CFEL SCIENCE

SEMINAR

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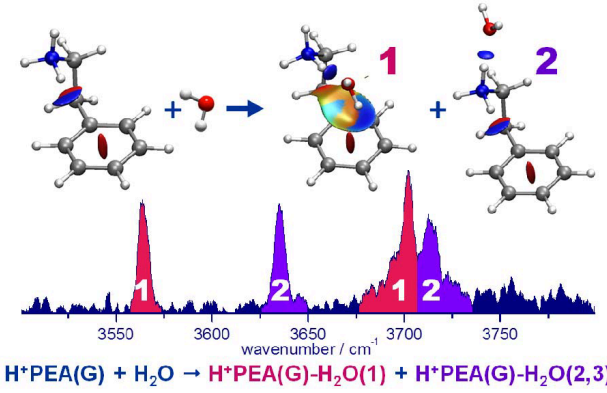
Binding motifs of a microsolvated neurotransmitter: IR spectroscopy of protonated phenylethylamine and its water clusters

Hydration has a drastic impact on the structure and function of flexible biomolecules, such as aromatic ethylamino neurotransmitters. The structure of microhydrated protonated phenylethylamine (H^+PEA-$(H_2O)_n$, n≤4) is investigated by infrared photodissociation (IRPD) spectroscopy of cold cluster ions by using rare-gas tagging and dispersion-corrected density functional theory calculations.[1,2] Microhydration of this prototypical neurotransmitter gives an insight into the first step of the formation of its solvation shell, especially regarding the competition between intra- and intermolecular interactions. The spectra of Ar-tagged H^+PEA-H_2O reveal the presence of a stable insertion structure in which the water molecule is located between the positively charged ammonium group and the phenyl ring of H^+PEA, acting both as a hydrogen bond acceptor (NH^+…O) and donor (OH…π). Two other nearly equivalent isomers, in which water is externally H-bonded to one of the free NH groups, are also identified. The balance between insertion and external hydration strongly depends on temperature. The further characterisation of H^+PEA-$(H_2O)_n$-Ar clusters with n>1 reveals the progressive solvation of the ammonium group forming for n = 3 a single isomer, core of the solvation shell.



$H^+PEA(G) + H_2O \rightarrow H^+PEA(G)\text{-}H_2O(1) + H^+PEA(G)\text{-}H_2O(2,3)$

[1] A. Bouchet, M. Schütz, B. Chiavarino, M-E. Crestoni, S. Fornarini, O. Dopfer, Phys. Chem. Chem. Phys., 2015, 17, 25742-25754

[2] A. Bouchet, M. Schütz, O. Dopfer, ChemPhysChem 2016, 17, 232 - 243

Host: Melanie Schnell - CFEL Molecular Physics seminar