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Fast Folding Dynamics of an α -Helical Peptide with Bulky Side Chains

Material for Electronic Supplementary Information

| Temperature / °C | 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 |
|---------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| A (total) | 38.6 | 39.7 | 37.9 | 38.3 | 37.8 | 37.7 | 37.5 | 37.5 | 37.5 |
| Band 1 | | | | | | | | | |
| f | 0.484 | | | | | | | | |
| xc/cm ⁻¹ | 1625.5 | | | | | | | | |
| w/cm ⁻¹ | 28.7 | 29.1 | 29.1 | 29.9 | 30.0 | 30.2 | 30.2 | 30.7 | 30.7 |
| v _{LG} | 0.75 | 0.98 | 0.83 | 0.92 | 0.93 | 0.96 | 0.97 | 0.97 | 0.97 |
| Band 2 | | | | | | | | | |
| f | 0.115 | 0.092 | 0.084 | 0.064 | 0.051 | 0.034 | 0.019 | 0.005 | 0.005 |
| xc/cm ⁻¹ | 1613.6 | 1614.0 | 1614.1 | 1614.5 | 1614.7 | 1614.8 | 1614.4 | 1614.1 | 1614.1 |
| w/cm ⁻¹ | 26.4 | 21.7 | 22.6 | 20.6 | 20.1 | 18.2 | 15.8 | 10.3 | 10.3 |
| v _{LG} | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Band 3 | | | | | | | | | |
| f | 0.375 | 0.404 | 0.406 | 0.437 | 0.452 | 0.471 | 0.483 | 0.496 | 0.496 |
| xc/cm ⁻¹ | 1647.3 | 1646.5 | 1648.2 | 1648.2 | 1648.6 | 1648.7 | 1648.9 | 1649.1 | 1649.1 |
| w/cm ⁻¹ | 36.0 | 39.3 | 38.0 | 41.4 | 42.3 | 43.5 | 44.0 | 44.7 | 44.7 |
| v _{LG} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Band 4 | | | | | | | | | |
| f | 0.025 | 0.019 | 0.025 | 0.014 | 0.012 | 0.011 | 0.013 | 0.014 | 0.014 |
| xc/cm ⁻¹ | 1674.0 | 1674.0 | 1674.1 | 1674.2 | 1674.1 | 1673.9 | 1673.6 | 1672.9 | 1672.9 |
| w/cm ⁻¹ | 18.0 | 17.3 | 18.8 | 15.7 | 15.4 | 15.4 | 16.5 | 18.0 | 18.0 |
| v _{LG} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Table A Parameters obtained from the fits of the temperature dependent FTIR spectra of PHPG in D₂O to four “pseudo-Voigt” bands. A (total) is the total area of the amide I' band and f, xc, w and v_{LG} are the fractional area, centre frequency, full width at half maximum and Lorentzian/Gaussian contributions of each component band (v_{LG} = 0 represents a purely Gaussian band and v_{LG} = 1 a purely Lorentzian band).