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Title:Lowest-lying vibrational signatures in corticosteroids studied by terahertz time-domain and Raman spectroscopies
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Abstract:In the present work low-frequency vibrational spectra of progesterone, 17α-hydroxyprogesterone and cortisone have been studied by terahertz time-domain (THz-TDS) and Raman spectroscopies in the temperature range of 18-300 K and in the spectral range of 10-85 cmsup-1/sup. The observed spectral features were interpreted by simulation of vibrational motions of corticosteroids, which was performed using solid-state density functional theory (DFT) (by DMolsup3/sup). Assuming that there is a similarity of the crystal space structure of the molecular crystals under study, we made an attempt to demonstrate the influence of intermolecular bonds on the topology of the THz absorption and Raman spectra in this spectral range. © 2012 Elsevier B.V.
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