

2D-IR Spectroscopy: Protein Dynamics, Ultrafast Structure Determination and Steering Photochemistry

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We will briefly cover the basics of molecular vibrations and infrared spectroscopy. We will explore the information content of static and time resolved infrared spectra using examples from chemistry and biology. Based on this foundation, ultrafast 2D-IR spectroscopy will be introduced. In contrast to 1D spectroscopy, 2D-IR spectroscopy reveals cross-peaks between bands of the IR absorption spectrum. We will discuss different mechanisms of how such cross-peaks are generated, such as chemical exchange, spectral diffusion, anharmonic coupling and vibrational energy transfer and how they can be exploited to investigate molecular structure and dynamics on a time scale of ~100 fs and longer.

Augmenting IR pulse sequences with near-IR, Vis or UV pulses creates novel spectroscopies, such as transient 2D-IR, triggered exchange 2D-IR, surface specific 2D-IR or VIPER 2D-IR. We will discuss the information content and application range of these mixed IR / non-IR multidimensional spectroscopies, using examples from protein biophysics, photochemistry, surface chemistry and others.

If time permits, technical aspects and different approaches of collecting 2D-IR spectra will be explained, comparing their advantages and disadvantages.

References:

From ultrafast structure determination to steering reactions: mixed IR/non-IR multidimensional vibrational spectroscopies, Luuk J. G. W. van Wilderen, Jens Bredenbeck, *Angew. Chem. Int. Ed.* 54, 11624-11640 (2015).

Concepts and Methods of 2D Infrared Spectroscopy, Peter Hamm and Martin Zanni, Cambridge University Press (2011).