

Selected Publications

A. REMPI/ZEKE/MATI Spectroscopy on H-bonded Complexes

ZEKE spectroscopy of complexes and clusters (review)

K. Müller-Dethlefs, O. Dopfer, and T.G. Wright*, Chem. Rev. 94, 1845-1871 (1994)*

- review article including results of my PhD thesis
- first ZEKE and MATI spectra of hydrogen bonded complexes
- accurate ionization energies and complete sets of intermolecular vibrations

B. Rovibronic Spectroscopy of Hydrocarbon Anions

Electronic spectra of linear carbon anions

M. Tulej, D.A. Kirkwood, G. Maccaferri, O. Dopfer, and J.P. Maier, Chem. Phys. 228, 293-300 (1998)*

- development of new apparatus for photodetachment spectroscopy of anionic species
- first evidence for carbon anions as possible carriers of diffuse interstellar bands (DIB)

C. IR Photodissociation Spectroscopy and Microsolvation of Ionic Clusters

(I) Review Articles:

(a) High resolution spectroscopy of ionic complexes (review)

E.J. Bieske and O. Dopfer*, Chem. Rev. 100, 3963-3998 (2000)*

- review article including results of my habilitation thesis
- complete review of all high resolution studies of charged complexes
- ion-ligand interactions and their potentials
- sources and spectroscopic methods for ion-ligand complexes
- properties and general rules derived for ionic hydrogen (proton) and π -bonds

(b) Spectroscopic and theoretical studies of CH_3^+ -Rg_n clusters (Rg=He, Ne, Ar):

From weak intermolecular forces to chemical reaction intermediates (review)

O. Dopfer, Int. Rev. Phys. Chem. 22, 437-495 (2003)*

- review article of our experimental and theoretical results for CH_3^+ -Rg_n complexes
- solvation of reactive carbocations with nonpolar ligands
- ion-ligand potential energy surfaces
- structure and dynamics of p-bonded complexes (p-bonds versus H-bonds)
- model systems for S_N2 reactions (first spectroscopic evidence for double minimum potential)
- rare gas atoms as sensor for reactivity of molecular orbitals of fundamental ions
- open-shell effects on intermolecular forces (induction versus charge transfer)
- microsolvation process, isomers, cluster growth (influence of solvation on reactivity)
- quantum chemical calculation of potential energy surfaces
- multidimensional solution of rotation-vibration Schrödinger equation for nonrigid systems

(c) IR Spectroscopy of Microsolvated Aromatic Cluster Ions:

Ionization-Induced Switch in Aromatic Molecule-Solvent recognition (review)

O. Dopfer, Z. Phys. Chem. 219, 125-168 (2005)*

- review article of our experimental and theoretical results for biophysical interactions
- microsolvation of aromatic molecules in polar and nonpolar solvents
- H-bonds, π -bonds, charge-dipole interaction, proton transfer to solvent
- structure and intermolecular bonding motifs of biologically relevant interactions

(d) IR spectroscopic strategies for the structural characterization of isolated and microsolvated protonated aromatic molecules:

O. Dopfer, J. Phys. Org. Chem. xxx, xxx-xxx (2006)*

- review article of IR spectroscopic strategies für ions and their clusters
- protonated aromatic molecules: structure, protonation site, reactivity, microsolvation
- influence of functional groups on reactivity

(II) Ion-Ligand Interactions of Biophysical Interest:

(a) Microhydration of protonated biomolecular building blocks:

IR spectra of protonated Imidazol-water_n complexes

H.-S. Anrei, N. Solcà and O. Dopfer*, *ChemPhysChem* **7**, 107-110 (2006)

(b) Prototype microsolvation of aromatic hydrocarbon cations by polar ligands:

IR spectra of benzene⁺-L_n clusters (L=H₂O, CH₃OH)

N. Solcà and O. Dopfer*, *J. Phys. Chem. A* **107**, 4046-4055 (2003)

- first spectroscopic study for benzene⁺-water interaction and water solvation network
- prototype for interaction between aromatic cation and polar solvent
- first spectroscopic study for hydration of protonated biomolecules

(III) Spectroscopy of Fundamental Carbocations:

IR spectra of C₃H₃⁺-N₂ dimers: identification of proton-bound c-C₃H₃⁺-N₂ and H₂CCCH⁺-N₂ isomers

O. Dopfer*, D. Roth, J.P. Maier, *J. Am. Chem. Soc.* **124**, 494-502 (2002)

- C₃H₃⁺ isomers (relevance for hydrocarbon plasmas, combustion, soot formation soot, astrochemistry)
- first unambiguous spectroscopic detection of c-C₃H₃⁺ in the gas phase

(IV) Protonation of Aromatic Molecules:

(a) Protonated Benzene: IR Spectrum and Structure of C₆H₇⁺

N. Solcà and O. Dopfer*, *Angew. Chem. Int. Ed.* **41**, 3628-3631 (2002), **VIP Artikel**

(b) Protonation of gas-phase aromatic molecules:

IR spectrum of the fluoronium isomer of protonated fluorobenzene

N. Solcà and O. Dopfer*, *J. Am. Chem. Soc.* **125**, 1421-1430 (2003)

(c) Separate spectroscopic detection of carbenium and fluoronium isomers of protonated fluorobenzene

N. Solcà and O. Dopfer*, *Angew. Chem. Int. Ed.* **42**, 1537-1540 (2003), **VIP Artikel**

(d) Spectroscopic identification of oxonium and carbenium ions of protonated phenol in the gas phase:

IR spectra of weakly bound C₆H₇O⁺-L dimers (L=Ne, Ar, N₂)

N. Solcà and O. Dopfer*, *J. Am. Chem. Soc.* **126**, 2732-2741 (2004)

- first spectroscopic studies on gas-phase protonation of aromatic molecules
- first spectroscopic and unambiguous structure determination of protonated benzene
- competition between ring and substituent protonation (substitution effects on reactivity)

(V) Proton Wires:

(a) IR spectrum and structure of protonated ethanol dimer:

implications for the mobility of excess protons in solution

N. Solcà and O. Dopfer*, *J. Am. Chem. Soc.* **126**, 9520-9521 (2004)

(b) Hydrogen-bonded Networks in Ethanol Proton Wires:

IR Spectra of (EtOH)_qH⁺-L_n clusters (L=Ar/N₂, q≤4, n≤5)

N. Solcà and O. Dopfer*, *J. Phys. Chem. A* **109**, 6174-6186 (2005)

- first spectrum of a protonated alcohol dimer and larger clusters
- smallest building block of an alcohol proton wire
- influence of solvation on properties of proton bridges

(VI) Picosecond Time-resolved Spectroscopy

Real-time Observation of Ionization-Induced Hydrophobic ⇌ Hydrophilic Switching

S. Ishiuchi, M. Sakai, Y. Tsuchida, A. Takeda, Y. Kawashima, M. Fujii*, O. Dopfer*, K. Müller-Dethlefs*,

Angew. Chem. **117**, 6305-6307 (2005), *Angew. Chem. Int. Ed.* **44**, 6149-6151 (2005)

- first three-colour ps experiment
- first direct real-time observation of an intermolecular isomerization reaction in a cluster ion
- competition between intermolecular ⇌ and H-bonds