

SYHR 3: High resolution spectroscopy - modern trends and new techniques III

Zeit: Donnerstag 16:30–18:30

Raum: VMP 8 R05

Hauptvortrag SYHR 3.1 Do 16:30 VMP 8 R05
Automated fitting of High Resolution spectra from the MW to the UV — ●W. LEO MEERTS — Molecular- and Biophysics Group, Radboud University Nijmegen, NL 6500 Nijmegen

The usefulness of an evolutionary algorithm (EA) based approach to the automated evaluation of molecular parameters from various kind of spectra is shown. The applicability of the method ranges from rotationally resolved electronic spectroscopy of large molecules to nuclear magnetic resonance (NMR) spectroscopy of molecules, which are partially oriented in an anisotropic liquid-crystalline environment.

The application of both the genetic algorithm (GA) and the evolutionary strategy algorithm (ES) approaches for the assignment of complex spectra and the necessity of fitting meta parameters, which are not related to the parameters of the model describing the spectra are discussed. Examples for the possible applications will be discussed.

Hauptvortrag SYHR 3.2 Do 17:10 VMP 8 R05
High resolution spectroscopy using supersonic planar plasma expansions — ●HAROLD LINNARTZ — Laboratory for Astrophysics, Leiden Observatory, University of Leiden, Leiden, the Netherlands

Transient molecules - typically radicals, ions and ionic complexes - belong to the chemically most reactive species. They are considered to be important intermediates in processes ranging from combustion to interstellar chemistry. The high reactivity, however, also complicates systematic spectroscopic gas phase studies.

In this talk the use of planar plasma sources [1] is reviewed, capable of producing molecular transients with high densities at low rotational temperatures in a Doppler free environment. Fully rotationally resolved spectra of rovibronic and rovibrational transitions are presented for exotic and highly unstable molecules. It is demonstrated how sensitive detection techniques, such as cavity ring down spectroscopy and plasma modulation techniques, can be used to record fully resolved spectra in direct absorption.

[1] H. Linnartz, 'Cavity ring down spectroscopy of molecular transients of astrophysical interest' in *Cavity Ring-down Spectroscopy: Techniques and Applications*, Eds. G. Berden and R. Engeln, Publisher: John Wiley & Sons, Ltd. (2009).

Hauptvortrag SYHR 3.3 Do 17:50 VMP 8 R05
Discussion of the Results of the Symposium — ●DAVID PRATT¹, HAROLD LINNARTZ², WOLFGANG STAHL³, GERHARD SCHWAAB⁴, JENS-UWE GRABOW⁵, BERNHARD ROTH⁶, GIANGAETANO PIETRAPERZIA⁷, and W. LEO MEERTS⁸ — ¹University of Pittsburgh — ²University of Leiden — ³RWTH Aachen — ⁴Ruhr University Bochum — ⁵Gottfried-Wilhelm-Leibniz-Universität Hannover — ⁶Heinrich-Heine-Universität Düsseldorf — ⁷Universita di Firenze — ⁸Radboud University Nijmegen

The possibilities and limits of new techniques and current trends in high resolution molecular spectroscopy will be discussed by the contributors to the Symposium. Discussion contributions from the audience are highly welcome.