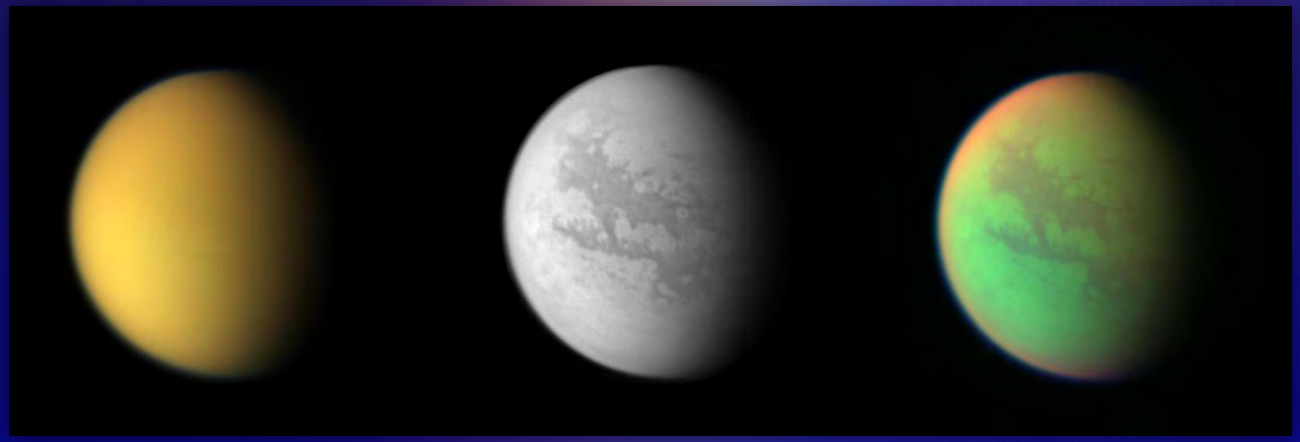
Analysis of High Resolution Laboratory Propane Spectra (ν_{21}, 922 cm^{-1}) and the Interpretation of Titan's Infrared Spectra



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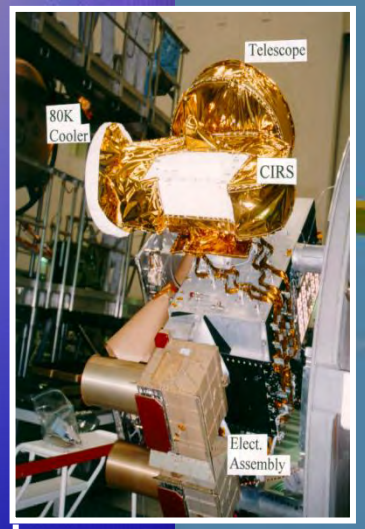
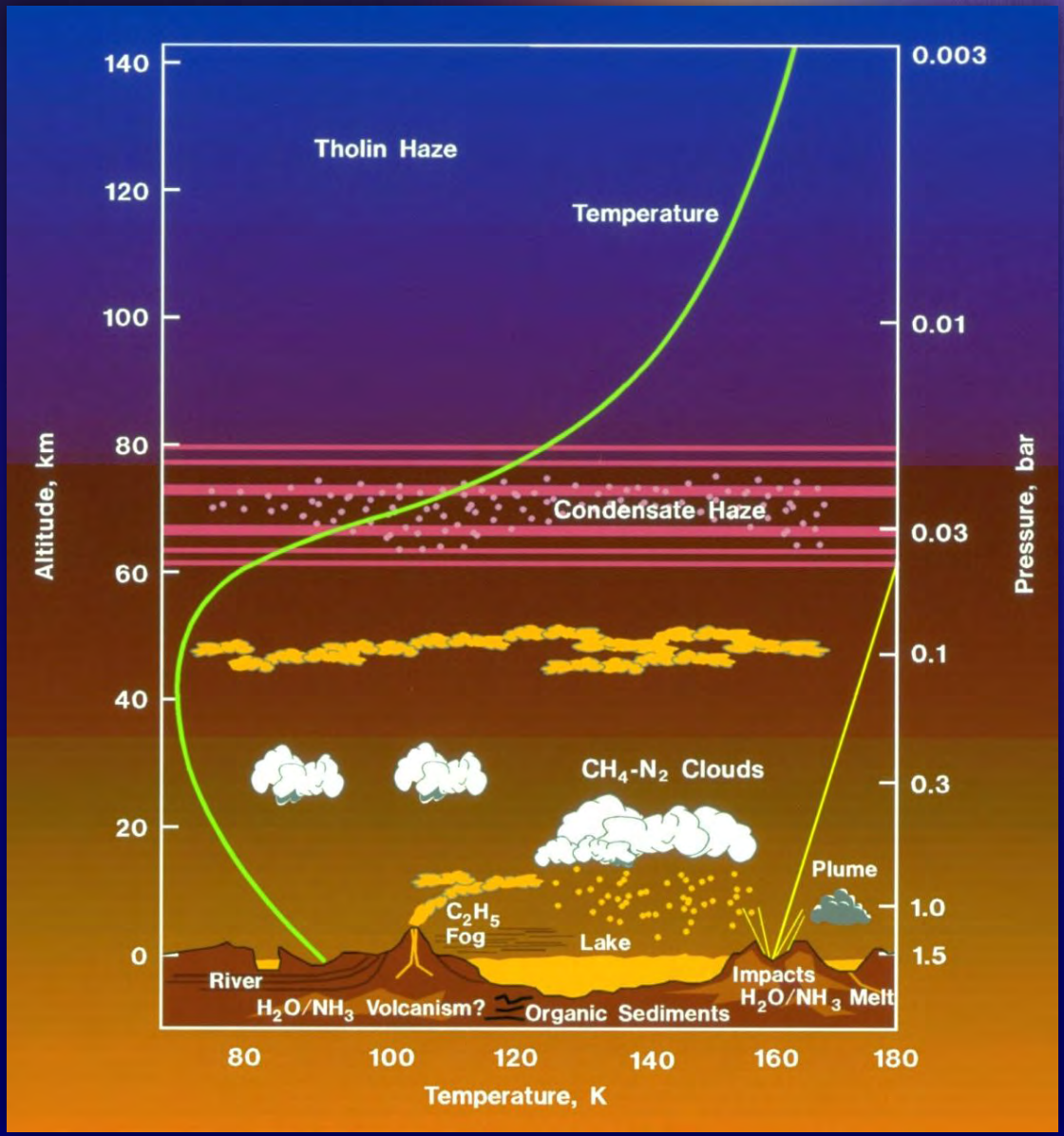
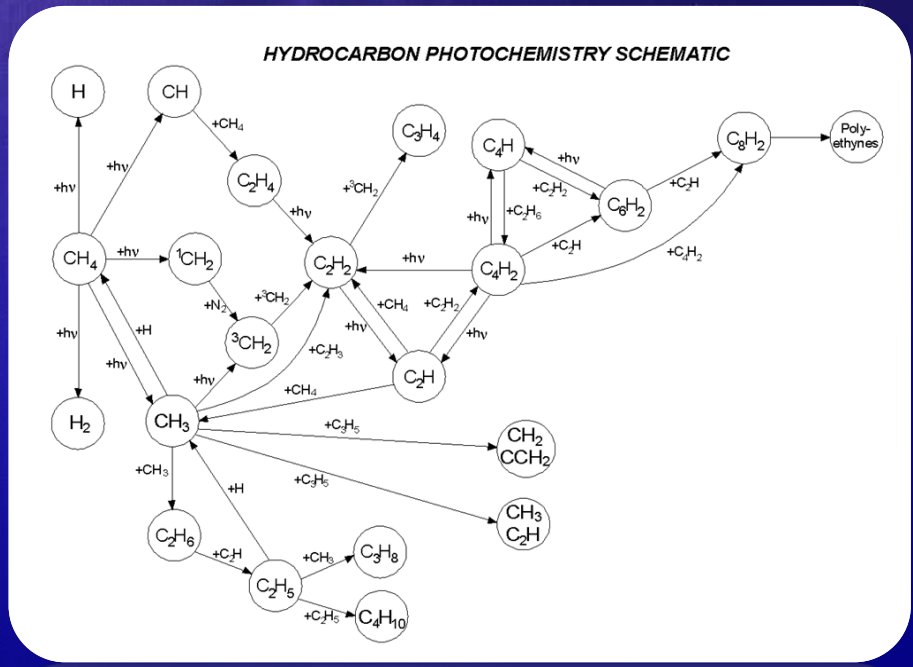
Cassini/CIRS

- CIRS = Composite Infrared Spectrometer
- records the infrared spectrum of targets in the Saturnian system
- provides details on their chemical composition and thermal structure
- its mapping of Titan's atmosphere has confirmed the presence of many chemical species and has detected new isotopic varieties

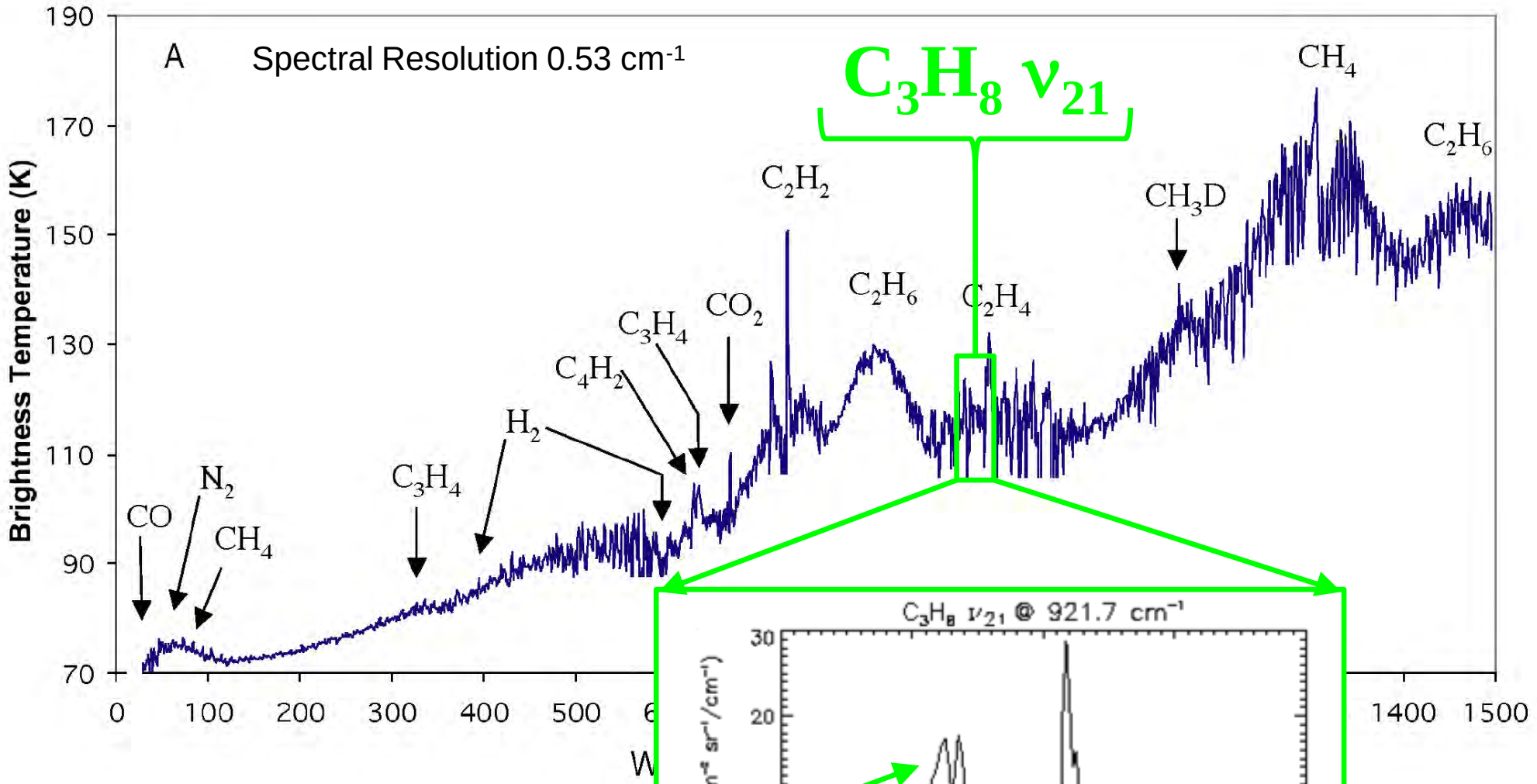


Atmospheric Photochemistry on Titan





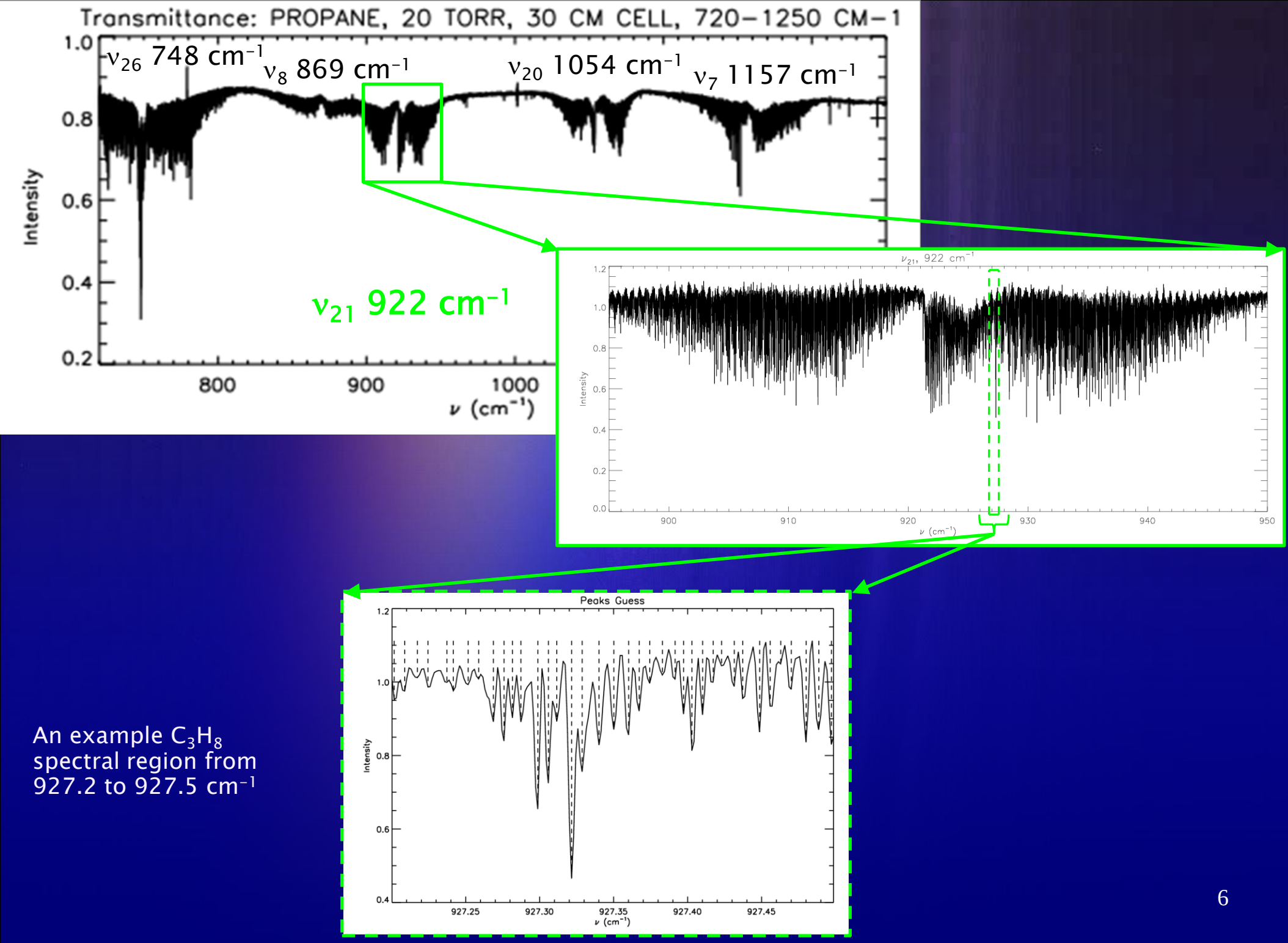
Cassini/CIRS Titan Spectrum



C_3H_6 ν_{19} ?

Data Collection

- McMath-Pierce Fourier Transform Spectrometer (FTS) at Kitt Peak National Observatory (KPNO)
- "Warm data": April 26, 1984
  "Cold data": May 15, 1989
  by D. E. Jennings *et al.*
- Resolution: 0.005 cm^{-1}
- Gas cell length: 2400 cm 30 cm
- Pressure: .558 torr 3.2 torr
- Cell temperature: 293 K 175 K

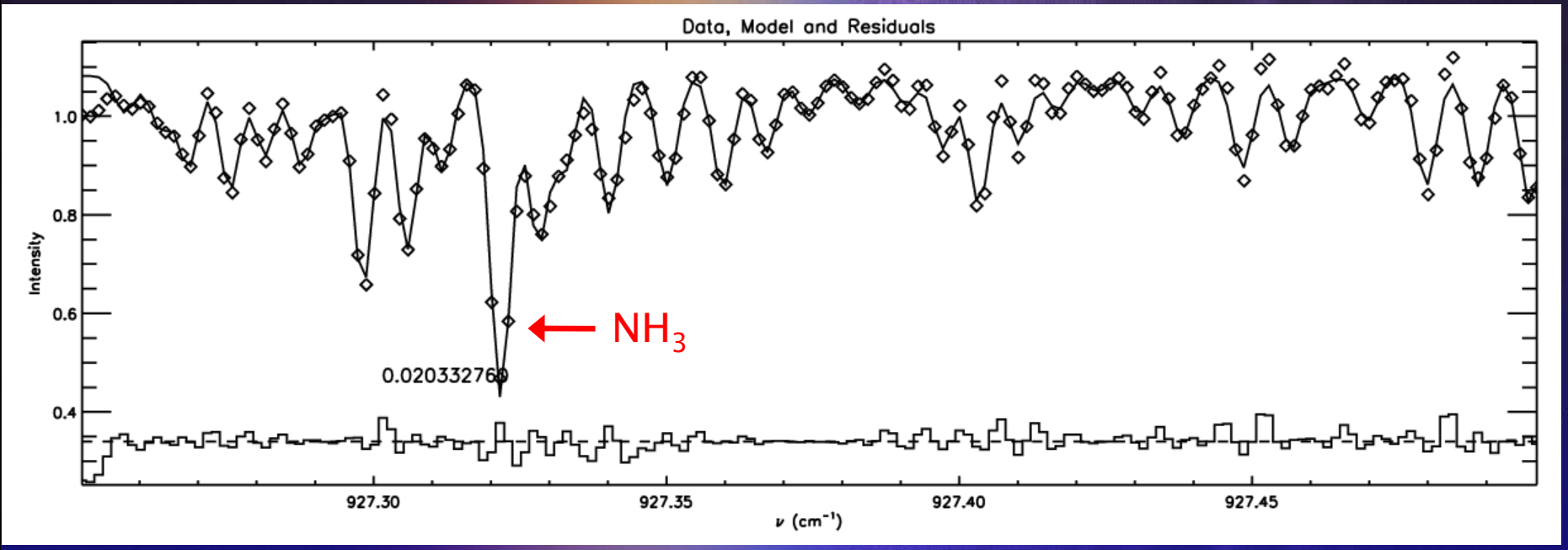


An example C_3H_8 spectral region from 927.2 to 927.5 cm^{-1}

Results

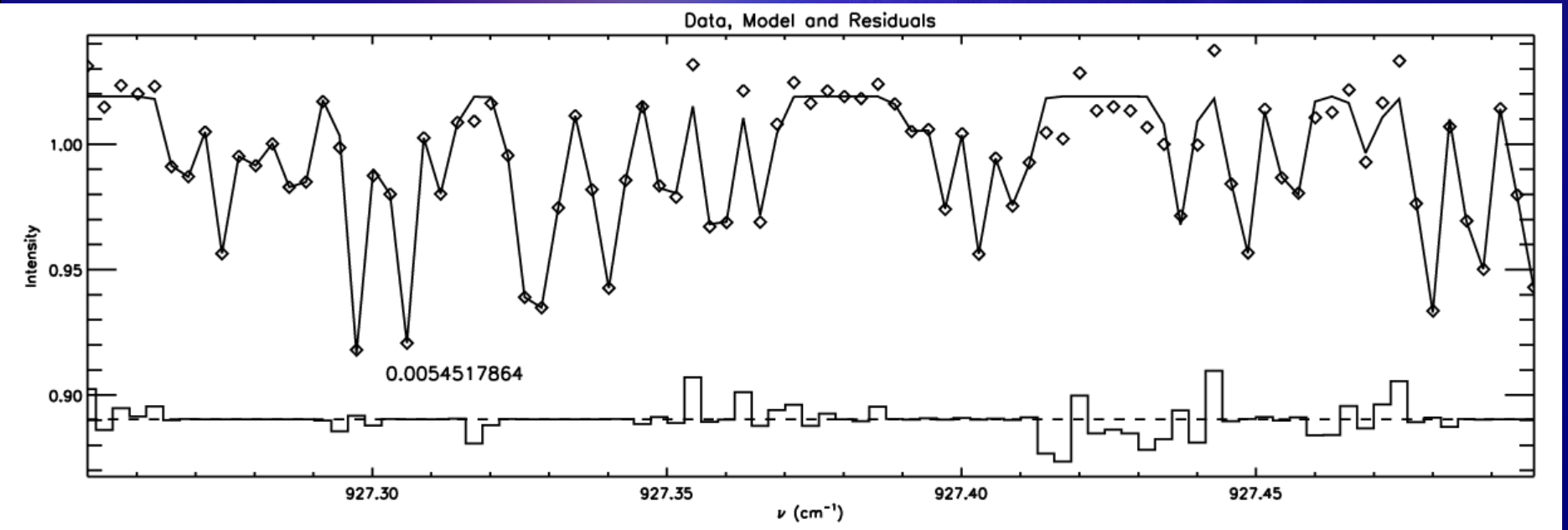
- Gas transmittance $T_\nu = e^{-\tau_\nu}$
  - Observed $F_\nu * T_\nu$ (F_ν = Instrumental line shape)
- Optical depth $\tau_\nu = p\,\Delta z\,S_{line}\,L_\nu$
  - $p, \Delta z, L_\nu, S_{line}$: pressure (atm), path length (cm), lineshape, line intensity (cm^{-2}/atm)
- Characterizing line shape
  - $L_\nu = G_\nu$ (Gaussian) results reported herein

  L_ν = Voigt, speed-dependent-Voigt in the future
- Derived quantities:
  - ν_0 = Linecenters (cm^{-1})
  - S_{line} = Line intensities (cm^{-2}/atm)
  - $\delta\nu$ = Half-widths (cm^{-1})



Warm Data

Example C_3H_8 spectral regions from 927.25 to 927.5 cm^{-1}



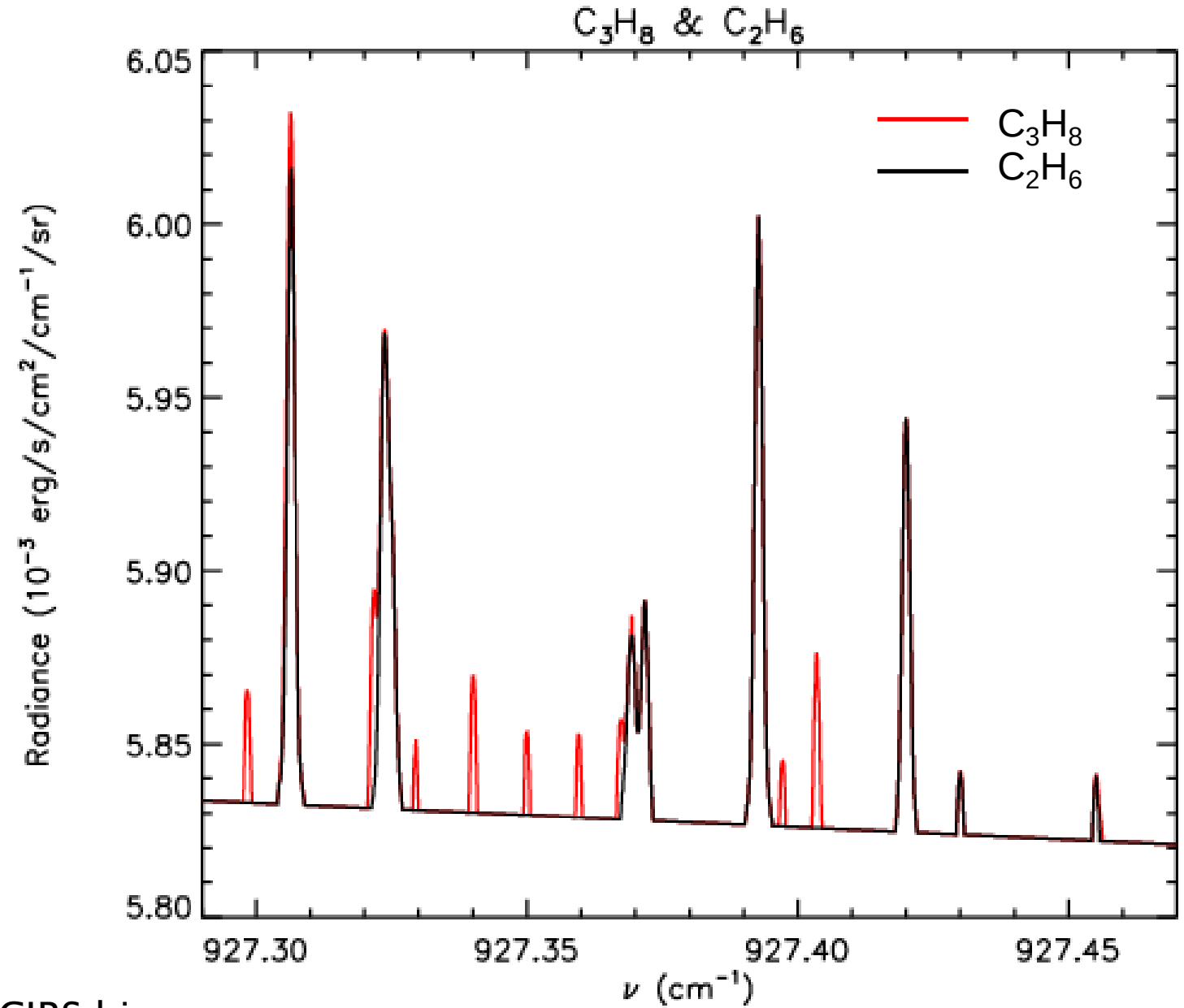
Cold Data

Estimated error
± 0.001 cm^{-1}

Linecenters (cm^{-1})	Relative Intensities	
	Warm Data	Cold Data
927.268	0.00032	0.00145
927.275	0.00044	0.00203
927.281	0.00024	0.00089
927.287	0.00031	0.00113
927.298	0.00099	0.00327
927.305	0.00078	0.00327
927.311	0.00032	0.00130
927.329	0.00088	0.00247
927.340	0.00067	0.00266
927.350	0.00051	0.00063
927.359	0.00051	0.00108
927.367	0.00034	0.00148
927.397	0.00044	0.00131
927.403	0.00073	0.00192
927.410	0.00042	0.00150
927.416	0.00023	0.00060
927.438	0.00036	0.00157
927.448	0.00052	0.00215
927.456	0.00042	0.00157
927.469	0.00028	0.00074
927.479	0.00060	0.00287
927.488	0.00061	0.00260
927.497	0.00068	0.00145

Estimated error
5–10%

Titan Model Spectrum



~1/3 CIRS bin

Next Steps

- Find calibrated intensities and lower state energies for the ν_{21}, 922 cm^{-1} band
- These bands of C_3H_8 still need to be analyzed:
  - ν_8, 869 cm^{-1}
  - ν_{20}, 1054 cm^{-1}
  - ν_7, 1157 cm^{-1}
- Subtraction of the ν_{21} band will potentially reveal underlying species (e.g. C_3H_6)
- Analyze spectra of more molecular species of interest to Titan

Acknowledgments

- I would like to thank Dr. Hewagama, for serving as my mentor, and Dr. Nixon, for serving as my advisor on this project.
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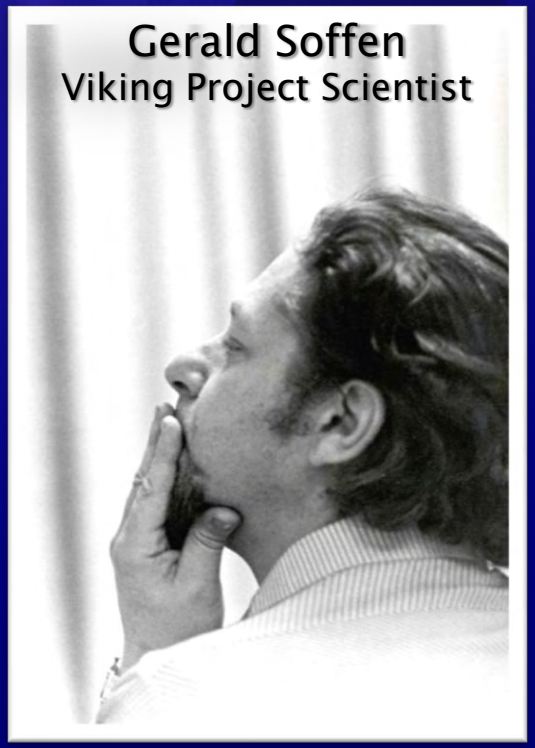
- This presentation was made possible in part by a Travel Grant from the Gerald A. Soffen Fund for the Advancement of Space Science Education (http://www.nasa-academy.org/soffen/travelgrant/)



End of Presentation

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Any Questions?

Additional Material

Levenberg-Marquardt Method

The degree of the model fit is characterized by χ^2.

$$\chi^2 = \sum_{i=1}^{N_D} \frac{(D_i - M_i)^2}{\sigma_i^2}$$

where D_i, M_i, σ_i, are the data, model, and error values, respectively, for the i^{th} element. The spectral model for the lines is a function of the set of parameters $\{P_j\}$: $G_k(\nu_i) = G_k(\{P_j\}, \nu_i)$ In the LMM, the parameter values are iteratively changed to search for a minimum in χ^2. In our case, the model consists of a complement of Gaussian functions that represent the spectral lines.

The bandshape is represented by the contribution of this set of lines and is given by

$$M_i = O_S - \sum_{k=1}^{N_L} |I_{0k}| e^{\frac{-(\nu - \nu_{0k})^2}{\delta\nu^2}}$$

The vector of parameters $(O_S, \delta\nu, \{\nu_{0i}\}, \{I_{0i}\})$ has $2N_L+2$ elements, where $2N_L$ refers to the parameters $\{\nu_{0i}\}$, $\{I_{0i}\}$ characterizing each of N_L spectral lines and the +2 refers to the offset correction term (O_S) and half-width $(\delta\nu)$ which is common to all lines.