

This report describes one of the first attempts to compare time-of-flight neutron spectra of BPTI, lysozyme and myoglobin to in vacuo simulations. Low temperatures turned out to emphasize low frequency vibrations against frozen out diffusive motions. Compared to 80 K it is “thus likely that at least part of the quasielastic scattering seen at 300 K is due to increased transitions between conformational substates, rather than damped harmonic modes”. The general understanding is that increasing temperature increases the amplitude of molecular transitions in contrast to resolution effects or enhanced damping of vibrational motions.