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Gibbs energies, enthalpies, and entropies of water and lysozyme at the inner edge of excess hydration

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Abstract

The aim of this study is to simultaneously monitor the excess partial Gibbs energies, enthalpies, and entropies of water and white egg lysozyme and demonstrate how these quantities correlate with the coverage of the protein macromolecules by water molecules. Isothermal calorimetry and water sorption measurements were applied to characterize the hydration dependencies of the excess thermodynamic functions. The excess partial quantities are found to be sensitive to changes in the water and protein states. At the lowest water weight fractions (w1), changes in the excess functions are primarily attributable to the addition of water. The transition of lysozyme from a glassy (rigid) to a flexible (elastic) state is accompanied by significant changes in the excess partial quantities. When the charged groups on the protein are covered, this transition occurs at w1 = 0.05; when the coverage of both polar and weakly interacting surface elements is complete, the excess partial quantities become hydrated at w1 > 0.5. At the highest water content, water addition has no significant effect on the excess quantities. At w1 > 0.5, changes in the excess functions solely reflect changes in the state of the protein. © 2013 AIP Publishing LLC.

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