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Title:DFT calculation analysis of terahertz time-domain spectra of polyalanines
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Abstract:Density functional theory (DFT) calculation was applied to simulate the far infrared (far-IR) spectra in the 700-0 cm-1 region of α-helical l-alanine oligomer models with the number of peptide bonds (n) of 24-8. The simulation for the model with n = 24 is in reasonable agreement with the dichroic IR spectra in the 700-60 cm-1 region already reported [K. Itoh and T. Shimanouchi, Biopolymers 9 (1970) 383], indicating the high reliability of the calculation. Terahertz (THz) time-domain spectroscopy was used to measure the far-IR spectra in the 160 - ca. 5 cm-1 region for poly-l-alanine in powder and film states. On treatment of the α-helical poly-l-alanine film with formic acid for 5 min a parallel band at 127 cm-1 and perpendicular bands at 116 and 82 cm-1 shift to 116, 109 and 73 cm-1, respectively, with concomitant intensity diminution, and on further treatment for 1 h the bands disappear and the far-IR spectrum in the region of 160 - ca. 5 cm-1 becomes almost transparent. On the other hand, the film treated with formic acid for 1 h still gives rise to the amides I and II bands due the α-helical structure with appreciable intensity. The calculated frequencies and intensities of bands corresponding to the observed bands at 127, 116 and 82 cm-1 decrease with decreasing the number of peptides bonds from 24 to 8, suggesting that the observed frequency lowering and intensity diminution are due to the decrease in the average number of the l-alanine residues forming the α-helix. After the treatment for 1 h the average number becomes too small to give the far-IR bands, resulting in the almost transparent spectral feature. The simulation also predicted the appearance of the accordion-like modes of the α-helical rod at 23 (n = 24), 26.5 (n = 20), 32 (n = 16), 39 (n = 12) and 48.5 cm -1 (n = 8) and the bending modes at 14 (n = 24), 19 (n = 20) and 27 cm-1 (n = 16). The observation of these modes, which should be called as "collective modes" in the strict sense of the word, will give information about static as well as dynamical structures of the α-helical sequences in polypeptides and proteins.
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