



UNIVERSITY OF COPENHAGEN



Spectroscopy and Reactions relevant to (Exo)Planetary Atmospheres

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PhD physics Odense, 1992;

Post doc Canada, 1992-1996

Lecture-Prof., Otago New Zealand, 1996-2009

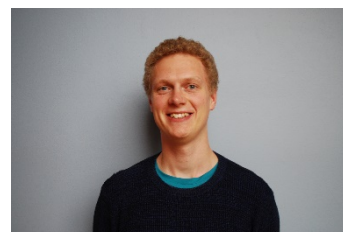
Prof., CHEM, KU, since 2009



Jing



Emil



Casper



Nanna



Research Focus

- **Experimental and theoretical spectroscopy of molecules (radicals) and molecular complexes.**

Vibrational, Rotational and Electronic spectra.

Theory: combine own codes + ab initio codes for potential and dipole surfaces

- **Theory of atmospheric (gas-phase) reactions.**

Bi-molecular and uni-molecular reactions.

Compare with experiments from other groups.



Leibniz Institute for
Tropospheric Research



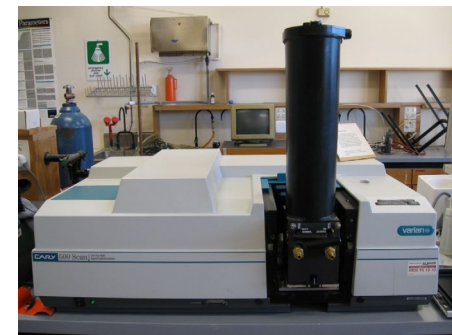
We often combine theory and experiment.

Spectroscopy - Experiments

- FT-IR & UV-vis Spectrometers**

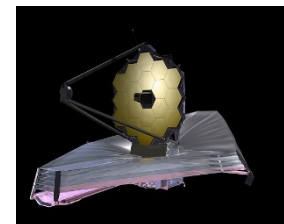
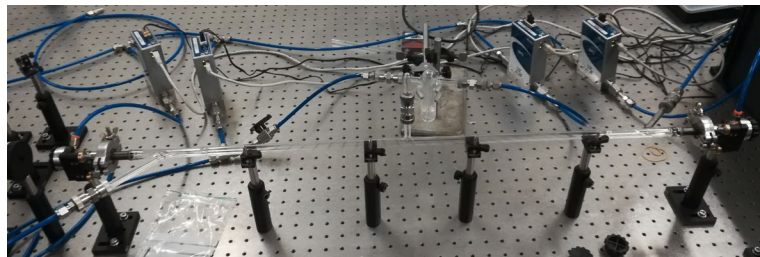
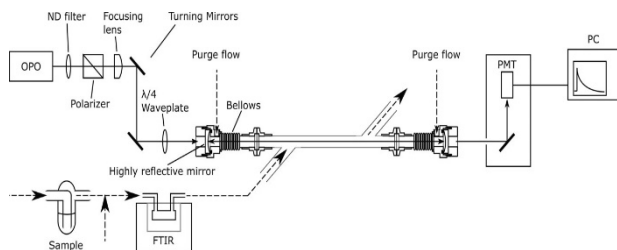


FT-IR, range 400-12000 cm^{-1}
 resolution down to 0.1 cm^{-1} .
 UV-vis, range $\sim 200\text{-}3000$ nm
 resolution about 0.01 nm.



Including variable pathlength (0.1-16 m) cells to increase signal

- Integrated CRD/FT-IR spectrometer (also PAS)**



Range $\sim 10000\text{-}16000$ cm^{-1} , resolution down ~ 5 cm^{-1} .

Very sensitive, equivalent to pathlength about 20 km signal

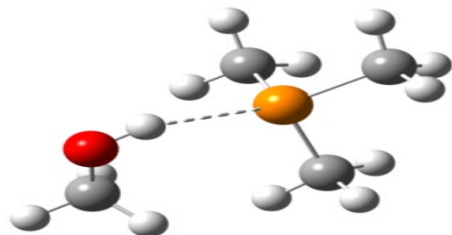


Spectroscopy - Experiments

- Matrix isolation cryostat**

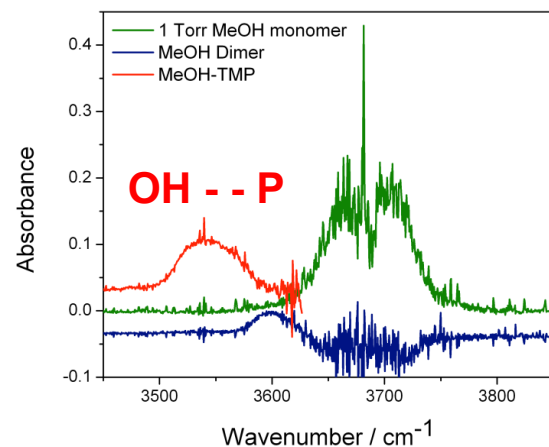
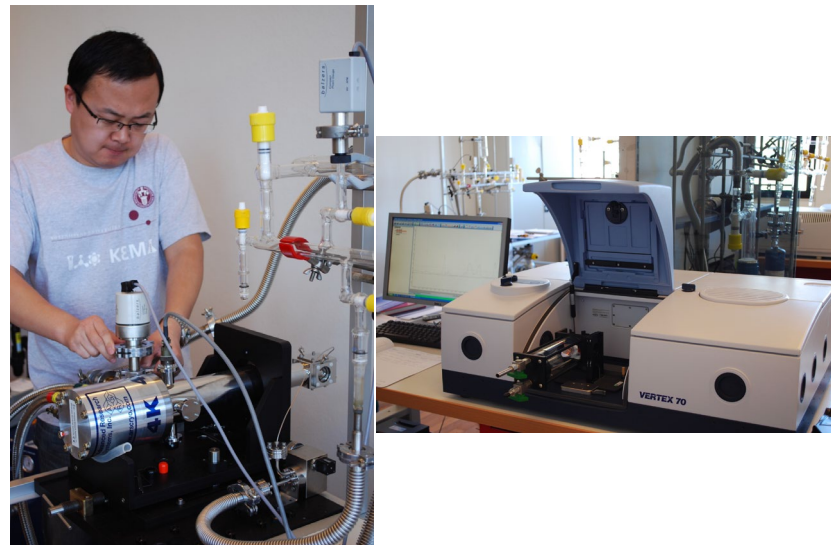
Sample down to about 10 K

Facilitate aggregation, complexes.



Discovered a new hydrogen bond ☺
OH - - P exist despite both H and P
having partial positive charge.

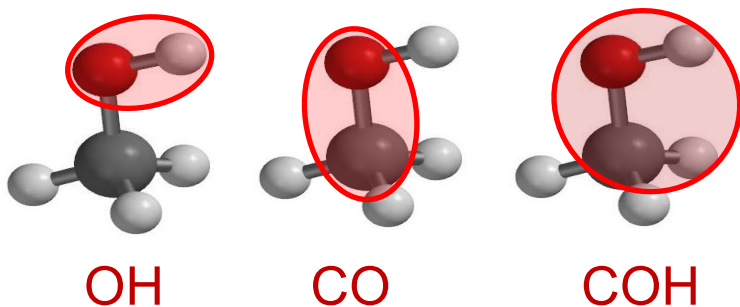
Calculated vibrational spectra, to
compare, identify and determine
strength of this hydrogen bonding.



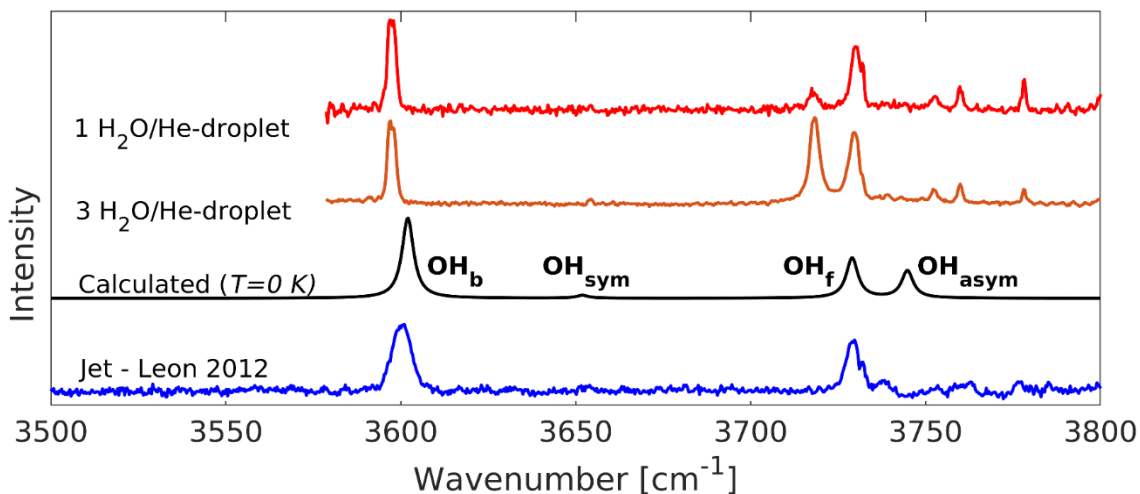
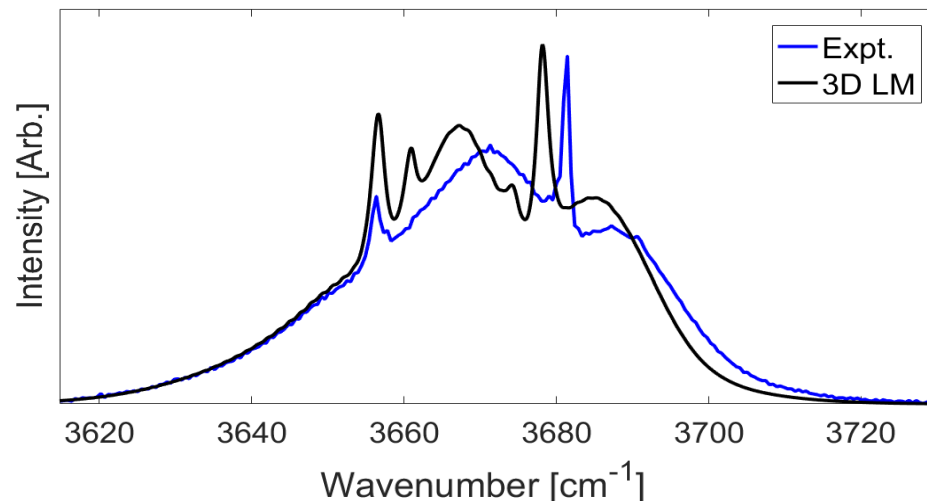
Spectroscopy - Theory

OH-stretching in alcohols

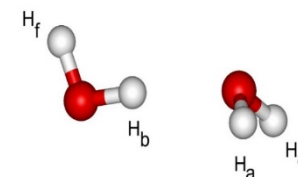
Include 3 local modes (LM),
reduced dimensionality



1-propanol – 5 conformers



Water Dimer 12D

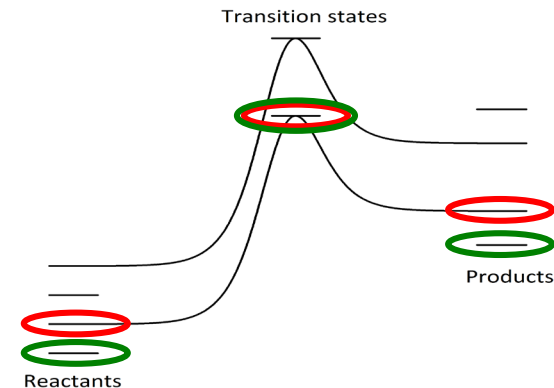


Water vapour continuum
Atmospheric absorption
of radiation.

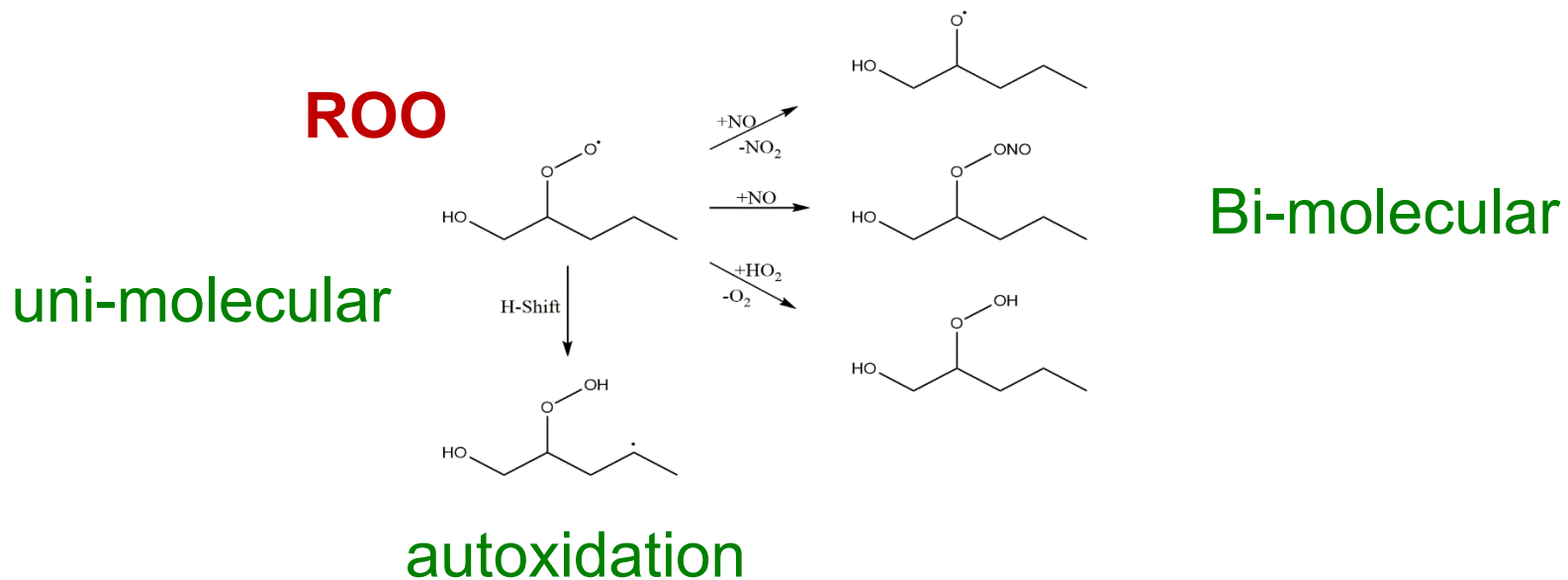


Reactions - Theory

Based on TST theory and use ab initio to get reaction surfaces and energetics

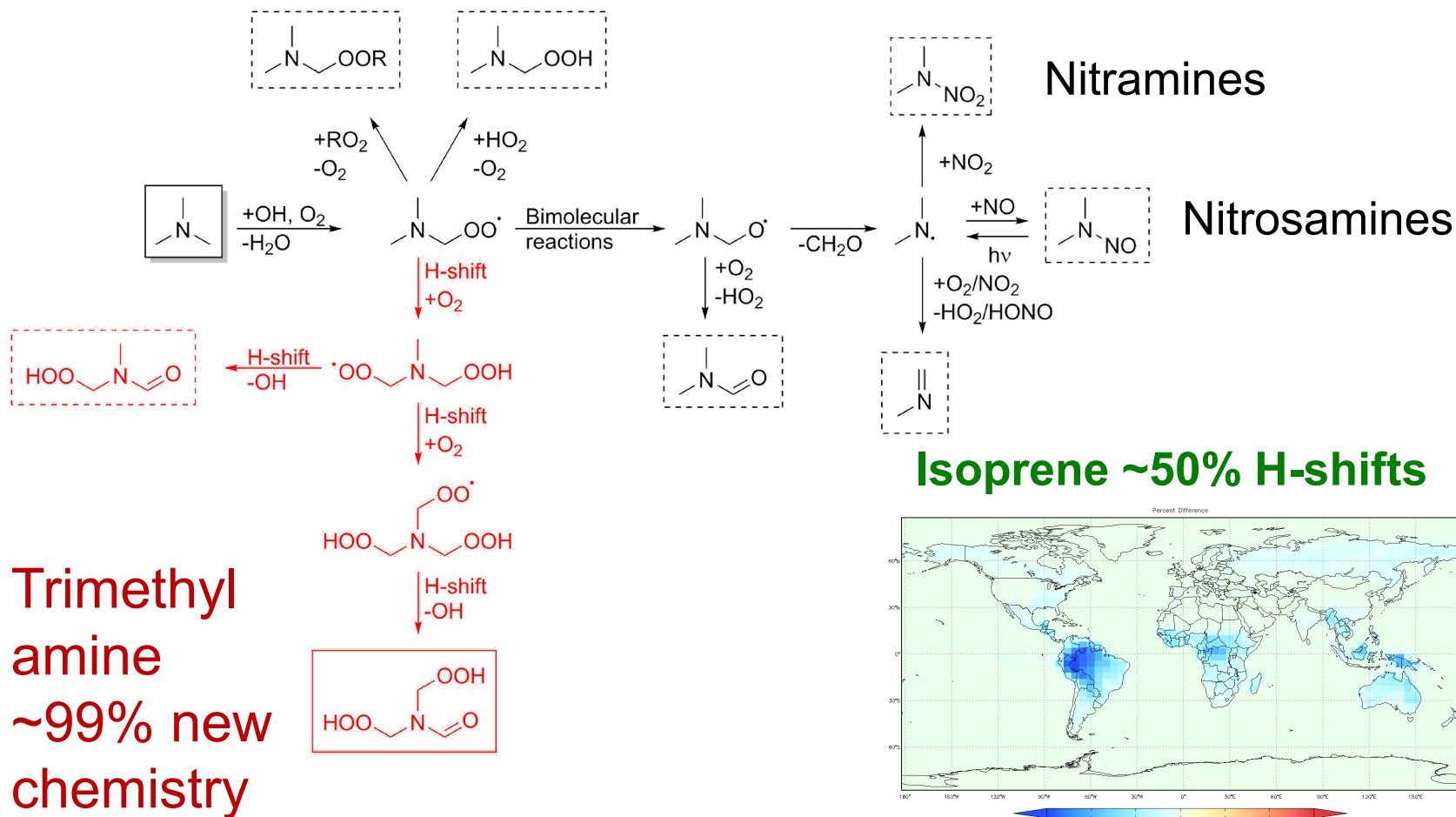


Oxidation reactions important in Earth's atmosphere

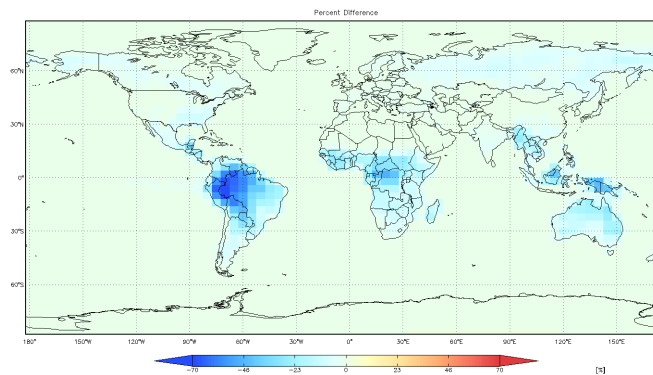


Amine Oxidation in the Atmosphere

Modeling existing and **find new chemistry** in atmosphere



Isoprene ~50% H-shifts



Recycling of OH



OSSO in the Venusian atmosphere

Atmospheric reaction mechanisms, rates and new compounds ☺

A new abundant sulfur oxide, OSSO, in the Venusian atmosphere.

