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Crystal Structure and Hydrogen-bonding System in Cellulose III₁ from Synchrotron X-ray and Neutron Fiber Diffraction. Masahisa Wada¹, Henri Chanzy², Yoshiharu Nishiyama², Paul Langan³,
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The crystal and molecular structure, together with the hydrogen-bonding system in cellulose III₁, has been determined using synchrotron and neutron fiber diffraction data. The X-ray data were used to determine the C and O atom positions. The resulting structure has a one-chain monoclinic unit cell with an asymmetric unit that contains only one glucosyl residue, and with the hydroxymethyl group in the *gt* conformation. The positions of H atoms involved in hydrogen bonding were determined from a Fourier difference analysis using neutron diffraction data collected from hydrogenated and deuterated samples. The hydrogen-bonding system is well defined with no evidence of disorder. A bifurcated hydrogen bond links a donating secondary alcohol O3 atom to a ring O5 atom (major) and a primary alcohol O6 atom (minor) of an adjacent residue in the same chain. Two well-defined hydrogen bonds are present between neighboring chains, perpendicular to the chain direction.