

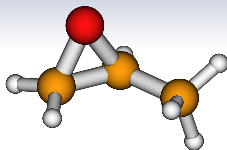
Infrared Spectra of Water Bending Bands of Propylene Oxide-Water Complexes: Sequential Solvation of a Chiral Molecule in Water

Xunchen Liu Yunjie Xu

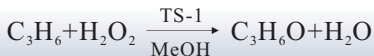
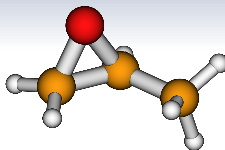
66th International Symposium on Molecular Spectroscopy

Department of Chemistry, University of Alberta, Edmonton, Canada, T6G 2G2

Propylene Oxide (PO)



Propylene Oxide (PO)

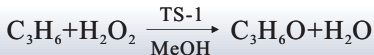
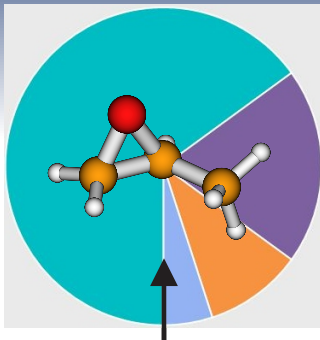


Hydrogen Peroxide to Propylene Oxide
(HPPO) production technology

4 Billion Pounds
Top 30 Chemicals

Propylene Oxide (PO)

Polyurethane (PU)

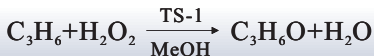


Hydrogen Peroxide to Propylene Oxide (HPPO) production technology

4 Billion Pounds
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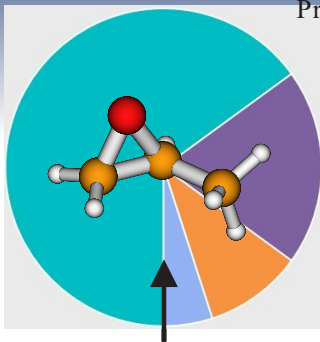
Propylene Oxide (PO)

Polyurethane (PU)



Hydrogen Peroxide to Propylene Oxide (HPPO) production technology

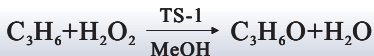
Propylene Glycol (PG)



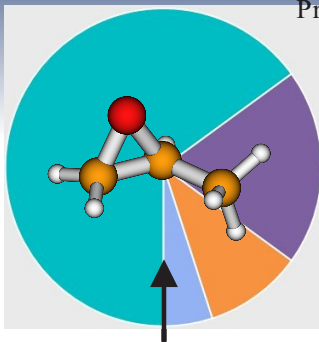
4 Billion Pounds
Top 30 Chemicals

Propylene Oxide (PO)

Polyurethane (PU)



Hydrogen Peroxide to Propylene Oxide (HPPO) production technology



Propylene Glycol (PG)



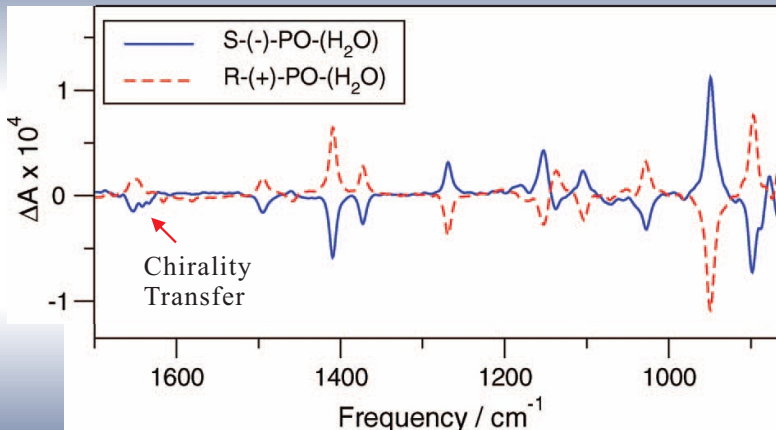
Propylene Glycol Ethers



4 Billion Pounds
Top 30 Chemicals

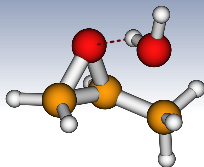
Chirality Transfer in Aqueous Solution

Optical activity from Water Bending

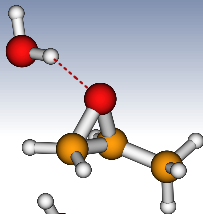




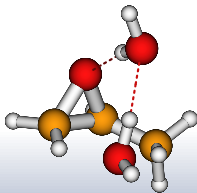
syn-dimer



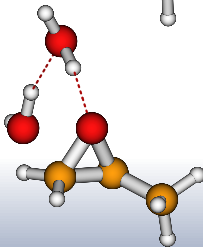
anti-dimer



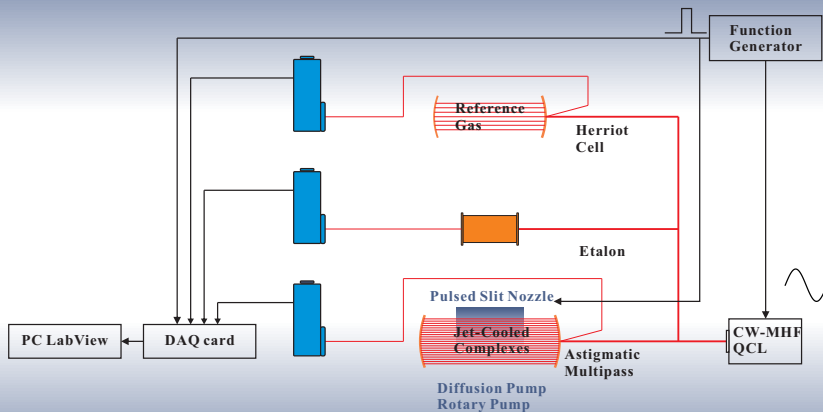
syn-trimer



anti-trimer

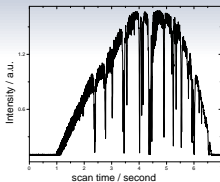
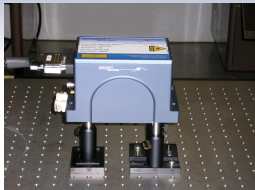


Quantum Cascade Laser Multipass Absorption Spectrometer

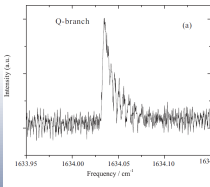
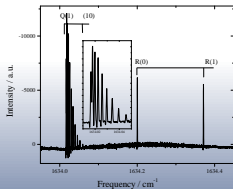


0.2% H₂O with 0.5% PO in 10 atm He backing gas

High Resolution Mid-IR Spectroscopy at $\text{H}_2\text{O } \nu_2$ Bending Region with External-Cavity Quantum Cascade Laser



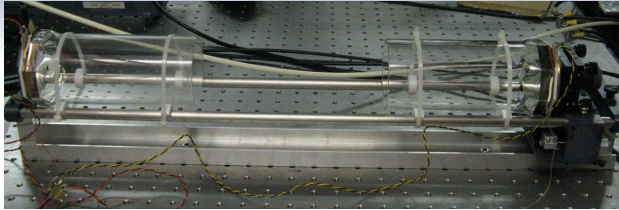
- continues-wave frequency broad coverage up to 100 cm^{-1}
- $< 0.001 \text{ cm}^{-1}$ line width



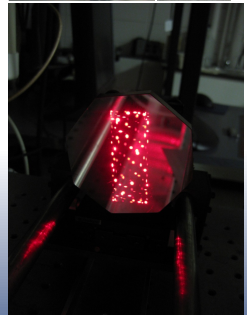
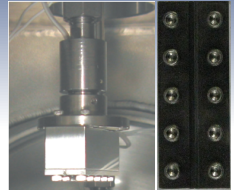
- MPA cell vs. cavity enhanced absorption cell
- rapid scan vs. wavelength modulation method

Astigmatic Multipass Cell

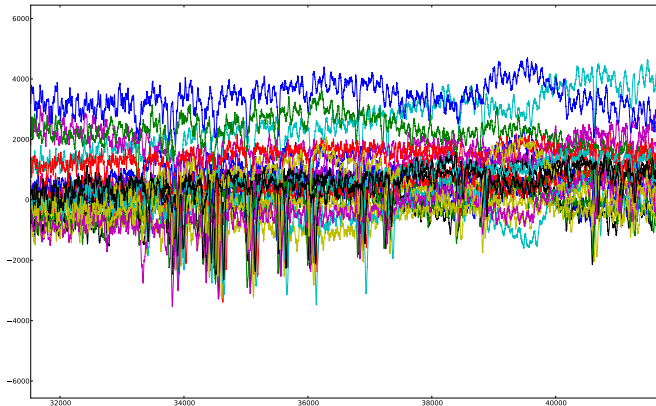
Supersonic Jet Expansion from Slit Nozzle



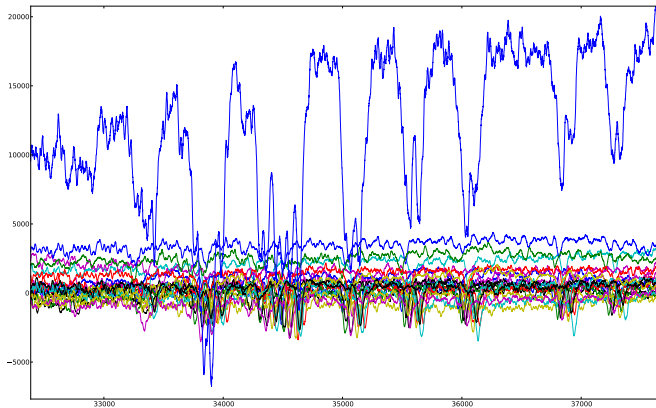
- Astigmatic multipass cell
mirror distance 55 cm, aligned for 366 passes
- supersonic jet expansion
home-made slit-nozzle



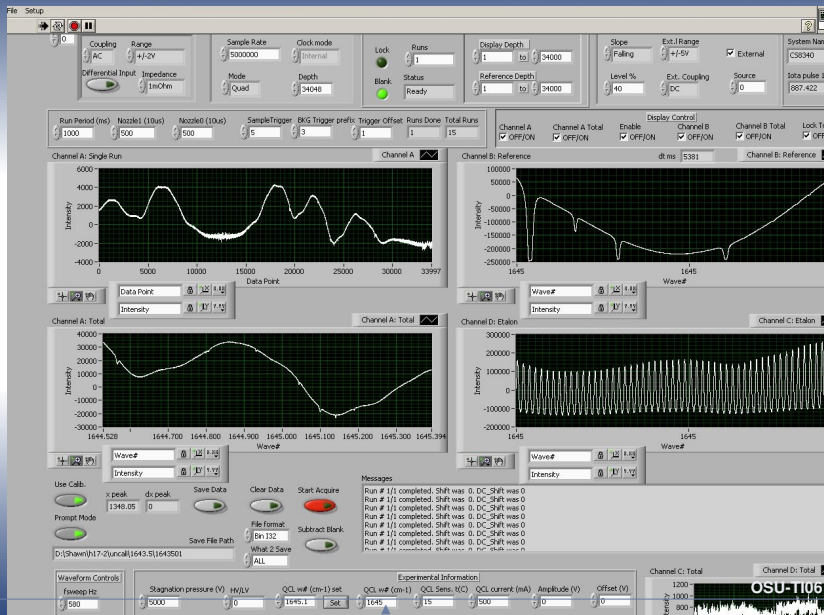
Frequency Drift of External Cavity Quantum Cascade Laser



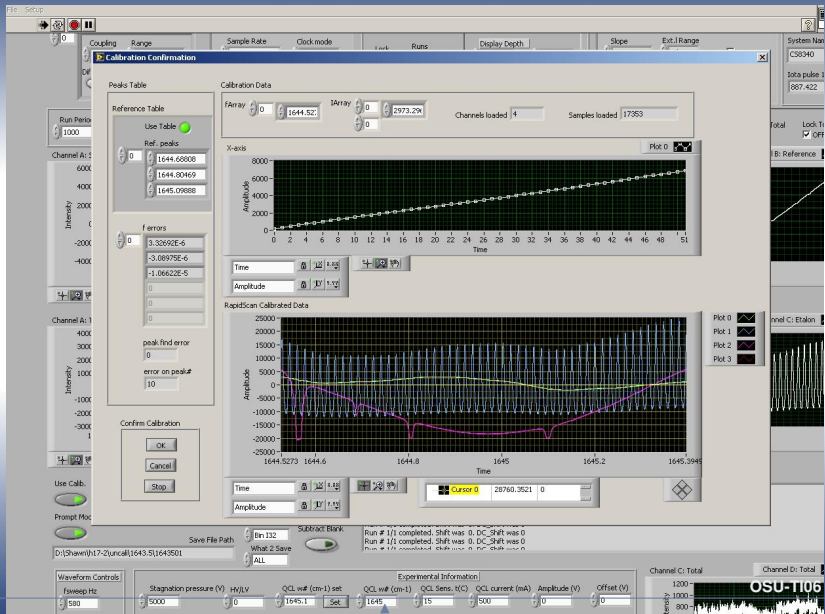
Frequency Drift of External Cavity Quantum Cascade Laser



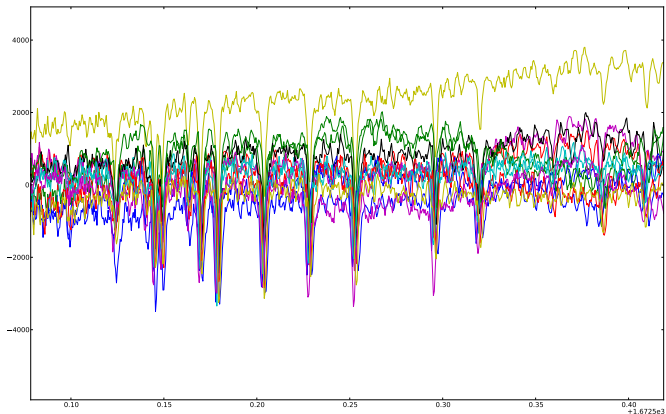
Calibration of Each Scan in LabView



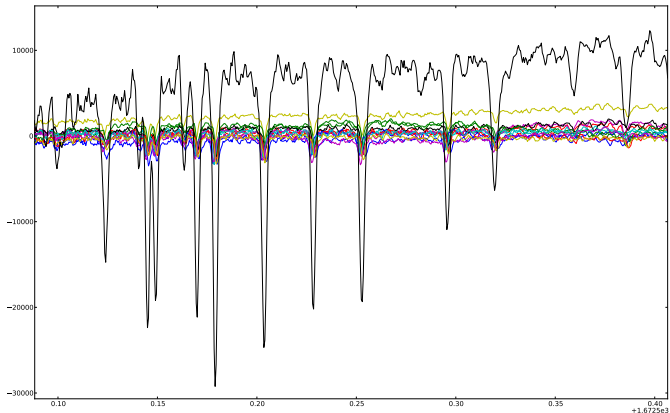
Calibration of Each Scan in LabView



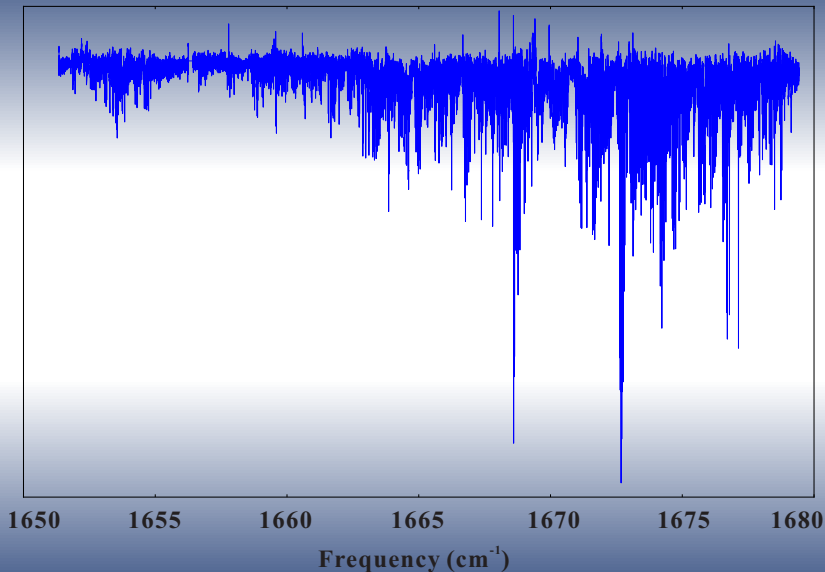
Improved Averaging



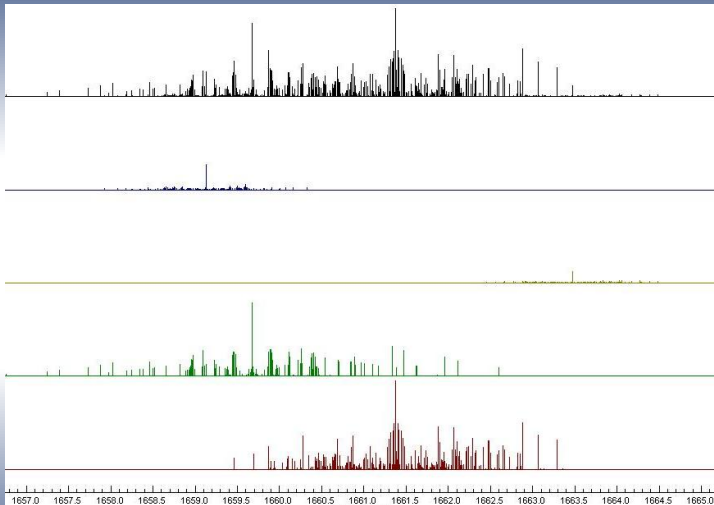
Improved Averaging



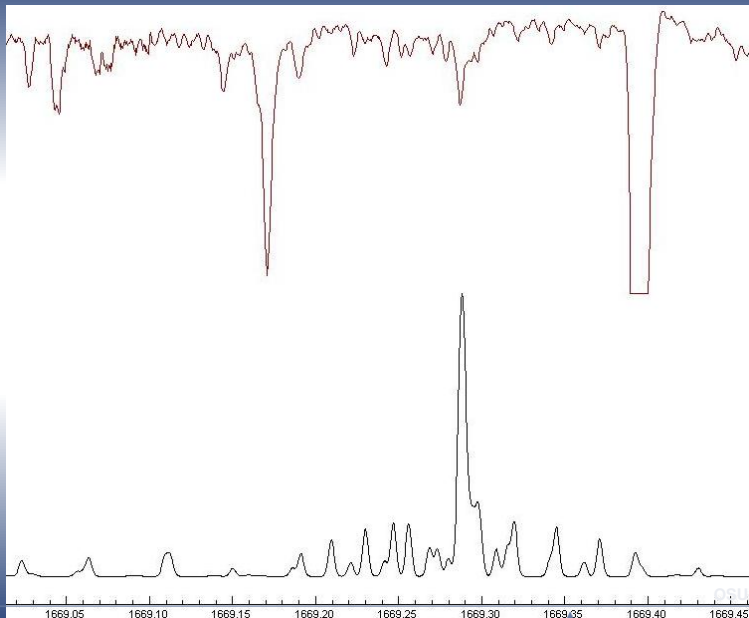
Infrared Spectrum 1650 cm^{-1} - 1680 cm^{-1}



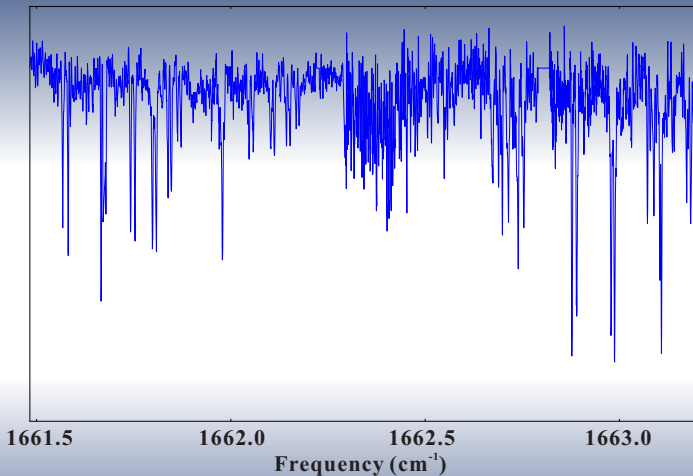
Simulation of *syn*- and *anti*-PO-(H₂O)_{1,2}



A Tentative Assignment



Doublets Features

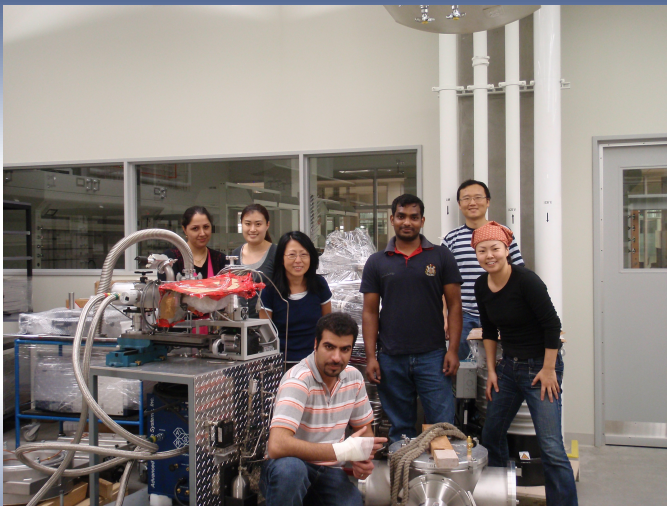


Methyl group internal rotation?

Summary and Future Work

- High resolution infrared spectra are measured for PO-H₂O complexes
- Fixing the laser head, and then measure the spectrum using new LabView program
- Implement the MW-IR double resonance components into the current spectrometer

Acknowledgement



Xu and Jäger groups

Thank you for
suggestion and comments