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Increased Acidity of Trifluoroacetic Acid in Amorphous Solid Water and Charge-Delocalized Hydroniums

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We studied the ionic dissociation of trifluoroacetic acid (TFA) in amorphous solid water (ASW) using reflection absorption infrared spectroscopy, low energy sputtering, and H/D isotopic exchange experiment. TFA readily dissociated to hydronium and counter ions in ASW at 60 K, which indicates a significant increase of the acidity as compared to that in aqueous solution at room temperature. The acid dissociation in D₂O-ASW produced a Zundel continuum band in the 1000–3000 cm⁻¹ region and an accompanying lowered intensity of the O–D stretching band of D₂O. The reduced intensity of D₂O was several times larger than that expected for 1:1 stoichiometric proton transfer from TFA to water. Excess protons released from the acid migrated through as many as 20 water layers in ASW. These observations indicate that excess protons are highly mobile and dynamically delocalized in the hydrogen-bonded water chain. Such characteristics of excess protons may be related to the increased acidity of TFA and the appearance of the Zundel continuum absorption in IR spectra.

Significance statement

The observation of efficient ionization of trifluoroacetic acid in amorphous solid water leads to an intriguing question: “can acids be more acidic in ASW than in liquid water?” The highly mobile nature of excess protons in ASW and its entropy-increasing effect may provide a clue to answer this question.

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