HIGH RESOLUTION MICROWAVE SPECTROSCOPY AND STRUCTURE OF THE WEAKLY BOUND $\mathrm{Xe}\cdots\mathrm{OCS}$ COMPLEX

DANIEL A. OBENCHAIN, SVEN HERBERS, PETER KRAUS, DENNIS WACHSMUTH, JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany*.

The rotational spectrum of the weakly bound complex between xenon and carbonyl sulfide has been measured using a coaxially oriented beam resonator arrangement (COBRA) Fourier transform microwave spectrometer in Hannover. There are nine naturally occurring isotopes of xenon in addition to the many possible isotopologues of carbonyl sulfide, which allows for a detailed analysis of the structure of the van der Waals complex and subsequent comparisons to other rare gas van der Waals complexes with carbonyl sulfide that have already been reported.

Of the nine isotopes of xenon, two have non-zero nuclear spins, $^{131}\mathrm{Xe}$ (I=3/2) and $^{129}\mathrm{Xe}$ (I=1/2). In the case of the $^{131}\mathrm{Xe}$, a hyperfine structure was observed in all transitions, revealing a non-zero field gradient at the xenon nucleus in the complex. High-level ab initio calculations were carried out to identify an accurate method for the prediction of the structure of the complex and the nuclear quadrupole coupling constants of $^{131}\mathrm{Xe}$. The van der Waals interaction energies of xenon and carbonyl sulfide will be discussed.