectrum of the AA Tau disk (Carr & Najita 2008).*

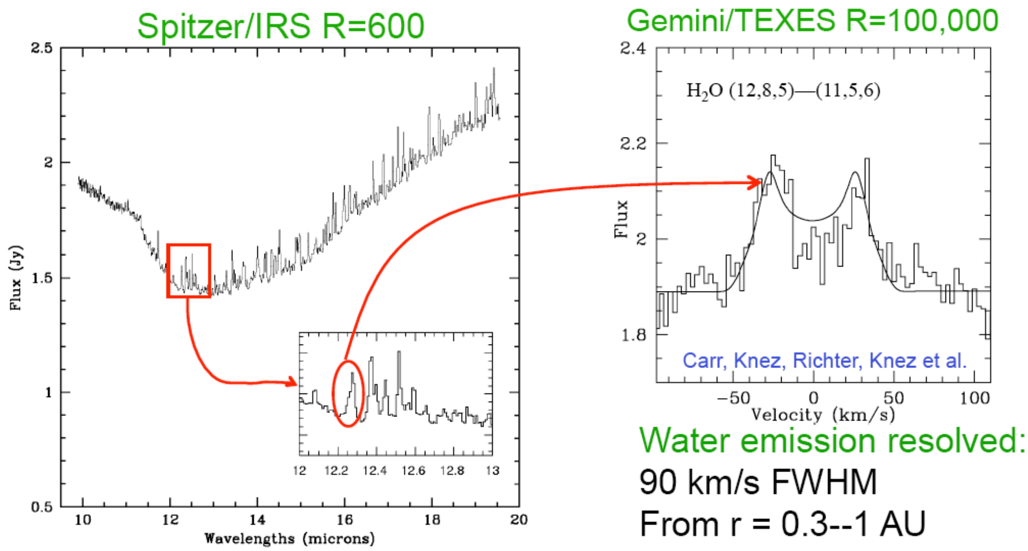

Figure 2. *Insight provided by high spectral resolution of H_2O. Under assumption of Kelperian motion, line width provides location in disk around RW Aur A (Knez et al. 2007).*

sensitivity is achieved when the resolution element matches the line width, but in the (background-limited) mid-IR region, higher-resolution observations can be binned to maximize the sensitivity. Secondly, because most lines are well resolved at these high resolutions (Fig. 2), the line profile can be related directly to the radial location of a molecule under the assumption of Keplerian rotation in the disk. Thus, in combination with the actual spatial resolution provided for some molecules by a giant telescope, a picture of the molecular spatial distributions within disks can be constructed. A resolution as good as $R=10^5$ (3 km s^{-1}) is needed to accomplish this goal. Multiple transitions from molecules permit determination of gas temperatures and optical depths. Thirdly, high spectral resolution provides the practical advantage of permitting astrophysical lines to be more readily separated from telluric (atmospheric) features.

3. Mid-IR Performance at a Giant Groundbased Telescope

We consider a baseline giant groundbased telescope (GSMT, ELT) with an aperture diameter of ~30 m and located at a quality mid-IR site defined as one with good thermal characteristics, low precipitable water vapor, and excellent seeing. The mid-IR sensitivity of a spectrograph with resolution $R=10^5$ when used at such a telescope will be phenomenal, providing several orders of magnitude increase in speed over existing 8-10-m class telescopes used at comparable spectral resolution. In fact, the sensitivity for unresolved lines will rival that of the 6.5-m JWST mid-IR spectrograph (R=2000), but with the substantial advantages that come with much higher spectral (×50) and angular (×5) resolutions. JWST will access some important spectral regions blocked from view from the ground, but the complementarity and synergy of these facilities are strong.

The shot noise of the (background) thermal emission from the sky and the telescope sets the fundamental limit to the mid-IR sensitivity. The high sensitivity of an $R=10^5$ spectrograph at a 30-m telescope results both from the large aperture and the high dispersion, which substantially decreases the thermal background per resolution element compared to that at lower resolutions. We have estimated the sensitivities (signal-to-noise ratio 10 in 100 s integration time) for unresolved emission lines for this configuration based on the system assumptions listed in Table 2. The resultant line and continuum sensitivities for point sources are listed in Table 3.

Table 2. *Assumptions used to calculate background-limited line sensitivity.*

Parameter	Assumed Value
Telescope D	30 m
System emissivity	13%
Nod efficiency	83%
Detector QE	60%
R at <14 μm	120,000
R at >14 μm	$(1.68\times10^6)/\lambda$
Slit efficiency	70%
PWV	1 mm
Airmass	1.4
Atmos. Temp.	260 K
Optical Efficiency	20%

Table 3. *Mid-IR point-source sensitivities[1] for $R=10^5$ at a 30-m telescope*

Wavelength (μm)	NELF[2] (10^{-16} ergs s^{-1} cm^{-2})	NEFD[3] (mJy)
8	2	64
10	2	82
12	1.8	87
18	3.4	190
20	3.9	220
22	7.3	410
24	17	930

[1]S/N = 10, t = 100 s
[2]Noise-equivalent line flux
[3]Noise-equivalent flux density

4. Science Observations

A high-resolution mid-IR spectrograph on a 30-m-class telescope will provide the tool needed to efficiently survey enough (~100) protoplanetary disks to construct the first observational inventory for understanding the origin and evolution of pre-biotic molecules. The key observations include abundances, distributions, temperatures, and excitation conditions. The targets will be disks around young (<5 Myr) stars with masses in the range ~0.2-8 M_{sun} that are past the optically thick accretion phase, i.e., primarily Class II disks. They are members of the pre-main-sequence classes known as T Tauri (< 2 M_{sun}) and Herbig Ae/Be (2-8 M_{sun}) stars. The sample will be within 200 pc, and can be drawn from the lists of several hundred known members of each class that have been studied extensively across the spectrum. Observations with

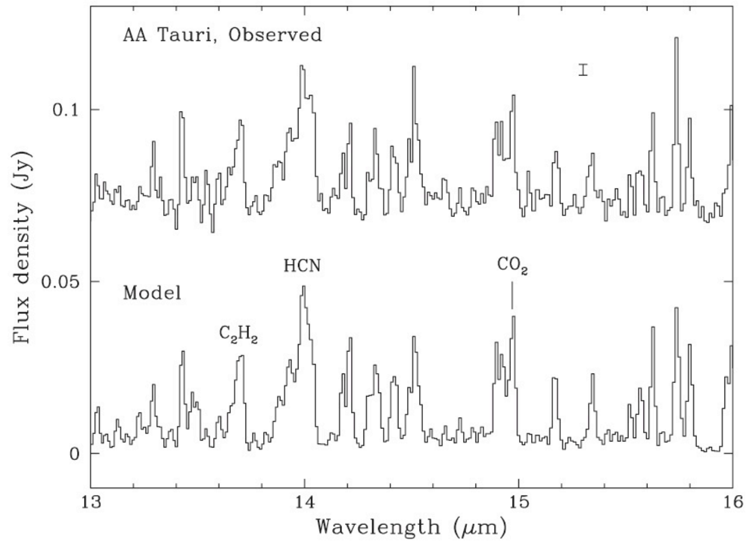

Figure 3. *Spitzer spectrum (subset of Fig. 1 spectrum) of the T Tau star AA Tau (Carr & Najita 2008) The observed spectrum (top) is offset from the model spectrum (bottom).*

Spitzer IRS indicate that mid-IR molecular emission is common in protoplanetary disks; roughly 90% of the ~60 classical T Tau stars observed so far with Spitzer IRS show water and/or other simple molecules (Carr & Najita 2008, Salyk et al. 2008; J. Carr, personal communication). This will be rich territory to explore with high resolution. This program will achieve its maximum benefit when carried out in conjunction with a similar study (not discussed here) of Class I protostars, which are the progenitors of the Class II sources and therefore represent the molecular starting point for these sources.

To assess how well the mid-IR line sensitivities indicated in Section 3 can serve our goals of exploring pre-biotic molecules in protoplanetary disks, we refer to recent mid-IR Spitzer spectra of the T Tauri star AA Tau (Carr & Najita 2008) located 140 pc away. Figure 3 shows the 13-16 μm part of the broader spectrum shown in Fig. 1. The Spitzer spectrum indicates that the flux of the unresolved R-branch HCN line (R13) is 1.4×10^{-15} ergs s^{-1} cm^{-2}. If this line is spread out over 60 km s^{-1}, as implied by the models of Carr & Najita (2008) which give the HCN extent (~1 AU) and inclination (45°) for the disk of AA Tau (0.6 M_{sun}), the average flux per resolution element (3 km s^{-1}) is 7×10^{-17} ergs s^{-1} cm^{-2}. The sensitivities listed in Table 3 then imply an average signal-to-noise ratio >20 per resolution element for the fully resolved line. This is excellent. Because the data would be background limited, it would be possible to bin to lower spectral resolution if higher signal-to-noise were required. A diffraction-limited 30-m-class telescope will provide an angular resolution $\lambda/D = 0.07$ arcsec at 10 μm. At 140 pc, the HCN emission in AA Tau disk would only subtend 0.01 arcsec and would not be resolved. However, AA Tau has a relatively low mass (~0.6 M_{sun}); more massive stars will excite the molecules at larger radii, supporting the expectation that these distributions can be resolved spatially in other sources.

In the example of the HCN line in AA Tau, the line is well resolved (20 resolution elements wide), because it originates in the inner disk, relatively close to the star. However, we emphasize that many of the lines of pre-biotic importance are expected to originate in the 1-10 AU zone and have widths several times lower than that; high-spectral resolution will be crucial in those cases to acquire any velocity information or, in some cases, to even detect the molecule. We expect a broad panoply of other organic molecules of pre-biotic interest to be present, but considerable detailed modeling constrained by observations such as those indicated here will be needed to describe their abundances and distributions. Models by Markwick et al. (2002) for interpreting the mm spectrum by Dutrey et al. (1997) of the 5 Myr-old, 0.65 M_{sun} mass T-Tau star DM Tau emphasize the richness of this territory; the top 20 molecules, prioritized by column density, are listed in Table 4 for three distances from the star.

Table 4. *Predicted abundances for some molecules in protostellar disks (truncated version of Table 3 in Markwick et al. 2002)*

	$R = 1$ AU		$R = 5$ AU		$R = 10$ AU	
	Species	log N (cm^{-2})	Species	log N (cm^{-2})	Species	log N (cm^{-2})
1	He	25.2	He	24.8	He	24.7
2	H_2O	22.2	H_2O	21.5	CH_4	21.0
3	CH_4	21.5	CH_4	21.1	CO	21.0
4	CO	21.5	CO	21.0	H	20.6
5	H	21.0	H	20.9	N_2	20.4
6	N_2	21.0	N_2	20.6	NO	19.4
7	HCN	20.4	NH_3	20.2	O_2	19.2
8	C_3H_4	20.4	CO_2	20.1	HCN	17.7
9	C_4H_2	20.0	C_3H_4	20.0	HNC	17.7
10	NH_3	20.0	C_4H_2	19.5	CH_3CN	17.2
11	HC_3N	20.0	C_3H_3	19.5	O	17.1
12	C_2H_2	19.3	O_2	18.9	C_3H_4	16.9
13	CH_3CN	19.3	HC_3N	18.9	C_3H_3	16.7
14	CO_2	18.9	CH_3CN	18.9	H_2CO	16.6
15	HNC	18.7	C_2H_2	18.8	C_2H_2	15.7
16	CH_3OH	18.5	NH_2	18.7	H_2CS	15.0
17	CH_3	18.4	HCN	18.6	N	15.0
18	O_2	18.4	HNC	18.1	CS	14.6
19	SO_2	18.3	CH_3OH	17.9	CH_2CO	14.6
20	CH_2CO	18.3	CH_2CO	17.9	SO	13.5

Acknowledgements
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