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Anharmonicity and Fragility of Protic Ionic Liquids JENNY KIM, National Institute of Standards and Technology, AUSTEN ANGELL, KAZUHIDE UENO, Arizona State University, MADHU TYAGI, CHRISTOPHER SOLES, KEVIN MASSER, National Institute of Standards and Technology — Supercooled liquids are often characterized by their fragility which is associated with physicochemical properties. However, the origin of fragility is still controversial. Superfragile liquid, decahydroisoquinoline (DHiQ) is chosen as a parent molecule to systematically investigate the relationship between anharmonicity and fragility of supercooled liquids. Earlier study by Ueno et al. (J. Phys. Chem. B 2012, 116) demonstrated that the protonation of DHiQ by different Bronsted acids results in the loss of superfragility. To understand the nature of fragile liquids, we conducted inelastic/quasielastic (IE/QE) neutron scattering measurements to examine low frequency vibrational dynamics (boson peak) and the relaxation behavior of DHiQ (high fragility) and DHiQ-based ionic liquids with intermediate (formate, Fm) and low (trifluoromethansulfonimide, TFSI) fragilities. With the protonation, molecular acids will be hydrogen-deficient and the scattering will be dominated by cation, [DHiQ$^+$]. This strategy simplifies our interpretation in terms of understanding the fitting result from IENS/QENS spectra. By protonating DHiQ with stronger acids, large shift in low frequency vibrational modes and smaller mean square displacements were examined at temperatures higher than Tg. We illustrate how the degree of protonation and ionicity plays a role in the loss in superfragility of DHiQ.

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