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## Molecular Dynamics simulations indicate solvation and stability of single-strand RNA at the air/ice interface, supporting a primordial RNA world on Ice

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Outstanding questions about the RNA world hypothesis for the emergence of life on Earth concern the stability and self-replication of prebiotic aqueous RNA. Recent experimental work has suggested that solid substrates and low temperatures could help resolve these issues. Here, we use classical molecular dynamics simulations to explore the possibility that the substrate is ice itself. We find that at -20 C, a quasi-liquid layer at the air/ice interface partially solvates a short (8-nucleotide) RNA strand such that the phosphate backbone anchors to the underlying crystalline ice structure through long-lived hydrogen bonds. The hydrophobic bases, meanwhile, are seen to migrate toward the outermost layer, exposed to air. Our simulations also reveal two key kinetic differences with respect to aqueous RNA. First, hydrogen bonds between solvent water molecules and phosphate diester moieties, believed to shield the RNA from hydrolysis, are much longer-lived for RNA on ice, compared to aqueous RNA at the same temperature. Second, contact between solvent water and ribose 2-OH' groups, considered a precursor to nucleophilic attack by deprotonated 2-OH' on the phosphate diester, is significantly less frequent for RNA on ice. Both differences point to lower susceptibility to hydrolysis of RNA on ice, and therefore increased opportunities for polymerization and self-copying compared to aqueous RNA. Moreover, exposure of hydrophobic bases at the air/ice interface offers opportunities for reaction that are not readily available to aqueous RNA (e.g., base-pairing reaction with free nucleotides diffusing across the air/ice interface). These findings thus offer the possibility of a role for an ancient RNA world on ice distinct from that considered in extant elaborations of the RNA world hypothesis. This work is, to the best of our knowledge, the first molecular dynamics study of RNA on ice.