Dynamics of an Antimicrobial Oligopeptide: Low-Temperature Adiabatic Calorimetry and Neutron Scattering

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The evolution of the energy landscape of proteins from the harmonic regime to complex hydration-dominated interactions above 200 K has been studied extensively. Parallel work on small and intermediate peptides is less developed. We are studying the dynamics of an antimicrobial 15-residue oligopeptide (CM15), a hybrid from Cecropin A and Melittin. As a system intermediate in size between small peptides and proteins, data on CM15 can contribute valuable information to our understanding of glass-like transitions in proteins.

We have performed low-temperature adiabatic calorimetry and neutron scattering measurements for the dry peptide and a 49 % water hydrated sample. For the calorimetric measurements, a laboratory-made adiabatic calorimeter for small samples was employed and for neutron scattering a time-of-flight instrument, MIBEMOL, was used at Laboratoire Leon Brillouin, France. We covered the 100 to 270 K region, recording spectra from CM15 at 9 temperatures plus a continuous scan from 195 to 270 K. We also measured spectra for the nominally dry sample.
The mean-square mobilities determined from the integrated intensities show that in this oligopeptide the dynamic transition occurs at a higher temperature, closer to that observed in glutathione. In inelastic spectra, up to 200 K, we observed, around 3 meV, a region of excess intensity over Debye behavior. Well-defined spectra up to 50 meV quantify the T and Q dependent evolution of bands of damped vibrational modes, suitable for detailed comparison with current heat capacity measurements. Results of the measured heat capacities of the 3 samples (dry, 49 %, and 451 % water) will be shown for the temperature range 6 - 300 K. The calculated mobilities as a function of temperature for the dry and 49 % hydrated samples will be presented, as well as the heat capacities calculated from the vibrational density of states.

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