LOW TEMPERATURE-INDUCED CONFORMATIONAL CHANGE OF MODEL COMPOUNDS

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Conformational equilibrium is a central concept in the structural chemistry of polyatomic molecules such as peptides and proteins. This equilibrium can be affected by environmental conditions such as temperature and pressure. Structural flexibility of these molecules plays an important role in biological phenomena. The structural flexibility of proteins becomes slower with decreasing temperature resulting in a glass transition. The glass transition temperature (T_g) of proteins has been investigated using DSC methods, however, there have been few studies of protein structural change under low temperature. To enhance conceptual understanding of this transition, it is useful to investigate the conformational behavior of simple model compounds at low temperature because of the ease of vitrification in such systems. We have investigated the low temperature-induced conformational behavior of aqueous tetraethylammonium halides (Et_4NX, X=halide ion) solutions having the $trans-gauche.trans-gauche$ ($tg.tg$) and $trans-trans.trans-trans.trans$ ($tt.tt$) equilibrium using vibrational spectroscopy. A remarkable result is that going from the liquid to crystal states the population of $tt.tt$ conformer of Et_4N^+ ion becomes a dominant conformer. On the other hand, the population of $tt.tt$ conformer of Et_4N^+ in the glassy state is less than in crystal state. Based on this result, the increase of $tt.tt$ conformer as seen in the crystal state was restricted by the vitrification. If the $tg.tg$ and $tt.tt$ conformers of Et_4N^+ ion correspond to the folded- and unfolded-structures of protein, respectively, our results indicate that the vitrification of aqueous protein solution might restrict protein unfolding.

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