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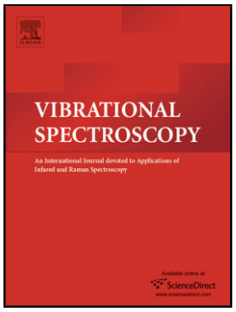

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Isomeric Xylene molecules in the terahertz-far infrared regime: computational chemistry and spectral modeling view

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Abstract

The theoretical assignments of spectral peaks of liquid phase *ortho-*, *meta-*, and *para*-xylene recorded with far-infrared (FIR) and THz spectroscopy in the spectral range between 50 cm^{-1} and 550 cm^{-1} is done with density functional theory (DFT) calculations. As THz spectroscopic techniques drastically evolved in recent years, the critical focus of this paper lies on the applicability of theoretical concepts, used as computational standard in near- and mid-IR spectra, to the FIR-THz region. An evaluation of the choice of functionals, basis sets, and appropriate scaling factors as well as the tractability of the liquid phase in a polarizable continuum model is performed. Alongside a new analysis procedure based on spectral Hard Modeling has been developed. DFT line spectra are fitted to experimental FIR spectra where a quantitative track record allows for meaningful comparisons. With all these tools we are able to reproduce experimental spectra in an optically appealing way and we can explain trends for each spectrum as well as across the row of the isomers.