Analyse kohärent gekoppelter Amid Zustände in Peptiden und Proteinen

Teilprojekt B6 (Hamm)

Vorarbeiten: Spektroskopie

Max-Born-Institut

Mitarbeiter

Dr. Sander Woutersen

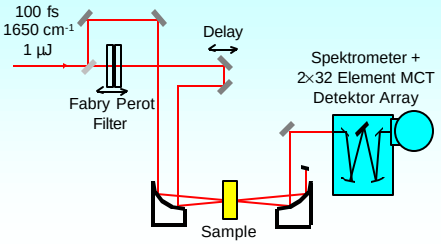
Dipl Phys. Julian Edler

Literatur:

- S. Woutersen, P. Hamm
  Structure determination of trialanine in water using polarization sensitive 2D vibrational spectroscopy
  J. Phys. Chem. B **104** (2000) 11316-11320.
- S. Woutersen, P. Hamm
  Structural dynamics of small peptides by time dependent 2D-IR spectroscopy.
  in *'Ultrafast Phenomena XII'*, eds. T. Elsaesser, S. Mukamel, M. M. Murnane, N. F. Scherer (Springer, Berlin 2000), p499-503
- S. Woutersen, P. Hamm.
  Isotope-edited two-dimensional vibrational spectroscopy of trialanine in aqueous solution.
  J. Chem. Phys. 114 (2001) 2727-2737.
- S. Woutersen, Y. Mu, G. Stock, P. Hamm
  Hydrogen-bond lifetime measured by time-resolved 2D-IR spectroscopy: N-Methylacetamide in methanol.
  Chem. Phys. Special Issue (2001) in press.
- S. Woutersen, Y. Mu, G. Stock, P. Hamm
  Subpicosecond Conformational Dynamics of Small Peptides probed by 2D Vibrational Spectroscopy
  Science, submitted

Dieses Projekt von der Deutsche Forschungsgemeinschaft im Normalverfahrens gefördert (HA 2297/3, Aug 1999- Aug. 2001) und soll in den SFB übergeführt werden.

2D-IR Setup



Vergleich

2D-IR	2D-NMR
2D-IR	**COSY**
Zeitabhängige 2D-IR	**Austauschspektroskopie und NOESY**
Exziton Cross Relaxation	**Nuclear Overhauser Effect**
Exziton spektrale Diffusion	**'Motional Narrowing Limit'**
Zeitskala : 1 ps	**1 ms**

Trialanin: Struktur

Korrelationsspektroskopie

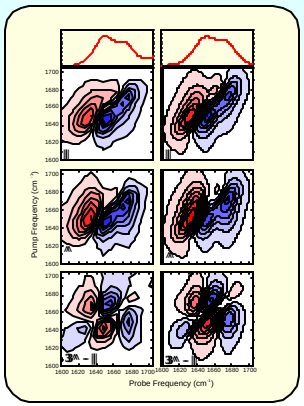
(b,q) → **(F, Y)**

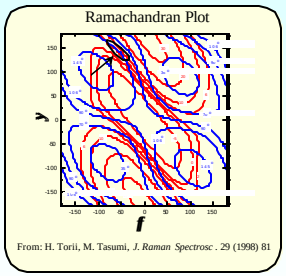
Result from Global Fit:

- Coupling b = 6 cm^{-1}
- Angle q = 106°

Unique Structure:

- F = -60°, Y = 140°
- poly(Gly) II



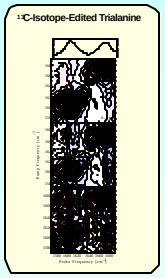


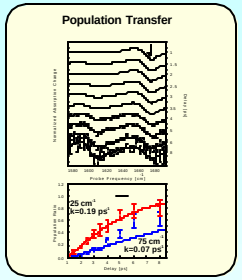
From: H. Torii, M. Tasumi, *J. Raman Spectrosc.* 29 (1998) 81

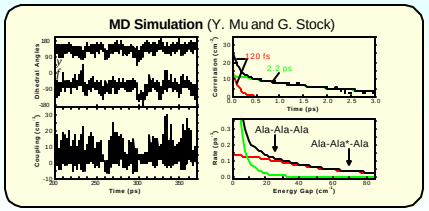
	f(°)	y(°)	b (cm^{-1})
Experiment	-60	140	6
MD Simulation	-68	141	5

Konformationsdynamik

'Vibrational Overhauser Effect Spectroscopy'



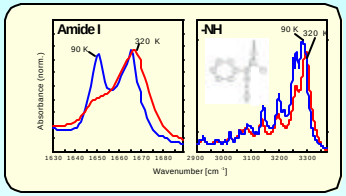


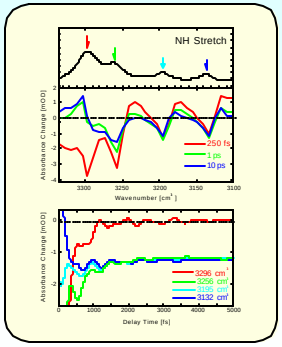


	t(fs)	D(cm^{-1})
Experiment	110	5.2
MD Simulation	120	4.1

Kohärente Wellenpackete

in kristallinem Acetanilide





- Kohärente Anregung von Phononen
- Ultraschneller Zerfall des freien Exzitons