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Measurements of the Thermal Contraction of Liquids as Applied to Nanoscale-Sized Solvent Channels in Cryogenically Cooled Protein Crystals

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Abstract: Protein crystals (length $\sim 10\text{-}10^3 \mu\text{m}$) are composed of an ordered array of protein molecules (length $\sim 10\text{-}100 \text{ nm}$) in which the interstitial spaces (length $\sim 10\text{-}100 \text{ nm}$) between the proteins are filled with disordered aqueous based liquid. Cooling the crystals to $\sim 100\text{K}$ damages the crystal, in part because the contraction of the disordered liquid in the nanoscale-sized interstices does not match the contraction of the protein molecule lattice. To reduce the crystal damage from cooling, the contraction of the disordered liquid can be modulated by changing its composition using small molecules commonly called cryoprotectants. Here we explore the dependence of the thermal contraction of binary solutions of water and various cryoprotective molecules (50% w/w) on the identity of the cryoprotectant. We use a buoyancy-based approach to measure the density of $\sim 1 \text{ mL}$ solutions at 77K and compare to the density at room temperature. We find correlations between the contraction and physical parameters of the cryoprotectants, and discuss these results in the context of the model for cooling-induced damage described above.



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