C_3H_8 Pseudo-Linelist 2560-3280 cm^{-1}

Based on lab measurements of Harrison & Bernath

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Infrared absorption cross sections for propane (C_3H_8) in the 3 μm region

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ABSTRACT

Infrared absorption cross sections for propane have been measured in the 3 μm spectral region from spectra recorded using a high-resolution FTIR spectrometer (Bruker IFS 125 HR). The spectra of mixtures of propane with dry synthetic air were recorded at 0.015 cm^{-1} resolution (calculated as 0.9/MOPD using the Bruker definition of resolution), at a number of temperatures and pressures appropriate for atmospheric conditions. Intensities were calibrated using two propane spectra (recorded at 278 and 293 K) taken from the Pacific Northwest National Laboratory (PNNL) IR database.

C_3H_8 Pseudo-Linelist (PLL)

Covers 2765 – 3080 cm^{-1} at 0.005 cm^{-1} spacing (63001 lines) based on Harrison's lab measurements.

[This is different from the pseudo-linelist covering 690-1550 cm^{-1} described by Sung et al. [2013], which was based on Sung's own lab measurements.]

Assumes:

- ABHW = 0.07
- SBHW = 0.14

Line intensities and E" are retrieved.

Assumed partition function following Sung et al. [2013]

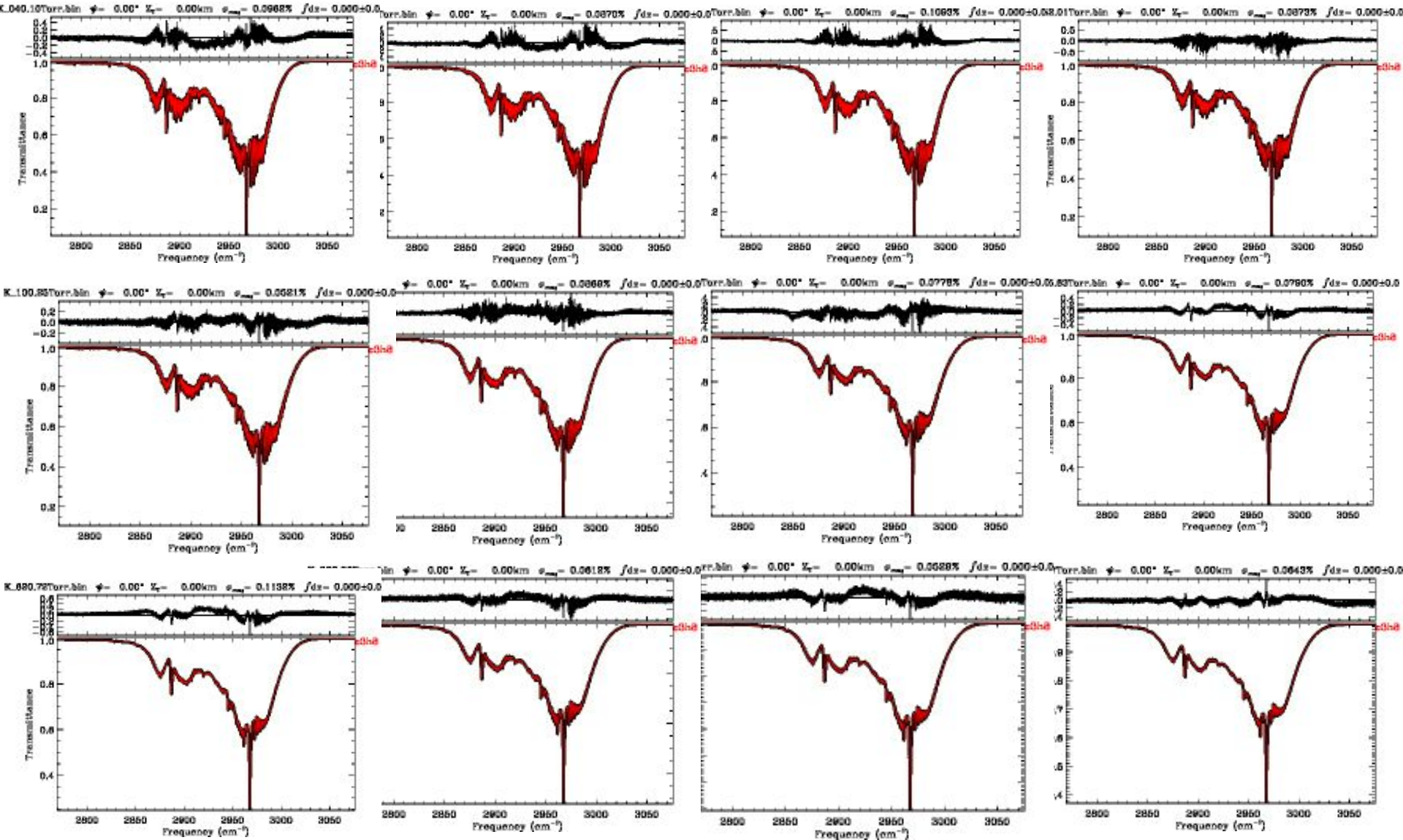
- Vibrational: Used 25/27 vibrational modes (dropping the torsional modes at 216 & 268 cm^{-1})
- Rotational: $(296/T)^2$

Retrieved VMR Scale Factors (VSF)

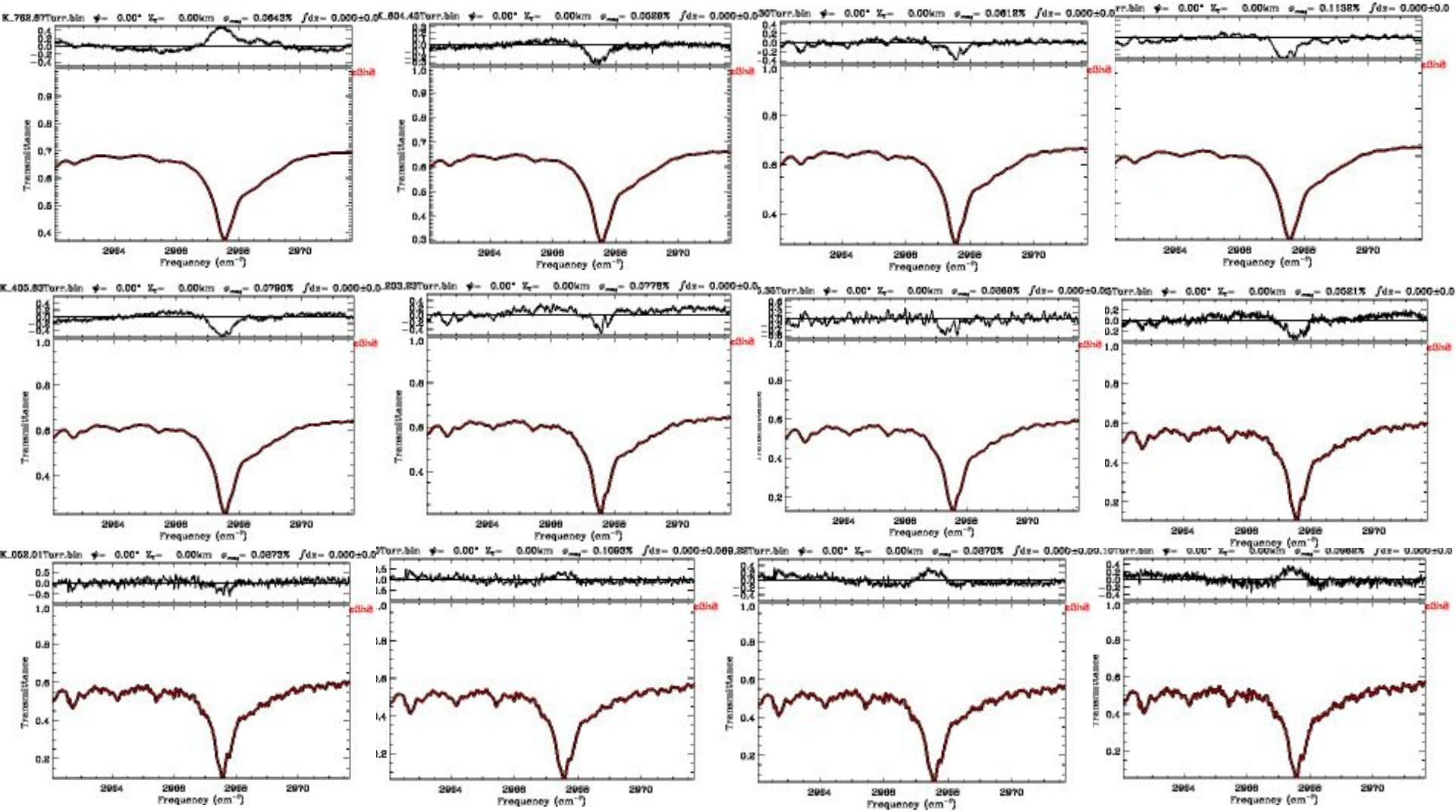
Spectrum	RMS %	VSF	VSF_error
C3H8_195K_040.10Torr.bin	0.0962	1.0263	2.9E-03
C3H8_195K_069.22Torr.bin	0.0870	1.0260	2.6E-03
C3H8_195K_098.30Torr.bin	0.1093	1.0267	3.3E-03
C3H8_215K_052.01Torr.bin	0.0873	0.9776	2.6E-03
C3H8_215K_100.25Torr.bin	0.0521	0.9782	1.6E-03
C3H8_215K_275.35Torr.bin	0.0869	0.9789	2.6E-03
C3H8_252K_203.23Torr.bin	0.0778	0.9632	2.3E-03
C3H8_252K_405.63Torr.bin	0.0790	0.9668	2.4E-03
C3H8_250K_620.72Torr.bin	0.1132	0.9644	3.4E-03
C3H8_269K_369.30Torr.bin	0.0612	0.9837	1.8E-03
C3H8_269K_604.45Torr.bin	0.0529	0.9828	1.6E-03
C3H8_296K_762.67Torr.bin	0.0643	1.0373	1.9E-03

C_3H_8 scale factors are all consistent within 4% (and 2% rms)
Spectral fits are typically better than 0.1% rms.

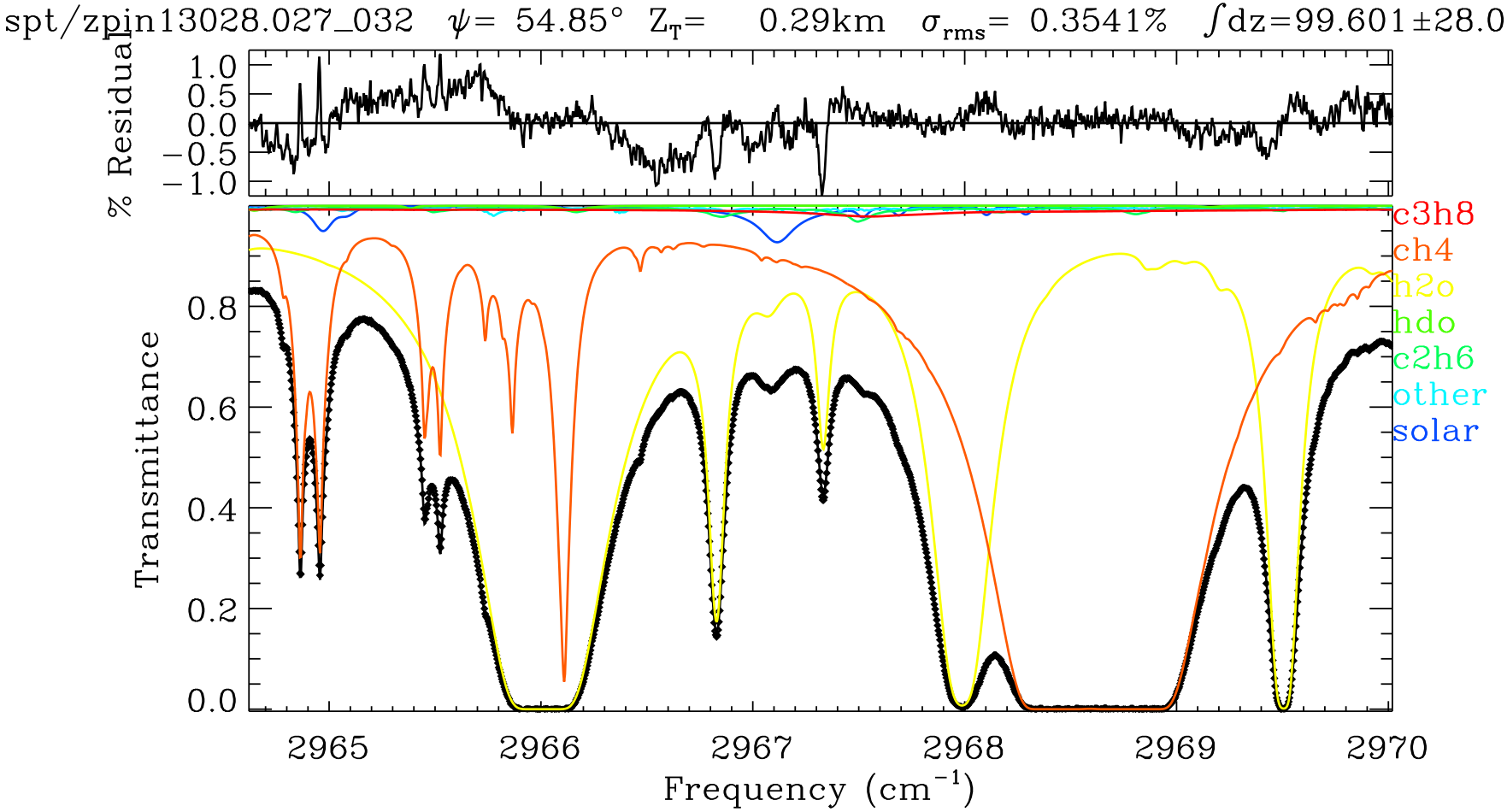
Fits to Lab spectra: Full Band



Fits to lab spectra: Q-branch

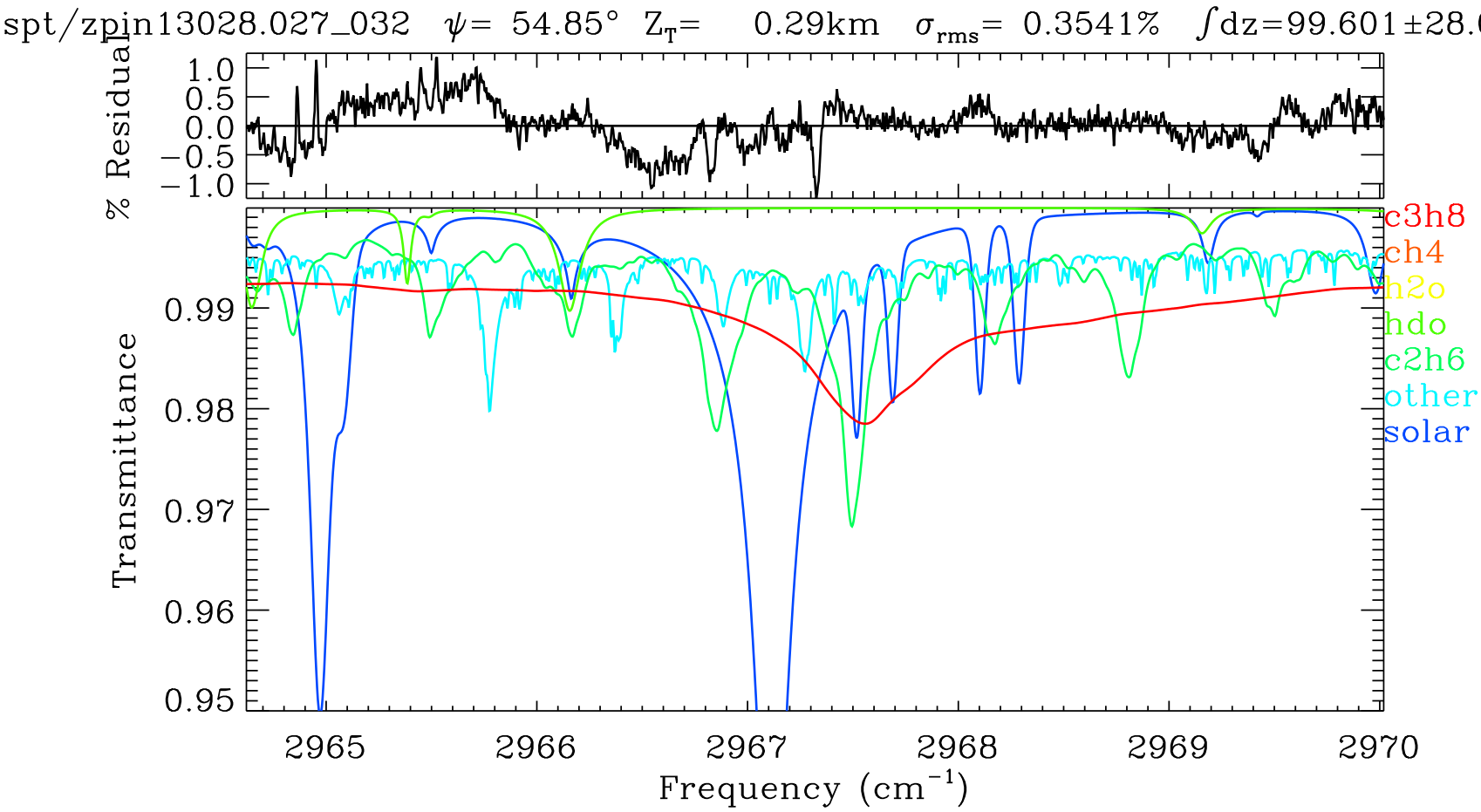


Fits to MkIV ground-based



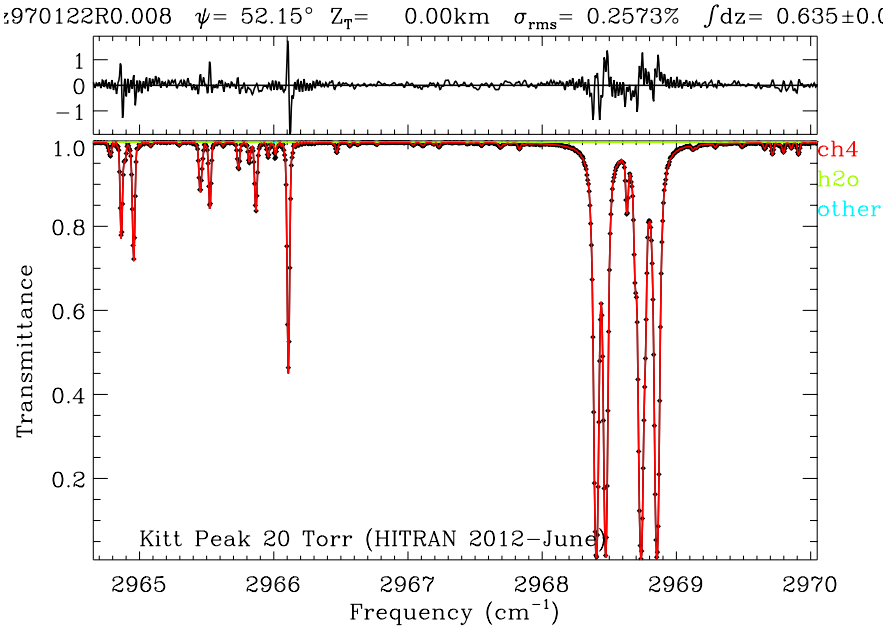
C_3H_8 Q-branch lies in wings of strong CH_4 lines at 2968-2969 cm^{-1} and so the retrieved C3H8 is very sensitive to assumptions about CH_4 widths, pressure shifts, and line mixing.

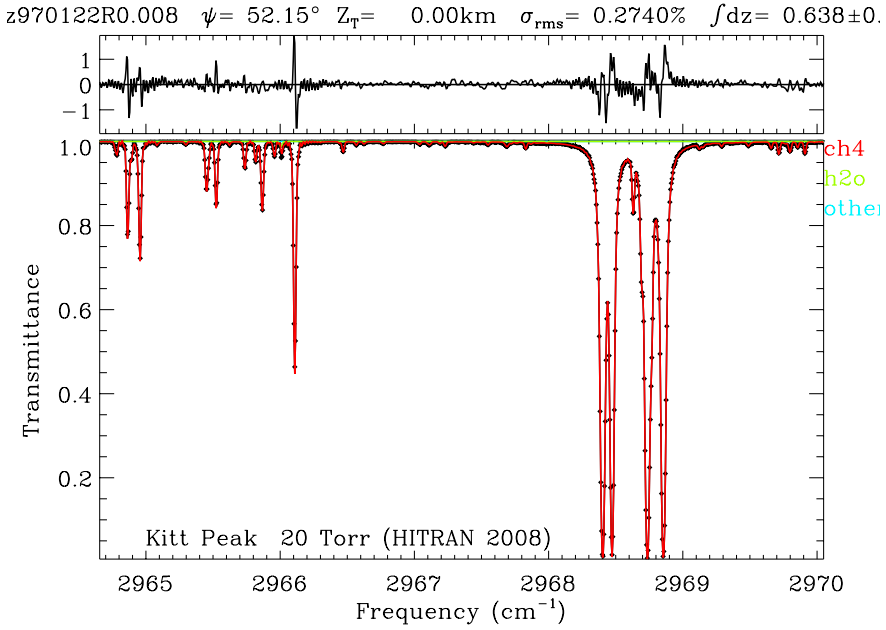
Fits to MkIV ground-based (zoom)

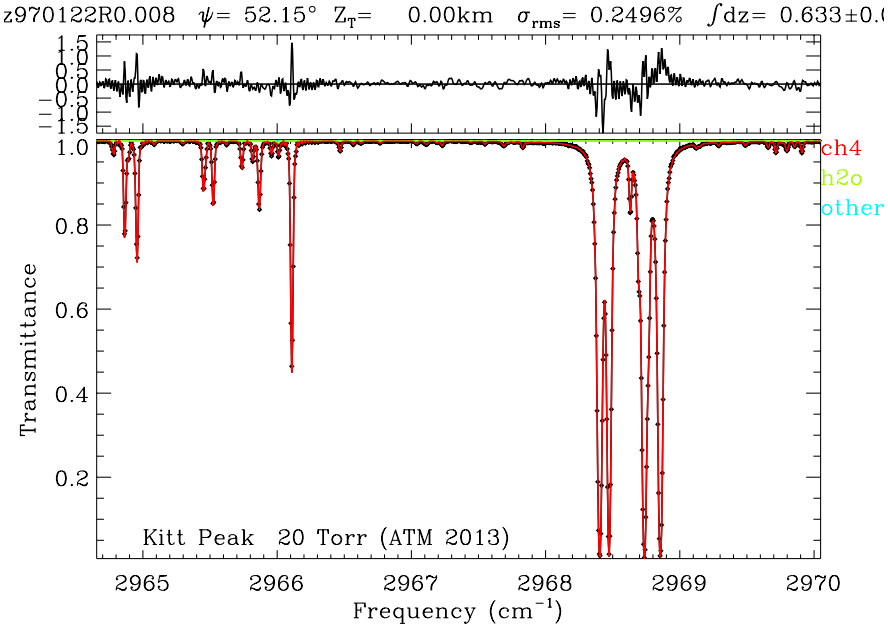


Same as previous figure, but y-zoomed to see the C_3H_8 absorption contribution

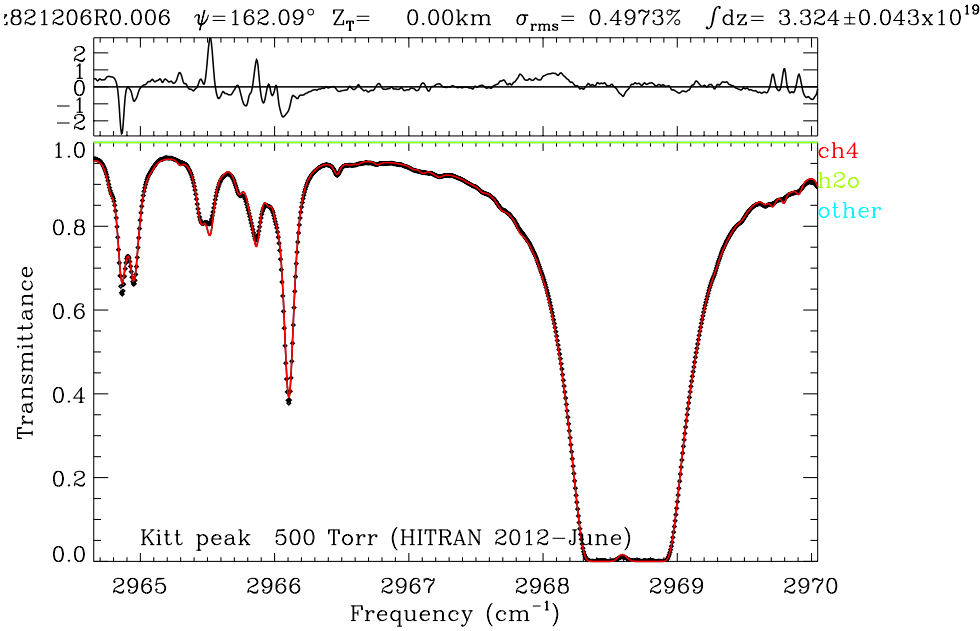
Kitt Peak
20 Torr CH_4

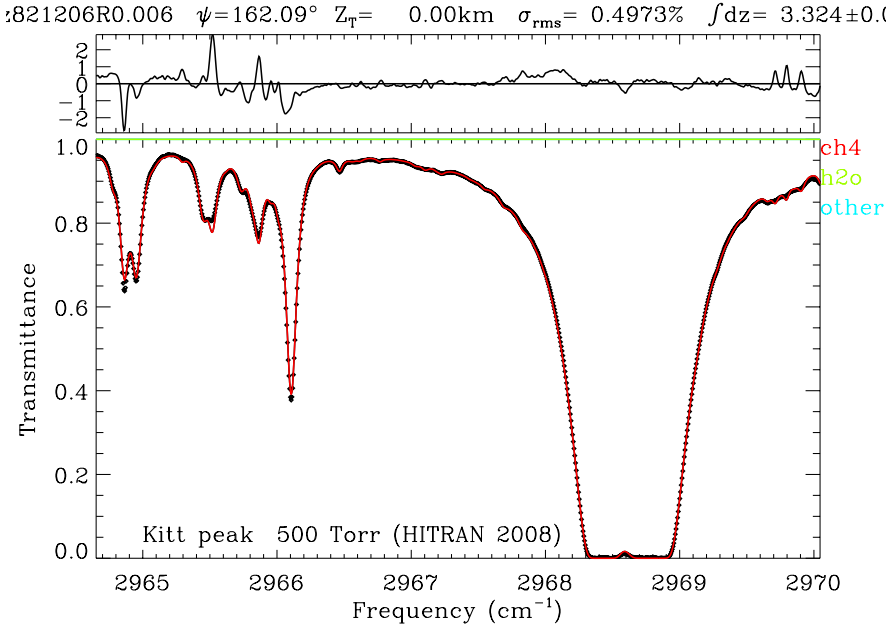


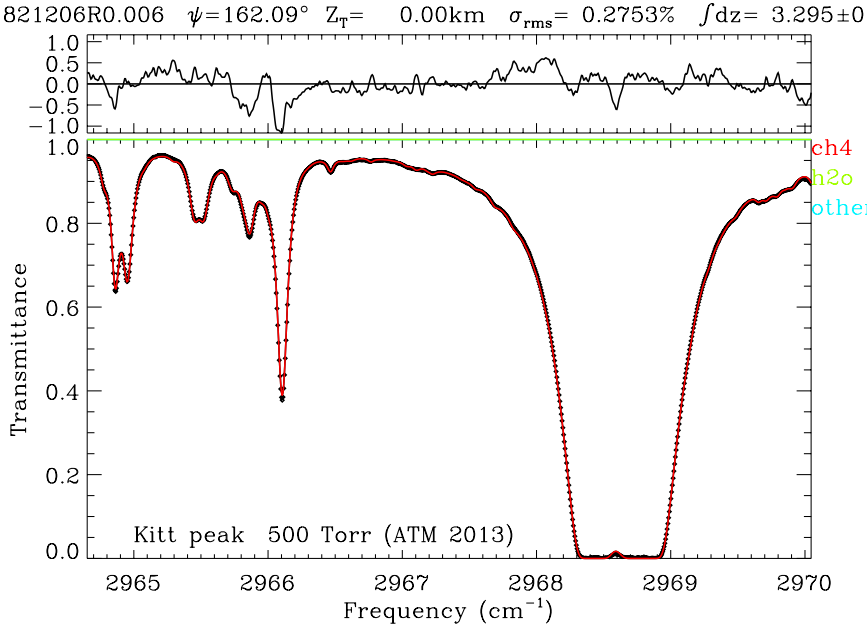




Kitt Peak CH4 500 Torr







Sung et al. [2013]

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FT-IR measurements of cold C_3H_8 cross sections at 7–15 μm for Titan atmosphere

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ABSTRACT

We present absorption cross sections of propane (C_3H_8) at temperatures from 145 K to 297 K in the 690–1550 cm^{-1} region. Pure and N_2-broadened spectra were measured at pressures from 3 Torr to 742 Torr using a Bruker IFS125 FT-IR spectrometer at JPL. The gas absorption cell, developed at Connecticut College, was cooled by a closed-cycle helium refrigerator. The cross sections were measured and compiled for individual spectra recorded at various experimental conditions covering the planetary atmosphere and Titan. In addition to the cross sections, a propane pseudoline list with a frequency grid of 0.005 cm^{-1}, was fitted to the 34 laboratory spectra. Line intensities and lower state energies were retrieved for each line, assuming a constant width. Validation tests showed that the pseudoline list reproduces discrete absorption features and continuum, the latter contributed by numerous weak and hot band features, in most of the observed spectra within 3%. Based on the pseudoline list, the total intensity in the 690–1550 cm^{-1} region was determined to be 52.93 (±3%) × 10^{-19} cm^{-1}/(molecule cm^{-2}) at 296 K; this value is within 3% of the average from four earlier studies. Finally, the merit of the pseudoline approach is addressed for heavy polyatomic molecules in support of spectroscopic observation of atmospheres of Titan and other planets. The cold cross sections will be submitted to the HITRAN database (hitran.harvard.edu), and the list of C_3H_8 pseudolines will be available from a MK-IV website of JPL (http://mark4sun.jpl.nasa.gov/data/spec/Pseudo).