Phase Transitions, Hydrogen Bond and Crystal Dynamics of *p*-Methylbenzyl Alcohol as Studied by Single Crystal X-ray Diffraction and ^{2}H NMR

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The title compound (*p*MBA) was found to undergo a first-order phase transition at 211 K (T_{c1}). Another transition with subtle enthalpy change appeared at 172 K (T_{c2}). Crystal structure determinations at various temperatures revealed that the transition at T_{c1} was accompanied by remarkable changes in the molecular conformations around the CH_2-C and O-CH_2 bonds and a reversal of the direction of the O-H···O hydrogen bond. Experiments of ^{2}H NMR were carried out on *p*MBA-d where the hydroxyl hydrogen of *p*MBA was selectively deuterated. Analyses of the ^{2}H NMR spectra and the temperature dependence of T_1 of the ^{2}H NMR indicated occurrence of jumping motions of ^{2}H between asymmetric potential wells at temperatures lower than T_{c1}.

Key words: Crystal Structure; Phase Transition; ^{2}H NMR; Crystal Dynamics; Hydrogen Bond.