CH_3COOH (Acetic Acid) Empirical Pseudo-Line-List

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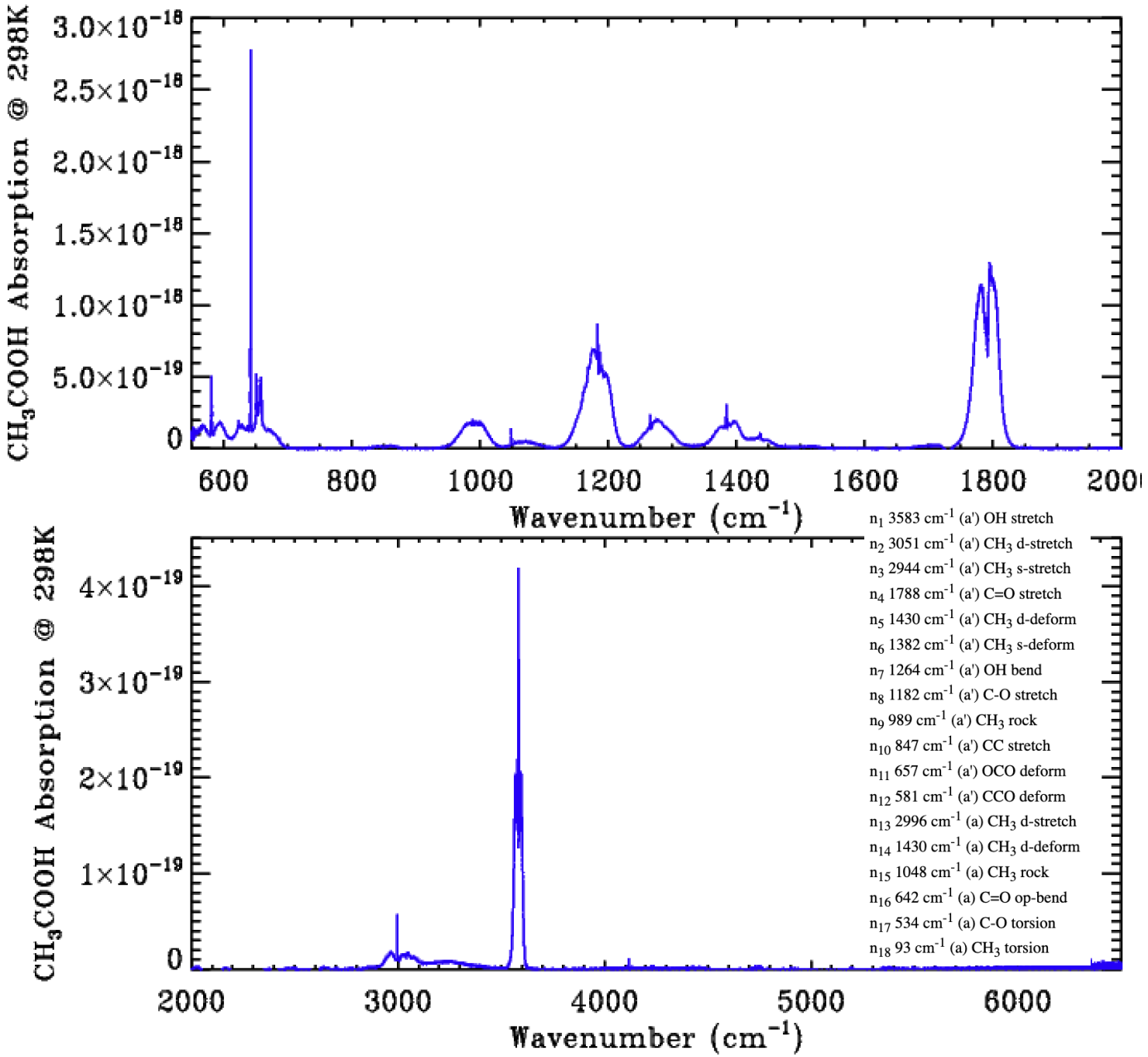
In 2011 a CH_3COOH EPLL was created based solely on two PNNL spectra at 298 & 323K (278K spectra do not exist). This EPLL had a uniform grid spacing of 0.01 cm^{-1}. The entry to $GGGPATH/history/ll.history states:

gct_20110509.101
Added an EPLL of CH3COOH (Acetic Acid) containing 118868 lines covering all important absorption bands in the 551-3623 cm-1 range. Based on PNNL spectra at 298 and 343K.

In 2021 it was realized that 27 Kitt Peak lab spectra, nominally of H_2O, were contaminated with CH_3COOH (and HCOOH). These KP spectra were much higher spectral resolution than the PNNL spectra, but the CH_3COOH amounts were unknown.

In 2022 a new CH_3COOH empirical pseudo-linelist was developed with line positions and relative intensities based on the Kitt Peak lab spectra (all 296K) and total intensities and E" based on PNNL lab spectra at 298K and 323K.

CH_3COOH cross-sections at 298K



The strongest and most distinctive feature is the ν_{16} Q-branch at 642 cm^{-1}. Unfortunately, this is buried beneath CO_2 absorption in spectra of the Earth's atmosphere. It is also below the cut-on limit of many HgCdTe detectors.

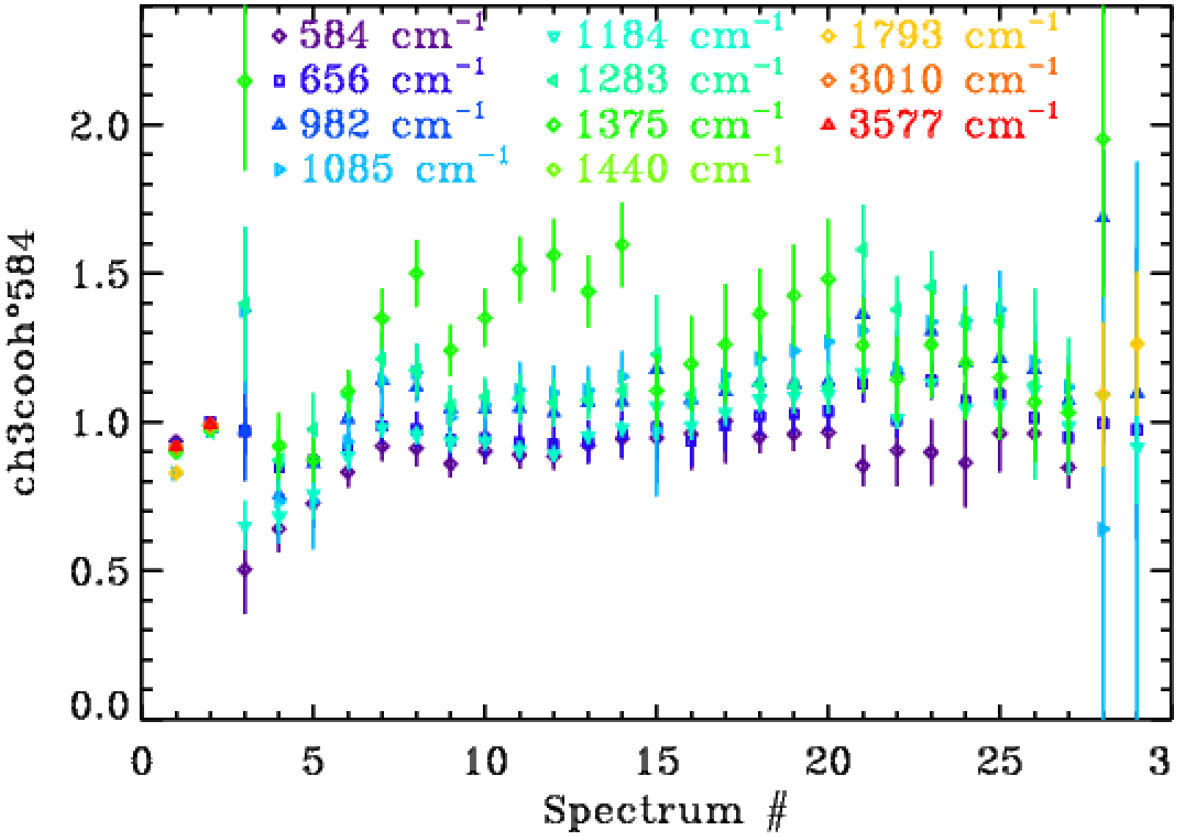
The second strongest band, the ν_4 centered at 1788 cm^{-1}, is buried beneath H_2O in ground-based spectra of the Earth's atmosphere.

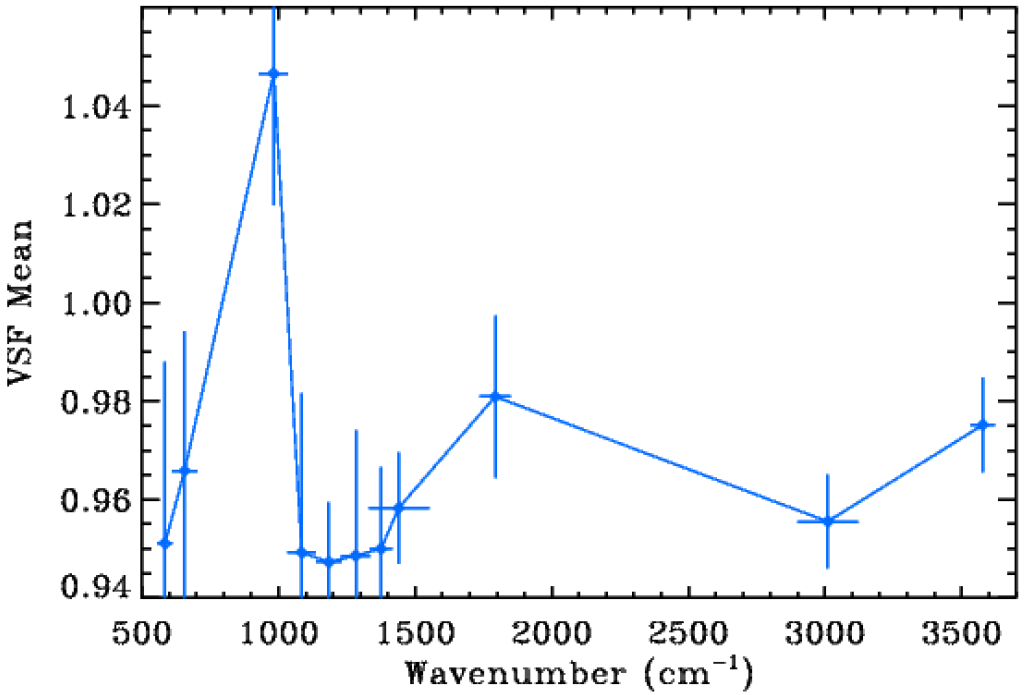
The third strongest band, the ν_8 centered at 1182 cm^{-1}, seems the best choice for ground-based observations of the Earth's atmosphere.

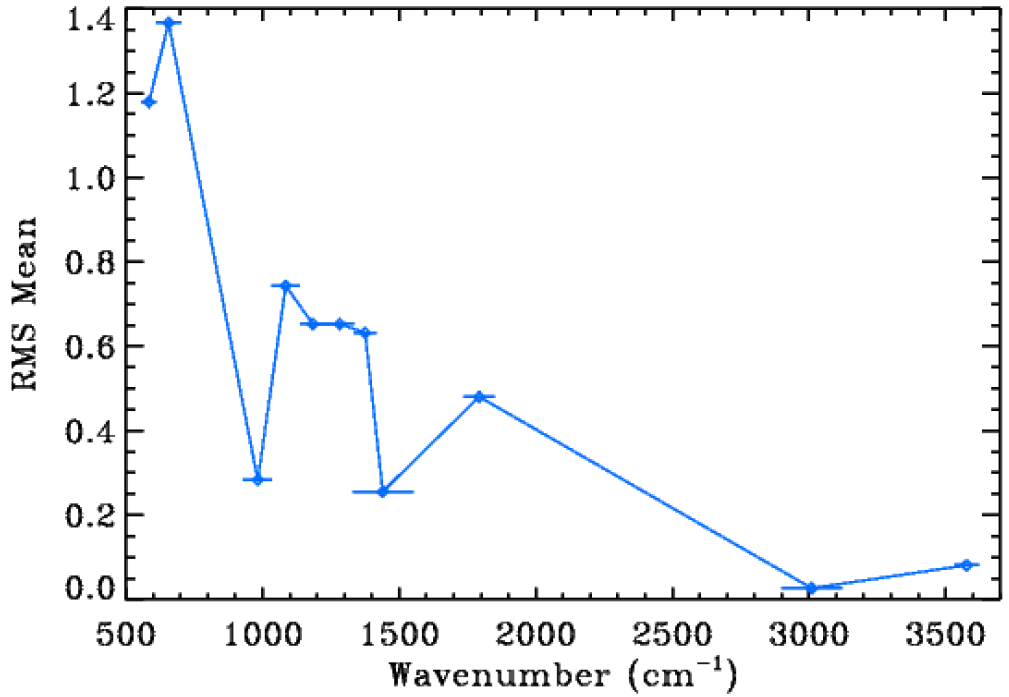
The fourth strongest band, the ν_1 centered at 3583 cm^{-1}, is blacked out by CO_2 and H_2O in Earth ground-based atmospheric spectra.

CH_3COOH VSFs retrieved from lab spectra

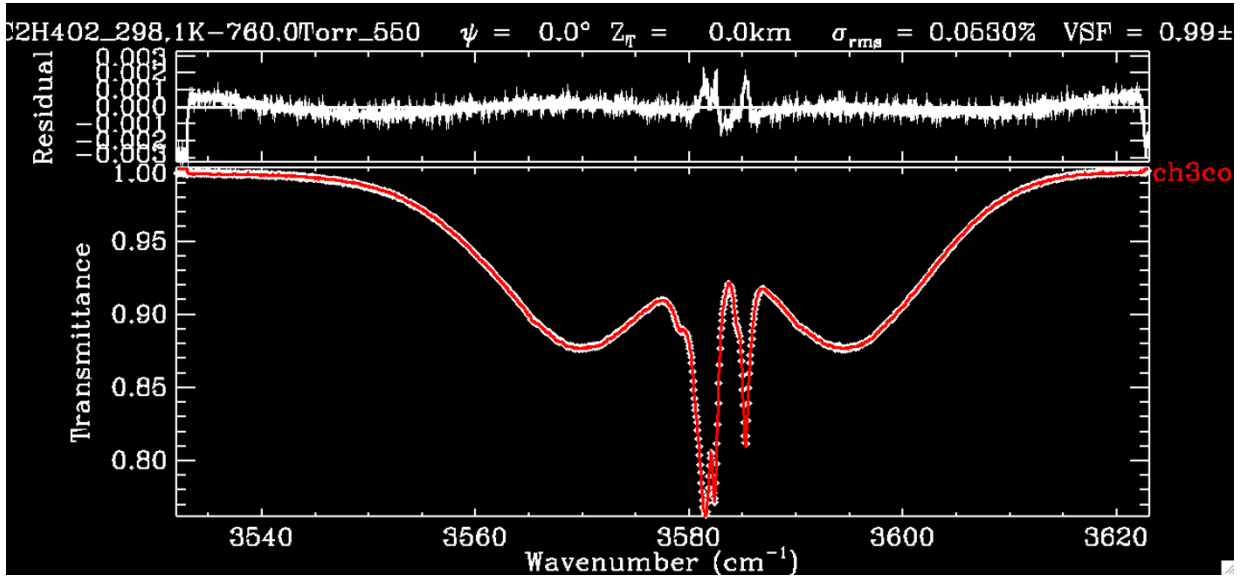
Spectra # 1 and 2 are the PNNL spectra.
Spectra #3 and #28 have low CH_3COOH amounts and therefore have large window-to-window variations in the Kitt Peak spectra due to the interfering absorbers and the continuum level variations.

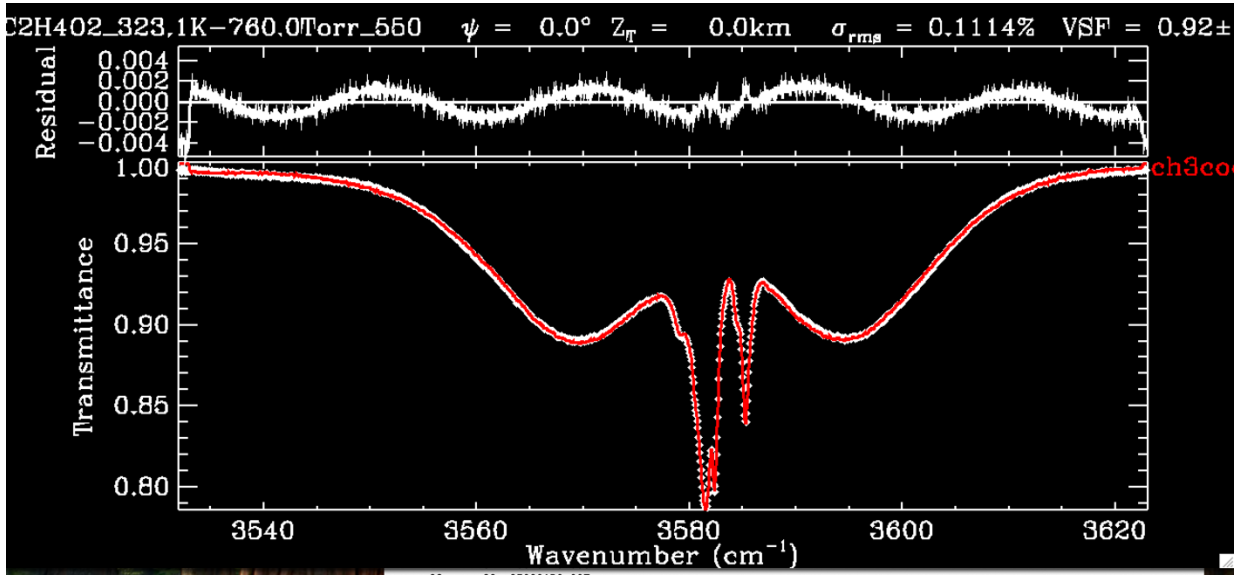


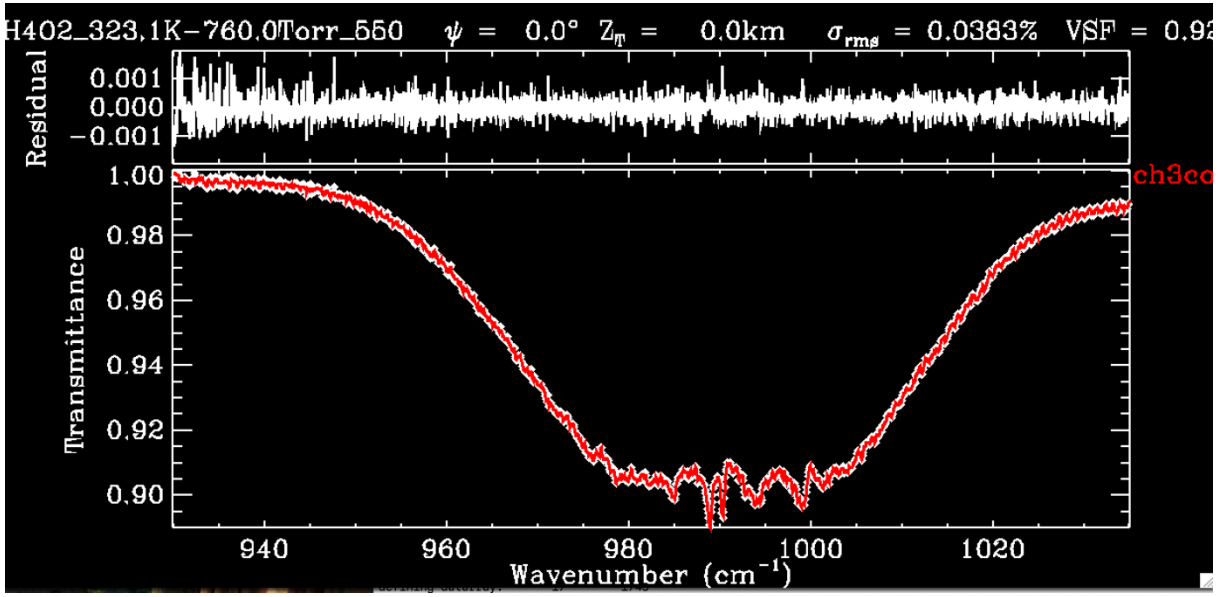


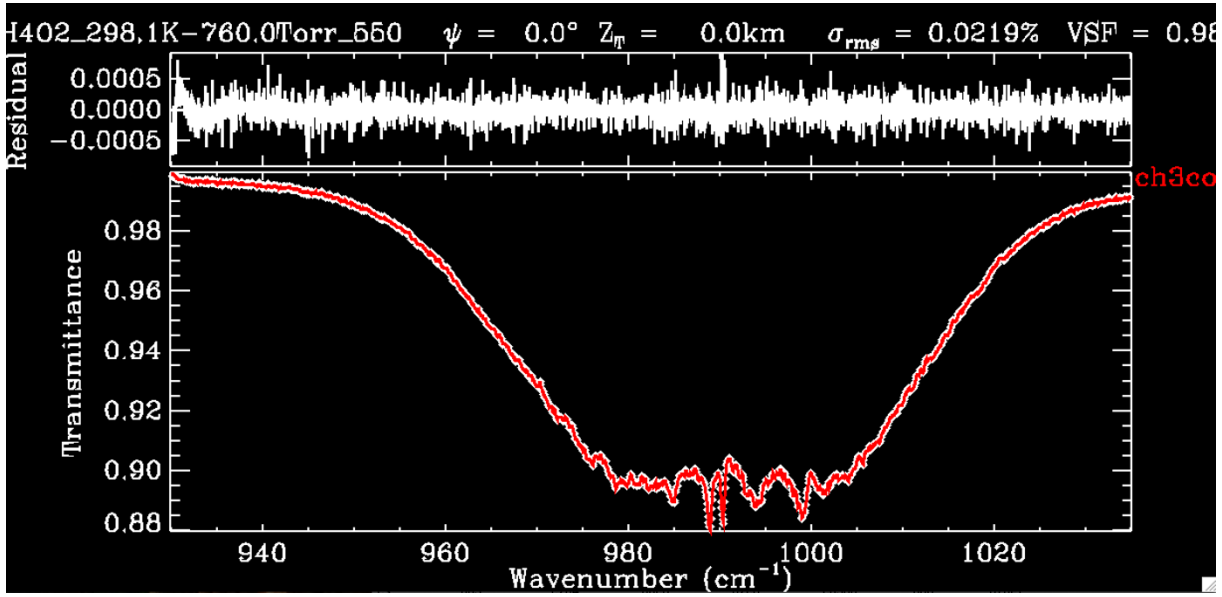


Examples of fits to PNNL spectra

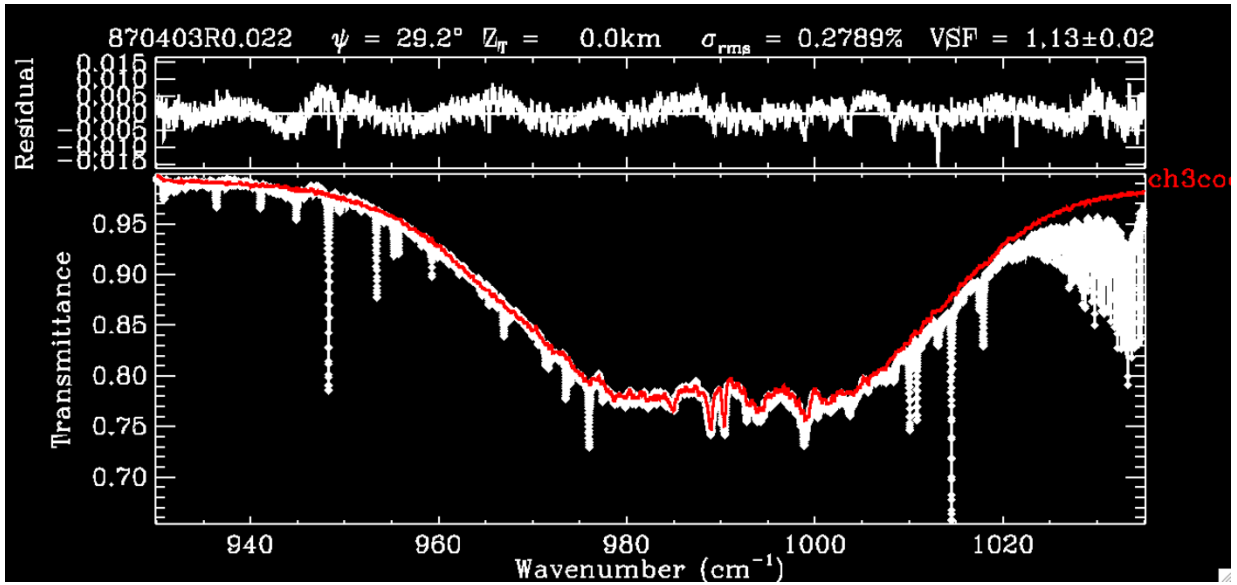


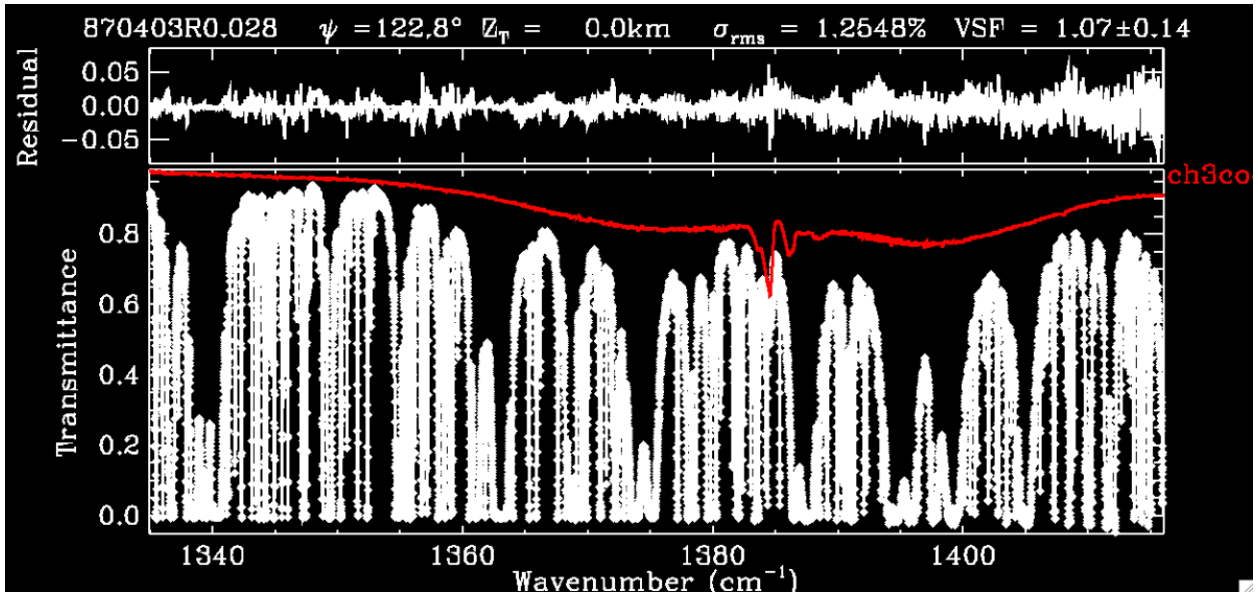


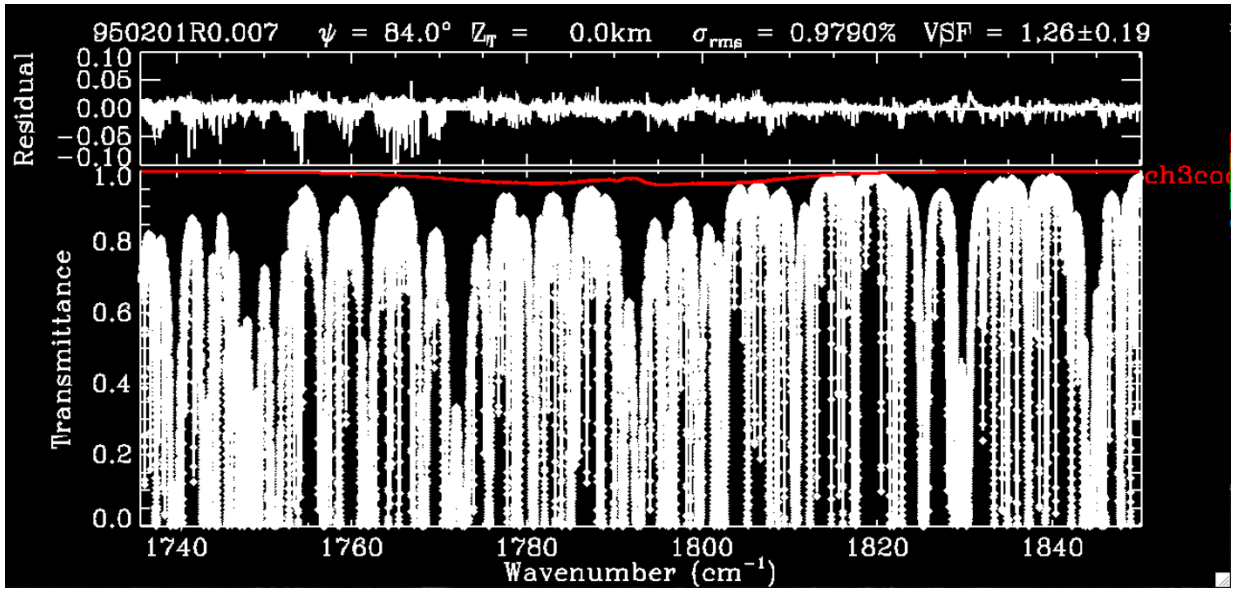




Examples of fits to Kitt Peak Lab spectra







Examples of fits to Kitt Peak Lab spectra in 1180 cm^{-1} window