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The structure of ice crystallized from supercooled water[1]

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The freezing of water to ice is fundamentally important to fields as diverse as cloud formation to cryopreservation. Traditionally ice was thought to exist in two well-crystalline forms: stable hexagonal ice and metastable cubic ice. It has recently been shown, using X-ray diffraction data, that ice which crystallizes homogeneously and heterogeneously from supercooled water is neither of these phases. The resulting ice is disordered in one dimension and therefore possesses neither cubic nor hexagonal symmetry and is instead composed of randomly stacked layers of cubic and hexagonal sequences. We refer to this ice as stacking-disordered ice I (ice I_{sd}). This result is consistent with a number of computational studies of the crystallization of water. Review of the literature reveals that almost all ice that has been identified as cubic ice in previous diffraction studies and generated in a variety of ways was most likely stacking-disordered ice I with varying degrees of stacking disorder, which raises the question of whether cubic ice exists. New data will be presented which shows significant stacking disorder (or stacking faults on the order of 1 in every 100 layers of ice I_h) in droplets which froze heterogeneously as warm as 257 K. The identification of stacking-disordered ice from heterogeneous ice nucleation supports the hypothesis that the structure of ice that initially crystallises from supercooled water is stacking-disordered ice I, independent of nucleation mechanism, but this ice can relax to the stable hexagonal phase subject to the kinetics of recrystallization. The formation and persistence of stacking disordered ice in the Earth's atmosphere will also be discussed.

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