Structured water around ions-FTIR difference spectroscopy and quantum-mechanical calculations.

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Rok wydania

2001

Czasopismo

Physical Chemistry Chemical Physics

Numer woluminu

3

Strony

4228-4234

DOI

10.1039/B103551G

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Saturated solutions of LiCl, NaCl, KCl, NH_4Cl, NH_4Br, NH_4I, $CaCl_2$ and $MgCl_2$ against pure water are recorded using attenuated total reflection FTIR difference spectroscopy. All ions show distinct effects on the water bands which result in several positive and negative bands. For the anions, band shifts to higher frequencies are found in the sequence F^-, Cl^-, Br^-, I^-. An opposite shift is observed for the cations in the sequence NH_4^+, K^+, Na^+, Li^+. With the shift of the band envelope to lower wavenumbers, bands are visible which are due to the effect of Fermi resonance ($\nu_1 + 2\nu_2$). Quantum-mechanical calculations using the GAUSSIAN 94 program package with the 6311G + + (3df,3pd) basis set were performed for the ions and one water molecule. Bands were calculated for water–ion formations in C_{2v} and C_s symmetry. The observed and calculated frequency shifts correspond to changes in the geometry and charge separation of the water molecules opposing the ion.

Adres publiczny

https://doi.org/10.1039/B103551G

Strona internetowa wydawcy

https://www.rsc.org/