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Low-Frequency Raman Spectroscopy of Trialanine.[1] RACHEL M. STEPHENSON, ANGELA R. HIGHT WALKER, NIST — The effect of sample conditions on the structural conformation of trialanine has been investigated with visible Raman spectroscopy. Trialanine is used here as a simple protein-mimetic system in order to more easily isolate the backbone amide vibrational modes, low-frequency tortional modes and modes from hydrogen bonding. Crystalline trialanine is known to exist with both parallel (p-Ala_3) and antiparallel (ap-Ala_3) β-sheet crystal structures, depending on the solvent composition during crystallization. The ap-sheet form of trialanine co-crystallizes with water, which is easily removed under vacuum, offering a further opportunity to examine the effect of solvation on the vibrational spectra, especially when also compared with trialanine in solution. By collecting Raman spectra in different sample phases, and at different concentrations, pH and temperatures, the vibrational modes most sensitive to the secondary structure can be identified. The collected data will be compared to the literature, including other vibrational spectroscopic data and high-level simulations.

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