A POSSIBLE ROLE OF BIFURCATED HYDROGEN BONDS IN FORMING THE LOW-FREQUENCY VIBRATIONAL SPECTRA OF AMINO ACIDS

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The notion of bifurcated hydrogen bond is used for explanation of some amino acid (α-Gly, β-Ala) spectra peculiarities in a low-frequency region. The energy and vibrational spectra of crystal fragments, that contain bifurcated H-bonds, are calculated by the quantum-chemical methods MNDO, AM1, and PM3. The results show that the potential of a hydrogen atom is formed mainly by the tetrahedral geometry of the bonds formed by the nitrogen atoms, with which this H-atom is covalently bound, and H-bonding causes only a deformation of the minimum without forming a double-minima potential. The H-atom has a tendency to be aligned to the line of one of the N–H–O bounds.