The 74th INTERNATIONAL SYMPOSIUM
ON MOLECULAR SPECTROSCOPY

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Mini-Symposia

ASTROCHEMISTRY AND ASTROBIOLOGY IN THE AGE OF ALMA
Organized by Laurent Marguès (Université Lille) and Anthony Remijan (NRAO). Featuring discussions on the advances ALMA has made and will be making in these fields. ALMA technology has already re-energized the fields and the next series of ALMA development programs will make the array the most powerful spectroscopic instrument on the planet for astrochemical and astrobiological discoveries. Invited Speakers: Jes Jorgensen (Niels Bohr Institute), Brett A. McGuire (NRAO), Nami Sakai (RIKEN), Charlotte Vastel (Institut pour la Recherche en Astrophysique et Planéologie)

HIGH-HARMONIC GENERATION AND XUV SPECTROSCOPY
Organized by Robert Baker (Ohio State), Scott Sayres (Arizona State), and Josh Vura-Weis (UHUC). Featuring advances in high-harmonic generation and the spectroscopy it enables. The ionization-recombination process itself is a sensitive probe of small-molecule electronic structure. Furthermore, the XUV pulse can be used as an element-specific probe of electron dynamics at femt-o-attosecond timescales. Invited Speakers: Lou DiMauro (Ohio State), Wen Li (Wayne State), Arvinder Sandhu (University of Arizona)

NON-COVALENT INTERACTIONS
Organized by Helen Leung (Amherst College), Mark Marshall (Amherst College), and Yunjie Xu (University of Alberta). Non-covalent interactions have profound influence on chemical and biological systems. Interactions in chiral contact pairs have provided the basis for a new method of chiral analysis. We focus on spectroscopic and theoretical characterization of non-covalent molecular interactions and how they can be utilized to explore new frontiers. Invited Speakers: Maria Sanz (King’s College London), Joseph Francisco (University of Pennsylvania), Kenneth Leopold (University of Minnesota)

Picnic (Tuesday)

The Symposium picnic will be held on Tuesday evening at Ikenberry Commons. The cost of the picnic is included in your registration (at below cost to students), so that all may attend the event. The Cobblestone Society is the host for refreshments for one hour. Please see your packet for additional details.

Sponsorship

We are pleased to acknowledge the many organizations that support the 74th Symposium. Principal funding comes from the National Radio Astronomy Observatory (NRAO). We also acknowledge the many efforts and contributions of The University of Illinois in hosting the meeting, including financial contributions from the Departments of Chemistry, Electrical and Computer Engineering, and Astronomy.

Our Corporate Sponsors are Bristol Instruments, Elsevier/JMS, Ideal Vacuum Products, Journal of Physical Chemistry/ACS, and Lumibird (The new name of Quantel-Keypsys group). Please see the back of this book for their advertisements.

We are also pleased to acknowledge...
4:09 – 4:24

HYDROXYL GROUPS INTERNAL ROTATION IN THE METHANEDIOL MOLECULE. DFT STUDY INCLUDING DISSIPATION INTERACTION.

ULAZDIRM Sapeshika, Physics, University of Illinois at Chicago, Chicago, IL, USA; GEORGE PETSIC- VICH, Physics, Belarussian State University, Minsk, Belarus; ALEX MALEVICH, Mechanics and Mathematics, Belarussian State University, Minsk, Belarus; VALERY SATSUBEKOVICH, Physics, Belarussian State University, Minsk, Belarus.

Methanediol (MD) molecule is of considerable interest to the field of astrophysics[1]. Studies present calculations of the geometry and IR spectrum of the molecule, however, torsional spectra has yet to be computed. This work presents calculations of 2D PES MD at B3LYP D3B2-pV5Zc-pVQZ and B3LYP-D3B2-cc-pVQZ levels. Computations used optimized geometries for all electronic parameters at each node with set torsion angles. Computational parameters were calculated using Wilson’s vector formalism. Potential energy calculations were performed at nodes of equidistant grids, number of nodes used 15 x 15 and 45 x 45. The energy values of the torsion levels were determined using DUR method.

Figure on the right (a) 2D PES for torsion movement of hydroxyl groups of MD molecule calculated in the B3LYP-D3 approxi- mation. (b) Torsional spectrum of MD molecule for the temperature of 300 K (upper spectrum) and 30 K (lower spectrum). [1] C. Barri- ena, P. Redondo, H. Martinez, A. Largo, Astr.J., 784:132 (2014) 1-7.

4:27 – 4:42

CH3, INTERNAL ROTATION IN 9-METHYLANTHACENE

MASAABI BABA, Division of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan; MASATOSHI MISANO, Applied Physics, Fukuoka University, Fukuoka, Japan; JON T. HOUGEN, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD, USA.

We observed the rotationally resolved fluorescence excitation spectrum of the S1 \rightarrow S0 transition of jet-cooled 9- methylanthacene. The potential energy curve for CH3 internal rotation is six-fold symmetrical. The barrier to rotation (V0) is ~ 120 cm^-1 [2], which is considerably larger than that of toluene (~ 5 cm^-1) [1]. The V0 value is the energy difference between two isomers ‘staggered’ and ‘ eclipsed’. The main contribution to V0 is expected to be hyperconjugation, which is the t-t interaction between the aromatic v orbital and methyl sp2 orbital.

The final goal of this work is to quantitatively elucidate the vibrational and rotational energy levels for CH3 internal rotation. It is essential to observe the high-resolution and high-precision electronic spectrum. We recently search the best effective Hamiltonian to reproduce the experimental results. We are now developing a new laser control system with optical frequency comb locked to GPS, and an ab initio method which provides the reliable potential energy curve.