SURVEYING THE HYDROGEN BONDING LANDSCAPE OF AN ACHIRAL, α-AMINO ACID: CONFORMATION SPECIFIC IR AND UV SPECTROSCOPY OF 2-AMINOISOBUTYRIC ACID

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2-Aminoisobutyric acid (Aib) is an achiral, α-amino acid having two equivalent methyl groups attached to C_α. Extended Aib oligomers are known to preferentially adopt a 3_{10}-helical structure in the condensed phase.[a] Here, we take a simplifying step and focus on the intrinsic folding propensities of Aib by looking at a single, capped Aib structure and then extending to longer oligomers in the gas phase, free from the influence of solvent molecules and cooled in a supersonic expansion. Resonant two-photon ionization and IR-UV holeburning will be used to record single-conformation UV spectra using the Z-cap as UV chromophore. Resonant ion-dip infrared (RIDIR) spectroscopy provides single-conformation IR spectra in the OH stretch, NH stretch, amide I and amide II regions. Two conformational isomers have been identified for the smallest unit in the study, Z-Aib-OH, and four conformational isomers were seen for Z-Aib-Aib-OH, with widely-varying IR spectral patterns. In addition to investigating the conformational dependence on oligomer length, this work also studies the steric and electrostatic impact of different capping groups, R-X where X = -OH, -OMethyl, and -OtButyl. These caps are considered here for the case of Z-Aib-Aib-X. Extension to larger Z-$(Aib)_n$-X oligomers will shed light on the extent to which the solution phase preference for 3_{10}-helix formation is retained in the gas phase, and when its onset first appears. When possible ^{13}C isotopomers will be used to assist with the assignments and modulate the coupling between amide I fundamentals.

[a] Toniolo, C.; Bonora, G. M.; Barone, V.; Bavoso, A.; Benedetti, E.; Di Blasio, B.; Grimaldi, P.; Lelj, F.; Pavone, V.; Padone, C., Conformation of Pleionomers of α-Aminoisobutyric Acid. *Macromolecules* **1985**, *18*, 895-902.