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标题: Hydration and temperature interdependence of protein picosecond dynamics
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摘要: We investigate the nature of the solvent motions giving rise to the rapid temperature dependence of protein picoseconds motions at 220 K, often referred to as the protein dynamical transition. The interdependence of picoseconds dynamics on hydration and temperature is examined using terahertz time domain spectroscopy to measure the complex permittivity in the 0.2-2.0 THz range for myoglobin. Both the real and imaginary parts of the permittivity over the frequency range measured have a strong temperature dependence at >0.27 h (g water per g protein), however the permittivity change is strongest for frequencies <1 THz. The temperature dependence of the real part of the permittivity is not consistent with the relaxational response of the bound water, and may reflect the low frequency protein structural vibrations slaved to the solvent excitations. The hydration necessary to observe the dynamical transition is found to be frequency dependent, with a critical hydration of 0.19 h for frequencies >1 THz, and 0.27 h for frequencies <1 THz. The data are consistent with the dynamical transition solvent fluctuations requiring only clusters of similar to 5 water molecules, whereas the enhancement of lowest frequency motions requires a fully spanning water network.
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