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Probing protein hydration by the difference O H (O D) vibrational spectroscopy: Interfacial percolation network involving highly polarizable water-water hydrogen bonds

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Abstract

The difference DO-H (HO-H, DO-H) IR and NIR vibrational absorption spectroscopy has been applied to aqueous solutions of native and thermally unfolded Bovine Serum Albumin (BSA). Subsequent global Gaussian analysis of the obtained and matching published data for the BSA "dry films" (J. Grdadolnik and Y. Maréchal, Biopolymers, 62 (2001) 40–53) disclosed two kinds of intensive and very broad O H (O D) sub-bands, centered at 3260 and 2840 cm^{-1} (for O D, at 2350 and 2050 cm^{-1}, accordingly). These bands are assigned to the stretching vibrations of water molecules involved in strong protein-water and water-water hydrogen-bonding, respectively, latter probably resulting in two dimensional (2D) percolating networks with migrating protons, as suggested recently by G. Careri (Progr. Biophys. Mol. Biol. 70 (1998) 223–249). For the BSA solution sample, upon the protein denaturation at ca. 65–70 °C, a partial liberation of unexchangeable N H protons has been observed accompanied also by the partial release of bound interfacial water.

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Keywords

Protein hydration; Difference vibrational spectroscopy of water; Polarizable hydrogen bonds; Percolating 2D network

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> …Replacing H2O with D2O for comparing the stability of proteins would lead to the increase of transition temperature and the decrease of enthalpy (Makhatadze, Clore, & Gronenborn, 1995). The Raman spectra after isotope exchange was shown in Fig. 2E. Khoshtariya et al. (2003) showed two kinds of intensive and very broad O–H (O-D) sub-bands, centered at 3260 cm−1 and 2840 cm−1. The appearance of the extra band at about 2500 cm−1 was attributed to the stretching vibration of the O/D bond, and the higher Raman strength value near the band indicated that more replaceable hydrogen atoms were inside and on the surface of the protein molecule.…

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> …Sánchez-gonzález et al. (2008) had evaluated the protein and water structural changes in gelation of surimi. Khoshtariya, Hansen, and Leecharoen (2003) has probed protein hydration by analyzing the different O-H (O-D) vibrational spectroscopy, which indicated that O-H bond lied in 3260 and 2840 cm−1 and O-D bond lied in 2350 and 2050 cm−1 that were connected with the hydrogen bond and other interactions between protein and water. As shown in Supplementary Fig. S1C, these are Raman spectra of samples after exchanging isotope H/D.…

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