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Polymorphism and vibrational investigations (FT-IR and IINS) of glass-forming 2-phenylbutan-1-ol (BEP), 2-(trifluoromethyl)phenethyl alcohol (2TFMP) and 4-(trifluoromethyl)phenethyl alcohol (4TFMP)

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The complex polymorphism and vibrational dynamic of three glass-forming single-phenyl-ring alcohols (with and without fluorine atoms) have been studied by complementary methods. Glass of isotropic liquid and cold crystallization of metastable supercooled liquid state were detected. Temperature investigation of vibrational motions point at hydrogen bond as an important intermolecular coupling in these materials. Quantum chemical (DFT) calculations for isolated molecule as well as a hydrogen-bonded dimer provide a satisfactory description of experimental spectra. The particular position of the CF₃ group in a phenyl ring (ortho/para) does not influence the intermolecular interactions.

In neutron inelastic scattering, the glass of supercooled liquid (disordered) and ordered crystal phase at 5 K can be easily distinguished. Comparing low temperature spectra of ordered crystal phase with glass of isotropic liquid, one can easily notice broadening of vibrational modes caused by rotational and translational molecular disorder, frozen in glassy state. An additional significant difference below 40 cm⁻¹ provides an evidence for the excitations in glass of disordered phase being localized and anharmonic, other than collective phonon excitations propagating in the crystal with a long-range order of molecules. Low energy barrier for torsional motions of CH₃-CH₂-CH- and OH-C₂-CH- (functional groups connected to phenyl ring) are visible on neutron spectra in the lattice vibrational region.

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