Far−IR Spectroscopy Needs: Instrument Focus

Workshop on Spectroscopy Needs for
Atmospheric Sensing
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Outline

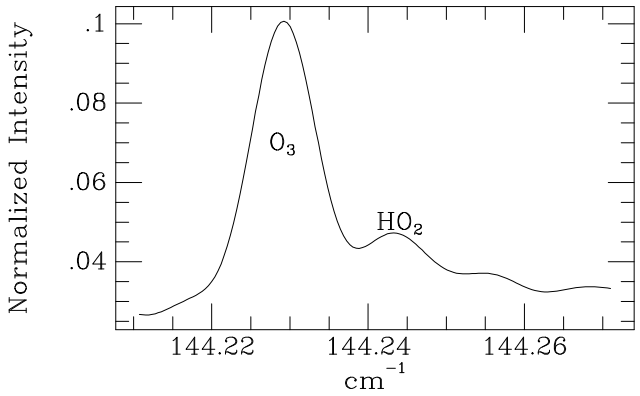
- Introduction
  - Types of measurements
- Instrument descriptions
  - Target species or measurement goals
- Spectroscopy needs
  - Problems with absolute radiance
  - Problems with target species
  - Problems with interfering lines

Introduction

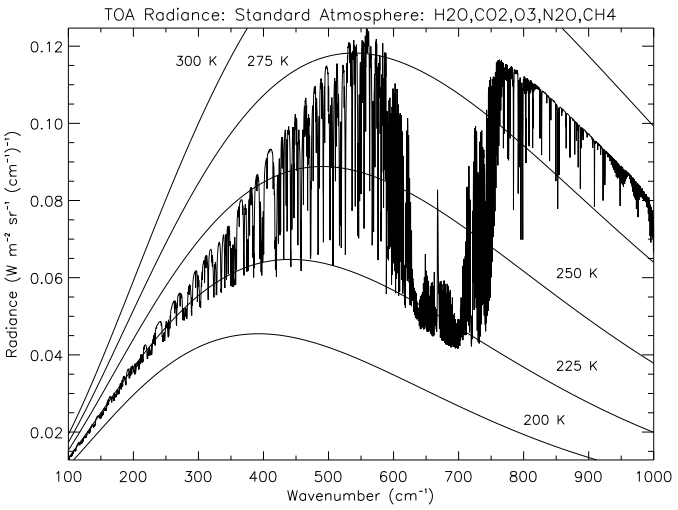
- Scope: Earth atmospheric sounders, viewing in the zenith, limb, or nadir direction.
  - We define the far−infrared as frequencies from 50−650 cm^{-1} (1.5−195 THz, or wavelengths from 200−15 μm).
  - Measurements in this region are often made with passive sensors using liquid helium cooled (4.2 K) photoconductors (although we include 2 heterodyne instruments), and observe the atmosphere in thermal emission rather than solar absorption.

Measurement Types

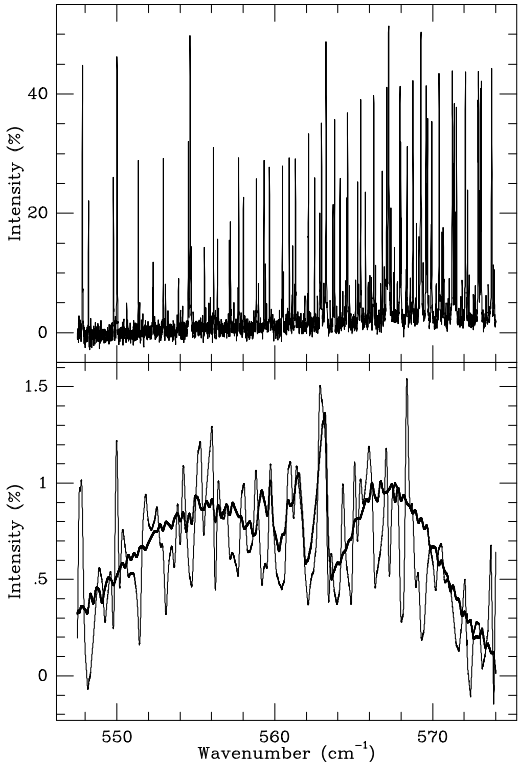
Single lines
(differential)



Radiometric
measurement
(total emission)



"Cross Sections"
(baseline counts!)



Single Lines

- Generally avoid saturated lines so that measurement is relatively insensitive to line broadening.
- Interference from weak lines of other species and wings of neighboring strong lines is a problem.
- Baseline (including continuum and far wings) can be fit and subtracted in narrow windows.

Cross Sections

- Feature is usually weak but very broad (30−100 cm^{-1} in width).
- Often have many overlying lines and bands, so that the relative line strengths and Q branch shapes (line mixing!) of all molecules in the window must be well known.
- It can be very difficult to separate baseline from the feature of interest.

Radiometric Measurements

- Concerned with very accurate measurements of total outgoing radiation.
- Spectral resolution is modest (0.1−0.6 cm^{-1}) but spectral coverage is broad (100−1000 cm^{-1}).
- May also do retrievals of temperature, pressure, and strong emitters like water and ozone.
- Calculations require strengths, positions, and broadening for H_2O, CO_2, and others, and a good continuum model.

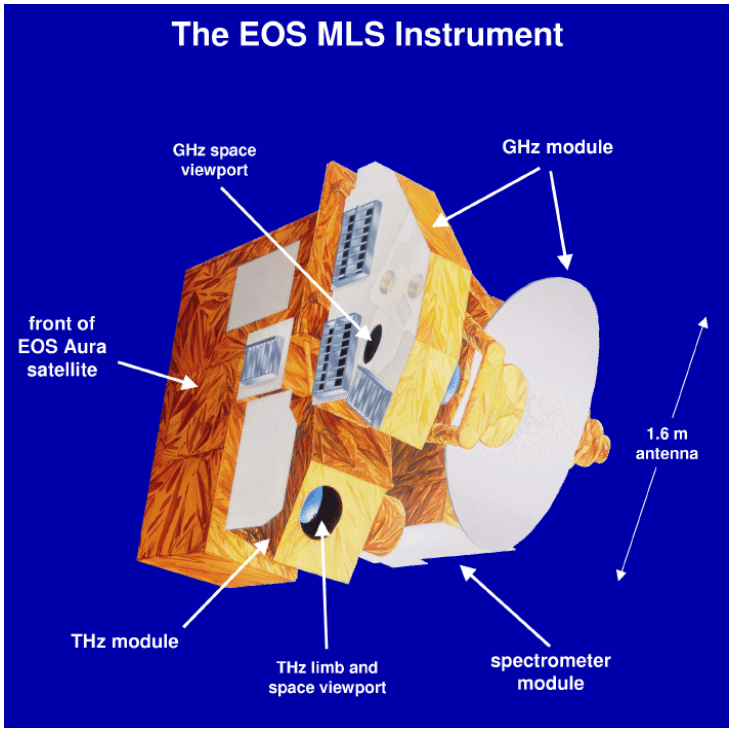
Instruments

- All instruments considered here produce spectrally resolved measurements (no broad−band radiometers.
- They fall into one of the following categories:
  - Heterodyne (narrow band, high spectral resolution).
  - Gratings (broad band with multiple orders or gratings, moderate resolution).
  - Fourier Transform spectrometers (FTS: broad band, moderate to high resolution.

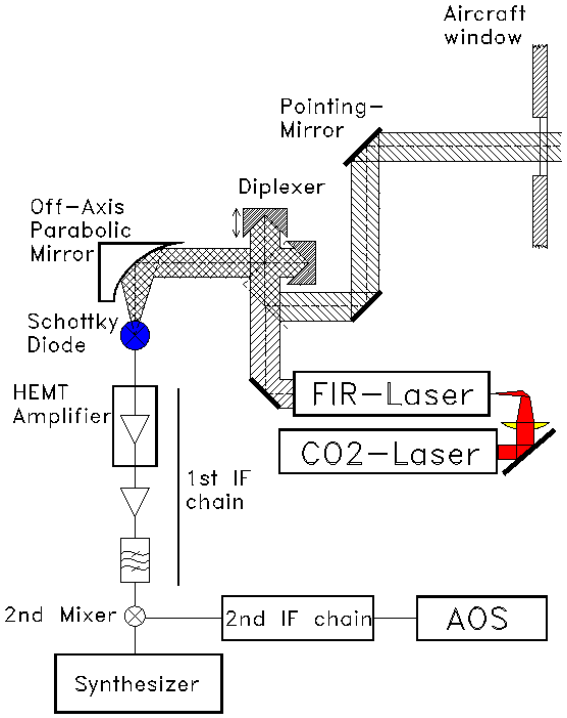
Heterodyne Instruments

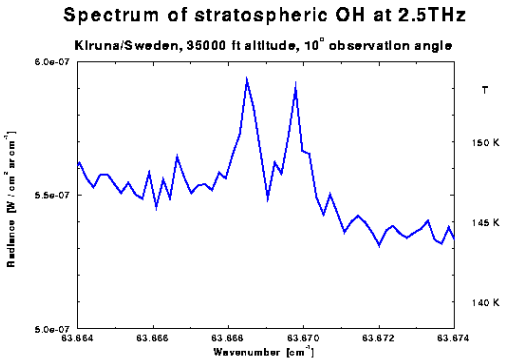
- Used to measure OH lines near 84 cm^{-1} (2.5 Thz).
- Examples include the Earth Observing System (EOS) Microwave Limb Sounder (MLS) 2.5 THz radiometer and the German Aerospace Center (DLR) THOMAS radiometer.
- Instruments produce very high resolution spectra of very narrow regions:
  - MLS has 25 channels over 0.04 cm^{-1}.
  - THOMAS has ~1400 channels over about 0.05 cm^{-1}

MLS and THOMAS



MLS (from web site)



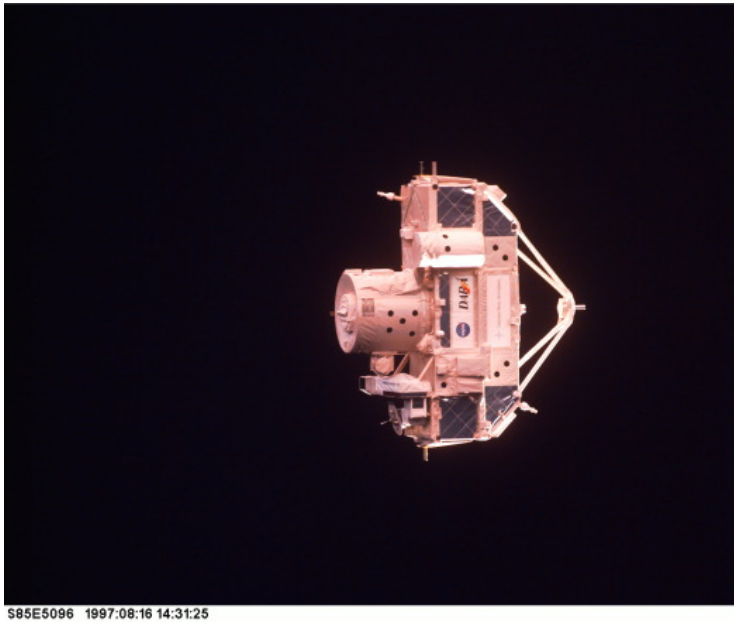


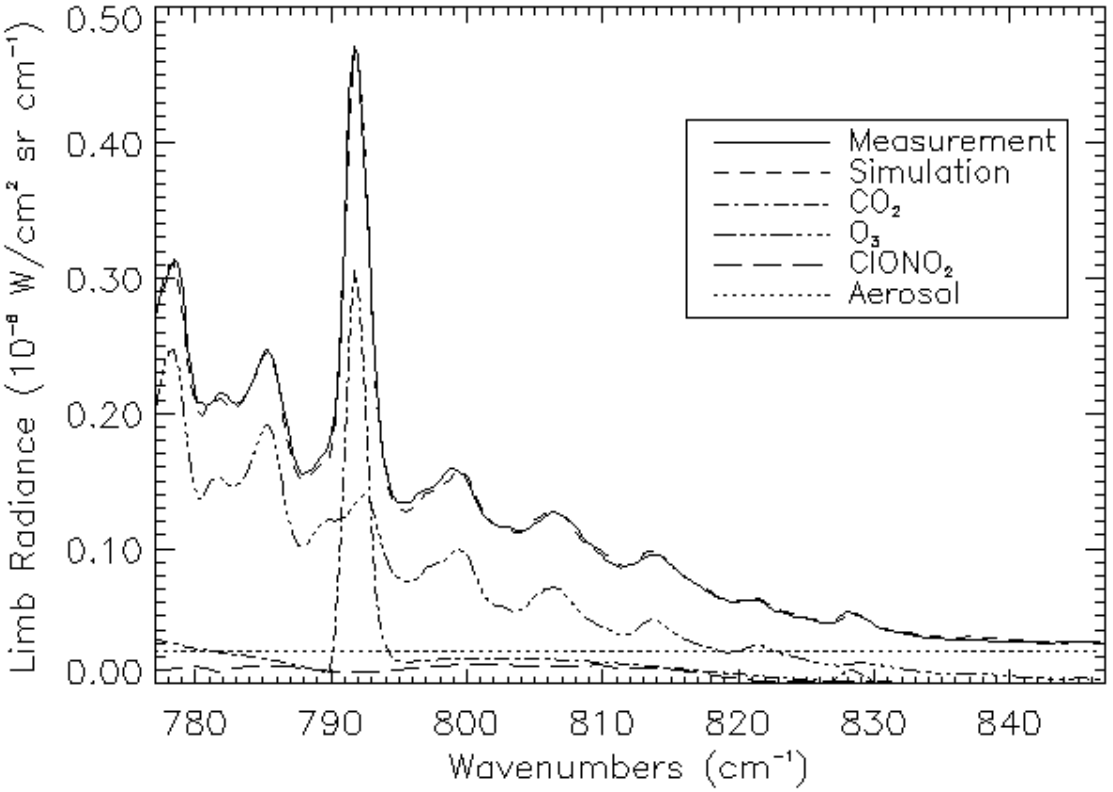
THOMAS (from web site)

Grating Instruments

- Cover a wider wavelength range than heterodyne.
- Observe many species simultaneously.
- Example: Cryogenic Infrared Spectrometers and Telescopes for the Atmosphere (CRISTA).
  - Covers 4−71 μm (2500−140 cm^{-1}): 4 spectrometers with resolving power ~500 (0.28−5 cm^{-1}).
  - Targets include CO_2, CO, NO, NO_2, H_2O, CH_4, N_2O, N_2O_5, O_3, CFC−11 and 12, HNO_3, HNO_4, CCl_4, $ClONO_2$, HF, HCl, $O(^3P)$, T, P, and aerosol.

CRISTA





CRISTA (as seen from the shuttle) and sample data (from web site).

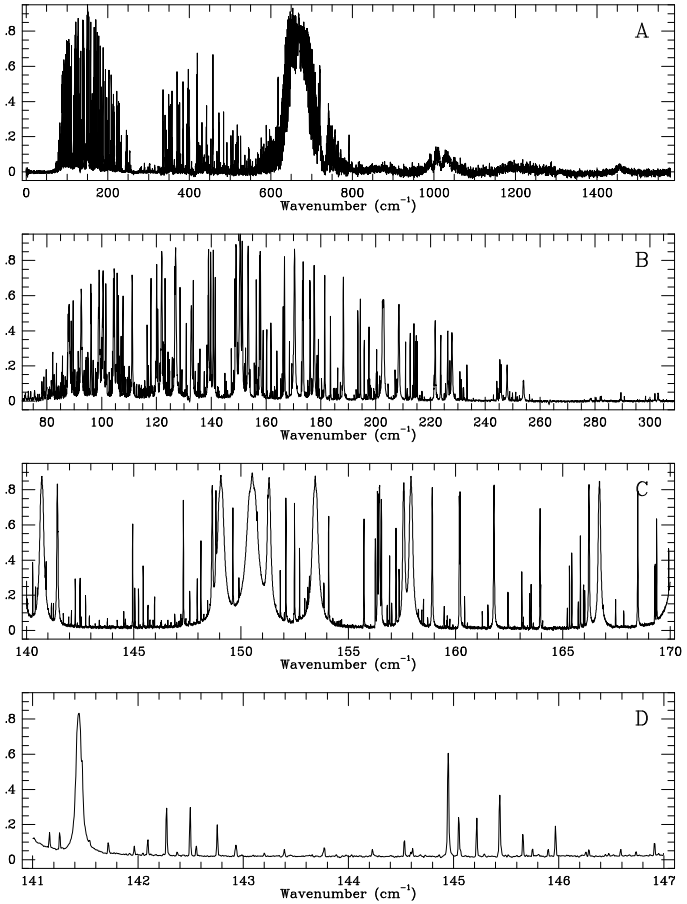
Fourier Transform Spectrometers

- Provide high resolution and broad spectral coverage.
- High resolution for line and band measurements:
  - IBEX (B. Carli et al.).
  - Smithsonian far−infrared spectrometer (FIRS−2).
- Moderate resolution for radiometric measurements:
  - Tropospheric Airborne FTS (TAFTS).
  - Far−infrared Sensor for Cirrus (FIRSC).
  - Far−infrared Spectroscopy of the Troposphere (FIRST).

FTS Summary

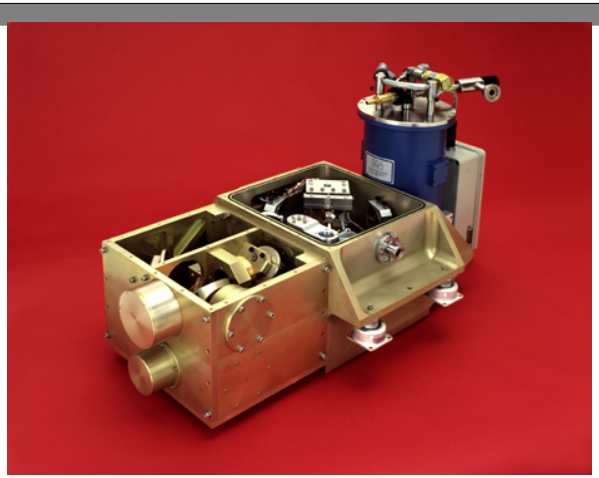
Instrument	Spectral band, cm^{-1}	Resolution, cm^{-1}
IBEX	10–50; 85–135	0.0025
FIRS–2	80–300; 330–1150	0.0080
FIRSC	10–35; 80–135	0.1000
TAFTS	80–800	0.1000
FIRST	100–1000	0.6000

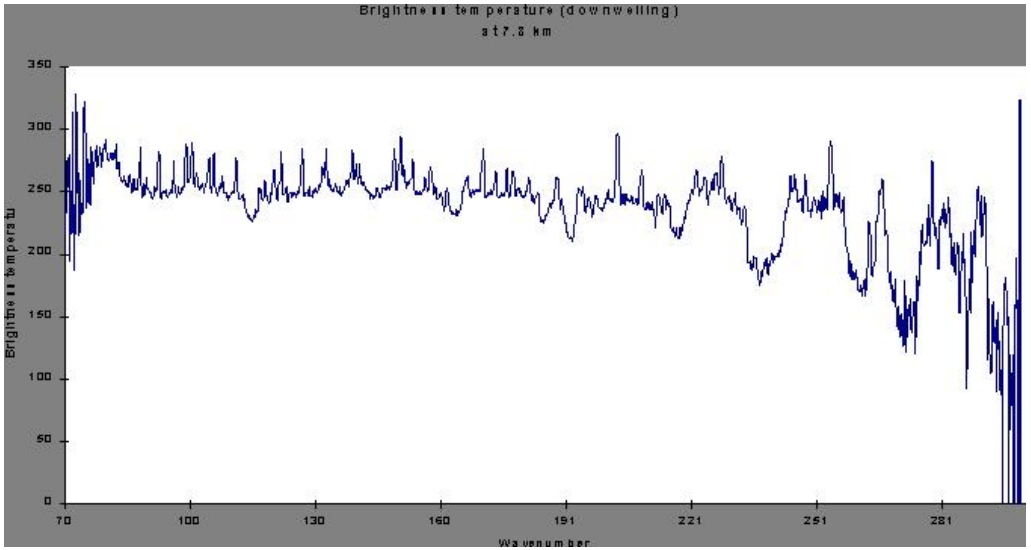
FTS Examples



FIRS−2

TAFTS





Known Spectroscopy Needs

- I will use FIRS−2 as a basis for defining problems with available spectroscopy from 50−650 cm^{-1}.
- The reference database is SAO2K; this is based mostly on HITRAN2000 with enhancements for the FIRS−2 spectral range.
- While this should also cover the requirements for the heterodyne instruments, the radiometric instruments require improved models for the continuum, better broadening for strong water lines, and maybe better CO_2.

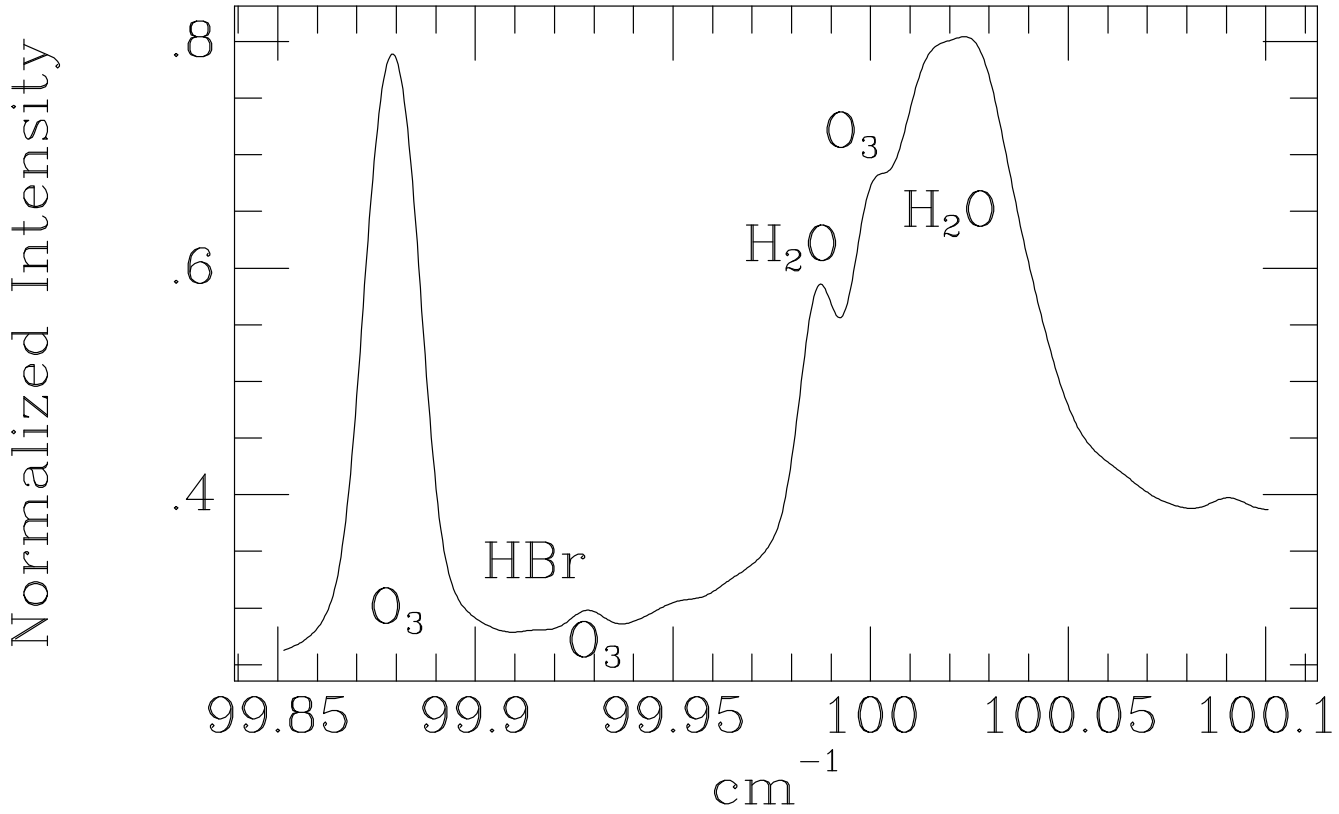
Species in good shape?

- No known problems for OH, HO_2, H_2O_2, HCl, HOCl, HF, NO_2, OCS, and HCN.
- HBr and HOBr: Would be OK except for interfering species.
- N_2O, CO_2(maybe), HNO_3, and O_3: Would be OK if did NOT interfere with others.

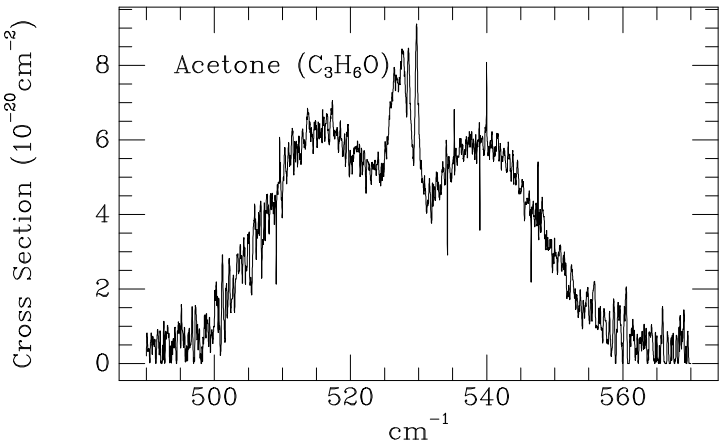
Interfering Species

- Line mixing in N_2O and CO_2 affects retrievals of $ClONO_2$ ($\nu 5$) and N_2O_5.
- Unlisted hot bands and combination/difference bands of HNO_3 affect retrievals of $ClONO_2$ ($\nu 6$).
- Hot bands (positions and strengths) and poor broadening parameters for O_3 affect retrievals for many weak species in the FIR (80−200 cm^{-1})

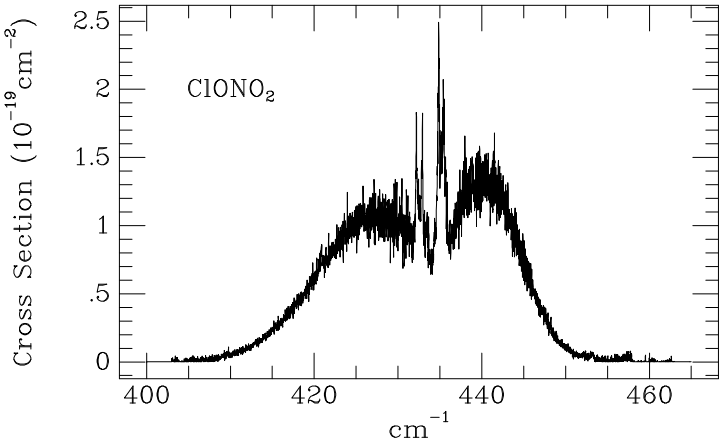
Example: O_3, H_2O, and HBr



Need Cross Sections



Acetone



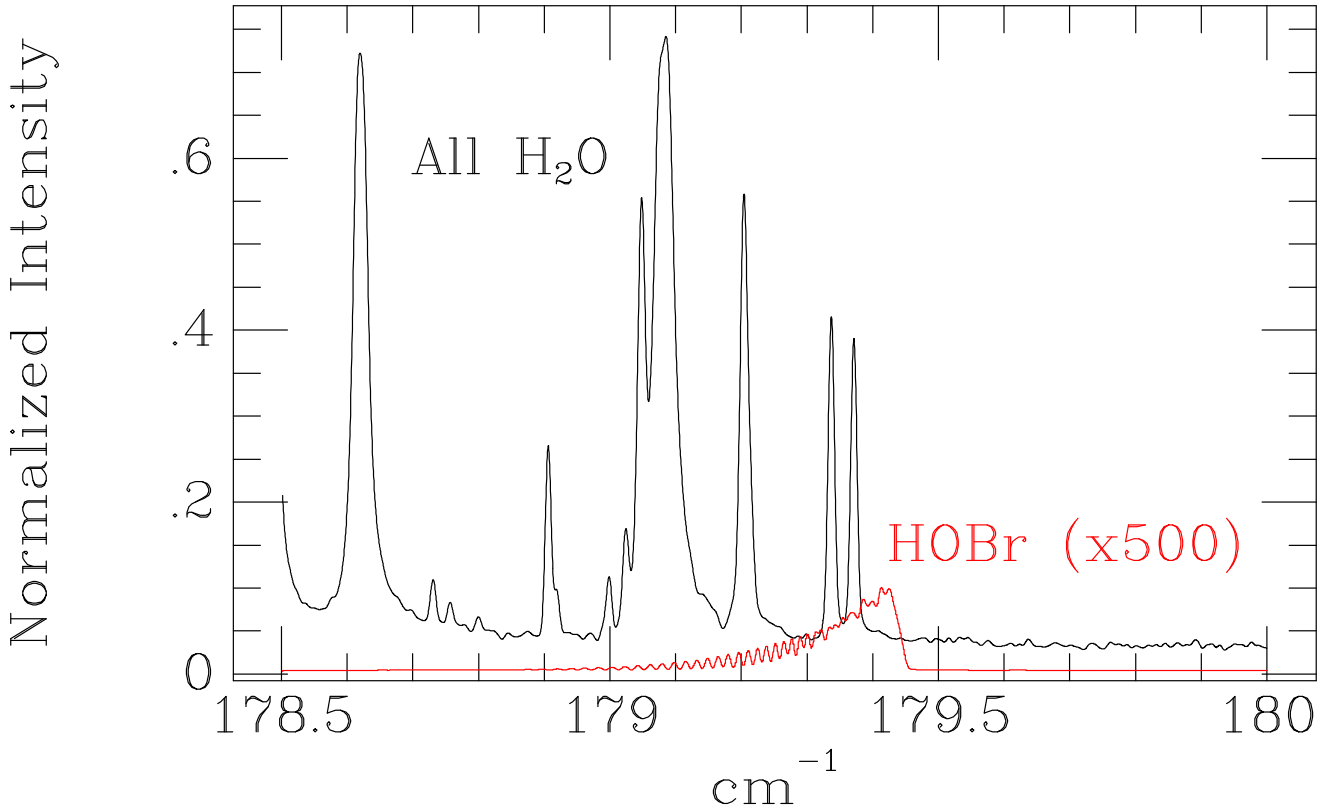
$ClONO_2$ ($\nu 6$)

- Also need N_2O_5 (300−650 cm^{-1})

Need Help!

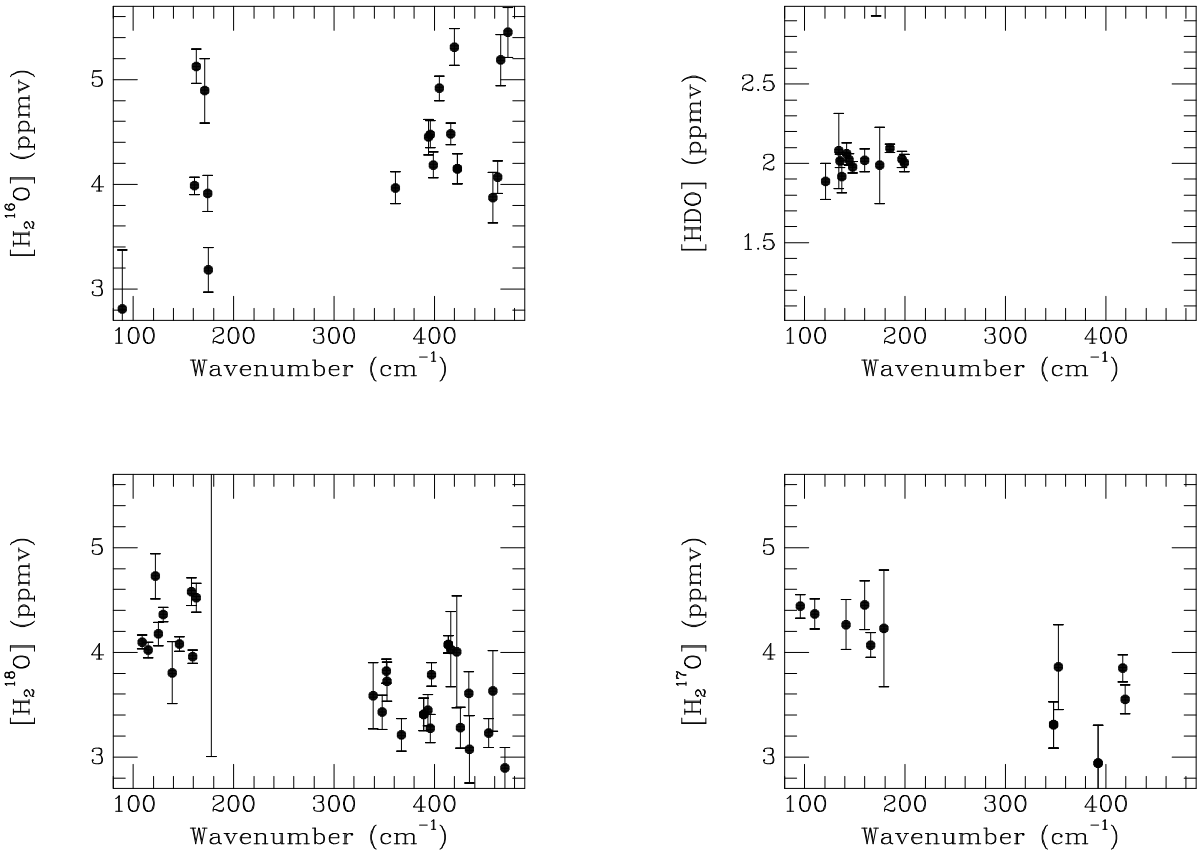
- All isotopes of water need significant improvement:
  - Wings of strong lines affect retrievals of weak species like HOBr.
  - High rotational states of $H_2{}^{16}O$ ($\Delta k=3$) need improved strengths and positions for retrievals.
  - All transitions for $H_2{}^{17}O$ and $H_2{}^{18}O$ (and maybe HDO) need better calculated strengths and positions.

Example 1: HOBr



Example 2: H_2O

- Example: this figure shows the mixing ratio retrieved for individual lines at a tangent height of 23 km, averaged over 6 balloon flights of the FIRS−2. Note the large scatter, as well as the systematic trend with frequency for $H_2{}^{17}O$ and $H_2{}^{18}O$. Note that this is from an earlier version of SAO2K



Summary

- Contact Ken Jucks for the list of problems with HITRAN2000 that we have fixed in SAO2K.
- We need good models of the water vapor continuum (and aerosol properties, but that is for another session!) and good positions (and pressure shifts), strengths, and widths for H_2O and CO_2 to interpret radiometric measurements.
- We need line mixing parameters for CO_2 and N_2O.

Summary (continued)

- We need measurements for hot and combination/ difference bands for HNO_3 (around 400−500 cm^{-1}).
- We need good linewidths for O_3 and positions and strengths for the hot bands.
- We need cross sections for $ClONO_2$ ($\nu 6$), acetone (~530 cm^{-1}) and N_2O_5 (300−650 cm^{-1}).

Summary (finally the end!)

- We need strengths and positions for H_2O weak lines and isotopes, and linewidths for the strong lines.
- Note that this list still includes many of the recommendations of the 1992 Langley Workshop!