

Water-Mediated Ion Pairing: Occurrence and Relevance - DTU Orbit (09/11/2017)

Water-Mediated Ion Pairing: Occurrence and Relevance

We present an overview of the studies of ion pairing in aqueous media of the past decade. In these studies, interactions between ions, and between ions and water, are investigated with relatively novel approaches, including dielectric relaxation spectroscopy, far-infrared (terahertz) absorption spectroscopy, femtosecond mid-infrared spectroscopy, and X-ray spectroscopy and scattering, as well as molecular dynamics simulation methods. With these methods, it is found that ion pairing is not a rare phenomenon only occurring for very particular, strongly interacting cations and anions. Instead, for many salt solutions and their interfaces, the measured and calculated structure and dynamics reveal the presence of a distinct concentration of contact ion pairs (CIPs), solvent shared ion pairs (SIPs), and solvent-separated ion pairs (2SIPs). We discuss the importance of specific ion-pairing interactions between cations like Li(+) and Na(+) and anionic carboxylate and phosphate groups for the structure and functioning of large (bio)molecular systems.

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