HYDROGEN BONDING, IR SPECTRUM, AND THE STRUCTURE OF METHYL-β-D-GLUCOPYRANOSIDE

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A theoretical study of the structure and vibrational spectrum of methyl-β-D-glucopyranoside is performed with allowance for the hydrogen bond effect on them. At the density functional theory level with the use of the B3LYP functional in the 6-31G(*d*) basis set the structural dynamic models of a free molecule of methyl-β-D-glucopyranoside and its simplest complexes with hydrogen bonding in the form of dimers with different structures are constructed. Energies are minimized; structures, electro optical parameters, force constants, and normal vibrational frequencies in the harmonic approximation and their intensities in IR spectra are calculated; the hydrogen bond energy is estimated. Based on the calculation, the conclusions are drawn about the structure of the methyl-β-D-glucopyranoside sample, the formation and interpretation of its IR spectrum, and the possibilities of the used density functional theory method.

Keywords: methyl-β-D-glucopyranoside, hydrogen bonding, H-complex, molecular simulation, quantum chemistry, density functional, normal vibrations, IR spectrum, frequency, intensity.