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TITLE: How does the Porosity of Interstellar Ice Affect Chemical Complexity and Deuteration Exchange?

ABSTRACT BODY:

Abstract Body: The porosity of interstellar water ice, Amorphous Solid Water (ASW), greatly enhances the ability of ice to uptake, then release small gas adsorbates. This provides the strongest evidence that interstellar ices must be porous, accounting for the differences between predicted and observed gas-phase abundances, and provides a mechanism to enhance reagent diversity for complex chemistry in the ice. However, no dangling OH (d-OH) bond features, to-date associated with ice porosity, have been reported in interstellar ice spectra, so some conclude that interstellar ices must be non-porous, given that the d-OH spectra disappear in laboratory studies when ASW is energetically processed. But are d-OH features and gas-uptake reliable experimental measures of ice porosity? Here we combine fundamental studies of ASW with observational data to determine ASW porosity and understand its role in the chemical evolution of interstellar ices.

We show upper-limit detections of d-OH in observational spectra towards a handful of sources (Fraser et al (2015)). Laboratory experiments on selective irradiation of d-OH features (Noble et al (2013), (2014)), combined with quantum chemical calculations (Lui et al (2015)), show that the d-OH bonds probe the density of defect sites in the surface and sub-surface structure. Consequently surfaces with d-OH bonds are significantly more reactive and therefore promote chemical complexity across extra-terrestrial regions where they are found, but do not reflect ice porosity.

Our neutron scattering data show that ASW ices actually contain cylindrical pores of around 10 Å diameter (Mitteldorfer et al (2014)). The pore collapse process can only be initiated by long range molecular diffusion at T > 121 K, and follows complex kinetics (Hill et al (2015a); such effects can be reproduced by molecular dynamics simulations of ASW ice-heating (Elkind et al (2015): Miller et al (2015)), and are directly linked to deuteration exchange. We explain the implications of these data for interstellar ice reactivity, ice growth (Hill et al (2015b)), and exchange reactions leading to ice deuteration (Fraser et al (2015)).

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