

Invited Lectures O

September 2, Friday, 11:00 – 12:30

Millimeter-wave jet spectroscopy of van der Waals complexes and small clusters containing helium and hydrogen

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The presence of molecular species like CO, H₂O, NH₃ in the interstellar medium (ISM) and their usefulness as indicators of molecular cloud properties has motivated considerable experimental and theoretical efforts aimed largely at understanding the interactions between these species and their main ISM collision partners, H₂ and He. The collisional excitations of the species involved strongly depend on important features of the multidimensional intermolecular potential energy surfaces (PES), such as barriers, anisotropies, binding energy, and structure in the most stable configurations.

High resolution spectroscopy of van der Waals complexes has proved to be a very effective tool for the elucidation of intermolecular PES, because the bound states of the complexes are sensitive to the interaction potential. The recent progress on the millimeter-wave studies of weakly bound molecular complexes, mostly those which contain H₂ and He, using intracavity OROTRON jet spectrometer along with double resonance technique will be presented. These experimental measurements provided rigorous tests of the accuracy of the *ab initio* PESs and computed bound states.

Another application, in which the intermolecular interactions with He and H₂ play an important role, is the doping of helium or *para*-hydrogen clusters with a probe molecule to perform high resolution spectroscopy. Such experiments directed on the detection of superfluid response of molecular rotation in the He and *p*-H₂ clusters will be also considered.

Getting Wet in the Gas Phase: Water Aggregates from Broadband Rotational Spectroscopy

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Over the past decade, rotational spectroscopy has experienced a major advance with the design and development of chirped-pulse Fourier transform microwave (CP-FTMW) spectrometers.^[1,2] This represented an unparalleled improvement in data acquisition speed and sensitivity which enabled the study of increasingly more complex systems. This presentation will focus on the application of broadband rotational spectroscopy to determine the structure of small bare water clusters^[2-5] and microsolvated molecules.^[6,7] Using H₂¹⁸O water substitution it was possible to obtain accurate structural information of these molecular aggregates up to the water decamer. Of particular interest is the water hexamer – the first three-dimensional water cluster – where three different structural isomers of low energy have been identified. Apart from structural studies, this talk will showcase the use of isotopic substitution experiments to reveal the internal cluster dynamics in small clusters as it has been recently reported.^[5]

References

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