Spectroscopic Needs for Microwave Atmospheric Sensing: Instrument Focus

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for NASA Workshop on
Spectroscopic Needs for Atmospheric Sensing
San Diego, California   22-26 October 2001

Organization of talk

- **Microwave remote sensing of the atmosphere**
  - some basic points
- **Near-term spectroscopy needs**
  - within next few years
- **Projected longer-term spectroscopy needs**

Prime (research) application areas for microwave atmospheric remote sensing

- **Stratospheric Chemistry**
  - *Is the ozone layer, and ozone chemistry, recovering as expected following international regulations?*
  - *How do stratospheric trace constituents respond to changes in climate and composition?*
- **Climate Research**
  - *How do water vapor feedback processes affect climate change?*
  - *What are the roles of ice clouds in climate variability?*
- **Tropospheric Chemistry**
  - *What are the effects of regional pollution on the global atmosphere?*
  - *Is the ability of air to 'cleanse itself' diminishing?*

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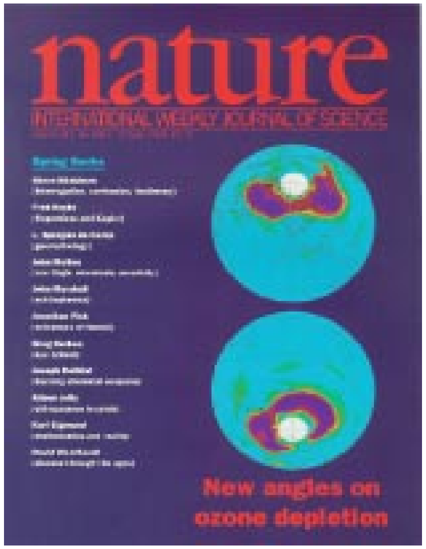
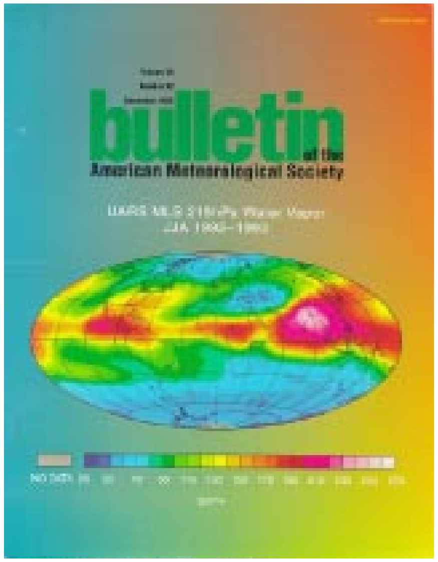
Maps of ozone-destroying chlorine monoxide





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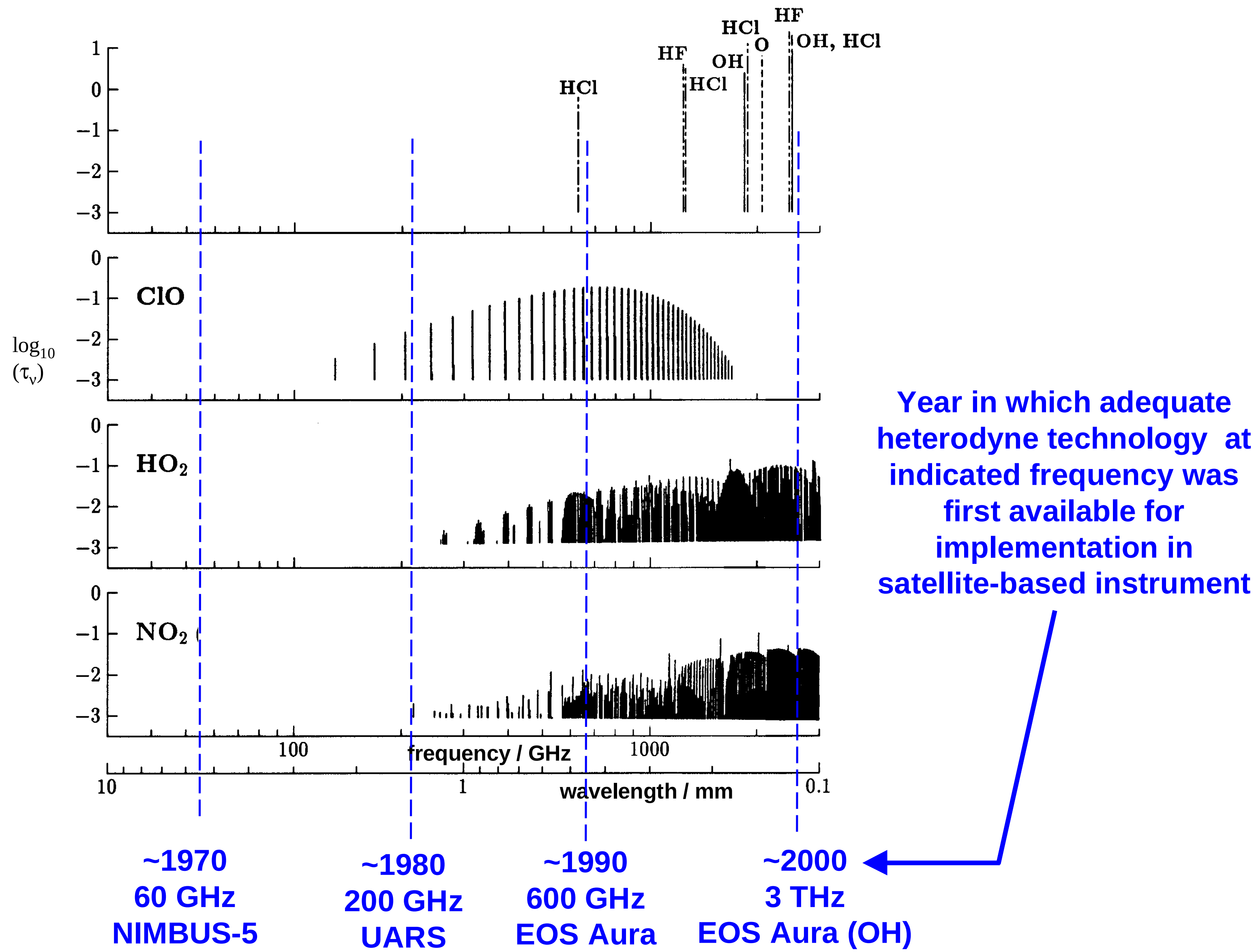
Maps of water vapor in the upper troposphere that are are not degraded by ice clouds

Features of Microwave Atmospheric Sensing
(some of which are shared with other techniques)

- **Many chemical species can be measured**
  - **including in the presence of ice clouds, dense aerosol, smoke**
  - resolved spectral lines, and simultaneous measurement of all spectral channels, provide robust measurements
- **Water vapor, cloud ice (including aspects of size distribution) and temperature can simultaneously be measured**
  - needed to improve understanding of upper trop processes affecting climate
- **Thermal emission is observed**
  - allows measurements at all times of day/ night and daily global coverage by satellite
- **Arbitrarily-fine spectral resolution**
  - allows very weak lines to be measured in the presence of nearby strong ones
  - allows vertical structure to be obtained from line shape
- **Excellent instrument calibration, calibration stability**
  - UARS MLS antenna reflectivity change - thought the major uncertainty in overall cal stability - was less than ~0.02% over an analyzed 6 years of space radiance data
- **Lab measurements yield very accurate spectral line strengths**
  - Dipole (and other) moments that set line strengths are measured by ‘counting’ - from Stark and Zeeman splitting - typically to 4 significant figures

Microwave Spectroscopic Needs for Atmospheric Remote Sensing

Molecular Spectra and Instrument Technology



Spectroscopy Support for Microwave Sensing

- Tremendous thanks to the spectroscopy community for your great support over many years in providing the spectroscopy data we need

- And to NASA for realizing the importance/criticality of spectroscopy and supporting it
  - Especially to Mike Kurylo, Phil DeCola and colleagues

The microwave atmospheric remote sensing spectroscopy 'bible'

JPL Publication 80-23, Rev. 4

Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

H.M. Pickett
R.L. Poynter
E.A. Cohen
M.L. Delitsky
J.C. Pearson
H.P. Müller

March 10, 1996

NASA

National Aeronautics and Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

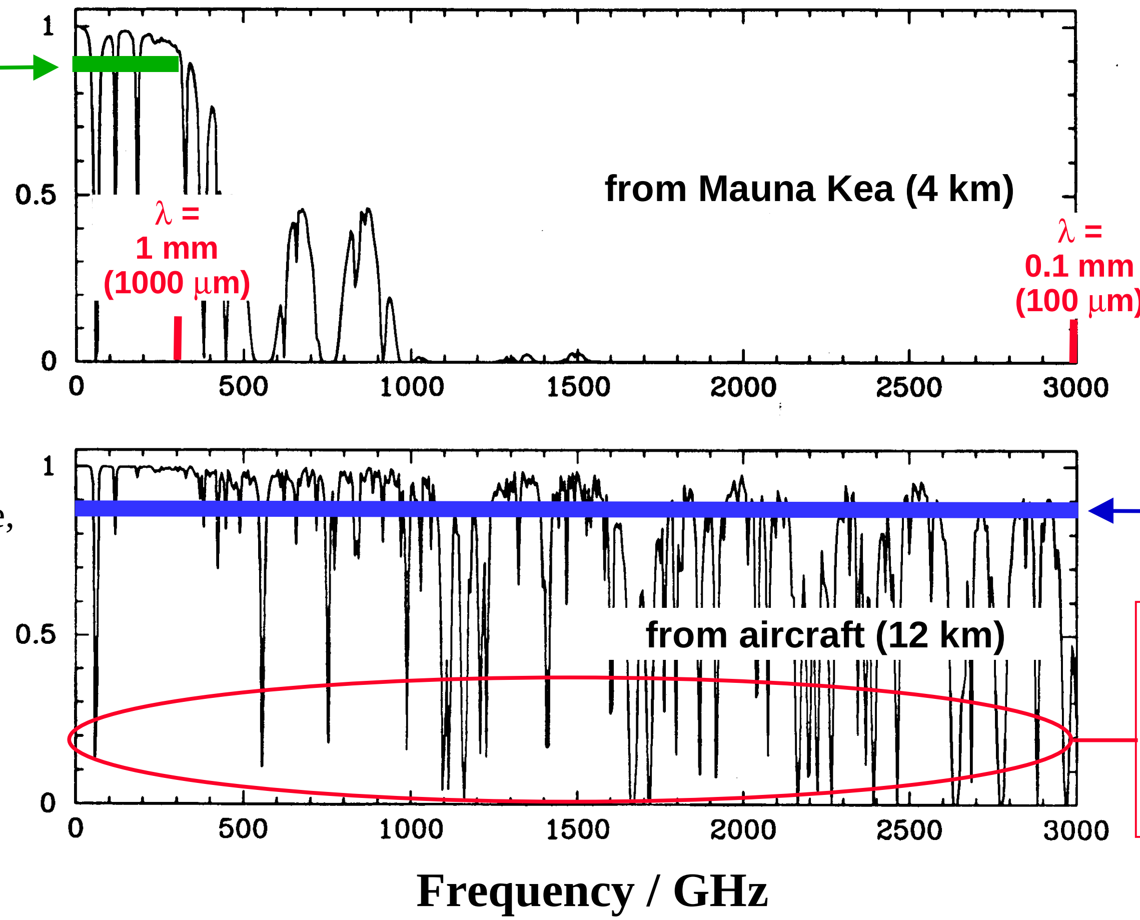
Atmospheric transmission at mm and submm wavelengths

spectral region below ~300 GHz is available for tropospheric remote sensing - and ground-based remote sensing of the upper atmosphere

entire spectral region is available for stratospheric (and mesospheric, thermospheric) remote sensing - but instrument must be located above ~10 km

Measured atmospheric zenith transmission

[Phillips and Keene, *Proc. IEEE 80*, 1662-1668, 1992]



strong absorption lines seen here are H_2O and O_2

A spectral line measurement 'Figure of Merit' for a molecule

- The measurement signal, for optically-thin spectral lines, is proportional to the absorption coefficient at line center. This can be written

$$\alpha_\nu^{ul} = \frac{2\pi}{3\varepsilon_o hc\,k}\cdot\frac{f\,\mu^2}{Q(T)}\cdot\frac{p_{air}}{T\,\Delta\nu}\cdot g_l\,g_u\,\phi_{ul}^2\cdot\left[e^{-E_l/kT} - e^{-E_u/kT}\right]\cdot\nu_{ul}$$

a factor involving fundamental constants

a factor involving molecular properties that are independent of a specific spectral line:

f = volume mixing ratio

μ = moment describing interaction with radiation

Q = partition function at temperature T

a 'line shape' factor (approximately constant for pressure broadening where $\Delta\nu \propto p_{air}T^{-x}$, $\Delta\nu$ being the linewidth parameter)

a factor with parameters of the quantum transition for the spectral line

g = state degeneracy
ϕ = matrix element
u => upper state
l => lower state

a factor describing the difference in populations of the two states involved in the transition

E = state energy

spectral line frequency. (this factor offsets increasing instrument noise with increasing frequency)

This factor gives a general 'Figure of Merit' for measurement of a molecule or atom by microwave techniques →

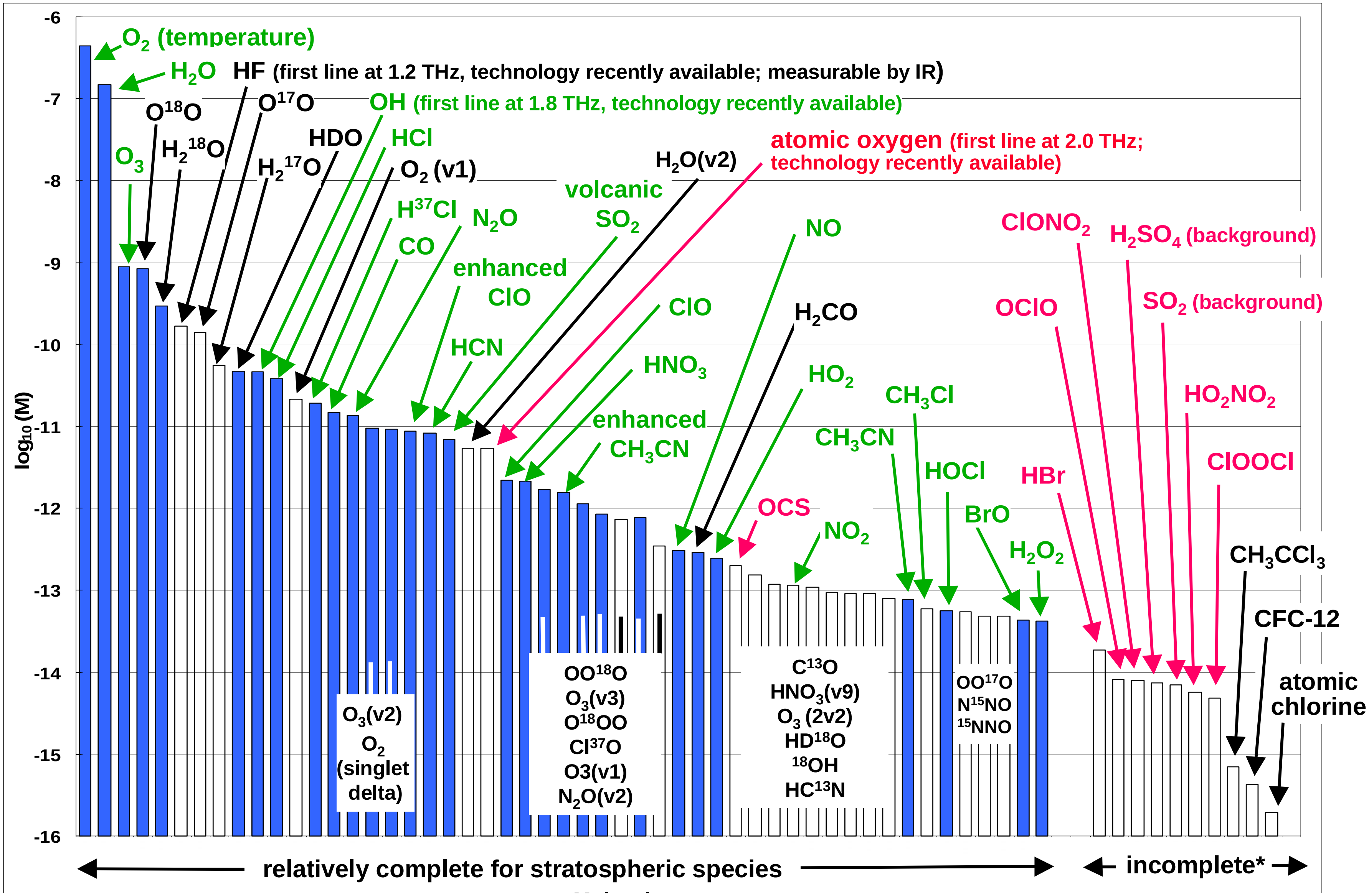
$$\text{Figure of Merit} \equiv \text{M} = \frac{f\,\mu^2}{Q(T)}$$

$\log_{10}(M)$ for stratospheric species (for typical abundances, T=225K)

blue bars indicate microwave atmospheric measurements to date

green indicates targets of current or upcoming satellite experiments

red => some other measurements that should be achievable with latest technology



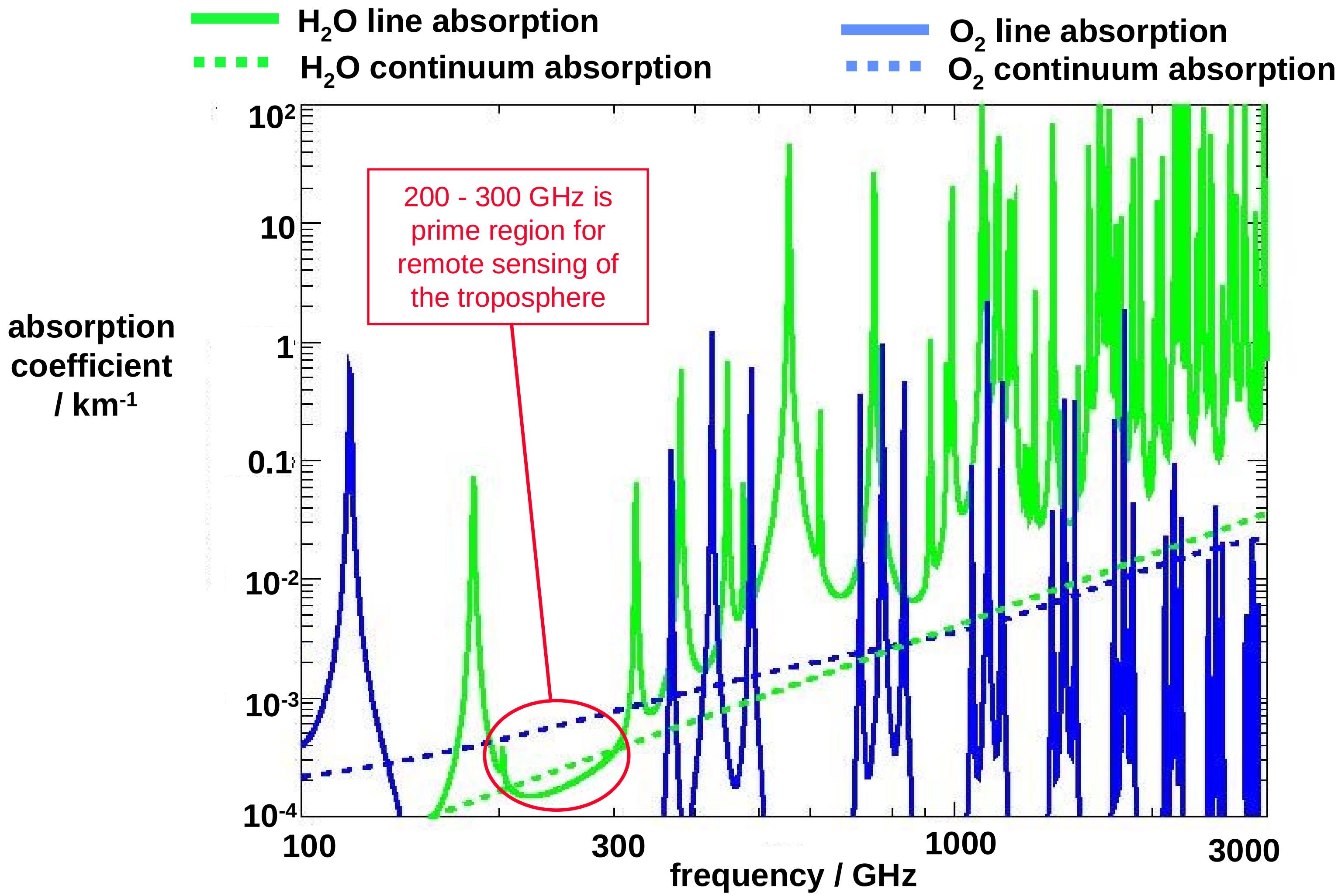
*a more complete list is in 'Microwave Limb Sounding' [ch. 8, *Atmospheric Remote Sensing by Microwave Radiometry*, M. Janssen, ed., 1993]

Microwave Spectroscopic Needs for Atmospheric Remote Sensing

O_2 and H_2O line and continua absorption

calculated by W.G. Read for 200 hPa, 220 K and 50% RH wrt ice (upper trop conditions)

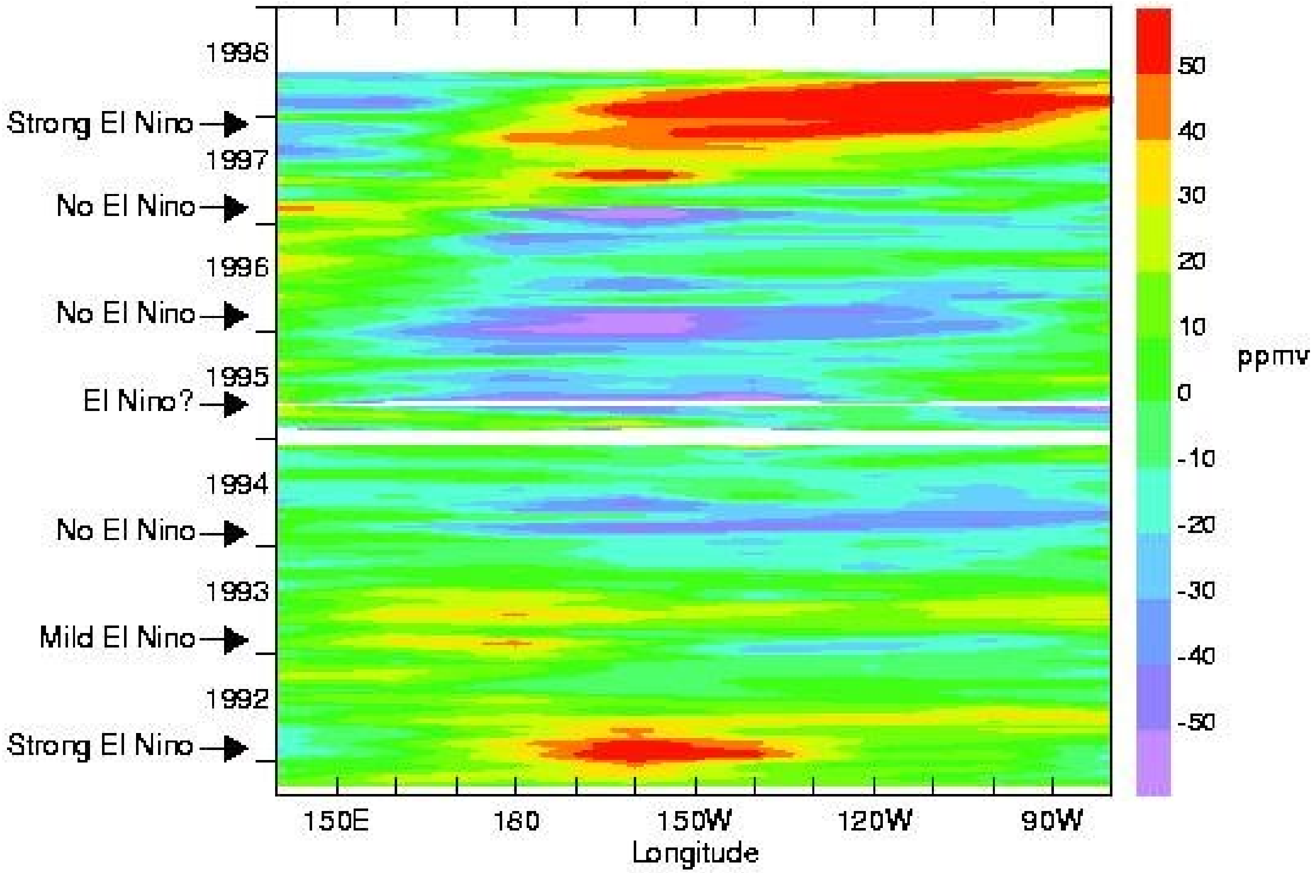
Inadequate lab data and theoretical models for these <u>continua</u> currently limit the accuracy of microwave measurements of upper trop H_2O and cloud ice



Upper tropospheric H_2O obtained from UARS MLS measurements of 205 GHz continuum emission

This image by W.G. Read [Waters et al., *JAS 56*, 194, 1999] shows correlation between tropical 215 hPa H_2O and El Nino sea surface temperature variations

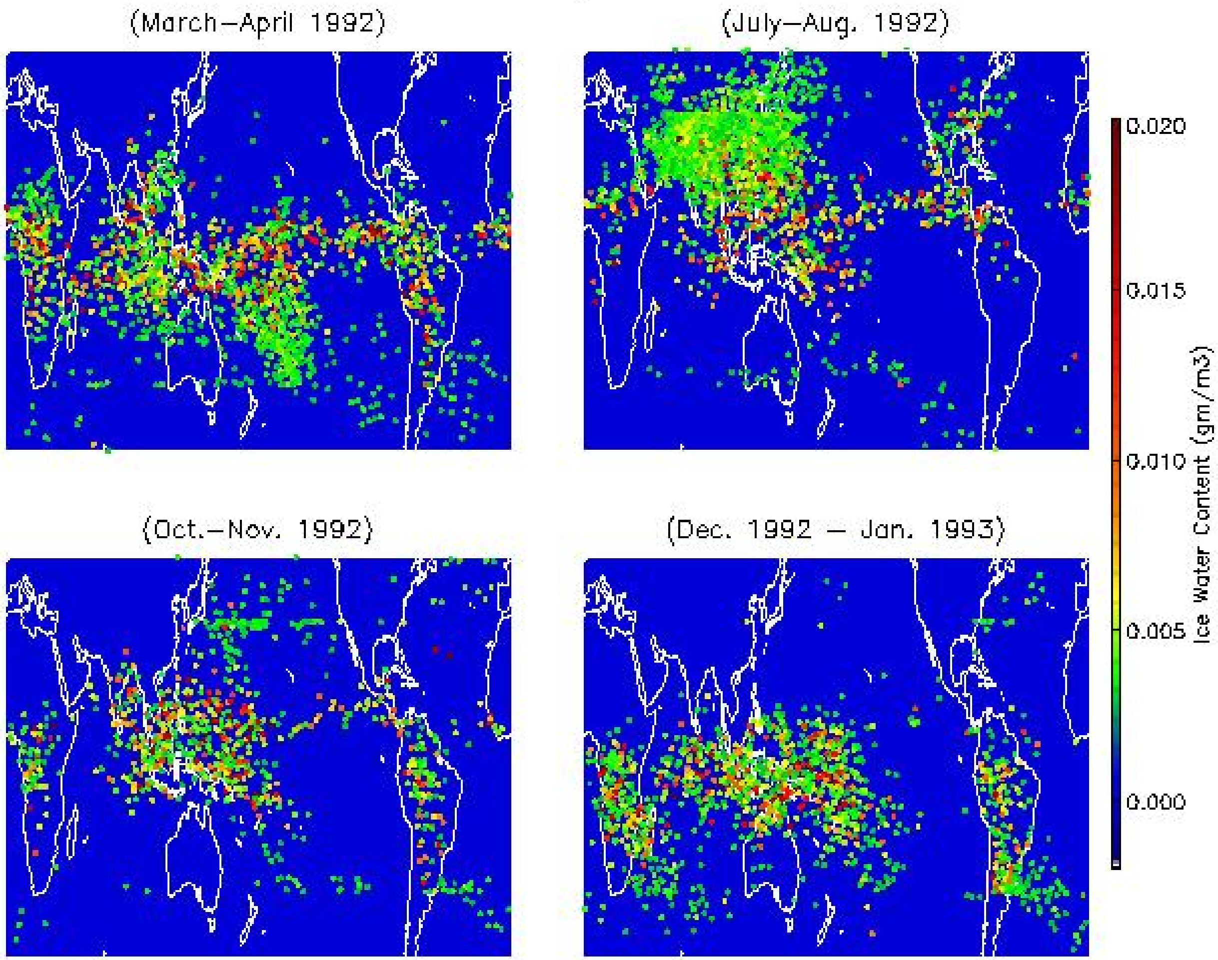
See Read et al: 'UARS MLS upper tropospheric humidity measurement: Method and validation' [JGR, in press (available at http://mls.jpl.nasa.gov)]



Near-tropopause cloud ice obtained from UARS MLS measurements of continuum at 186 and 203 GHz

This image by D.L. Wu [Waters et al., *JAS 56*, 194, 1999] shows initial results of cloud ice at 100 hPa retrieved using continuum emission at 186 and 203 GHz

Cloud ice is a prime target for measurement by EOS MLS



Current & Near-term Microwave Atmospheric Measurements (1)

- **green indicates spectral lines for which specroscopic parameters are not thought to limit measurement accuracy, or there is no identified way of improving existing accuracy of these parameters**
- ***red indicates lines (and continua) for which inadequate spectroscopic parameters are known to limit measurement accuracy, and there are identified or expected ways by which better parameters can be obtained***

molecule, spectral line frequency (in GHz)	ground based	aircraft and/or balloon-based	satellite-based UARS MLS (1991-2001)	MAS (3/92, 11/94)	Odin (2001 -)	EOS MLS (2003 -)	SMILES (2005 -)	comments
O_2								
60-65			♦	♦				
118.8					♦	♦		
487.2					♦			**line broadening parameters needed?**
2502.3		♦				♦		***line broadening parameters needed***
continuum		♦	♦			♦		***needed (+ N_2 cont) for trop H_2O, cloud ice measurements***
H_2O								
22.2	♦							
183.3			♦	♦		♦		
488.5, 556.9					♦			**line broadening parameters needed?**
2531.9		♦				♦		***line broadening parameters needed***
continuum		♦	♦			♦		***needed for tropospheric H_2O & cloud ice measurements***
O_3								
184.4			♦	♦				
206.1			♦			♦		
235.7, 237.1						♦		***primary lines for measuring tropospheric ozone***
239.1						♦		***better line broadening parameters needed***
242.3, 243.5						♦		
278.	♦							**line broadening parameters needed?**
486-504					♦			**line broadening parameters needed?**
541-581					♦			**line broadening parameters needed?**
625.4		♦				♦	♦	***broadening parameters w.req'd accuracy recently measured by B. Drouin***
2509.6		♦				♦		***line broadening parameters needed***

Current & Near-term Microwave Atmospheric Measurements (2)

- **green indicates spectral lines for which spectroscopic parameters are not thought to limit measurement accuracy, or there is no identified way of improving existing accuracy of these parameters**
- ***red indicates lines (and continua) for which inadequate spectroscopic parameters are known to limit measurement accuracy, and there are identified or expected ways by which better parameters can be obtained***

molecule, spectral line frequency (in GHz)	ground based	aircraft and/or balloon-based	satellite-based					comments
			UARS MLS (1991-2001)	**MAS** (3/92,11/94)	**Odin** (2001 -)	**EOS MLS** (2003 -)	**SMILES** (2005 -)	
$H_2{}^{18}O$								
203.4	◆							**UARS and EOS MLS detect wing of this line**
547.8					◆			**line broadening parameters needed?**
HDO								
209.9	◆							**line broadening parameters needed?**
486.5					◆			**line broadening parameters needed?**
OH								
2509.9, 2514.3		◆				◆		***line broadening parameters needed***
HCl								
625.9		◆				◆	◆	***broadening parameters w.req'd accuracy recently measured by B. Drouin***
CO								
230.5	◆					◆		***line broadening parameters needed***
576.3					◆			**line broadening parameters needed?**
N_2O								
201.0	◆					◆		
552.5, 577.6					◆			**line broadening parameters needed?**
652.8						◆		
ClO								
204.4	◆		◆	◆		◆		
278.6	◆							
575.4					◆			
649.5		◆				◆	◆	

Current & Near-term Microwave Atmospheric Measurements (3)

- **green indicates spectral lines for which specttoscopic parameters are not thought to limit measurement accuracy, or there is no identified way of improving existing accuracy of these parameters**
- ***red indicates lines (and continua) for which inadequate spectroscopic parameters are known to limit measurrment accuracy, and there are identified or expected ways by which better parameters can be obtained***

molecule, spectral line frequency (in GHz)	ground based	aircraft and/or balloon-based	satellite-based					comments
			UARS MLS (1991-2001)	MAS (3/92, 11/94)	Odin (2001 -)	EOS MLS (2003 -)	SMILES (2005 -)	
HCN								
177.3						♦		***line broadening parameters needed***
265.9	♦							***line broadening parameters needed***
SO_2								
200.8						♦		***line broadening parameters needed***
204.2			♦			♦		
624.9, 625.8							♦	***line broadening parameters needed***
626.2, 649.2							♦	***line broadening parameters needed***
660.5, 660.9						♦		***line broadening parameters needed***
HNO_3								
181.6						♦		
206.6			♦			♦		**UARS MLS measured HNO3 from wing emission of this line**
269.2	♦							
494					♦			**line broadening parameters needed?**
624.6, 650.3							♦	**line broadening parameters needed?**
CH_3CN								
183.9						♦		***line broadening parameters needed***
202.3			♦			♦		***line broadening parameters needed***
624.8, 626.4						♦		***line broadening parameters needed***

Current & Near-term Microwave Atmospheric Measurements (4)

- green indicates spectral lines for which spectroscopic parameters are not thought to limit measurement accuracy, or there is no identified way of improving existing accuracy of these parameters
- *red indicates lines (and continua) for which inadequate spectroscopic parameters are known to limit measurement accuracy, and there are identified or expected ways by which better parameters can be obtained*

molecule, spectral line frequency (in GHz)	ground based	aircraft and/or balloon-based	satellite-based					comments
			UARS MLS (1991-2001)	MAS (3/92, 11/94)	Odin (2001 -)	EOS MLS (2003 -)	SMILES (2005 -)	
HO_2								
265.8	♦							line broadening parameters needed?
579.8, 579.9					♦			line broadening parameters needed?
649.7						♦	♦	*broadening parameters w.req'd accuracy recently measured by B. Drouin*
660.5						♦		*line broadening parameters needed*
HOCl								
625.1						♦	♦	*line broadening parameters needed*
635.9						♦		*line broadening parameters needed*
^{81}BrO								
624.8, 650.2						♦	♦	*broadening parameters w.req'd accuracy recently measured by B. Drouin*
H_2O_2								
204.5			♦					
571.8					♦			line broadening parameters needed?
625.0							♦	line broadening parameters needed?
NO								
551.6					♦			line broadening parameters needed?
NO_2								
570.6					♦			line broadening parameters needed?
$O^{18}O$								
233.9						♦		*line broadening parameters needed*
$H^{37}Cl$								
625.0							♦	line broadening parameters needed?

Summary of Near-term Spectroscopy Needs (1)

- **Prioritized EOS MLS needs (see EOS Aura data validation plan)**
  - **Lab data and validated model for H_2O, O_2, N_2 continua absorption**
    - **work underway by Frank DeLucia and team**
  - **Collisional broadening parameters for following lines**

priority	*molecule*	*freq / GHz*	*comments*
1	BrO	624.8, 650.2	recently done by BJD/EAC (Brian Drouin / Ed Cohen)
1	HCl	625.9	recently done by BJD/EAC, along with 625.0 $H^{37}Cl$ line
1	HO_2	649.7, 660.5	underway/done by BJD/EAC
1	H_2O	2532	to be done by BJD/EAC
1	OH	2509, 2514	to be done by BJD/EAC
1	O_3	235.7, ..., 243.5	to be done by BJD/EAC
1		625 , 2509, 2543	done/to be done by BJD/EAC
1	O_2	2502	to be done by BJD/EAC
1	$O^{18}O$	233.9	to be done by BJD/EAC
2	CO	230.5	to be done by BJD/EAC
2	CH_3CN	183.9, ... , 660.7	to be done by BJD/EAC
2	HCN	177.3	to be done by BJD/EAC
2	HOCl	35.9	to be done by BJD/EAC
2	O_3	231.3, ..., 250.0	to be done by BJD/EAC
3	O_3	244.2, 247.8	to be done by BJD/EAC
3	SO_2	204.2, ..., 660.9	to be done by BJD/EAC

Summary of Near-term Spectroscopy Needs (2)

- **Projected needs for experiments other than EOS MLS**
  - Line broadening parameters for following (in alphabetical order)

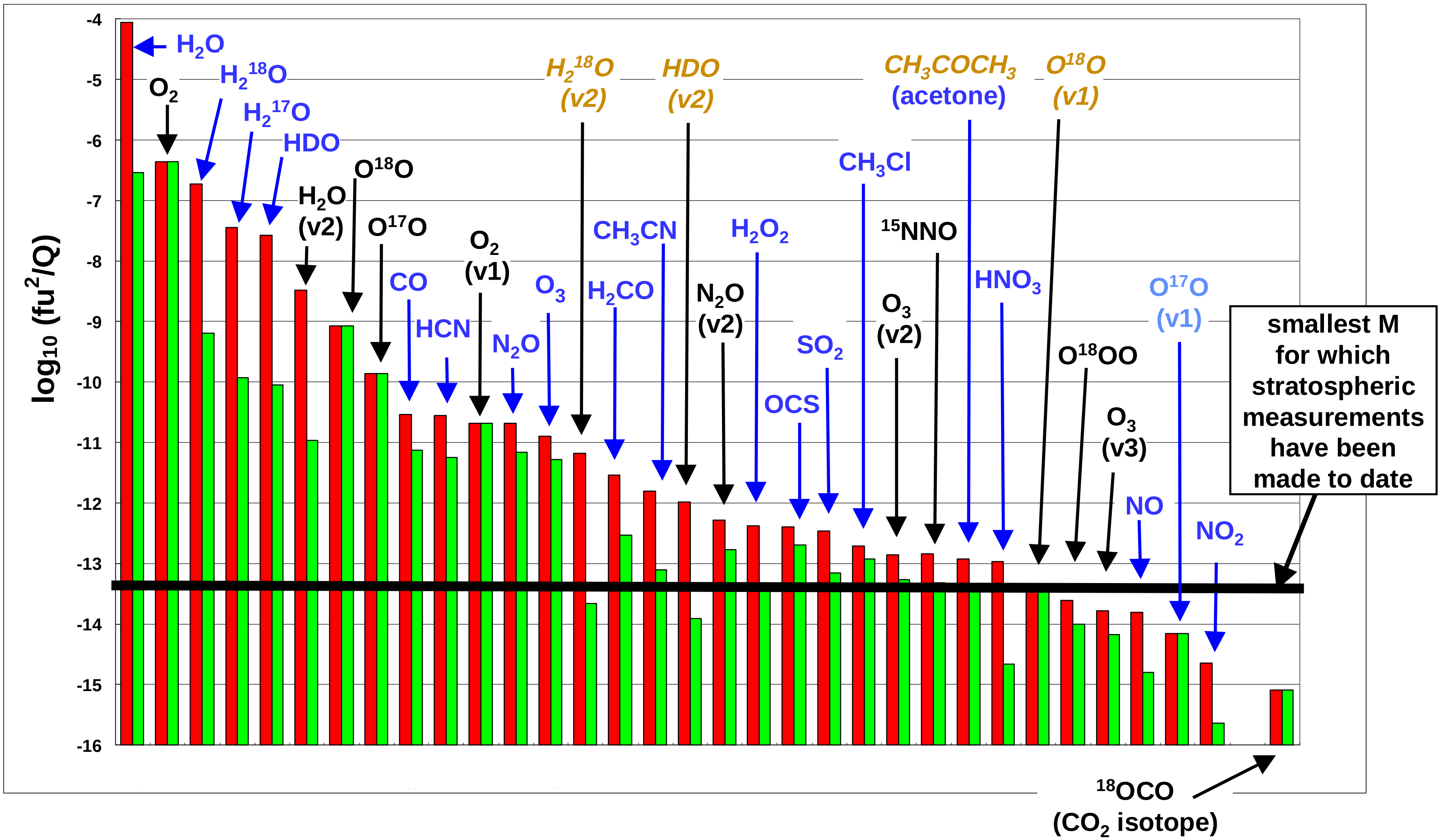
molecule	*freq / GHz*	*experiment*	*comment*
BrO	624.8, 650.2	SMILES	recently done BJD/EAC for EOS MLS
CO	576.3	Odin	
H_2O	488.5, 556.9	Odin	
$H_2{}^{18}O$	547.8	Odin	
HDO	486.5	Odin	
H_2O_2	571.8	Odin	
	625.0	SMILES	
$H^{37}Cl$	625.0	SMILES	recently done by BJD/EAC for EOS MLS
HNO_3	494	SMILES	
	624.6, 650.3	SMILES	also useful for EOS MLS
HOCl	625.1	SMILES	to be done by BJD/EAC for EOS MLS
HO_2	649.7, 660.5	SMILES	done /underway by BJD/EAC for EOS MLS
	579.8, 579.9	Odin	
NO	551.6	Odin	
NO_2	570.6	Odin	
N_2O	552.5, 577.6	Odin	
O_3	625.4	SMILES	recently done by BJD/EAC for EOS MLS
	486-504,541-581	Odin	some selected lines in these regions
SO_2	624.9, 625.8, ...	SMILES	also useful for EOS MLS

Likely Long-term Microwave Experiment Drivers

- **Continued stratospheric measurements**
  - with more efficient instruments
  - with (economical) flexibility for responding to new situations and needs
- **Better measurements for climate research**
  - especially in the upper troposphere
  - with better spatial resolution
- **Mid-upper tropospheric chemistry measurements**
  - applying MW ability to measure in/through ice, aerosol, smoke
  - applications for satellite, aircraft, ground-based instruments
    - regional-global issues for satellite
    - small-scale phenomena (e.g., burning, urban) for aircraft, ground-based

$\log_{10}$(M) for some mid-upper tropospheric species
(having spectral lines in the ~200-280 GHz range)

green bars are for minimum or typical abundances and T=225K
red bars are for maximum or polluted abundances and T=225K
blue font and arrows indicate desirable tropospheric measurements
brown italics indicate molecules that are not yet in JPL catalog



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Concept now being studied for a 3rd-generation MLS

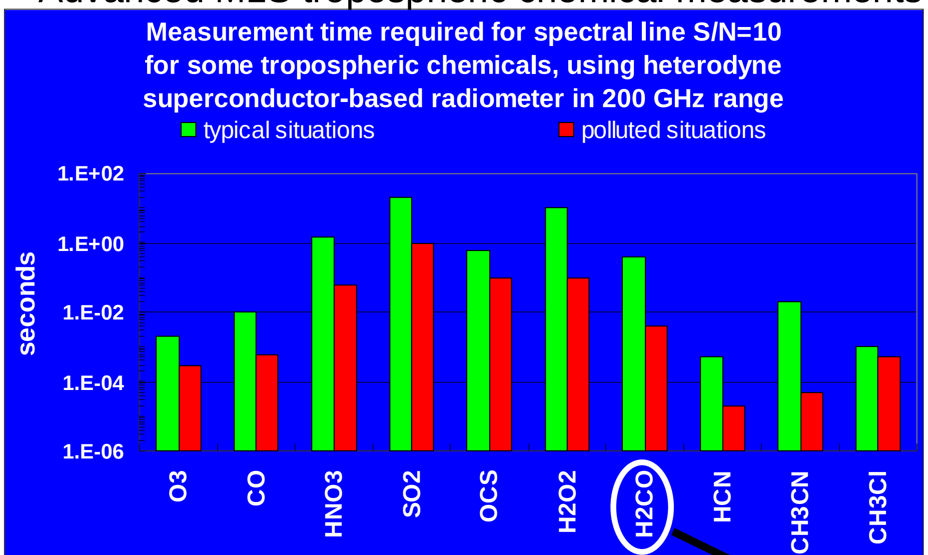
(probably to be proposed for a mission launching in ~2010)

- **Science Objectives**
  - **Continue MLS critical monitoring of stratospheric chemistry**
    - with improved precision
    - with in-orbit programmable measurement capability that
      - simplifies the instrumentation (e.g., fewer spectrometers required)
      - provides capability for efficiently responding to atmospheric events and evolving measurement priorities
  - **Continue MLS mid-upper trop H_2O, temperature and cloud-ice measurements for climate research**
    - with improved spatial resolution and precision
  - **New measurements for regional-global tropospheric chemistry issues**

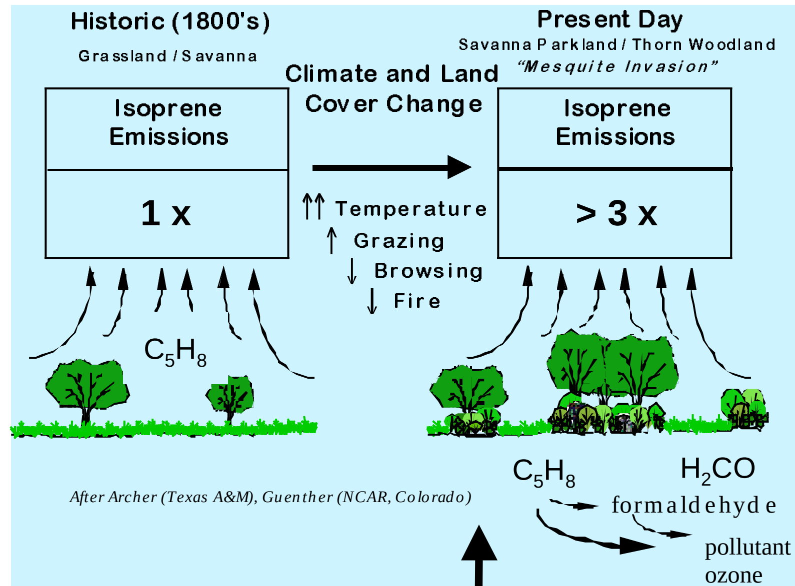
- **Instrument: 'Scanning MLS' (SMLS)**
  - FOV scans limb in both vertical and horizontal directions
  - Cooled radiometers
  - Programmable spectral coverage

Tropospheric chemistry: an important new application area for future microwave remote sensing

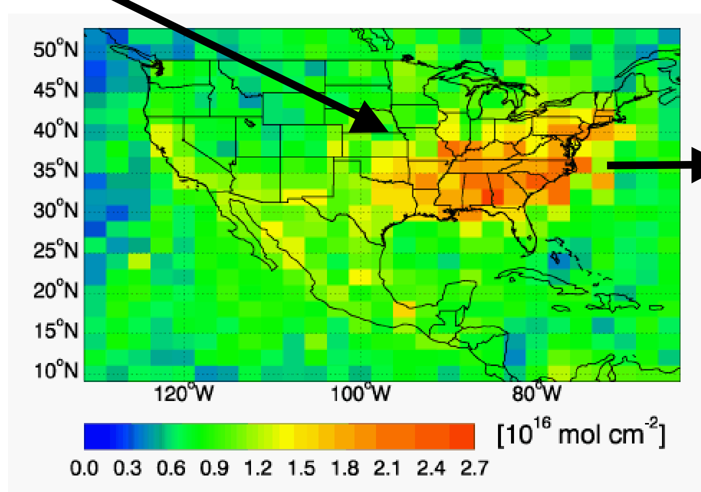
Advanced MLS tropospheric chemical measurements



Climate and land changes affecting chemistry



Formaldehyde (H_2CO), one of many tropospheric chemicals that can be measured by an advanced MLS. Maps at right are H_2CO columns measured by vis-near IR techniques. The MLS technique can provide improved spatial resolution, vertical profiles, and continuous day/night coverage. The enhanced abundances over southeast US are thought to arise, mainly, from isoprene (C_5H_8) emissions by oak forests.



Formaldehyde spotlights both ordinary pollution and natural emissions in an appropriate way

[Formaldehyde charts courtesy of Jack Kaye, NASA Hq.]

Some Projected Longer-term Spectroscopy Needs

- **Spectra that need adding to catalog**
  - **CH_3COCH_3 (acetone)** [**tropospheric measurement target]**
  - **$H_2{}^{18}O$ (v1)** [to determine its interference with targeted trop measurements]
  - **HDO (v2)** [to determine its interference with targeted trop measurements]
  - **$O^{18}O$ (v1)** [to determine its interference with targeted trop measurements]
  - extend spectra of several species (e.g., various states of HNO_3, H_2CO) to ~3 THz
  - others TBD

- **Linewidth parameters**
  - **$H_2{}^{18}O$** (203 GHz) **[$H_2{}^{18}O$ meas needed for near-tropopause dynamics issues]**
  - **HDO** (242 GHz) **[HDO meas needed for near-tropopause dynamics issues]**
  - **H_2CO** (252 GHz) **[tropospheric measurement target]**
  - **CH_3Cl** (239 GHz) **[tropospheric measurement target]**
  - **H_2O_2** (204, 252 GHz) **[tropospheric measurement target]**
  - **NO** (251 GHz) **[tropospheric measurement target]**
  - **OCS** (207 GHz) **[tropospheric measurement target]**
  - **HCN** (266 GHz) **[tropospheric measurement target]**
  - **CH_3COCH_3 = acetone** (200 GHz lines) **[potential trop measurement target]**
  - **atomic oxygen** (2.06 THz) **[stratospheric measurement target]**
  - **NO and NO_2** (lines in 2.0-2.5 THz range) **[stratospheric measurement targets]**
  - others TBD