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| Title: | Investigation of solvation of ammonium salts: A Raman spectroscopy and ab initio study |
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| Abstract: | The effect of dissolved salts on the hydrogen bonded network in water is extremely important to be understood, as it plays an important role in many aspects of structure and dynamics in aqueous solutions. We have undertaken a study of this phenomenon, using NH4Cl (AC) and (NH4)2SO4 (AS), as the salts for influencing the hydrogen bonded network in water. The effects of varying the temperature and concentration in these aqueous solutions of both the salts, on the Raman spectra were studied, over the wavenumber range 50–4000 cm−1. It was found that at 25 °C, with increasing AS concentration, a monotonic increase in intensity of spectral features on the low wavenumber side (~3200 cm−1 region) of the O–H stretching band was observed, whereas AC showed the opposite effect. A parameter (χstruct) is defined from the spectral data, which indicates that more hydrogen bonded network forms in presence of AS salt compared with AC salt, in aqueous solution. Temperature variation study also reveals that, presence of AC induces a more disordered network in aqueous solutions, than AS. To support these conclusions, we have performed ab initio calculation for the salt···nW species, where n = 1−8, using the MP2/6–31+G(d,p) level of theory. Solvent separated ion pair formation has been reported for NH4+ and Cl− ions, whereas NH4+ and SO42− ions remain as contact ion pair up to AS···8W cluster. This study helps understand the effect of salt water interaction at the molecular level and may have huge implications in atmospheric physics, geophysics, and ice crystallization. |
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