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Accession number:20120414706517

Title:Watching the low-frequency motions in aqueous salt solutions: The terahertz vibrational signatures of hydrated ions

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Source title:Journal of the American Chemical Society

Abbreviated source title:J. Am. Chem. Soc.

Volume:134

Issue:2

Issue date:January 18, 2012

Publication year:2012

Pages:1030-1035

Language:English

ISSN:00027863

E-ISSN:15205126

CODEN:JACSAT

Document type:Journal article (JA)

Publisher:American Chemical Society, 2540 Olentangy River Road, P.O. Box 3337, Columbus, OH 43210-3337, United States

Abstract:The details of ion hydration still raise fundamental questions relevant to a large variety of problems in chemistry and biology. The concept of water "structure breaking" and "structure making" by ions in aqueous solutions has been invoked to explain the Hofmeister series introduced over 100 years ago, which still provides the basis for the interpretation of experimental observations, in particular the stabilization/destabilization of biomolecules. Recent studies, using state-of-the-art experiments and molecular dynamics simulations, either challenge or support some key points of the structure maker/breaker concept, specifically regarding long-ranged ordering/disordering effects. Here, we report a systematic terahertz absorption spectroscopy and molecular dynamics simulation study of a series of aqueous solutions of divalent salts, which adds a new piece to the puzzle. The picture that emerges from the concentration dependence and assignment of the observed absorption features is one of a limited range of ion effects that is confined to the first solvation shell. © 2011 American Chemical Society.

Number of references:26

Main heading:Molecular dynamics

Controlled terms:Dynamics - Hydration - Ions - Molecular biology - Solutions - Terahertz spectroscopy

Uncontrolled terms:Aqueous salt solution - B-y Ions - Concentration dependence - Experimental observation - Hofmeister series - Hydrated ions - Ion effect - Ion hydration - Keypoints - Low-frequency motion - Molecular dynamics simulations - Solvation shell - Structure makers - Tera Hertz - Vibrational signature

Classification code:801 Chemistry - 801.4 Physical Chemistry - 802.2 Chemical Reactions - 803
Chemical Agents and Basic Industrial Chemicals - 804 Chemical Products Generally - 931.1
Mechanics

DOI:10.1021/ja207929u

Database:Compendex

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