MO 4: Verschiedenes

Zeit: Montag 17:00–17:30 Raum: VMP 6 HS-F

MO 4.1 Mo 17:00 VMP 6 HS-F

J- and H-bands of molecular aggregates: validity of the CES approximation — •Jan Roden[1], Alexander Eisfeld[1], and John Briggs[2] — [1]MPIPKS Dresden — [2]Uni Freiburg, Theoretische Quantendynamik

In molecular aggregates collective excitations of the constituting monomers lead to the formation of a narrow red-shifted absorption peak, the J-band, and a broad blue-shifted band with a lot of structure, the H-band [1]. Due to strong coupling to vibrations the understanding of the details of the aggregate absorption spectrum remains a difficult task. However, the "coherent exciton scattering"(CES) approximation is able to well reproduce the measured bandshapes of both the J- and the H-band in detail by taking the experimental spectrum of a single molecule as input. To better understand the excellent agreement of CES calculations and measured aggregate spectra and to investigate the validity of the CES approximation a comparison with direct diagonalisation of a model vibronic Hamiltonian, where only one undamped vibrational mode is taken into account, is performed [2]. Only in the H-band region, where previously good agreement of CES and measured spectra was obtained [3], CES does not conform to the direct diagonalisation spectra. This is shown to arise from use of the measured monomer spectrum which includes implicitly dissipative effects not present in the model calculation.

[1] T. Kobayashi, J-Aggregates, World Scientific, 1996
[2] J. Roden, A. Eisfeld, J. S. Briggs, Chem. Phys. 352 (2008) 258
[3] A. Eisfeld, J. S. Briggs, Chem. Phys. 324 (2006) 376

MO 4.2 Mo 17:15 VMP 6 HS-F

The Microwave Spectrum of Ethyl Acetate and Allyl Acetate — •Ha Vinh Lam Nguyen — Institute of Physical Chemistry, RWTH Aachen University, 52056 Aachen, Germany

Fourier transform microwave spectroscopic studies on ethyl acetate and allyl acetate in a molecular beam will be presented.

In the case of ethyl acetate the spectrum of the trans conformer has been completely assigned. The rotational and centrifugal distortion constants as well as the barriers to internal rotation of both methyl groups have been determined.

Allyl acetate is currently under study. First results on the structure and internal dynamics of this molecule will be reported.

The experimental data of both molecules will be compared with the results of ab initio calculations.