

MOLECULAR DYNAMICS AND PHASE
TRANSITIONS BEHAVIOR OF BINARY
MIXTURES OF FATTY ACIDS AND
CETYLTRIMETHYLAMMONIUM
BROMIDE AS STUDIED VIA DAVYDOV
SPLITTING OF MOLECULAR
VIBRATIONAL MODES

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S u m m a r y

The 1:1 solid phase complexes of stearic (SA) and behenic (BA) fatty acids (FA) with cationic surfactant cetyltrimethylammonium bromide (CTAB) are prepared from an equimolar ethanol solution of their binary mixtures. A supramolecular complexation between FA and CTAB molecules is proven with FTIR spectroscopy, X-ray diffraction (XRD), and differential scanning calorimetry (DSC). A single-phase layered crystalline structure of both CTAB:SA and CTAB:BA complexes is revealed by XRD. The greatly enhanced thermal stability of the CTAB:FA complexes over the pure FA (by about 40–50°C) is found with DSC along with a number of successive solid-solid phase transitions. The temperature-dependent FTIR study of the Davydov splitting for CH₂ rocking (720–730 cm⁻¹) vibrations revealed a significant difference in the conformational disorder of methylene chains and the molecular packing in successive solid phases of CTAB:SA and CTAB:BA complexes. Our research provides a molecular basis for a prospective application of such class of binary mixtures of oppositely charged cationic and anionic surfactants in thermo-sensitive supramolecular systems.