UNBOTTLEABLE MOLECULES GENERATED BY COLLISION INDUCED ELECTRON TRANSFER IN THE GAS PHASE: AN INTERSECTION OF EXPERIMENT AND THEORY

Helmut Schwarz

Institut für Chemie, Technische Universität Berlin, D-10623 Berlin,
FAX: ++49 30 314 21102; e-mail: Helmut.Schwarz@www.chem.tu-berlin.de

Over the last decade, neutralization-reionization mass spectrometry (NRMS)[1] has emerged as a powerful method for the generation and structural characterization of small, neutral molecules, which are believed to play a central role in many fields of chemistry, but are usually not accessible in the condensed phase. Systems that will be discussed in detail include the celebrated water oxide and ethylenedione molecules.

Further, experimental and computational studies of small, multiply charged cations (e.g. Olah's "superelectrophiles") [2] will be presented with emphasis on the generation of *thermochemically stable*, doubly- and triply-charged diatomic molecules by charge stripping (CS) mass spectrometry. [3] This area is of topical interest in chemistry and physics, and examples will be discussed for diatomic cations with *positive* proton affinities or of diatomic trications that are thermochmically stable towards Coulomb explosion.

References:

1. Schalley, C. H.; Hornung, G.; Schröder, D.; Schwarz, H. *Chem. Soc. Rev.* **1998**, *27*, 91.

2. Olah, G. H. *Angew. Chem.* **1993**, *105*, 805.

3. Schröder, D.; Schwarz, H. *J. Phys. Chem. A* **2000**, *104*, 11257.