2D-IR Spectroscopy

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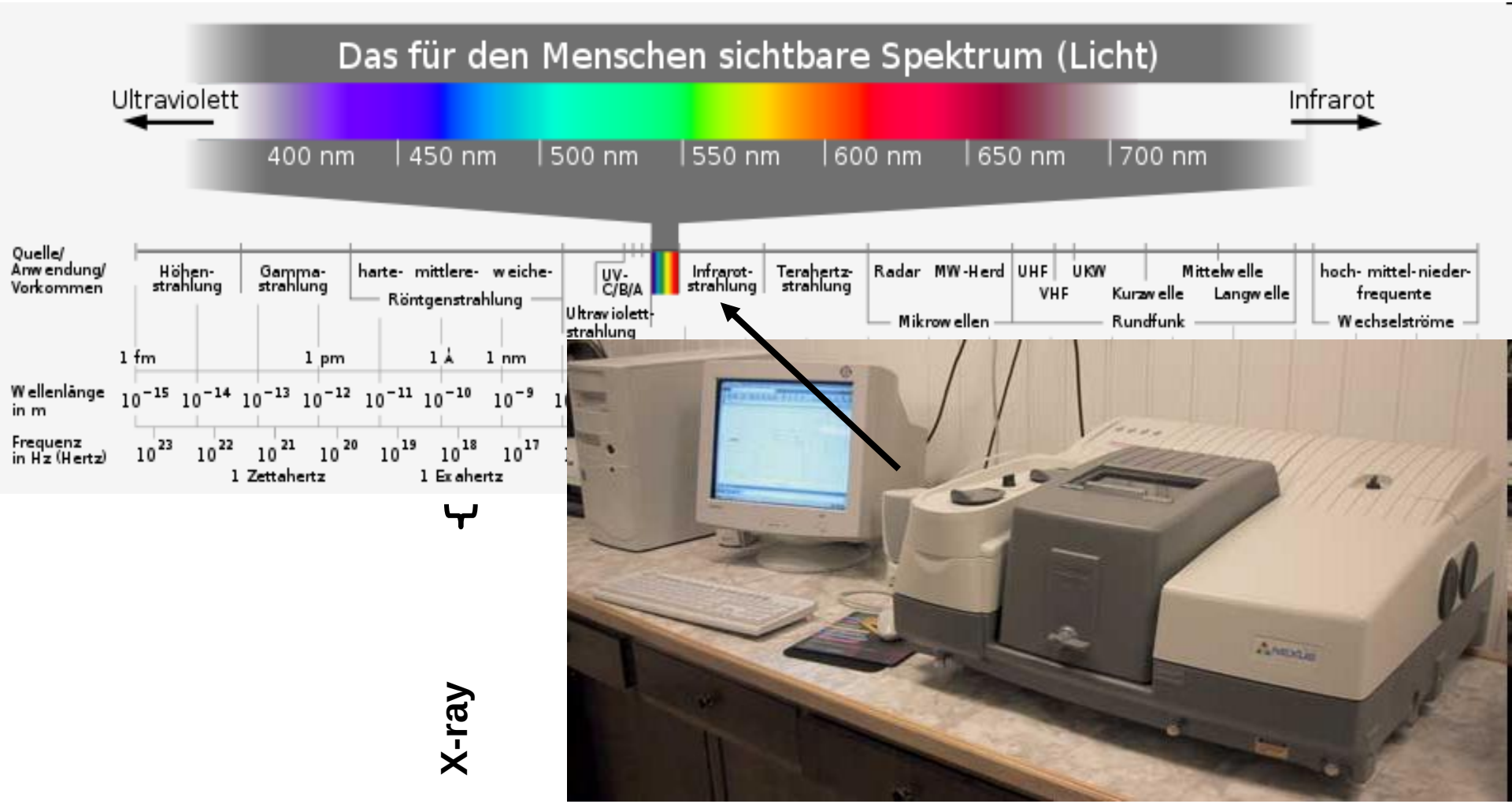
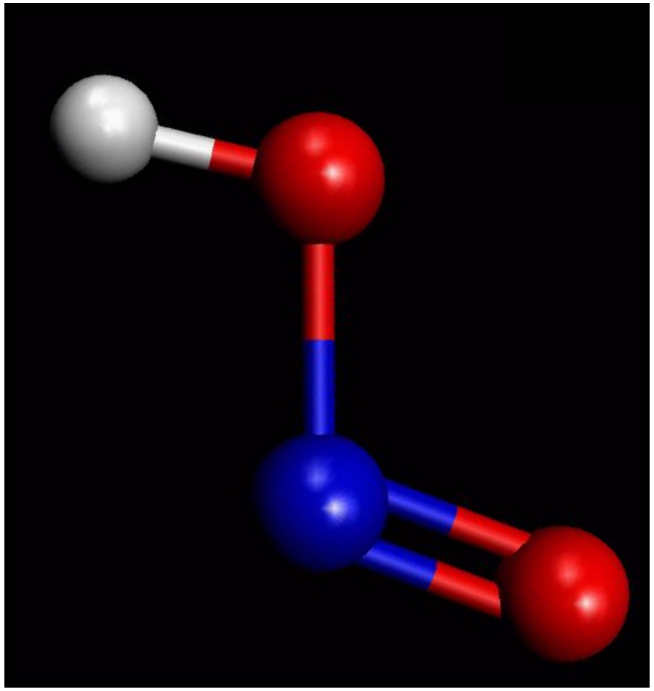
The Electromagnetic Spectrum

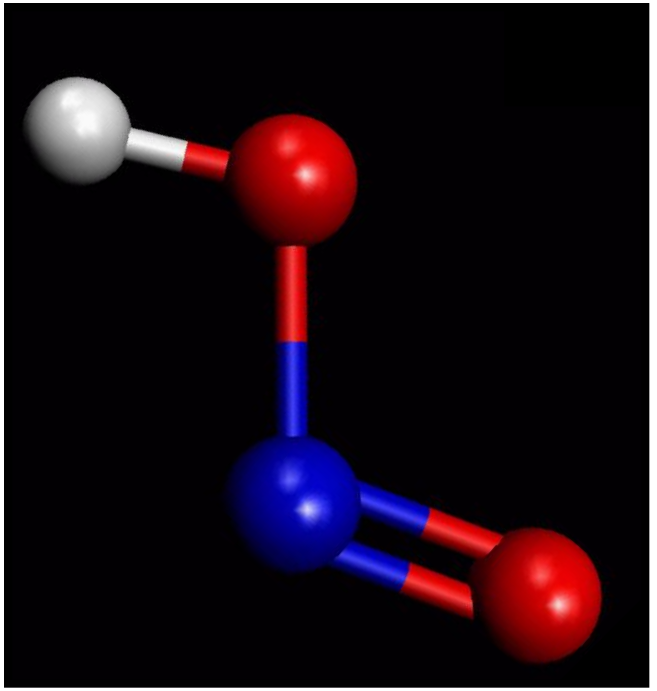


X-ray

Important for analytical and mechanistic studies in Molecular Sciences

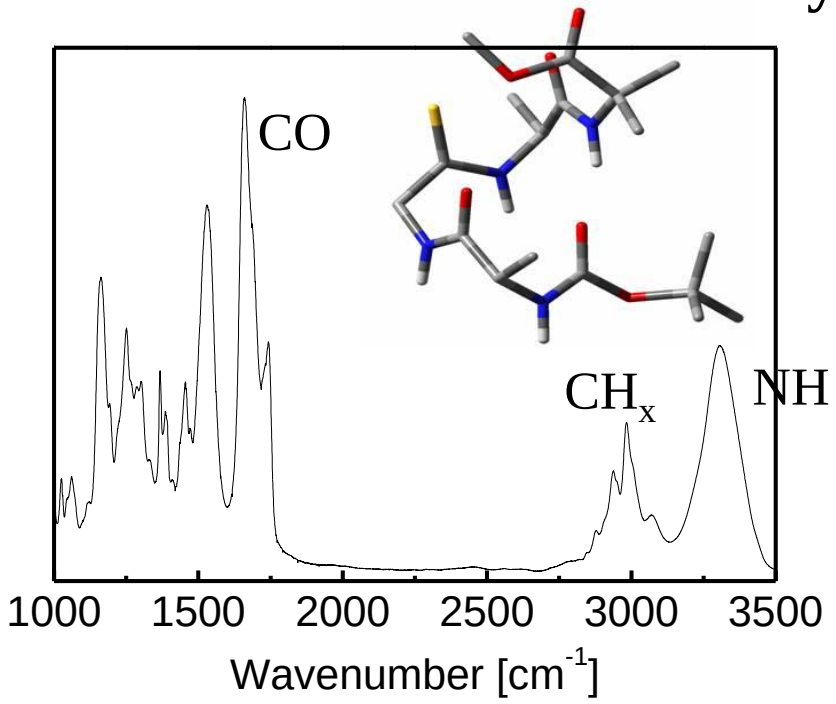
IR Spectroscopy: Vibrations of Molecules

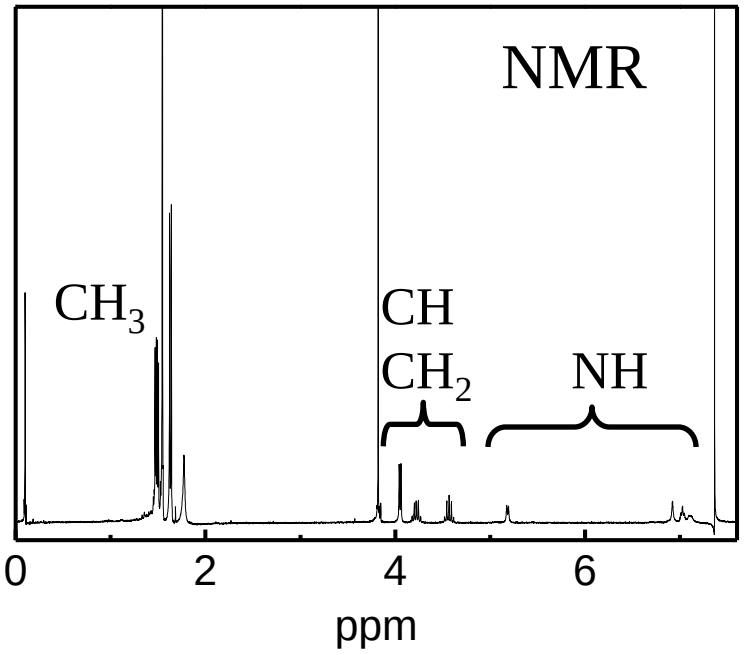




Vibrational *versus* NMR Spectroscopy

Boc-Ala-Gly-Ala-Aib-OMe



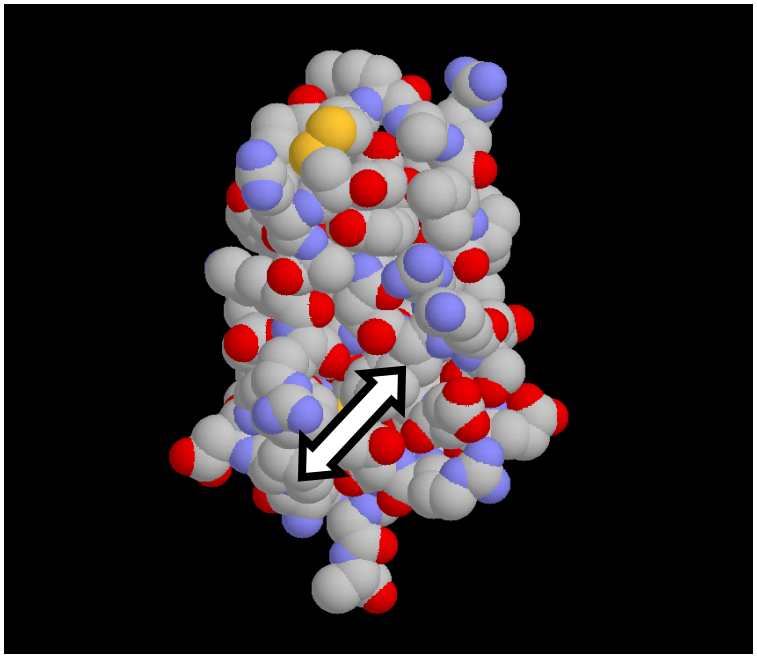


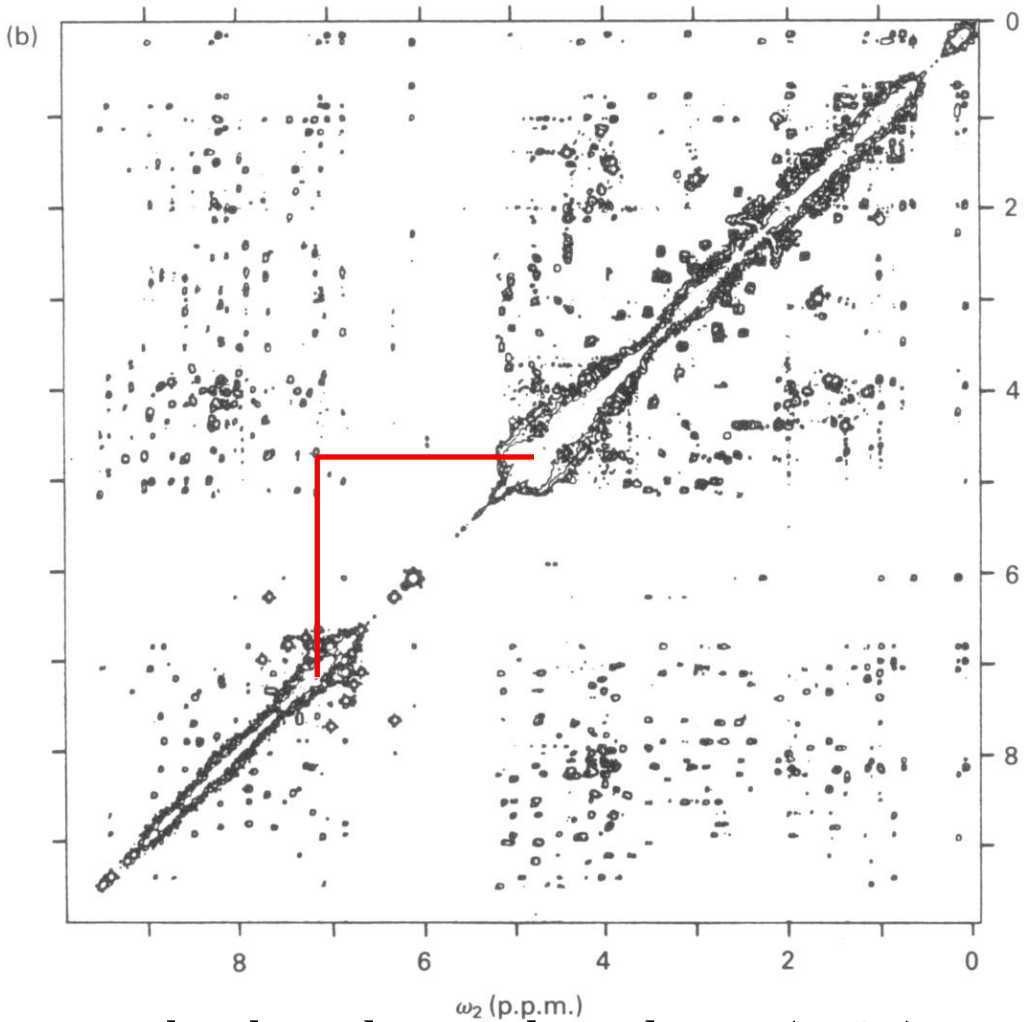
Principle information content:

- Certain molecular groups appear at certain frequencies
- Frequencies shifts and line broadening upon chemical environment
- Couplings reveal connectivity and 3D structure: (2D spectroscopy)

2D-NMR Spectroscopy

BPTI





Wüthrich et al. J. Mol. Biol. 155 (1982) 347

2D-NMR Spectroscopy

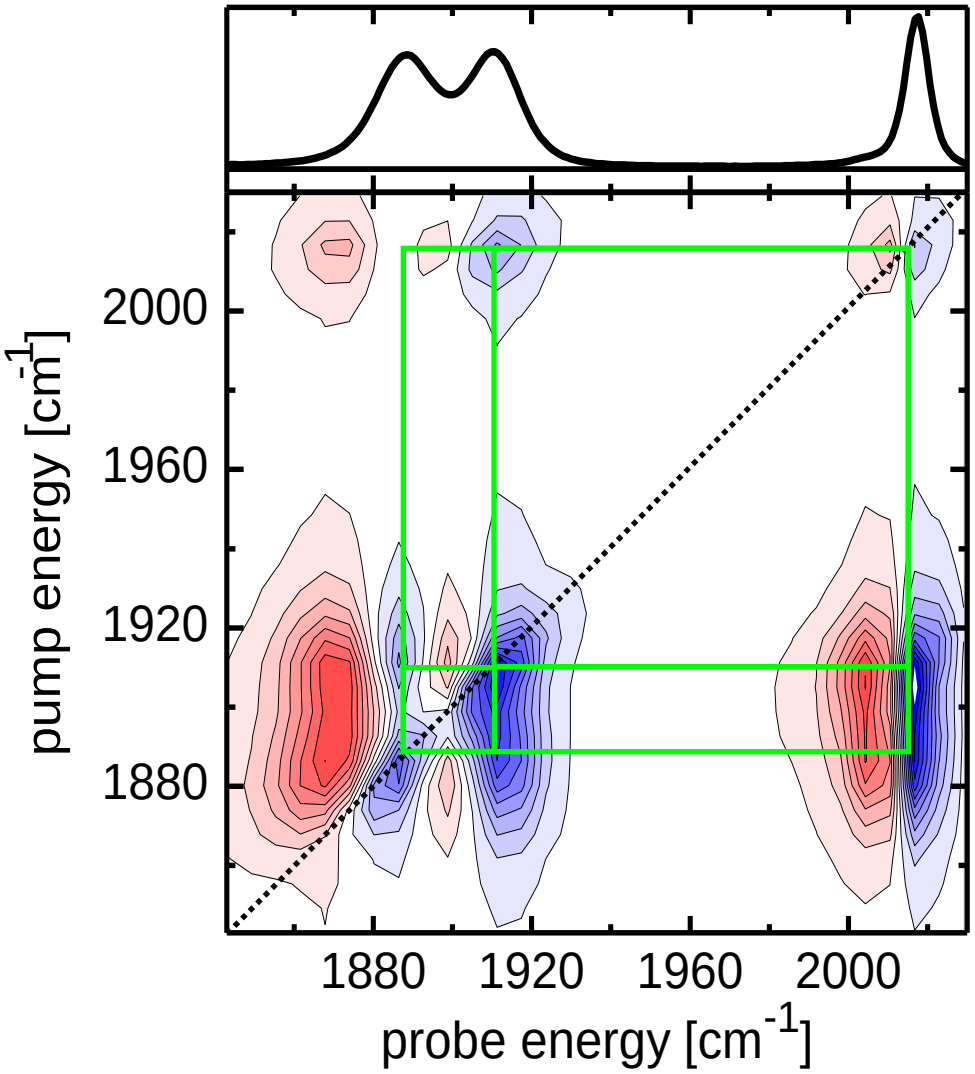
Richard Ernst (1976):

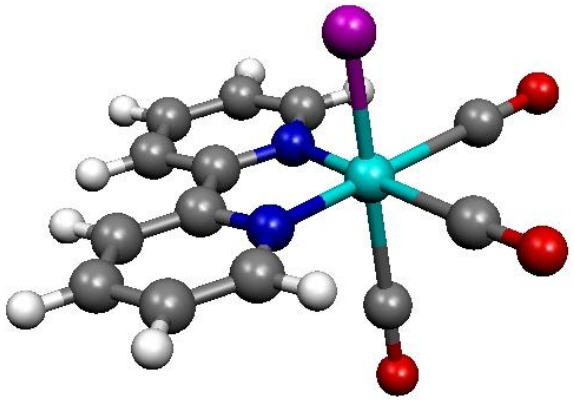
2*D* spectroscopy fascinates by its conceptual simplicity and by its general applicability. It seems to open one further dimension to the spectroscopist. Of ....

The basic principles which have been exploited are very general and can be applied to other coherent spectroscopies as well. Applications are conceivable in electron spin resonance, nuclear quadrupole resonance, in microwave rotational spectroscopy, and possibly in laser infrared spectroscopy.

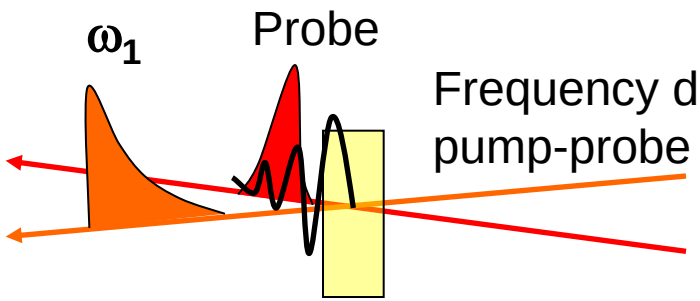
W. P. Aue, E. Bartholdi, and R. R. Ernst, *J. Chem. Phys*. 64 (1976) 2229

2D-IR Spectroscopy

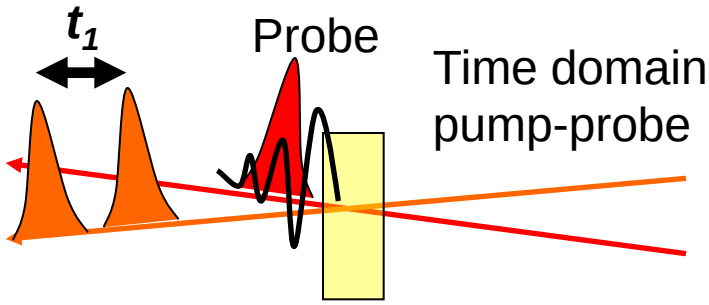




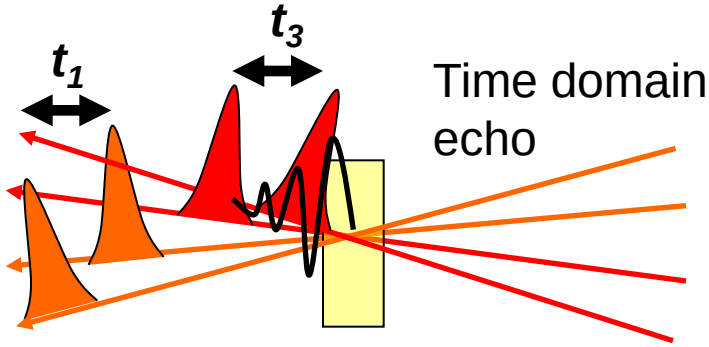
2D-IR Spectroscopy: Techniques



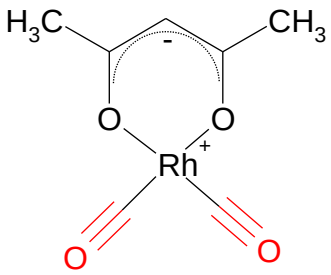
Frequency domain pump-probe

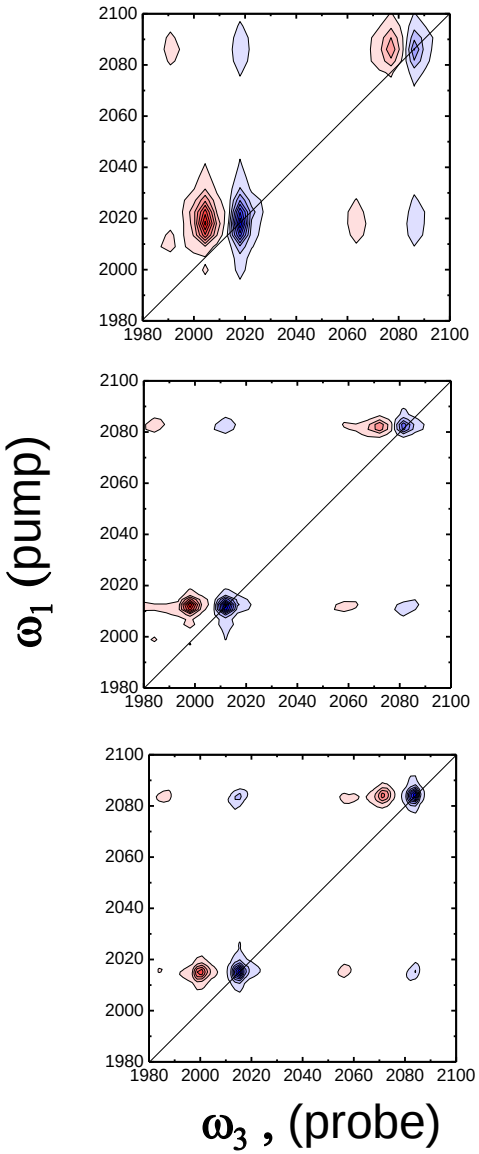


Time domain pump-probe



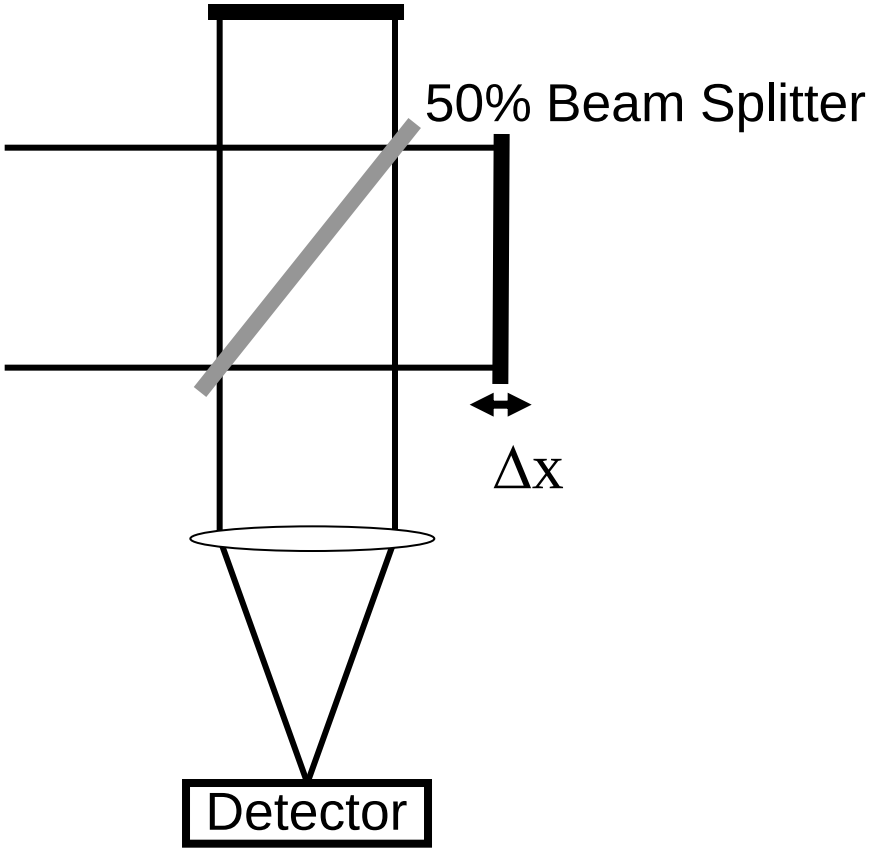
Time domain echo





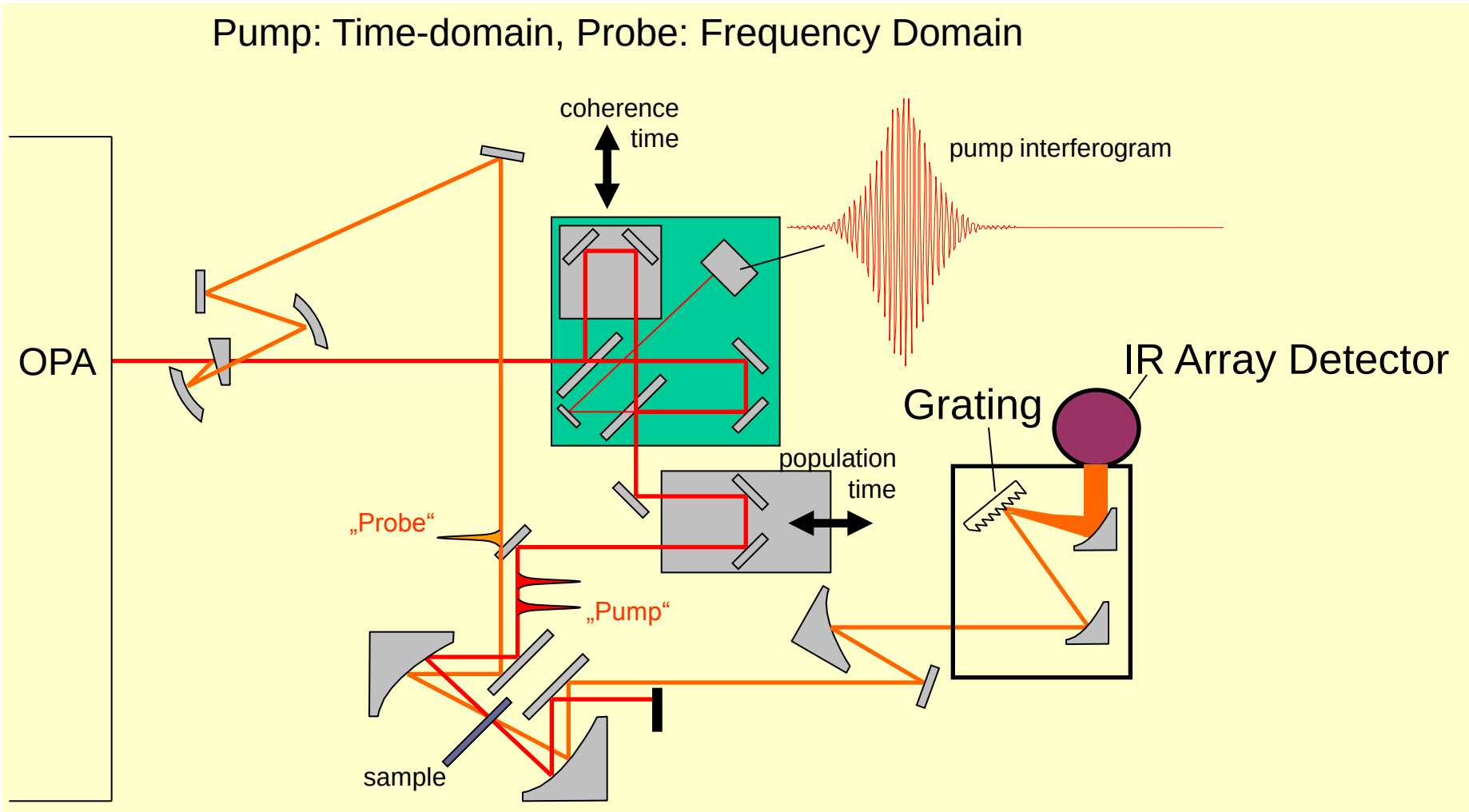
Frequency- versus Time-domain Spectroscopy: 1D

FTIR Spectrometer



1D spectrosocpy: short coherence length (incohrent light)
2D spectrosocpy: short pulses (femtosecond laser)

2D-IR: A simple Implementation

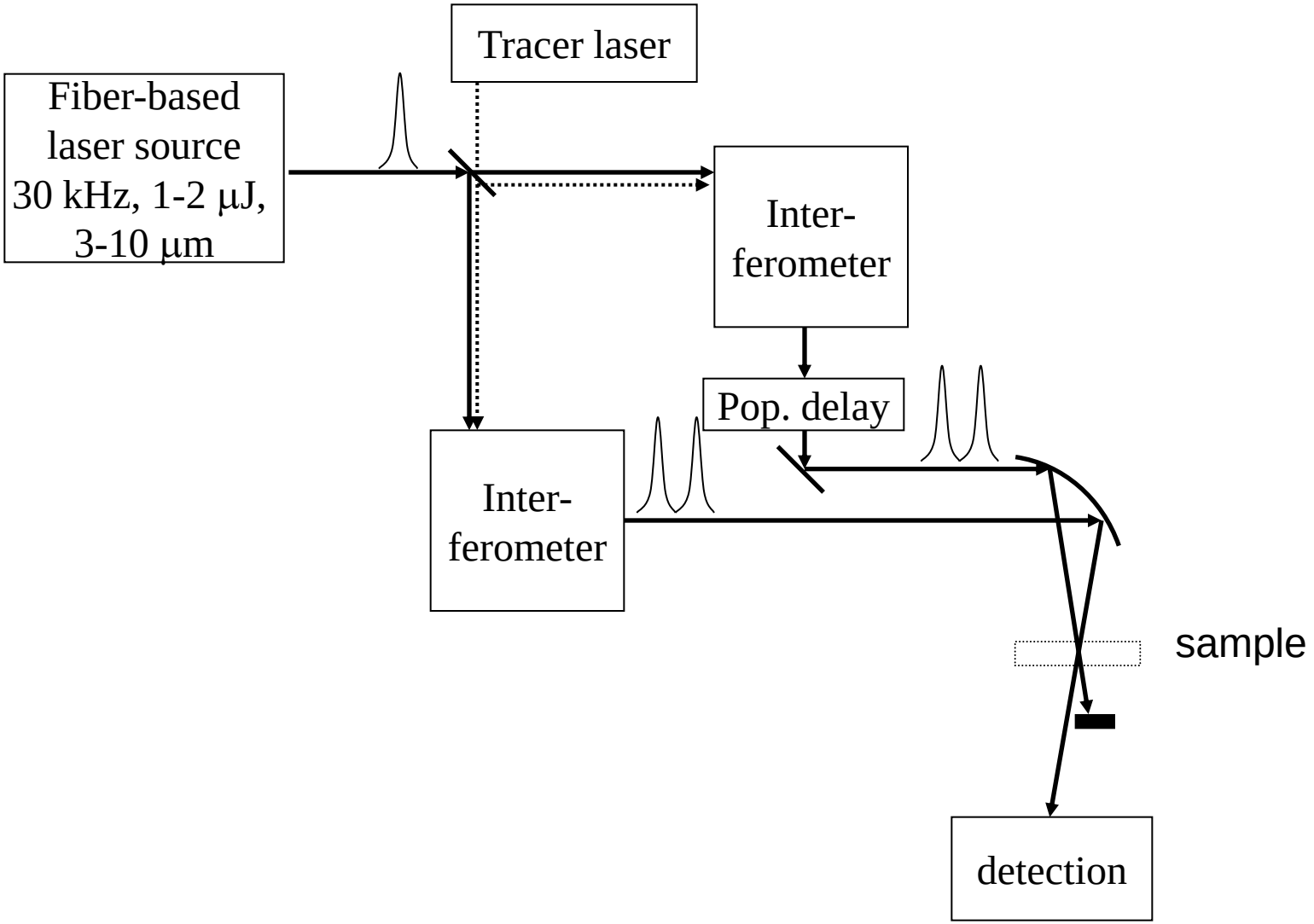


J. Helbing and P. Hamm, JOSA B 28 (2011)

Components

Amplified Ti:Sapphire System (e.g. Spectra Physics, Coherent)	CHF 350.000
● Optical Parametrical Amplifier: (e.g. Light Conversion, Spectra Physics)	CHF 80.000
● 2D-IR, Optics and Optomechanics: (e.g. Thorlabs, Newport, Edmund, Janos, Layertec)	CHF 30.000
● Spectrometer: (e.g. Jobin Yvon)	CHF 25.000
● IR Array Detector + Electronics: (Infrared Associates and Infrared Systems)	CHF 70.000
	CHF 555.000

Simplifying 2D IR to the essentials



Patent pending: P100283US01 (together with Martin Zanni, University of Wisconsin)

Components

Fiber-based IR laser + OPA
(30 kHz, 1-2 μJ, 3-10 μm) CHF ??

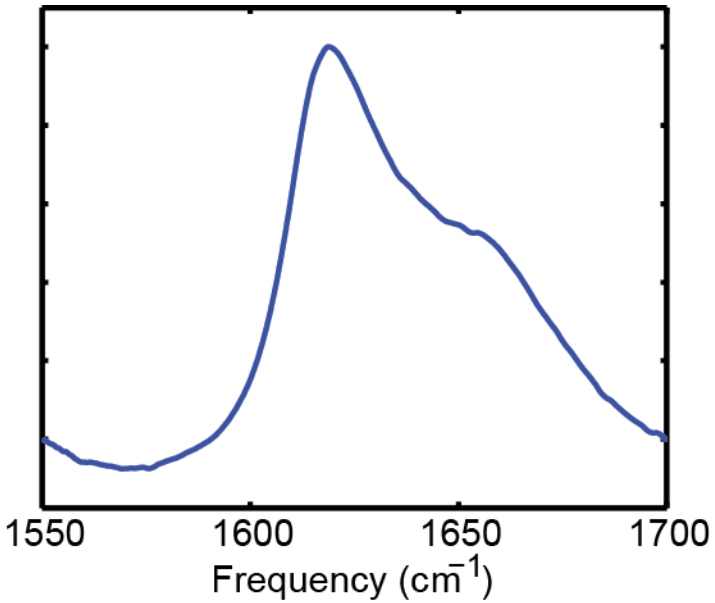
- 2 Interferometers as in any FTIR
(e.g. Bruker, Perkin Elmer, Agilent, Thermo, ABB) CHF 50.000
- Single IR Detector + Electronics: CHF 5.000

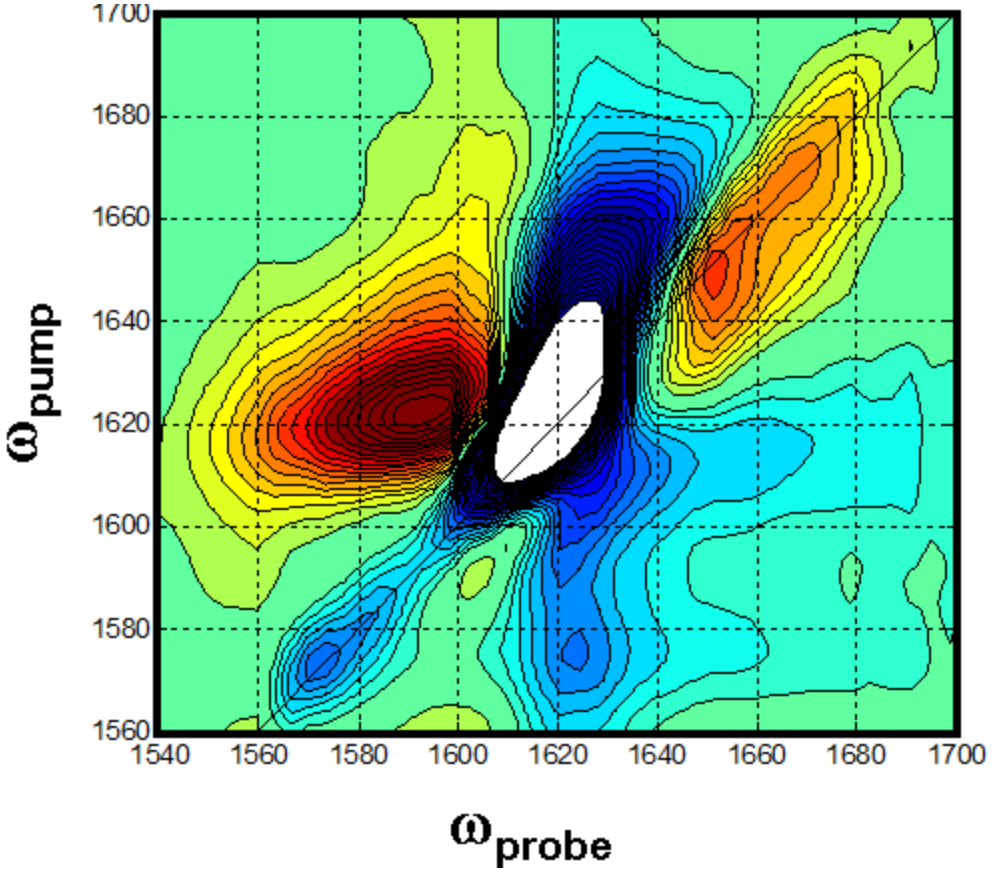
In comparison:

- Commercial FTIR Spectrometer CHF 25.000-125.000

If you had the choice, would you …

hIAPP: KCNTATCATQRL<u>A</u>NFLVHSSNNFGAILSSTNVGSNTY

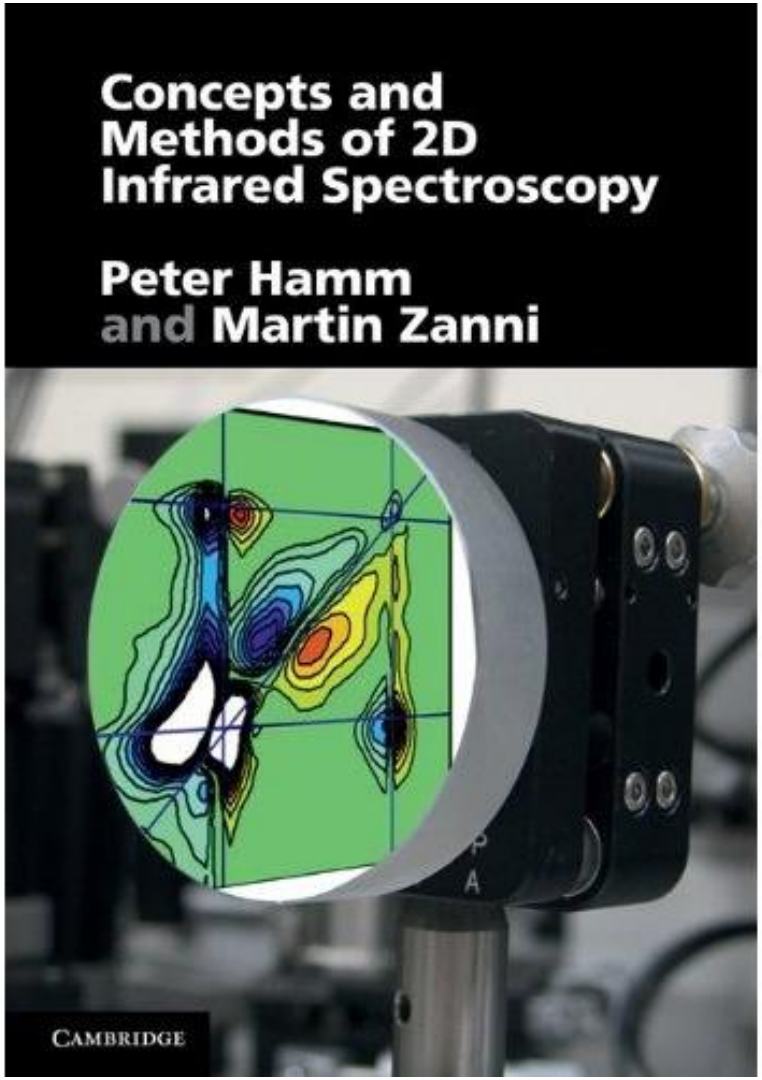


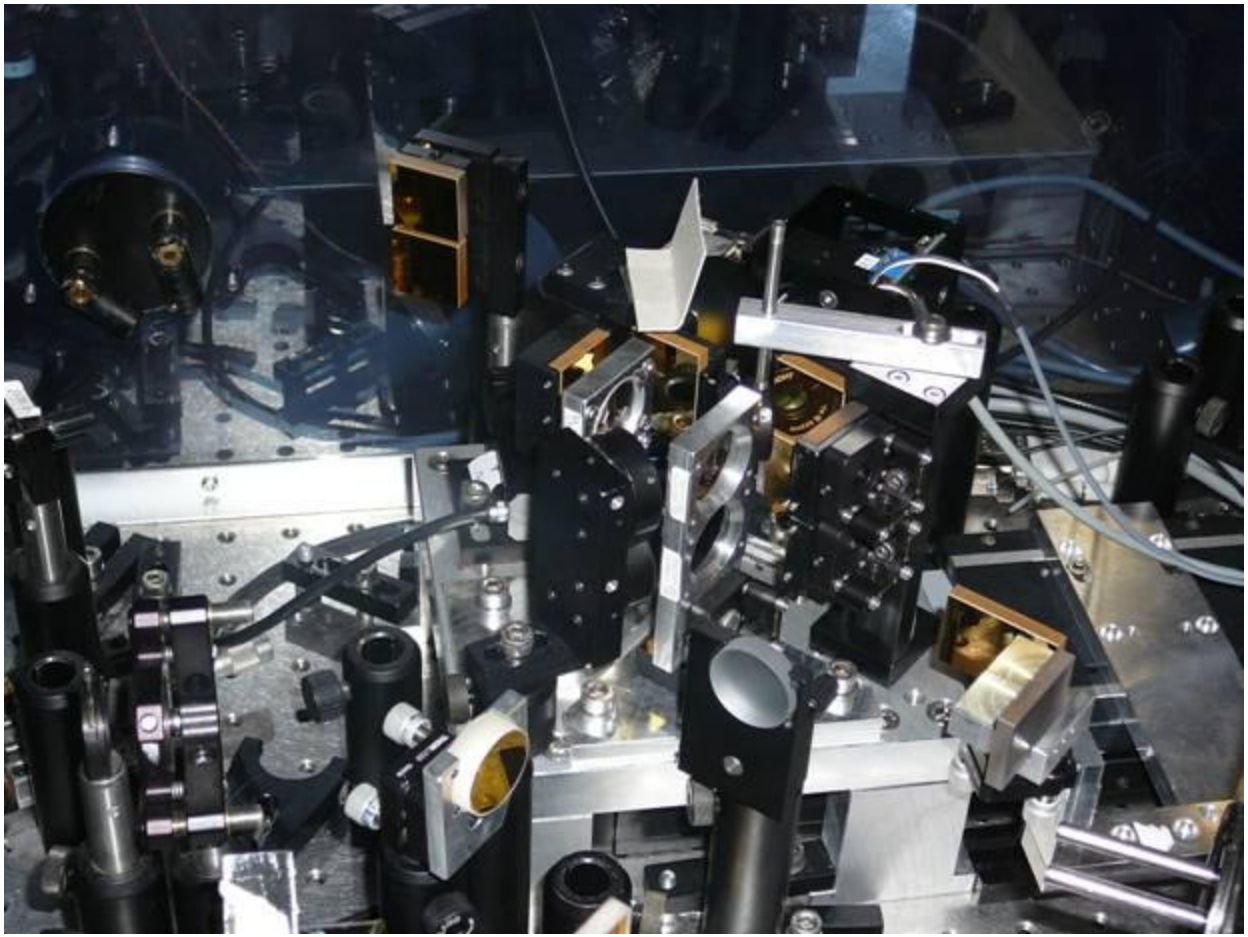


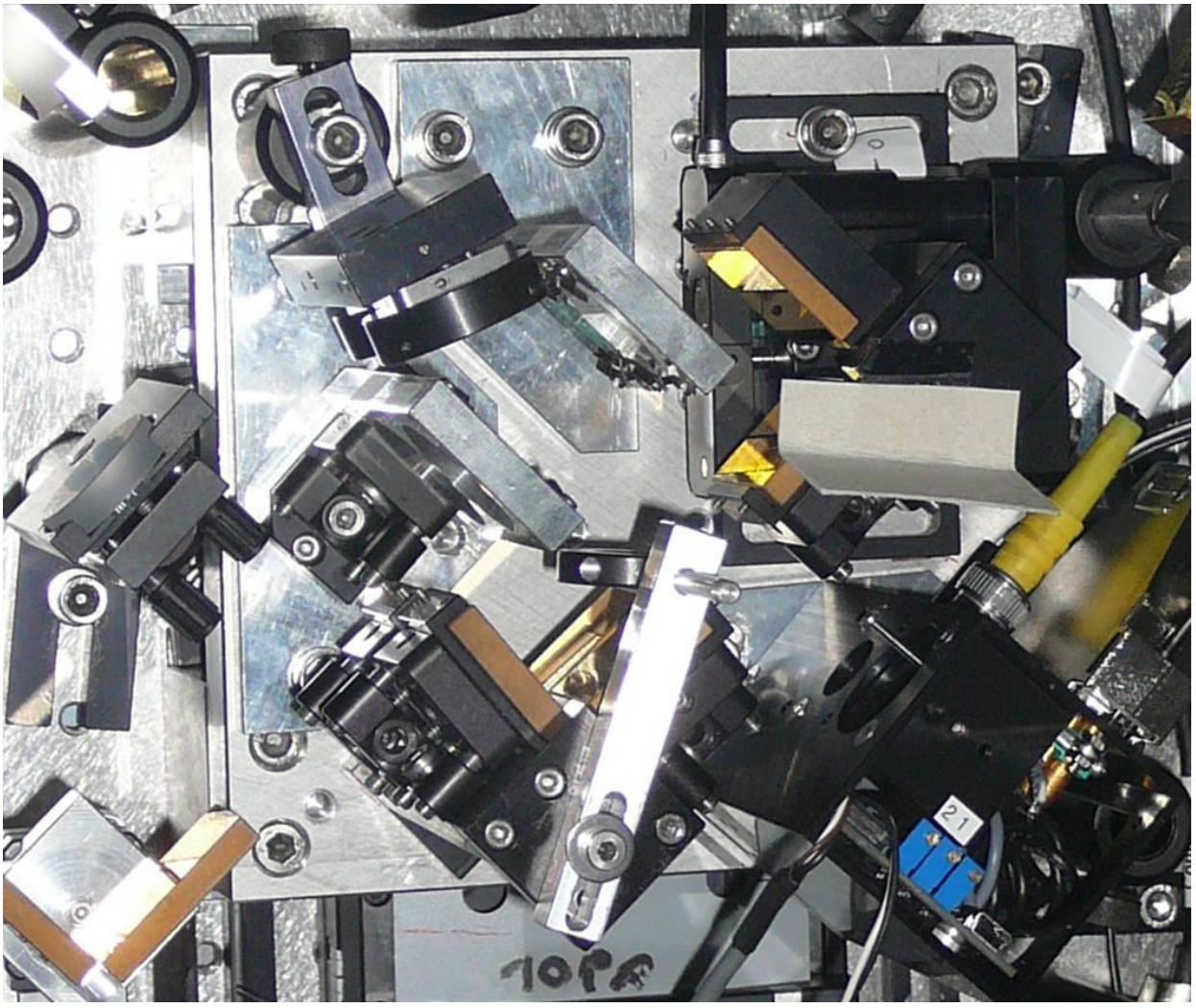
In the next 10 years, good chance that 2D IR will replace FTIR.

Courtesy of Martin Zanni

The Book


Concepts and
Methods of 2D
Infrared Spectroscopy
Peter Hamm
and Martin Zanni
CAMBRIDGE

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