

# Seminar invitation

Monday, October 2<sup>nd</sup> 2017 at 14:00, room 108

J. Heyrovský Institute of Physical Chemistry CAS, Dolejškova 3, Prague

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## Spectroscopic Snapshots of the Proton Transfer Mechanism in Water

How ions are solvated in solution has intrigued physical chemists since the development of the theory of electrolytic dissociation at the end of the nineteenth century. The anomalously high proton mobility of water, for example, can be explained by a periodic isomerization between the Eigen and Zundel binding motifs,  $\text{H}_3\text{O}^+(\text{aq})$  and  $\text{H}_5\text{O}_2^+(\text{aq})$ , respectively. However, the detailed mechanism is considerably more complex and not completely understood, in part, because the vibrational fingerprint of this process is masked by the diffuse nature of the key bands in bulk water. These rapidly interconverting structures from the condensed phase can be stabilized, isolated and studied in the gas phase in the form of protonated water clusters.

Infrared photodissociation (IRPD) spectroscopy not only serves as a powerful tool for studying the structure of the protonated water clusters  $\text{H}^+(\text{H}_2\text{O})_n$  and  $\text{D}^+(\text{D}_2\text{O})_n$ , but also to capture clear markers that encode the collective reaction coordinate along the proton-transfer event.<sup>1-5</sup> With the aid of isomer-selective infrared/infrared double resonance ( $\text{IR}^2\text{MS}^2$ ) spectroscopy the contribution of multiple isomers to the IRPD spectrum can be disentangled and assigned on the basis of a comparison to the results of electronic structure calculations. Recent advances in the vibrational spectroscopy of protonated water clusters are highlighted, with particular emphasis on the importance of probing a broad spectral range and of considering anharmonic as well as nuclear quantum effects to unambiguously identify the signal carrier.

<sup>1</sup> C.T. Wolke, J.A. Fournier, L.C. Dzuman, M.R. Fagiani, T.T. Odbadrakh, H. Knorke, K.D. Jordan, A.B. McCoy, K. R. Asmis, M.A. Johnson, *Science* **354** 1131 (2016)

<sup>2</sup> M.R. Fagiani, H. Knorke, T. Esser, N. Heine, C.T. Wolke, S. Gewinner, W. Schöllkopf, M.-P. Gaigeot, R. Spezia, M.A. Johnson, K.R. Asmis, *Phys. Chem. Chem. Phys.* **18** 26743 (2016)

<sup>3</sup> N. Heine, M.R. Fagiani, K.R. Asmis, *J. Phys. Chem. Lett.* **6** 2298 (2015)

<sup>4</sup> N. Heine, M.R. Fagiani, M. Rossi, T. Wende, G. Berden, V. Blum, K.R. Asmis, *J. Am. Chem. Soc.* **135** 8266 (2013)

<sup>5</sup> K.R. Asmis, N.L. Pivonka, G. Santambrogio, M. Brümmer, C. Kaposta, D.M. Neumark, L. Wöste, *Science* **299**, 1375 (2003)