Report on the 2001 San Diego Workshop on Molecular Spectroscopy for Atmospheric Sensing

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Purpose of the Molecular Spectroscopy Workshop:

- Review the status of current spectroscopic parameters for important atmospheric species
- Identify current and future spectroscopic needs for existing and planned atmospheric sensing technologies
- Prioritize the needs stemming from the above considerations
- Produce useful documentation as a guide for researchers in these fields

Organizers of 2001 San Diego Workshop

- Smithsonian Astrophysical Observatory
  - K. Jucks (Co-chair)
- NASA Headquarters
  - M. Kurylo
- Jet Propulsion Laboratory
  - L. Brown
- Computer Sciences Corporation
  - K. Thompson

History of Atmospheric Spectroscopy Workshops

- Workshop on Molecular Spectroscopy for Atmospheric Sensing, Oct. 23-26, 2001, San Diego, CA.

  http://www.aero.jussieu.fr/~sparc/News19/index.html, eds. Bhaswar Sen (JPL) and Ken Jucks (SAO)

- Spectroscopic Parameters for Upper Atmosphereic Measurements, Apr. 8-10, 1992, LaRC, Hampton, VA.

  http://atmoschem.jpl.nasa.gov/Sumry92Workshop_17Jul01.pdf, ed. Mary Ann H. Smith (LaRC)

- Spectroscopic Parameters for Upper Atmosphereic Measurements, Oct. 17-19, 1984, LaRC, Hampton, VA.

  NASA Conference Publication 2396, ed. Mary Ann H. Smith (LaRC)

- Spectroscopic Data for Measurements of Stratospheric Species, Oct. 29-30, 1979, LaRC, Hampton, VA.

  NASA Conference Publication 2136, eds. Aaron Goldman (Denver Univ.) and James Hoell (LaRC)

Reason for 2001 San Diego Workshop

Increasingly-sophisticated scientific questions addressed by in situ and remote sensing payloads have increased demands for higher precision, higher accuracy measurements:

- CO_2: precision: 0.1‰ ; accuracy: 0.3‰
  - Estimate spatial gradients in sources and sinks
- CO, CH_4: precision: 3‰
  - Estimate spatial gradients in sources and sinks
- δ(D)-HDO: precision: 10‰
  - Determine the processes that regulate upper tropospheric water vapor, and its' transport into the lower stratosphere

Improved spectroscopy of trace gases:

- Broadening parameters and its theoretical representation
- Line mixing and its theoretical representation
- Pressure-induced line shifts for ground-based measurements

http://atmoschem.jpl.nasa.gov

Workshop on Laboratory Spectroscopy Needs for Atmospheric Sensing

San Diego, California, 23-26 October 2001

Chair: Michael Kurylo, NASA / NIST
Organizer: Ken Jucks, SAO / Harvard, and Bhaswar Sen, NASA / JPL

The workshop provided a forum for discussion of a broad range of topics in laboratory spectroscopy required to meet
the needs of remote sensing and in-situ measurements of the Earth's atmosphere.

Invited talks focused on the various spectral regions: microwave, far infrared, near and mid-infrared, and ultraviolet/visible, as well as aerosols.

Poster sessions were held & displayed during the entire week.

Oral Presentations

Agenda | Conference Announcement | Previous Workshop Summary | Poster Sessions | Contact Information

Jet Propulsion Laboratory
California Institute of Technology
4800 Oak Grove Drive
Pasadena, CA 91009-8099

Feb. '02 Tom Wilson CL01-1611

Organization of 2001 San Diego Workshop

- Workshop was divided wavelength regions: microwave, far infrared, near and mid infrared, ultraviolet and visible.
- Separate session concentrating on aerosol spectroscopy.
- Each wavelength region had multiple sessions:

  oral session with two or more invited overview presentations

  poster session with presentations of specific laboratory and atmospheric sensing projects

  breakout groups charged with prioritizing the spectroscopic needs and desired precision of measurements.

  summaries presented by rapporteurs, followed by a final discussion

List of Overview Presenters/Rapporteurs

Aerosol presenters: Jim Sloan and Richard Neidzeila
Aerosol rapporteurs: Laura Iraci and Annmarie Eldering
Microwave presenters: Joe Waters and Frank Delucia
Microwave rapporteurs: Brian Druin and Bill Read
Far-IR presenters: Dave Johnson and Manfred Birk
Far-IR rapporteurs: Brenda Winnewisser and Marcos Sirota
IR presenters: Chris Webster, Peter Bernath, Jean-Marie Flaud, and Chris Benner
IR rapporteurs: Curtis Rinsland and Larry Rothman
UV/Vis presenters: Ernie Hilsenrath and Johannes Orphal
UV/Vis rapporteurs: Stan Sander and Klaus Pfeilsticker

http://atmoschem.jpl.nasa.gov/Oral_Presents.htm

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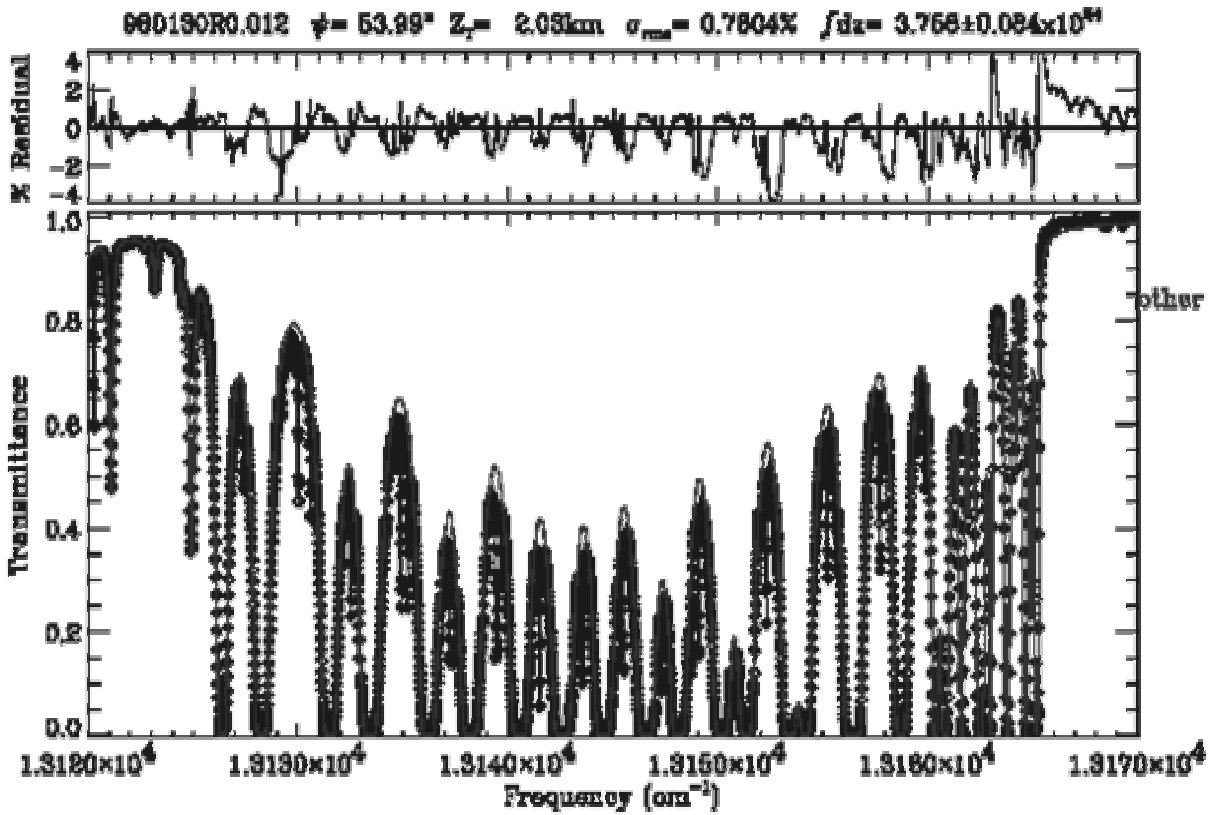
Oral Presentations	
Laboratory Studies of Aerosol Optical Properties R. F. Niedziela	**Prerequisites, Progress & Prospects: Determining Atmospheric Aerosol Chemical Composition by Remote Sensing** J.J. Sloan, A. Zassetski & T. Kurosu
IR and Near-IR Remote Sensing of the Atmosphere Peter Bernath	**Mid-IR and Near-IR in Situ Instrument Needs** Christopher Webster
Far-IR Spectroscopy Needs: Instrument Focus David G. Johnson	**Remote Sensing in the Far-IR** Manfred Birk
Microwave Spectroscopy and the Remote Sensing Problem Frank De Lucia	**Microwave Spectroscopic Atmospheric Sensing Needs** Joe Waters

Line Shape Error in O_2 A-Band (Q-R Branch) ?

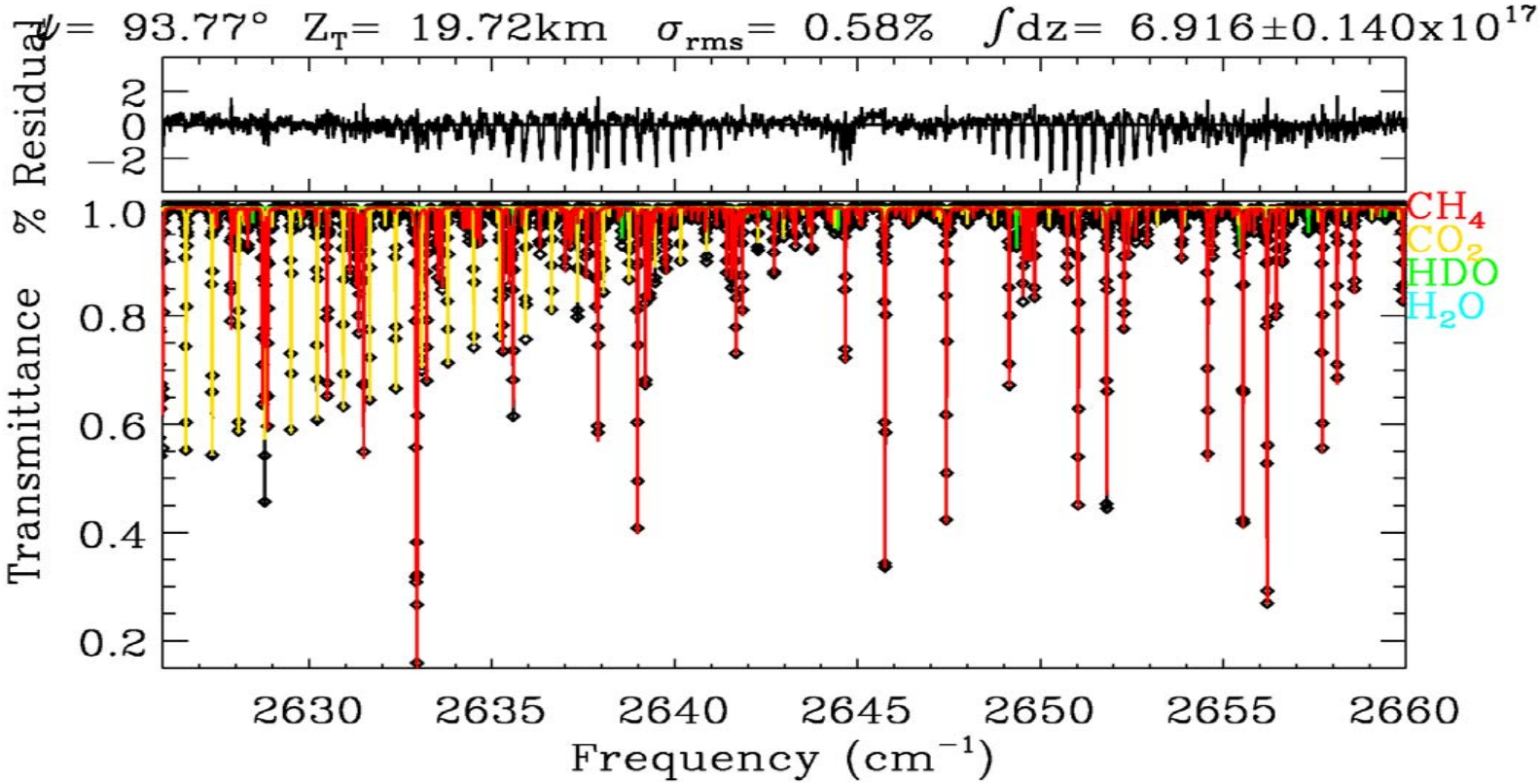
Kitt Peak spectrum taken on 980130. Diamonds are the measurements and the solid line is calculation using Voigt lineshape. Zero level offset and near ground temperature offset are fitted to minimize the residual. Amount of O_2 is fixed to atmospheric truth. O_2 A-band is important for determination of corrections for aerosols, clouds, and surface pressure.



Courtesy Z. Yang, CIT

Missing $2\nu_4$ band of HNO_3 ?

MkIV balloon spectra in the 2620-2660 cm^{-1} region show the presence of systematic residuals, that appear to exhibit P, Q, and R-branches. These residuals are up to 3% deep in spectra measured from Esrange, Sweden. in 991203. The presence of these residuals can cause problems in fitting gases (e.g. HDO, HBr, H_2S, CO_2 isotopologues) in this region.

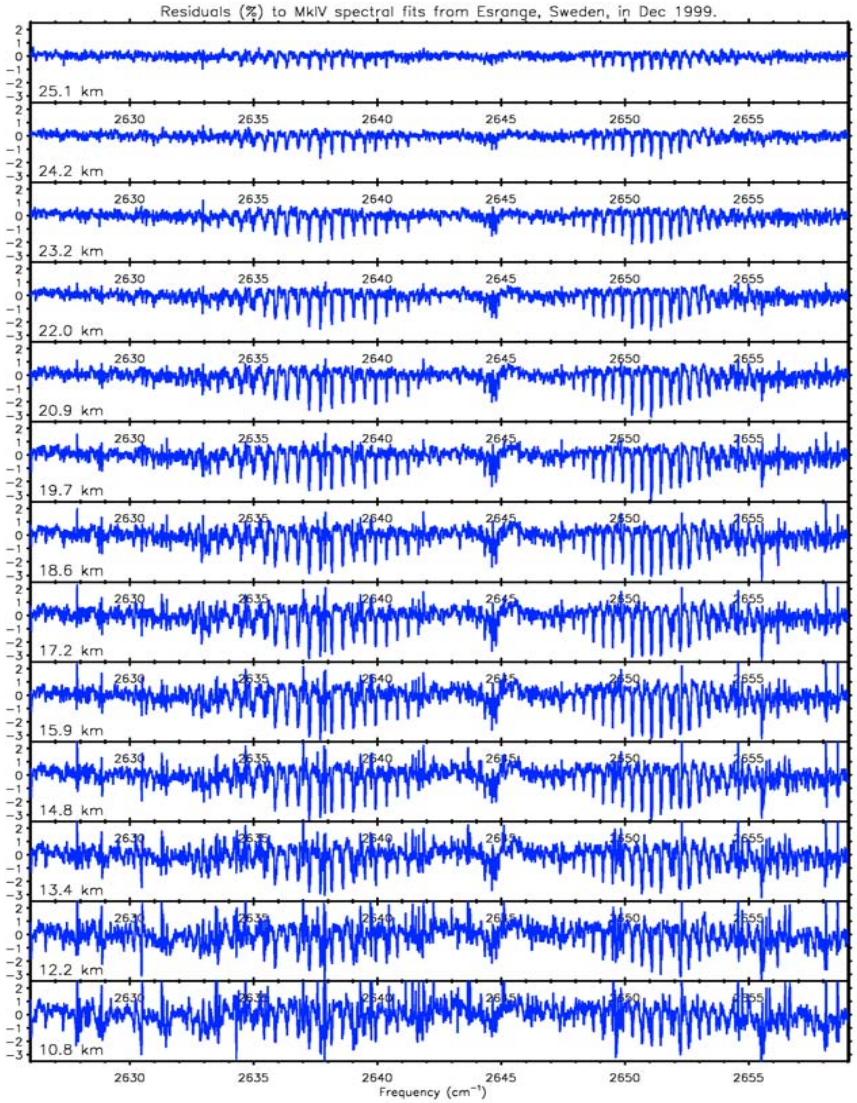


Missing $2\nu_4$ band of HNO_3 ?

The altitude variation of the depths of these residuals confirms that the concentration of the responsible absorber peaks in the lower strato-sphere at ~16 km.

HNO_3 is the most likely candidate since the band looks like the longer wavelength HNO_3 bands and each of the absorption dips is a manifold containing several lines. Since the HNO_3 ν_4 band is centered at 1326 cm^{-1}, a possibility is the $2\nu_4$ band.

Courtesy G.C. Toon, JPL



San Diego Workshop Recommendation Molecular Spectroscopy Panel

The need for a recommendation panel for molecular spectroscopic parameters:

- An advisory group will comprehensively review and provide detailed specific recommendations for generating complete sets of parameters.
- Regularly report the status of the database to the atmospheric sensing and spectroscopic communities.
- Form and overview sub-panels for different spectral region and/or molecules.
- The sub-panels will set guidelines for:
  - spectroscopic data submission
  - level of scientific review
  - quantitative assessment of the quality of the data and uncertainties.

San Diego Workshop Recommendation
Water Vapor Spectroscopy

The need for improvements to the spectroscopy of water vapor over the entire electromagnetic spectrum:

- Water vapor absorbs strongly from the microwave through the visible and is a significant contributor to the radiative budget of the atmosphere, atmospheric photochemistry, and convective transport.
- Accurate spectroscopic parameters for water are very important. Potential solutions for accurate water vapor spectroscopy include:
  - improved rotational/vibrational coupled non-rigid-rotor models
  - performing laboratory spectroscopy with multiple wavelength regions
  - using atmospheric spectra directly in order to obtain longer pathlengths and colder temperatures

San Diego Workshop Recommendation Pressure-Broadening Coefficients

The need for more thorough investigation of temperature dependent pressure broadening line shapes and intensities:

Uncertainties in pressure broadening coefficients can have a significant impact on the retrievals of molecules for instruments with high spectral resolution.

Pressure broadening uncertainties also affect the use of line shape for the inference of altitude in nadir and zenith observations.

There is an immediate need for pressure broadening line shape information, especially for water vapor, at all wavelengths.

San Diego Workshop Recommendation
Specific Examples

Things Missing:

near and mid ir cross sections of tropospheric species

near ir absorbers, strengths and broadening parameters (O_3, CH_4,)

self-consistent set of aerosol refractive indices across all wavelengths

solar spectrum: 115 nm – 2.5 μm (spectral resolution: 0.05 cm^{-1})

Things that need Improving:

accurate μwave dipole measurements of minor isotopomers of H_2O and O_3, along with dipole observations of BrO and acetone

μwave, far, and mid ir continuum, both from H_2O and dry air

H_2O and its isotopomers (ir strength and broadening parameters)

HNO_3 (ir absolute strengths; hot bands)

O_3 (ir widths)

$ClNO_3$ (ν_6 band)

ir cross sections of hydrocarbons, replacement halocarbons

ternery solution refractive indices at polar stratospheric temperatures

http://www.aero.jussieu.fr/~sparc/News19/index.html

S P A R C

Stratospheric Processes And their Role in Climate

A project of the World Climate Research Programme

Home | Initiatives | Organisation | Publications | Meetings | Acronyms and Abbreviations | Useful Links

Report on the Workshop on Molecular Spectroscopy for Atmospheric Sensing San Diego, USA, 23-26 October, 2001

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Introduction

Remote sensing and *in situ* measurements play critical roles in developing an understanding of the chemistry and physics of the Earth's atmosphere and of its susceptibility to change as a result of natural and anthropogenic forcings. Improvements in laboratory spectroscopic measurements are required to meet the needs of these endeavours, particularly in light of the increasing demands of current sensing technology and of the increased accuracy and precision required to address current atmospheric science issues. Nevertheless, the laboratory spectroscopy needs for atmospheric sensing have not been assessed since the early preparations for the UARS (Upper Atmosphere Research Satellite) observatory [1]. Accordingly a workshop on Molecular Spectroscopy for Atmospheric Sensing was organised in San Diego, CA during October 23-26, 2001 (http://atmoschem.jpl.nasa.gov/). The workshop brought together laboratory molecular spectroscopists and investigators who use spectroscopic techniques to probe atmospheric processes to stimulate discussion, to define the needs of the atmospheric sensing community, and coordinate these needs with the current capabilities of laboratory spectroscopy. The programme was balanced between invited oral presentations, posters, and discussions of the issues raised.