LOWEST ENERGY VIBRATIONAL MODES OF NINE NAPHTHALENE DERIVATIVES; EXPERIMENT AND THEORY

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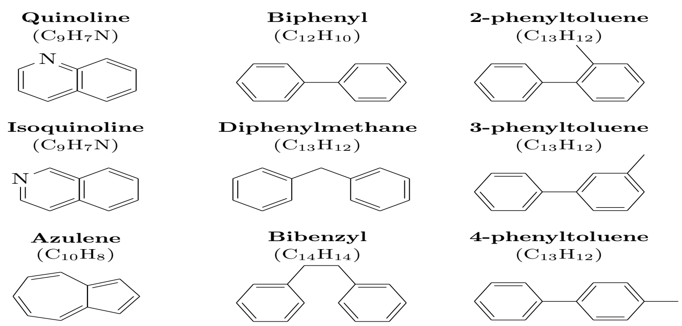
FIR gas phase absorption spectra of nine naphthalene derivatives (azulene, quinoline, isoquinoline, biphenyl, diphenylmethane, bibenzyl, 2-, 3-, and 4-phenyltoluene) have been recorded at medium resolution (0.5 cm^{-1}) using a Fourier transform Bruker IFS125 interferometer located on the AILES beamline of SOLEIL synchrotron. Assignments of these weak vibrational bands were performed using density-functional theory calculations carried out at the harmonic and anharmonic levels (B97-1/6-311G(d,p)). Molecular structure dependence of the FIR spectra is discussed based on the comparative study of several selected FIR modes.



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