Temperature dependence of the infrared spectra of ices

Figure S1 shows IR reflection–absorption spectra at different temperatures for the ice obtained after Ne matrix sublimation at 11 K (upper panel) and 13 K (middle panel), and for amorphous ice vapor-deposited at 11 K (lower panel). The prepared ices were heated at 0.1 K s\(^{-1}\) and spectra were measured in the range 50–160 K. The IR spectra of both the crystalline and amorphous ices obtained after Ne matrix sublimation remained quite stable until 90 K, and the amorphous ice crystallised at 130–160 K. This shows that after water ice forms at low temperature, further structural rearrangement (annealing) is unlikely unless the sample is heated sufficiently to induce hydrogen-bond rearrangement.

The IR spectra for the vapor-deposited amorphous ice continuously changed with heating to 130 K. Water began to desorb at 130–150 K (as denoted by a decrease in the absorption band strength), before crystallisation occurred at 160 K. These results show that the ices obtained after Ne matrix sublimation are more strongly hydrogen bonded than the vapor-deposited amorphous ice.
**Fig. S1.** Infrared reflection–absorption spectra of ices at different temperatures using H$_2$O with 3.5 mol% HDO, showing ices obtained after Ne matrix sublimation at 11 K (upper) and 13 K (middle), and vapor-deposited amorphous H$_2$O ice at 11 K (lower). The prepared ices were heated at 0.1 K s$^{-1}$ and spectra were measured at the preparation temperature of 11 or 13 K (black), 50 K (blue), 90 K (green), 130 K (orange), 150 K (red), and 160 K (brown).