H_2O spectroscopy evaluation 3220-3377 cm^{-1}

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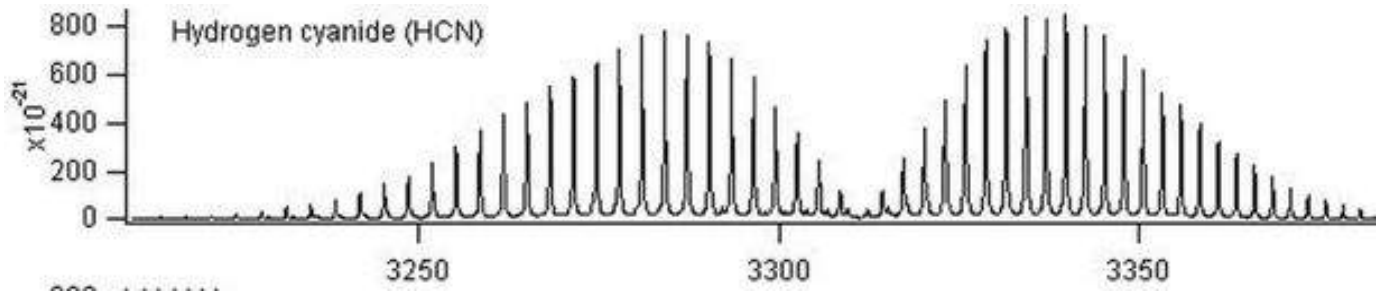
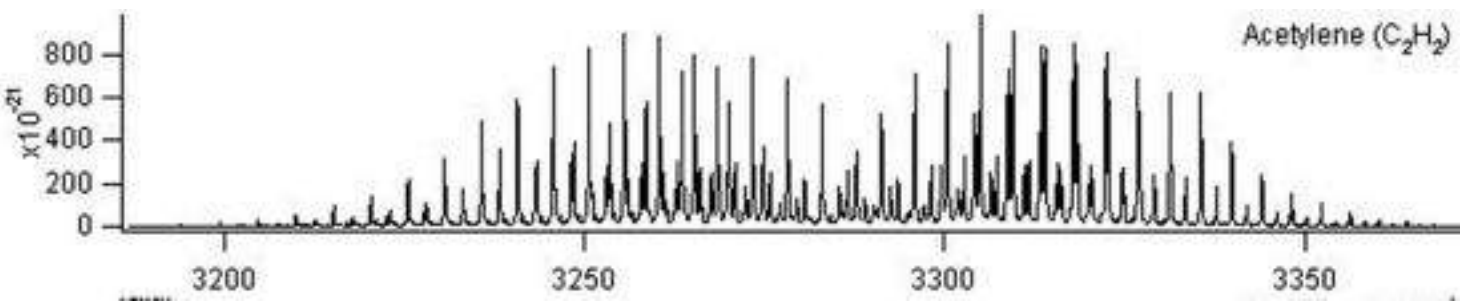
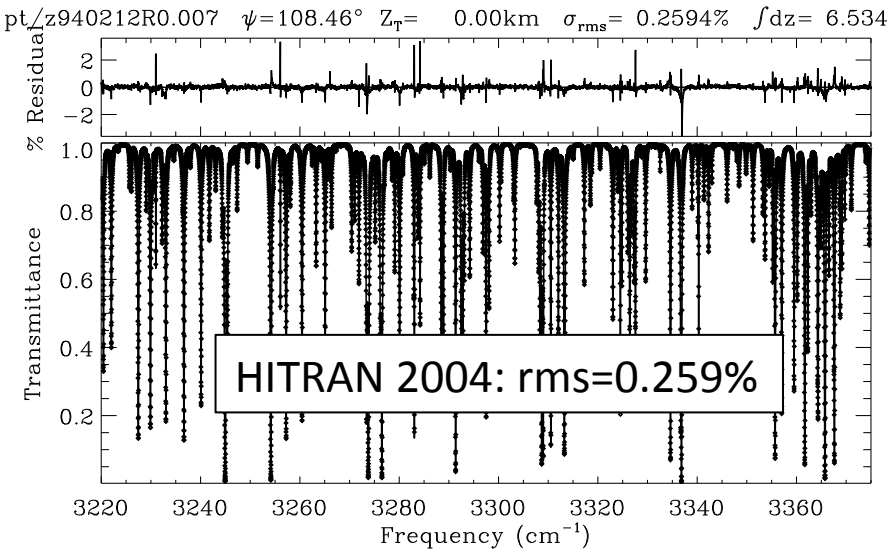
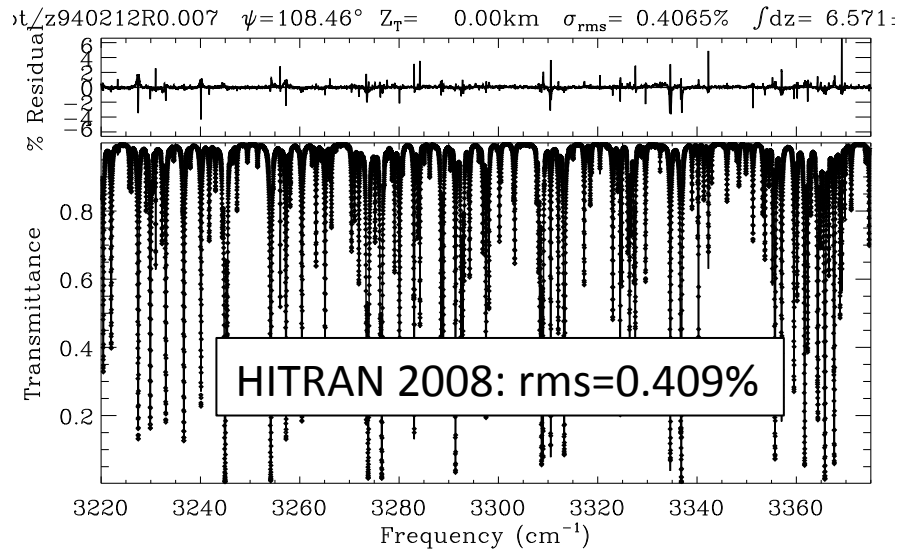
This region covers the 3 micron bands of C_2H_2, HCN, and CO_2 which are used for remote sensing of these atmospheric trace gases. In ground-based spectra, spectral interference comes primarily from H_2O. HCN and C_2H_2 absorption spectra (below) from PNNL.

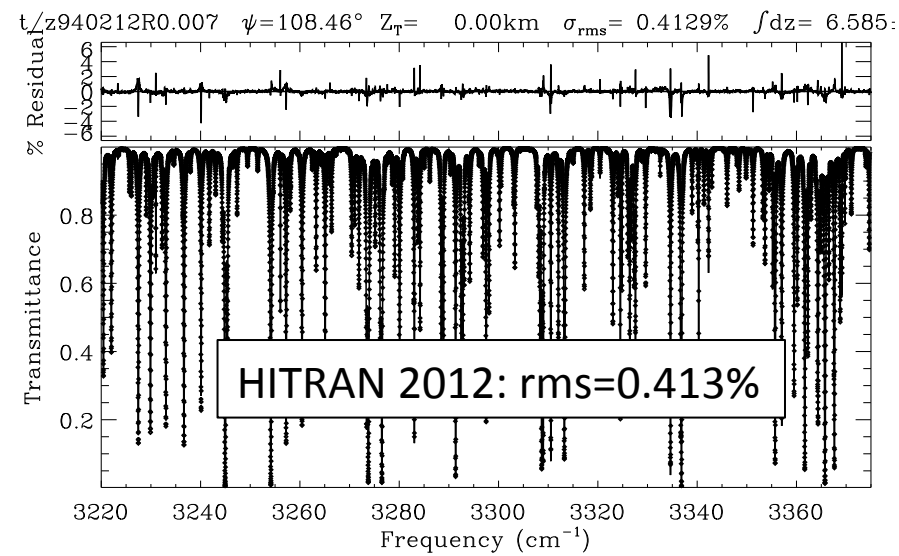


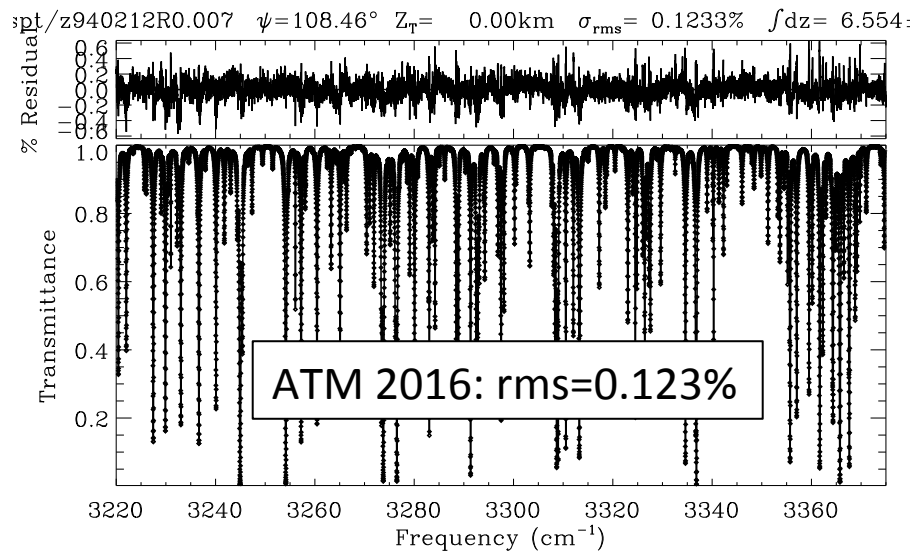


Fits to KP lab spectrum









144m path at 19.6C, 1.55 Torr of H_2O air-broadened to 557 Torr

Summary/Conclusions

The HITRAN 2004 H_2O linelist in this region was based on:
Toth R.A., Linelists of water vapor parameters from 500 to 8000 cm^{-1},
see http://mark4sun.jpl.nasa.gov/data/spec/H2O/Readme_H2O.pdf

After reading the HITRAN 2008 paper (excerpted below) I'm still not sure what caused the worsening of the spectral fits.

The HITRAN 2012 produces similar spectral fits to HITRAN 2008.

The ATM 2016 linelist is based on Toth's 2003 measurements, but with empirical tweaks (especially to widths and pressure shifts) to improve agreement with various Kitt Peak laboratory spectra and MkIV atmospheric solar spectra.

The 2004 edition of *HITRAN* [1] featured a major update in line positions and line intensities for all *HITRAN* water-vapor isotopologues between 500 and 8000 cm^{-1} based on the work of Toth [13], with the exception of the principal isotopologue which had calculated values from Coudert [14] up to 800 cm^{-1}. However, recently reported measurements of transitions in the ν_2 band in the 1000–2000 cm^{-1} range [15] suggest that Toth's data systematically underestimated the intensities of the strongest transitions in this region by between 5% and 10%. This conclusion is supported by independent *ab initio* calculations [16]. The intensities of the unblended strong lines have therefore been replaced using the new measurements; for four blended strong lines, those located at 1512.30732, 1539.05857, 1539.06079, and 1684.83515 cm^{-1}, the theoretical results are from variational calculations using an *ab initio* dipole surface [17]. There have been other recent measurements at shorter infrared wavelengths [15,18,19] as well as a comprehensive *ab initio* analysis of the line intensities [20]. The issue of whether or not adjustments are also needed for the line intensities at these wavelengths is currently being studied with a view to coming up with recommendations for a future edition of the database.