The Quest for Consistency and Accuracy of Spectroscopic Parameters in HITRAN:

Bridge between Archive and Application

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HITRAN Conference

Cambridge MA

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"Global Consistency"

- ► Bands
- ► Isotopologues
- ► Lines

} Intensities, Positions

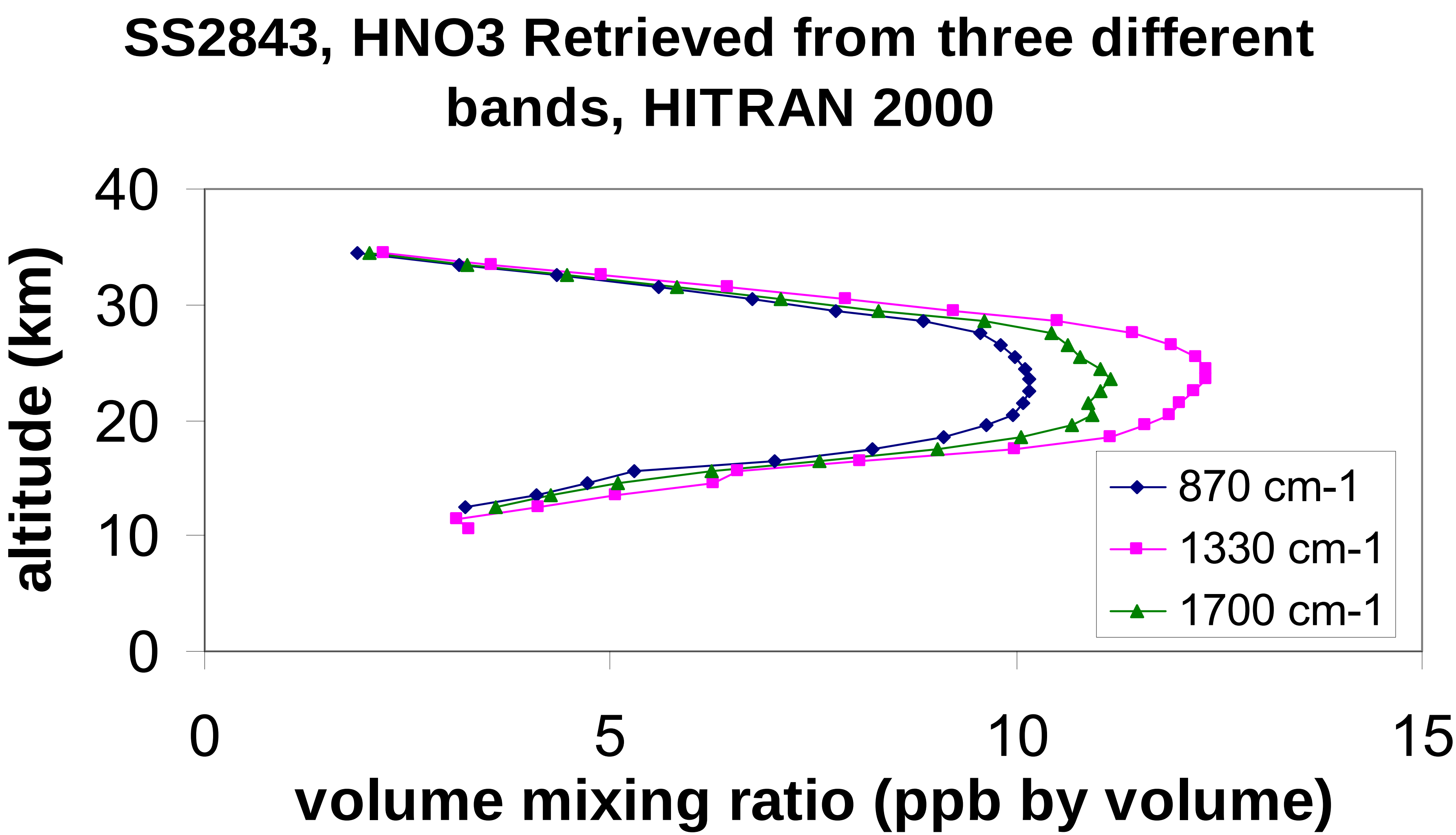
► Different Parameters $\left\{ \begin{array}{l} S \text{ vs } \gamma, \quad n, \\ \text{line-coupling} \rightarrow \gamma' \end{array} \right.$

► Why?

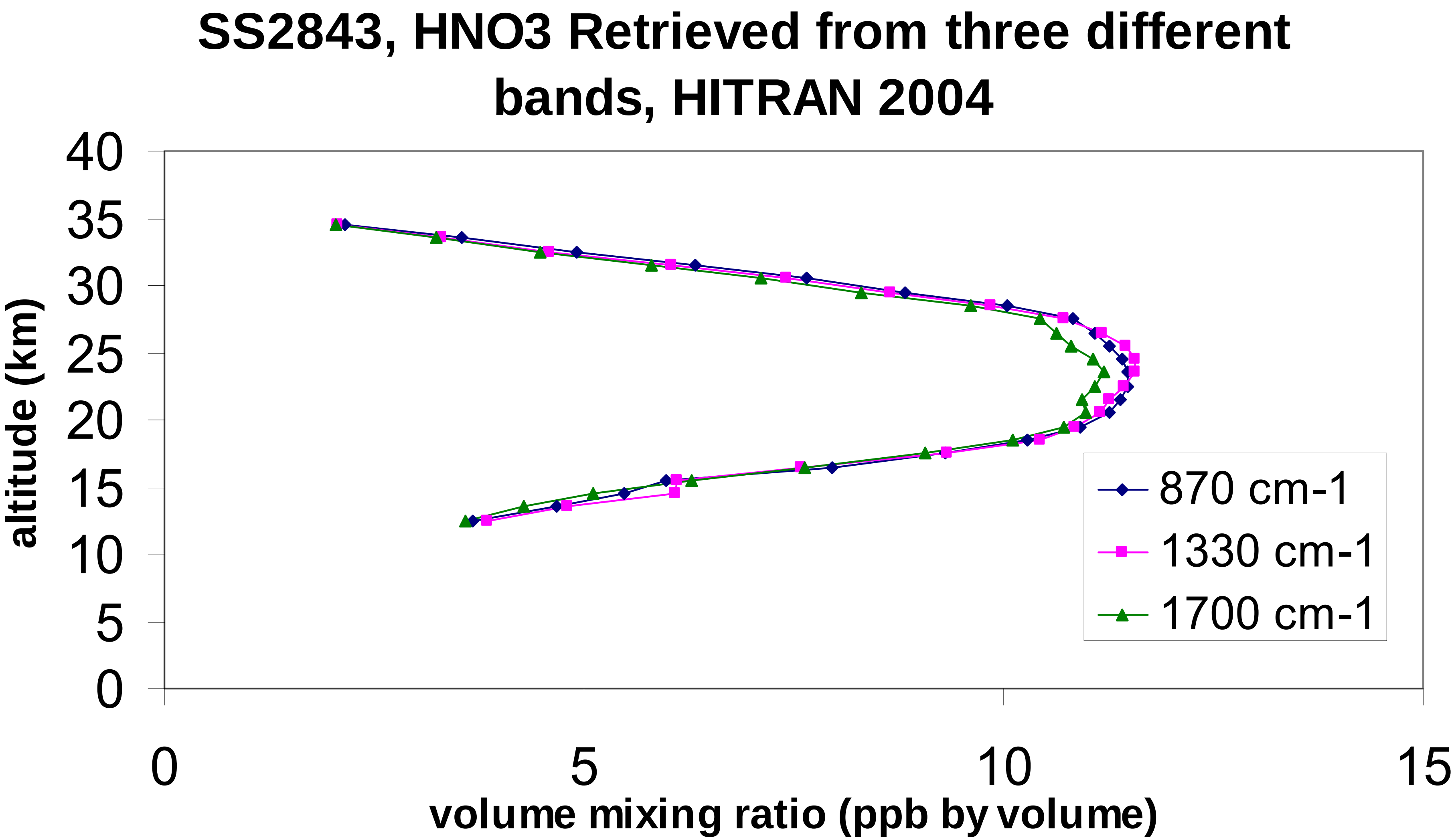

ASSFTS 12th Workshop
Atmospheric Science from Space using
Fourier Transform Spectrometry
When: May 18 - 20, 2005

Consistency of Retrievals using three Different Bands

SS2843: Arctic Occultation measured by ACE, late February 2004
(C. Boone and P. Bernath, U. Waterloo, private communication 2004)



Improvement of Consistency using HITRAN 2004

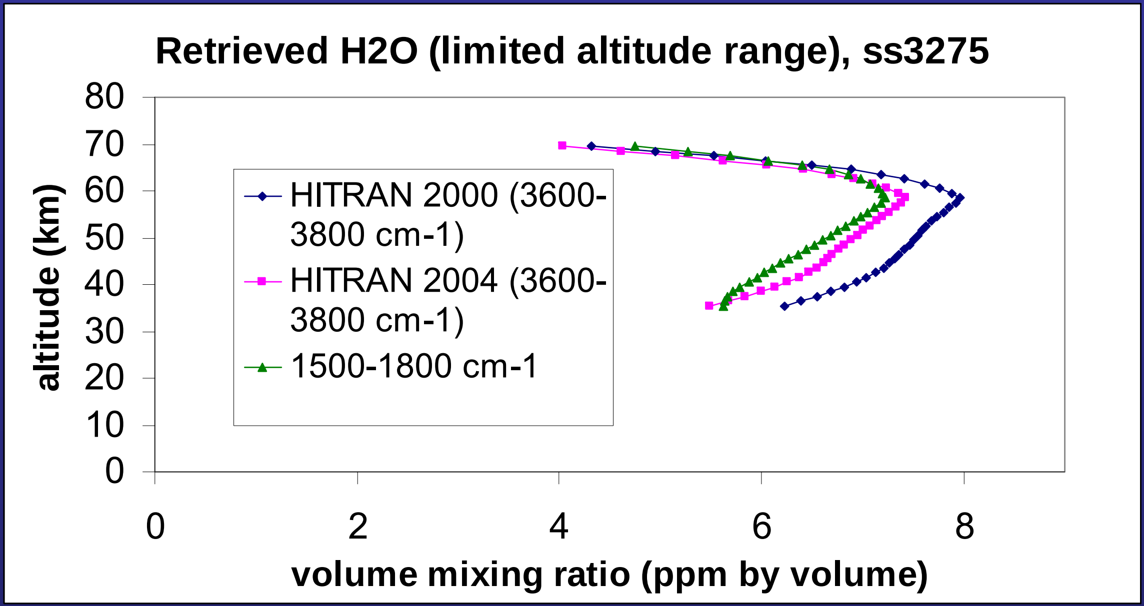


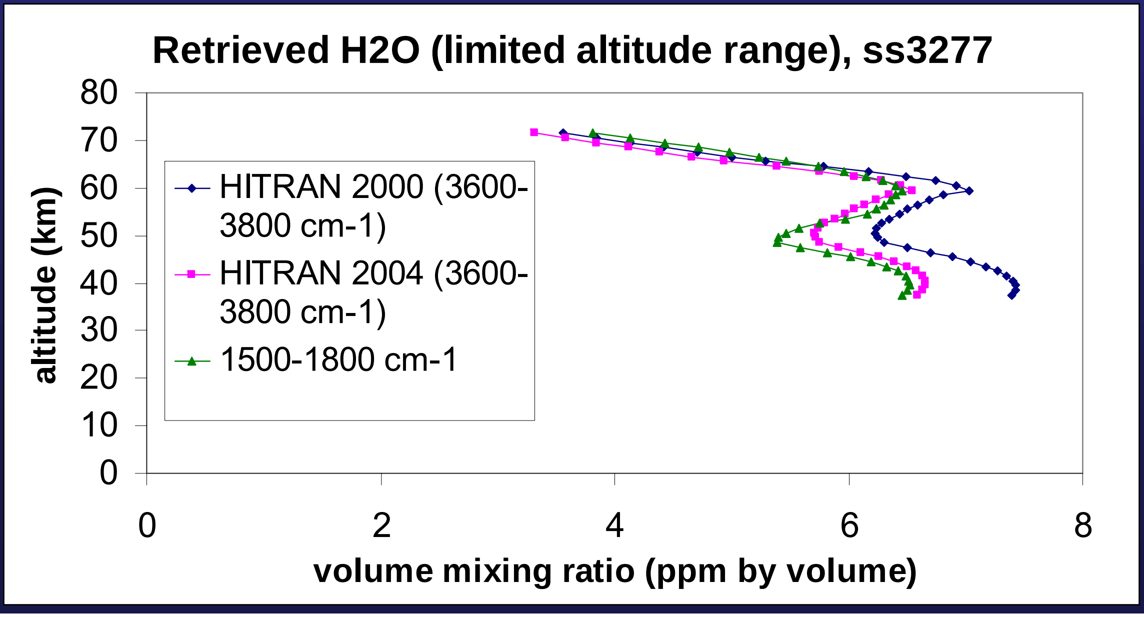
Consistency of Retrievals using two Different Bands

(C. Boone and P. Bernath, U. Waterloo, private communication 2004)

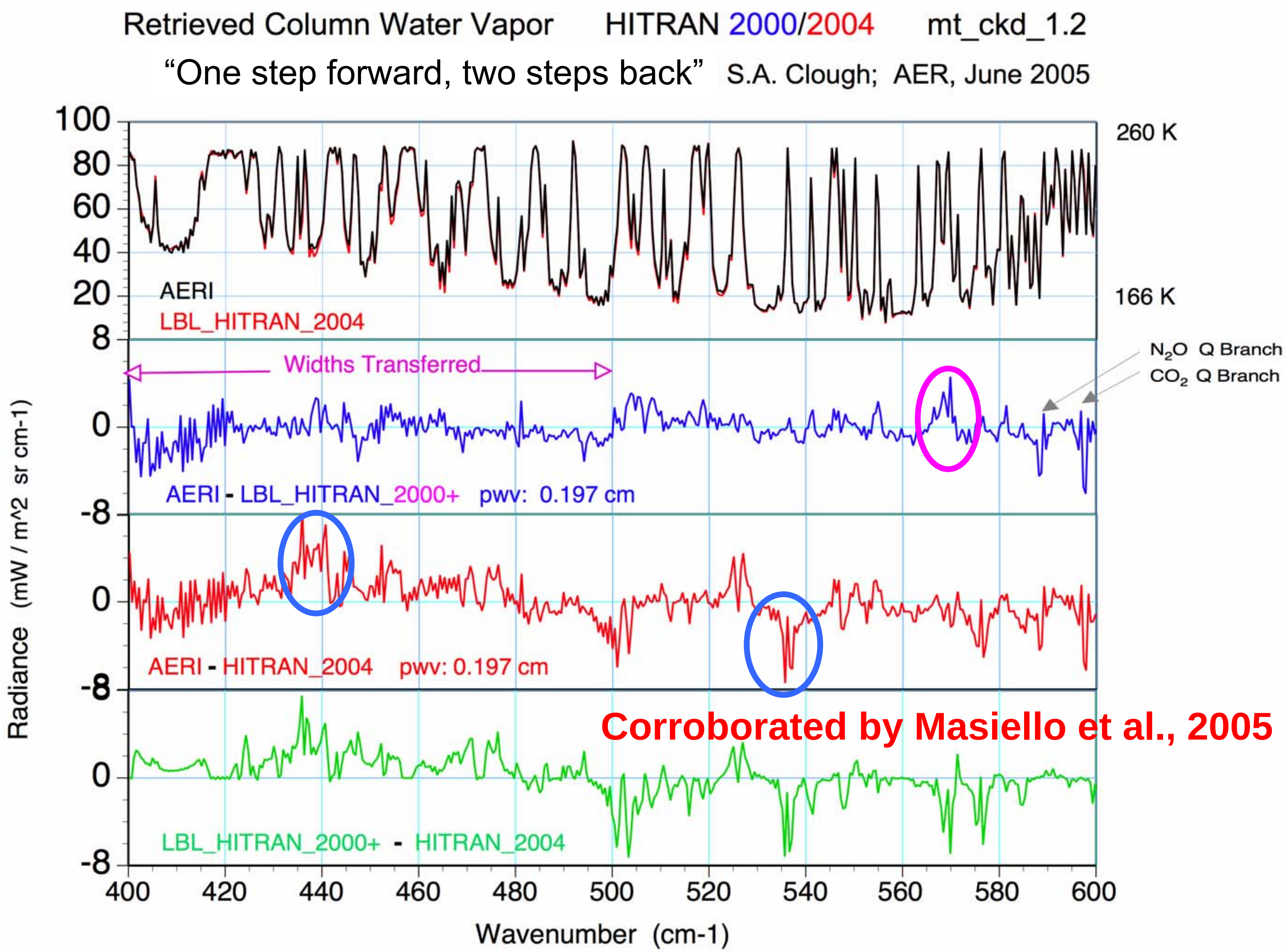
Occultations ~63° North measured by ACE

March 22, 2004

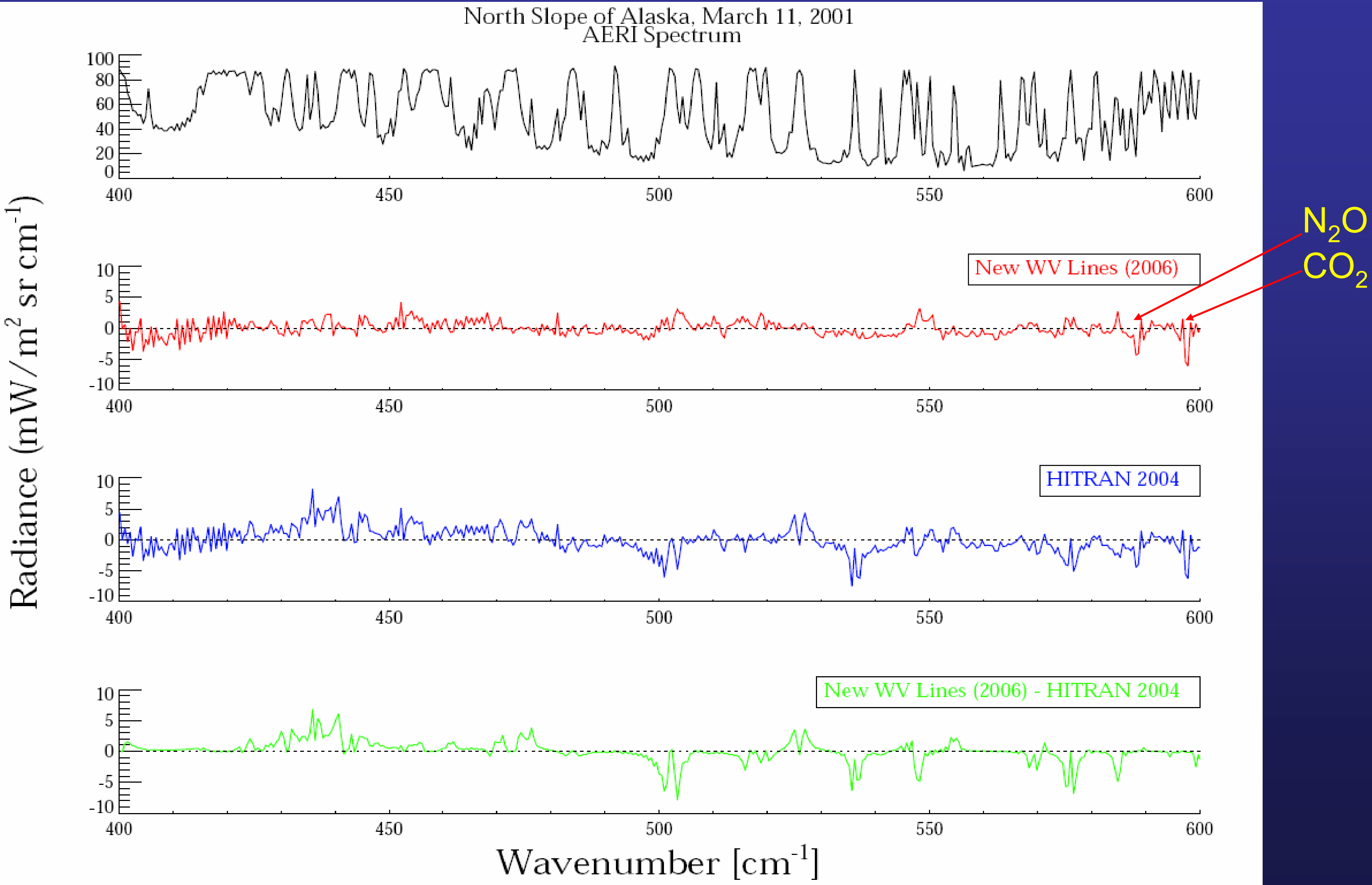




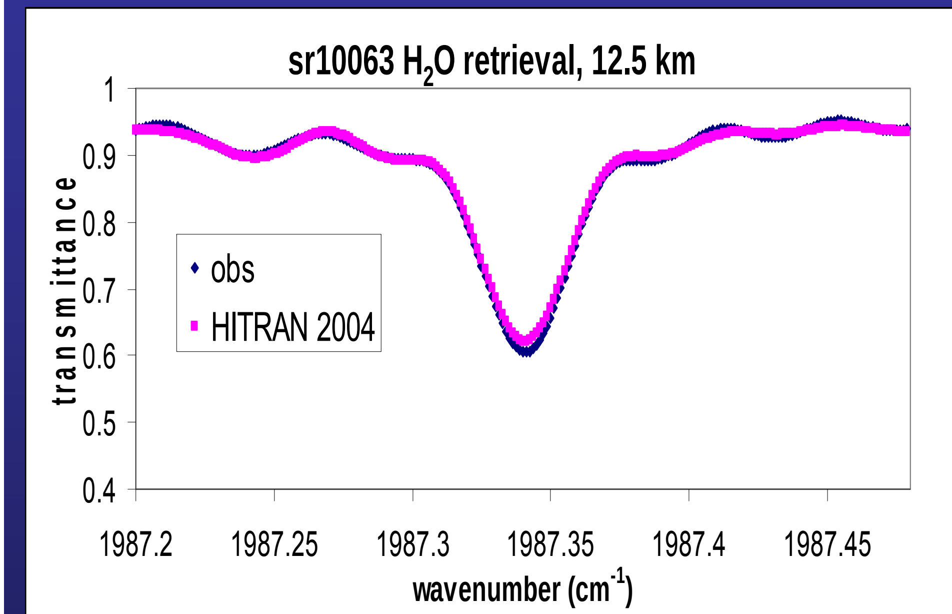
AERI_ER Validation in the Polar Window ARM NSA

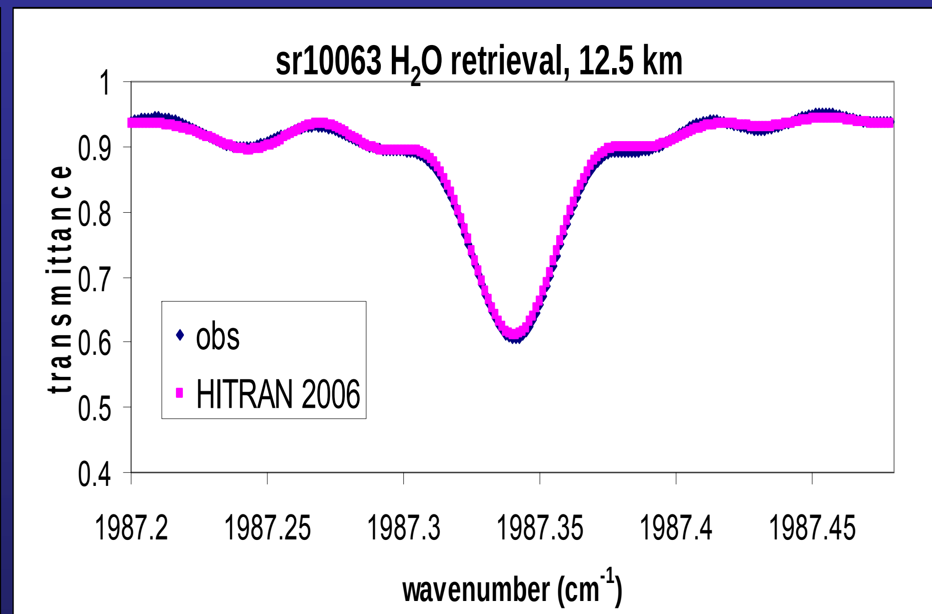


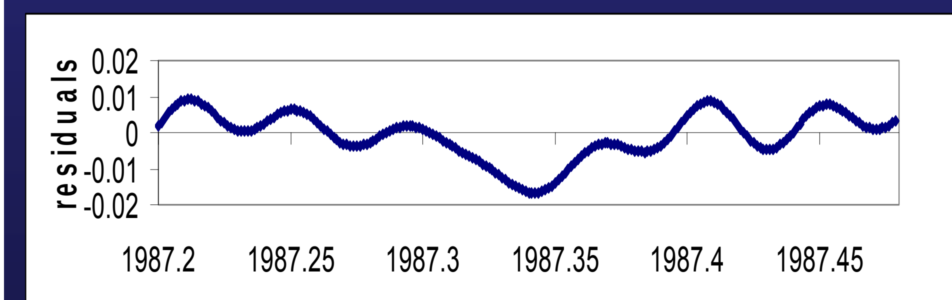
Validation (AER)

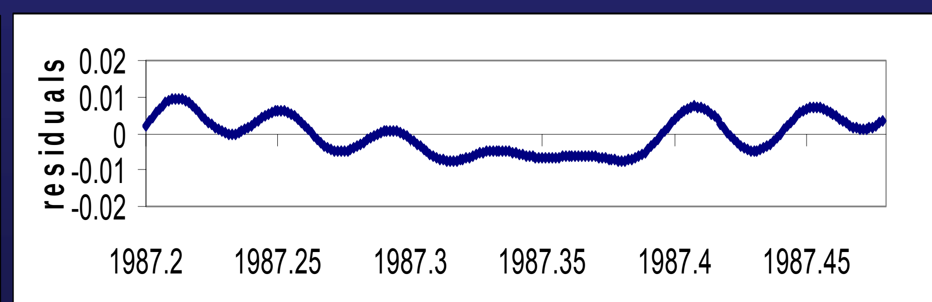


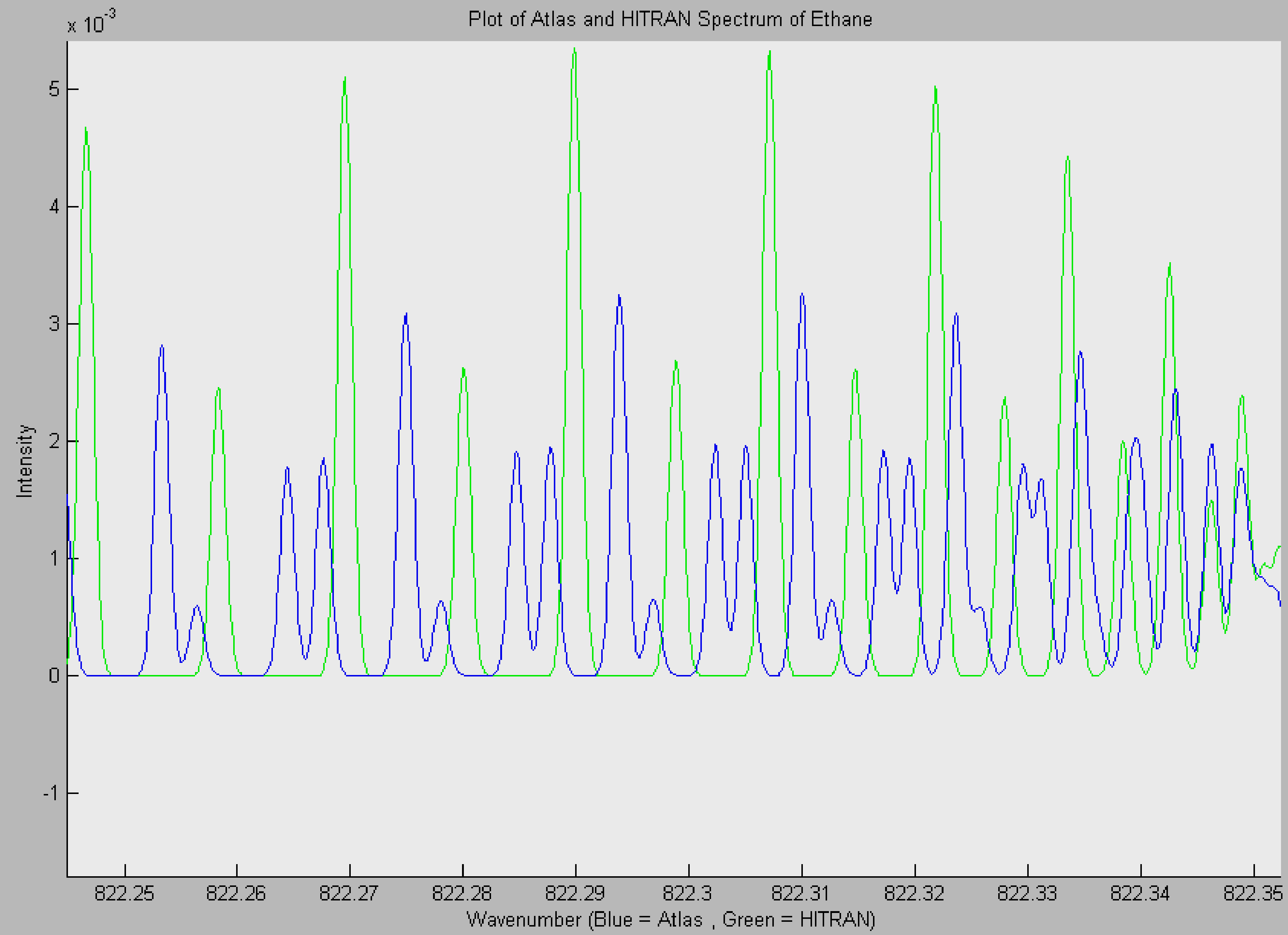
Validation (ACE)



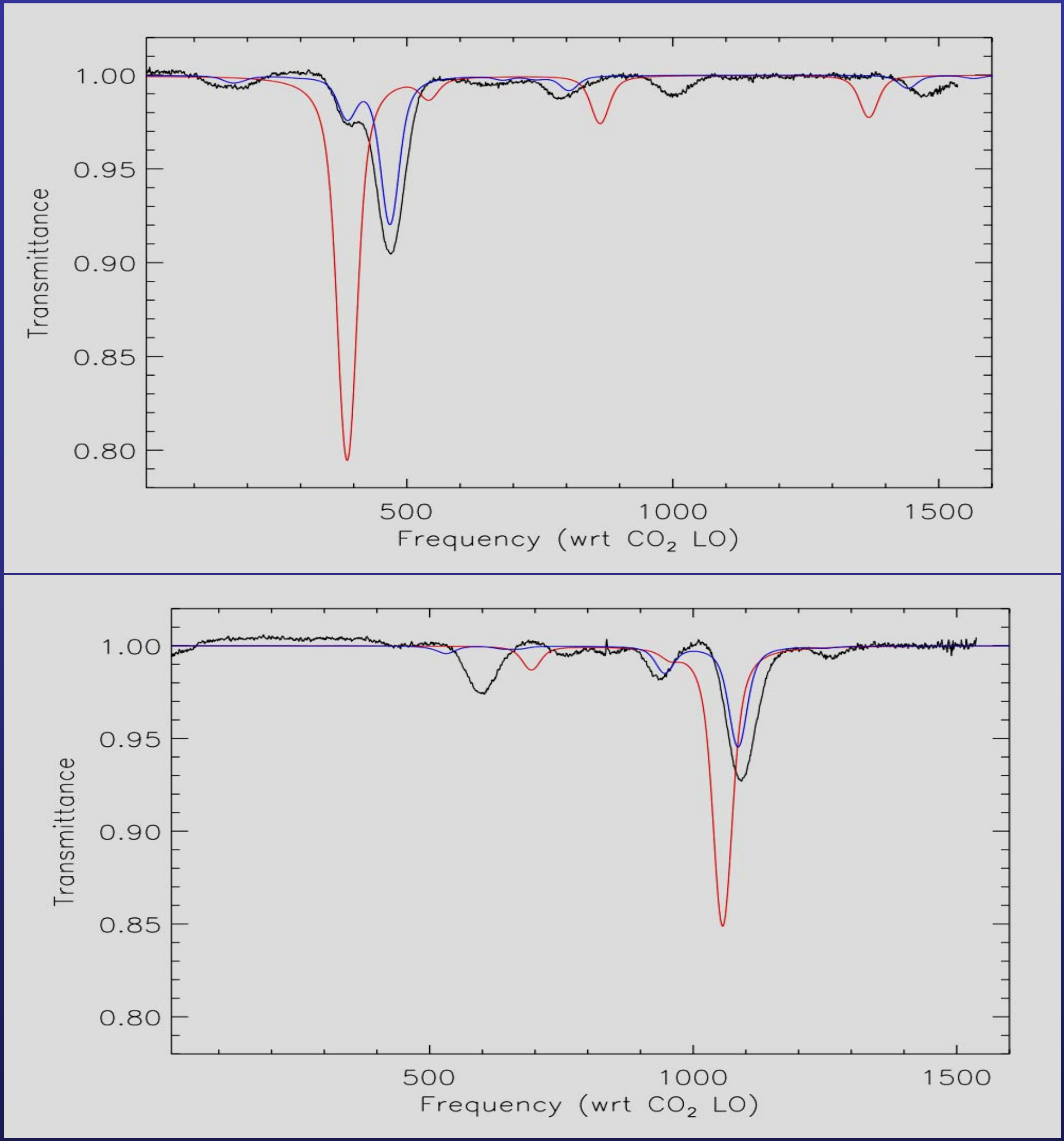






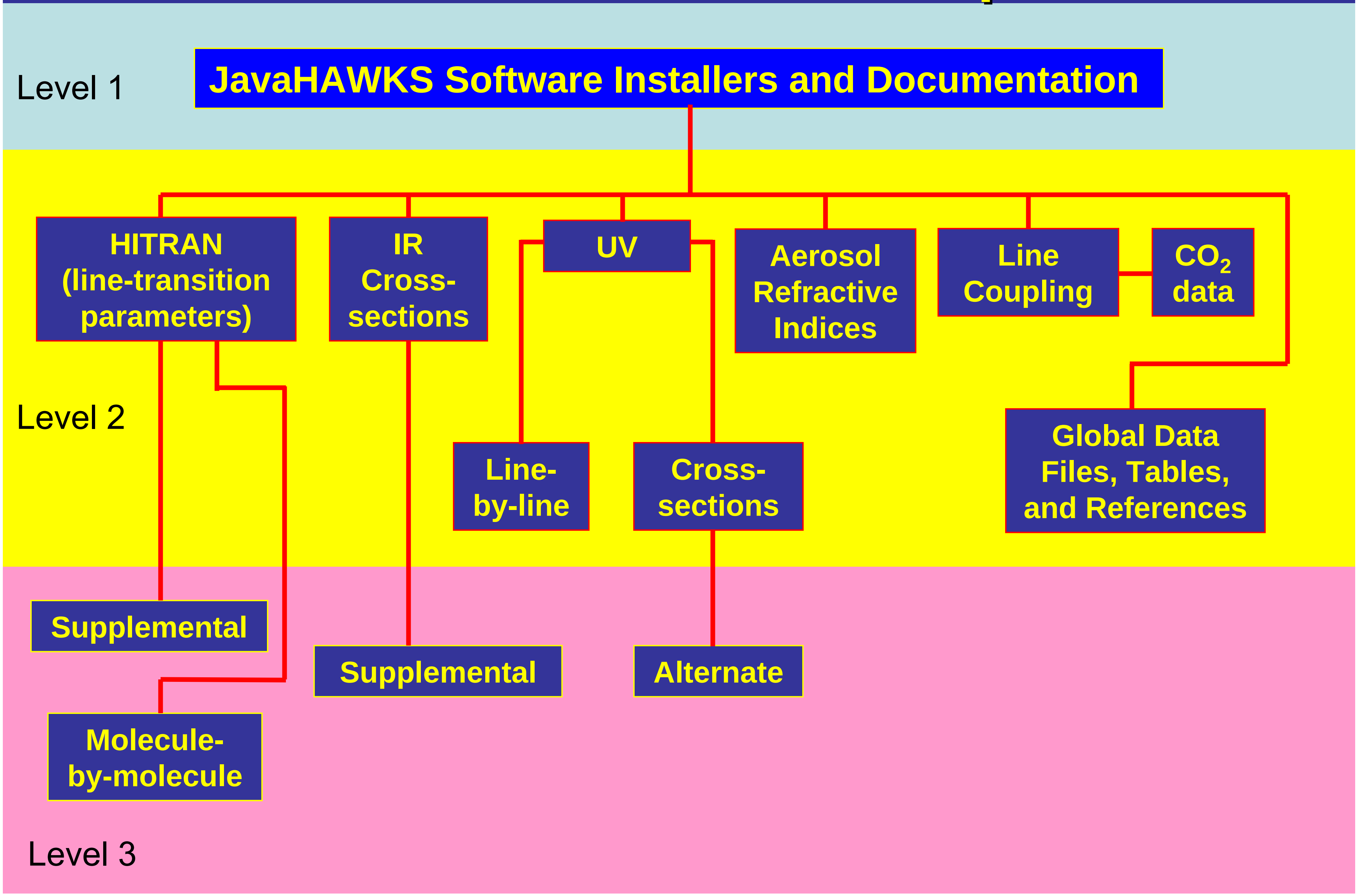


Plot of Atlas and HITRAN Spectrum of Ethane
x 10^-3
Intensity
5
4
3
2
1
0
-1
822.25
822.26
822.27
822.28
822.29
822.3
822.31
822.32
822.33
822.34
822.35
Wavenumber (Blue = Atlas , Green = HITRAN)



Ethane spectrum near 851.50514 and 856.47908 cm^{-1} measured at 0.00003 cm^{-1} resolution with LIRHS (black) compared with spectra modeled using line positions and intensities from HITRAN (red) and from the U. Tennessee/GSFC atlas (blue). Note that the line at 1000 MHz does not appear in either atlas and the line intensities, number of lines and the frequency values are different from the line atlases. Measurements were made with a 30 cm long cell and 0.5 Torr ethane pressure.

File Structure of HITRAN Compilation



HITRAN Line-by-line Parameters

Parameter	Field size	Definition
Mol	I2	**Molecule number**
Iso	I1	**Isotopologue no.**(1 = most abundant, 2 = second most abundant, …)
ν_{if}	F12.6	**Transition wavenumber in vacuum** [cm^{-1}]
S_{if}	E10.3	**Intensity** [cm^{-1}/(molecule·cm^{-2}) @ 296K]
A_{if}	E10.3	**Einstein *A*-coefficient** [s^{-1}]
γ_{air}	F5.4	**Air-broadened half-width** (HWHM) [cm^{-1}/atm @ 296K]
γ_{self}	F5.4	**Self-broadened half-width** (HWHM) [cm^{-1}/atm @ 296K]
E''	F10.4	**Lower-state energy** [cm^{-1}]
n_{air}	F4.2	**Temperature-dependence coefficient of** γ_{air}
δ_{air}	F8.6	**Air pressure-induced shift** [cm^{-1}/atm @ 296K]
v', v''	2A15	**Upper and Lower "global" quanta**
q', q''	2A15	**Upper and Lower "local" quanta**
ierr	6I1	**Uncertainty indices for** ν_{if}, S_{if}, γ_{air}, γ_{self}, n_{air}, δ_{air}
iref	6I2	**Reference pointers for** ν_{if}, S_{if}, γ_{air}, γ_{self}, n_{air}, δ_{air}
*	A1	**Flag for line-coupling algorithm**
g', g''	2F7.1	**Upper and Lower statistical weights**

160-character total

Table summarizing species

#	Molecule	No. of lines	#	Molecule	No. of lines	#	Molecule	No. of lines
1	H_2O	62894	14	HF	107	27	C_2H_6	4749
2	CO_2	62913	15	HCl	613	28	PH_3	11790
3	O_3	311481	16	HBr	1293	29	COF_2	70601
4	N_2O	47835	17	HI	806	30	SF_6	22901
5	CO	4477	18	ClO	7230	31	H_2S	10071
6	CH_4	251440	19	OCS	19920	32	HCOOH	24808
7	O_2	6428	20	H_2CO	2702	33	HO_2	38803
8	NO	102280	21	HOCl	16276	34	O	2
9	SO_2	38853	22	N_2	120	35	$ClONO_2$	32199
10	NO_2	104223	23	HCN	4253	36	NO^+	1206
11	NH_3	29084	24	CH_3Cl	31119	37	HOBr	4358
12	HNO_3	271166	25	H_2O_2	100781	38	C_2H_4	12978
13	OH	42373	26	C_2H_2	3517	39	CH_3OH	19899

Total = 1,778,549 !

Future Requirements of Database

- ► Extended Spectral Coverage (more bands)

  Emphasis on near-IR and Visible

  Weak transitions of combination bands (CH_4, etc)

- ► Additional Molecular Species
- ► Additional Parameters

  Other foreign-gas broadeners (H, He, etc)

  Line-shape parameters

  Temperature-dependence parameters

- ► Higher Temperature Capability
- ► Collision-Induced Absorption

  H_2-H_2, O_2-O_2, etc

$$\alpha_L(p,T) \cong \left[\gamma_{air}(p_0,T_0)(1-\chi) + \gamma_{self}(p_0,T_0)\chi\right] p \left(\frac{T_0}{T}\right)^{n_{air}}$$

$$\alpha_L(p,T) = \left[\gamma_{air}(p_0,T_0)(1-\chi)\left(\frac{T_0}{T}\right)^{n_{air}} + \gamma_{self}(p_0,T_0)\chi\left(\frac{T_0}{T}\right)^{n_{self}}\right] p$$

More Issues

- Improved database managing
- Improved documentation
- Validation, Comparisons, Recommendations, Acquisition
- Continuity, Funding

HITRAN International Advisory Committee

Et al

David

Marie

Iouli