Temperature and Pressure Effects on Conformational Equilibria of Model Compounds of Proteins in Aqueous Solutions: A Vibrational Spectroscopic Study

Takahiro Takekiyo

The hydration is an important factor for the conformational equilibria of simple organic molecules, such as haloalkane and haloacetone. The hydration is also an important factor for the structural stability of proteins in aqueous solutions. However, the detail relationship between the structural stability of proteins and hydration is not clarified due to the complicated structure of proteins. Oligopeptides are located between the simple organic molecules and the biopolymers such as proteins. The study of the hydration on conformational equilibria of oligopeptides is important to expand the thermodynamic interpretation for the hydration of simple organic molecules. Moreover, the study of the hydration on conformational equilibria of simple organic molecules and oligopeptides could also provide us with basic information for understanding the hydration effect on structural stability of proteins. However, the thermodynamic studies of the hydration on conformational equilibria of model compounds of proteins including oligopeptides have been hardly done. In this study, we measured the temperature and pressure effects on conformational equilibria of model compounds of proteins in aqueous solution by using vibrational spectroscopy (Infrared and Raman), and determined the difference in the partial molar enthalpy (ΔH)and the difference in the partial molar volume (ΔV) between the conformers. From obtained ΔH and ΔV, it was found that the contribution of the hydration for ΔH and ΔV of model compounds increases with increasing chain length of model compound. Moreover, from the pressure effect on the helix-coil transition of the helix formed oligopeptide without tertiary structure such as hydrophobic interaction, the population of the helix conformer increases with increasing pressure, and that of the coil conformer decreases. Our result is different from the pressure effect on the helix structure in proteins, which the helix structure in proteins breaks with increasing pressure. From these results, the helix formation oligopeptide having no tertiary structure stabilized under high pressure. Therefore, we suggested that the tertiary structure such as hydrophobic interaction contributes to the pressure denaturation of proteins.