

EINLADUNG

Im Rahmen der gemeinsamen Kolloquien der Fakultät für Chemie und Chemische Biologie der Technischen Universität Dortmund und des Projektes RAMSES hält

PD Dr. Patrick Weis

Institut für Physikalische Chemie, Karlsruher Institut für Technologie

einen Vortrag mit dem Thema

"Determination of gas phase structures with ion mobility spectrometry"

In the first part TIMS-based collision cross section of several, mostly anionic species will be presented such as porphyrin oligomers, fullerene anions up to C₁₅₀, and dye molecules. By comparing their experimental CCS data with predictions from theory it is possible to assign structures and rule out or confirm isomers. The calculations are based on a combination of density function theory for geometry optimization and trajectory method for CCS determination. The quality of these theory-based predictions critically depends on the method used and on the overall charge state as well as the charge distribution of the molecular ion considered. Fullerenes and small dye molecules are used as test cases since their structures are well known. As an application the identification of several isomeric intermediates by TIMS in a dual-gold-catalyzed reaction will be presented.

The second part of my talk will focus on the combination of ion mobility spectrometry with photodissociation and photo electron spectroscopy using a custom-built instrument.

Zeit: Montag, 27.05.2019, 13.00 Uhr

Ort: Campus Nord, Chemiegebäude, C2-03-528

Für die Dozenten der Chemie

Der Dekan

Betreuer: Prof. Clever (0231/755 8677)