

## MO 14: Cluster

Zeit: Donnerstag 8:30–10:30

Raum: 3G

MO 14.1 Do 8:30 3G

**Pulsed Molecular Beams of Nucleobases** — ●ADNAN SARFRAZ, KLAUS RADEMANN, and WOLFGANG CHRISTEN — Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 2, 12489 Berlin

Transfer of non-volatile and thermally unstable molecules into the gas phase is important for a variety of applications such as analytical mass spectrometry, optical spectroscopy and thin film growth. Supercritical fluids may be used to dissolve molecules at moderate temperature and pressure conditions. This property can be utilized for the molecular beam expansion of thermally labile molecules without the use of significant heat. Extending our previous work [1] we present mass spectra of five biologically relevant nucleic acids (adenine, guanine, cytosine, thymine, and uracil) in a pulsed molecular beam. The molecules are deposited onto a polycrystalline gold surface and studied using Atomic Force Microscopy as well as Thermal Desorption Spectroscopy.

[1] W. Christen, S. Geggier, S. Grigorenko, K. Rademann, *Rev. Sci. Instrum.* **75**, 5048 (2004).

MO 14.2 Do 8:45 3G

**Isomer specific spectroscopy of Benzene-Acetylene aggregates** — ●MATTHIAS BUSKER, THOMAS HÄBER, MICHAEL NISPEL, and KARL KLEINERMANN — Institut für Physikalische Chemie und Elektrochemie I, Heinrich Heine Universität Düsseldorf, Germany

The relatively strong CH- $\pi$  interactions in Benzene-Acetylene cocrystals have found broad interest due to their importance for the stabilization of supramolecular aggregates, crystal packing, molecular recognition and folding of proteins. We present new gas phase results on medium-sized clusters of Benzene(B) with Acetylene(A) by using mass-resolved Resonant Two Photon Ionisation (R2PI) and IR-UV double resonance spectroscopy for analysis. For BA<sub>1-2</sub> analysis see A. Fujii, S. Morita, M. Miyazaki, T. Ebata and N. Mikami, *J. Phys. Chem. A*, 2004, 108, 2652. The investigated B<sub>1</sub>A<sub>1-4</sub> and B<sub>2</sub>A<sub>1-2</sub> aggregates were structurally assigned based on comparison of their infrared spectra with ab initio calculated frequencies and intensities and by taking the shift of their electronic spectra into account. The obtained cluster structures were compared with the basic structural units of BA 1:1 cocrystals obtained via x-ray analysis (see R. Boese, T. Clark and A. Gavezzotti, *Helvetica Chimica Acta*, 2003, 86, 1085)

MO 14.3 Do 9:00 3G

**What microwave spectroscopy tells us about the benzene dimer** — ●UNDINE ERLEKAM<sup>1</sup>, MELANIE SCHNELL<sup>1</sup>, GERARD MEIJER<sup>1</sup>, GERT VON HELDEN<sup>1</sup>, JENS-UWE GRABOW<sup>2</sup>, and PHILIP R. BUNKER<sup>3</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, Berlin, Germany — <sup>2</sup>Institut für Physikalische Chemie, Leibniz-Universität, Hannover, Germany — <sup>3</sup>Steele Institute for Molecular Sciences, NRC, Ottawa, Canada

The benzene dimer is a model system for investigating dispersive intermolecular interactions between aromatic molecules. Numerous theoretical and experimental studies exist. Infrared and Raman spectra show different signatures for the two benzene rings in the dimer from which it can be concluded that they are symmetrically inequivalent. Different theoretical calculations find two different minimum structures for the benzene dimer. One is a “parallel-displaced” structure, and the other a distorted T-shaped one with “stem” and “top” benzene rings. The former structure has symmetrically equivalent rings, whereas the latter has symmetrically inequivalent rings in agreement with the Infrared and Raman studies.

We try to solve this conflict using microwave spectroscopy in the 3 to 6 GHz range. In agreement with the only previous microwave study we find a group of microwave transitions, which fit a symmetric top Hamiltonian. It consists of a quartet fine structure with a characteristic intensity and splitting pattern. To explore the origin of this splitting we have studied the microwave spectrum of the (C<sub>6</sub>H<sub>6</sub>)<sub>2</sub> and C<sub>6</sub>H<sub>6</sub>-C<sub>6</sub>D<sub>6</sub> isotopologs. Our experimental results will be presented and discussed in the light of the nuclear spin statistics.

MO 14.4 Do 9:15 3G

**Pure rotational spectra of PbSe and PbTe: potential function, Born-Oppenheimer breakdown, field shift effect and magnetic shielding** — BARBARA M. GIULIANO<sup>1</sup>, LUCA BIZZOCCHI<sup>1</sup>, STEPHEN COOKE<sup>2</sup>, DEIKE BANSER<sup>3</sup>, MAREIKE HESS<sup>3</sup>, JULIANE FRITZSCHE<sup>3</sup>, and ●JENS-UWE GRABOW<sup>3</sup> — <sup>1</sup>Università di Bologna, Dipartimento

di Chimica “G. Ciamician”, vie F. Selmi 2, 40126 Bologna, Italia — <sup>2</sup>University of North Texas, Department of Chemistry, Denton, TX 76203, United States of America — <sup>3</sup>Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie & Elektrochemie, Lehrgebiet A, Callinstrasse 3A, 30167 Hannover, Deutschland

We present the supersonic-jet Fourier-transform microwave spectra of 42 isotopologues of PbSe (16) and PbTe (26). Using our LASER-ablation jet source, vibrationally very highly excited states of up to  $v=13$  could be prepared. A multi-isotopologue analysis yields precise spectroscopic constants and Born-Oppenheimer breakdown correction coefficients. A significant contribution to the Born-Oppenheimer breakdown could be attributed to the finite size of the Pb nucleus, the so-called field-shift effect. From the magnetic hyperfine interaction in isotopologues containing dipolar nuclei the nuclear spin-rotation coupling constants and NMR shielding parameters were determined. Direct fits of a radial Hamiltonian yield analytic potential-energy and Born-Oppenheimer breakdown radial functions. Besides contributing to the understanding of the internuclear potential, electronic structure and chemical bond of intermetallic species, the study also demonstrates the wealth of information encoded in pure rotational spectra.

MO 14.5 Do 9:30 3G

**IR spectroscopy on isolated cobalt-alcohol cluster anions** — ●PHILIP BIALACH<sup>1</sup>, MARTIN WEILER<sup>1</sup>, MICHAELA BRAUN<sup>2</sup>, ARNE LÜCHOW<sup>2</sup>, and MARKUS GERHARDS<sup>1</sup> — <sup>1</sup>TU Kaiserslautern, Fachbereich Chemie, Schrödingerstr. 52, 67663 Kaiserslautern & H.-Heine Uni Düsseldorf, Institut für Physikalische Chemie I, 40225 Düsseldorf — <sup>2</sup>RWTH Aachen, Institut für Physikalische Chemie, Landoltweg 2, 52056 Aachen

As an example of a model system for investigating metal-anion/ligand compounds we report on clusters of cobalt and alcohols, e.g. methanol, ethanol and propanol. There are questions in understanding the change in physical and chemical properties with increasing cluster size. The metal anions are produced by laser ablation and the alcohols are attached in a supersonic beam. By applying IR-photodetachment or photofragment spectroscopy the OH stretching vibrations of mass-selected cobalt/n/alcohol/m/ cluster anions (n,m = 1-3, alcohol=methanol, ethanol, propanol) are investigated. By comparing the experimental results with predictions of ab initio and DFT calculations structural assignments can be obtained. Both the orientation of the OH groups with respect to the metal clusters as well as the orientation of the aliphatic side chains of the alcohols can be discussed.

MO 14.6 Do 9:45 3G

**Study of autodetachment effects in the photoemission of fullerene anions** — ●MATTIAS SVANQVIST, RAPHAEL KUHNEN, CHRISTINE WEHRSTEIN, and BERND V. ISSENDORFF — Fakultät für Physik, Universität Freiburg, Stefan Meier Straße 21, 79104 Freiburg

The electronic valence structure of fullerenes is determined by the delocalized  $\pi$ -band which can be seen as a spherical two-dimensional electron gas. This makes fullerenes interesting model systems for the study of excitation and relaxation processes in a highly correlated many-electron systems.

In photoelectron spectra of C<sub>60</sub><sup>-</sup> irradiated by ns-laserpulses evidence of electron Auger-like auto-detachment processes have been observed<sup>1</sup>. To verify this peak in the photoelectron spectra as indeed originating from an auto-detachment processes we have conducted a detailed study by scanning a wavelength range of 266 to 322 nm. This shows a linear dependence of the peak position in the binding energy spectras on the photon energy, as expected for auto-detachment, and allows to determine the excitation energy of the autodetaching state as about 3.5 eV.

<sup>1</sup>X.-B. Wang et al, *J. Chem. Phys.* **110**, 8217 (1999)

MO 14.7 Do 10:00 3G

**Oberflächenstreuung massenselektierter Molekülcluster: CO<sub>n</sub><sup>+</sup> und (CO<sub>2</sub>)<sub>n</sub><sup>+</sup>** — ●MUHAMMER BULAT, KLAUS RADEMANN und WOLFGANG CHRISTEN — Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 2, 12489 Berlin

Schwach gebundene Cluster aus Molekülen können durch Stöße mit Oberflächen effektiv angeregt werden. Diese Anregungsenergie kann

zur Fragmentation des Clusters führen. In einigen Fällen konnten auch stoßinduzierte Intraclusterreaktionen beobachtet werden [1]. Wir stellen Massenspektren für die großen- und energieabhängige Streuung der Molekülcluster  $\text{CO}_n^+$  und  $(\text{CO}_2)_n^+$  vor. Die Cluster werden durch Überschallexpansion erzeugt und mittels Elektronenstoß ionisiert. In einem Reflektron-Flugzeitmassenspektrometer ( $m/\Delta m > 2000$ ) erfolgt die Beschleunigung ( $U_0 \leq 6$  kV) und Größenselektion (Separationsvermögen  $> 200$ ) der Clusterionen [2]. Durch Variation der Reflektorspannung können die Cluster an dessen letzter Elektrode (Edelstahl) gestreut werden. Die Massenanalyse der bei der Streuung entstandenen Produktionen erfolgt über deren Flugzeit von der Edelstahloberfläche bis zum Detektor. Interessant ist das beobachtete Fragmentationsverhalten der untersuchten Moleküle: Im Gegensatz zu protonierten Clustern (z.B. Ammoniak, Methanol oder Wasser), die bei der Oberflächenstreuung eine Mehrfachfragmentation zeigen, wird bei CO und  $\text{CO}_2$  eine sequentielle Fragmentation beobachtet.

[1] W. Christen, U. Even, *J. Phys. Chem. A* **102**, 9420 (1998).

[2] W. Christen, K. Rademann, *Rev. Sci. Instrum.* **77**, 015109 (2006).

MO 14.8 Do 10:15 3G

**Lokalisation von K-Schalen-Photoelektronen und ICD-Elektronen in Neondimeren** — •K. KREIDT<sup>1,2</sup>, T. JAHNKE<sup>1</sup>, T.

WEBER<sup>3</sup>, T. HAVERMEIER<sup>1</sup>, R. GRISENTI<sup>1</sup>, X.-J. LIU<sup>4</sup>, Y. MORISITA<sup>5</sup>, S. SCHÖSSLER<sup>1</sup>, L. SCHMIDT<sup>1</sup>, M. SCHÖFFLER<sup>1</sup>, M. ODENWELLER<sup>1</sup>, N. NEUMANN<sup>1</sup>, L. FOUCAR<sup>1</sup>, J. TITZE<sup>1</sup>, B. ULRICH<sup>1</sup>, F. STURM<sup>1</sup>, C. STUCK<sup>1</sup>, R. WALLAUER<sup>1</sup>, S. VOSS<sup>1</sup>, I. LAUTER<sup>1</sup>, H.-K. KIM<sup>1</sup>, M. RUDLOFF<sup>1</sup>, H. FUKUZAWA<sup>4</sup>, G. PRÜMPER<sup>4</sup>, N. SAITO<sup>5</sup>, K. UEDA<sup>4</sup>, A. CZASCH<sup>1</sup>, O. JAGUTZKI<sup>1</sup>, H. SCHMIDT-BÖCKING<sup>1</sup>, S. K. SEMENOV<sup>6</sup>, N.A. CHEREPKOV<sup>6</sup> und R. DÖRNER<sup>1</sup> — <sup>1</sup>Institut für Kernphysik, J. W. Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — <sup>2</sup>DESY, Notkestrasse 85, 22607 Hamburg, Germany — <sup>3</sup>Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA — <sup>4</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan — <sup>5</sup>National Metrology Institute of Japan, AIST, Tsukuba 305-8568, Japan — <sup>6</sup>State University of Aerospace Instrumentation, 190000 St. Petersburg, Russia

Mit der COLTRIMS-Technik wurde der Zerfall von Neondimeren nach der K-Schalen Ionisation mit einer Photonenenergie von 881.2 eV untersucht. Dabei wurden sowohl die Ionen als auch die Elektronen mit einem Raumwinkel von  $4\pi$  gemessen. Am Aufbruch des Moleküls in die Fragmente  $\text{Ne}^+$  und  $\text{Ne}^{2+}$  wurde die Lokalisation der Photoelektronen sowie der ICD-Elektronen untersucht. Betrachtet wurde hierfür die Winkelverteilung dieser um die Molekülachse.