



21st May 2015 - 10:00

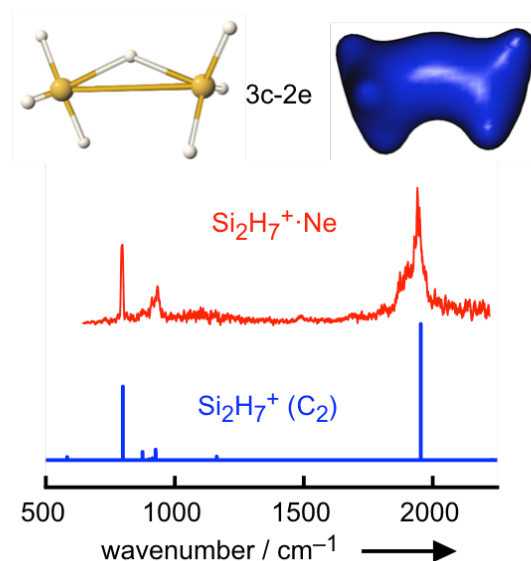
Building 99, Seminar Room I+II (EG)

Prof. Dr. Otto Dopfer

Institut für Optik und Atomare Physik, Technische Universität Berlin

Vibrational spectra and structures of silicon hydride cluster cations

Silanes (Si_xH_y) and their derivatives and ions are fundamental species in a variety of chemical disciplines, ranging from astrochemistry to materials science and the theory of chemical bonding. Although Si and C are both group IV elements, they drastically differ in their chemical bonding properties. In contrast to the well-known hydrocarbon analogues (C_xH_y), very little spectroscopic information is available for Si_xH_y species due to the lack of suitable precursors. Here, we systematically characterize the geometric and electronic structure of Si_xH_y cations by IR spectroscopy and quantum chemical calculations. IR spectra of Si_xH_y^+ produced in a supersonic plasma molecular beam expansion of SiH_4 are inferred from photodissociation of cold $\text{Si}_x\text{H}_y^+\text{-Ar/Ne}$ complexes obtained in a tandem quadrupole mass spectrometer coupled to an electron impact ionization source and an octopole ion trap. The clusters are characterized in their ground electronic states by quantum chemical calculations to investigate the effects of ionization and Ar/Ne complexation on their geometric, vibrational, and electronic structure. We present initial results for Si_2H_6^+ [1], Si_2H_7^+ [2] and Si_3H_8^+ [3] with low-energy isomers featuring unusual three-center two-electron (3c-2e) bonding. First results on protonated silanols will also be presented.



[1] M. Savoca, M.A.R. George, J. Langer and O. Dopfer, Phys. Chem. Chem. Phys. 15, 2774 (2013).

[2] M. Savoca, J. Langer and O. Dopfer, Angewandte Chemie 125, 1376 (2013).

[3] M.A.R. George, M. Savoca, O. Dopfer, Chem. Eur. J. 19 45 (2013).