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Title

Electron-phonon coupling in the molecular charge transfer crystal 2-(-methylbenzylamino)-5-nitropyridine

Source

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Abstract

Orientated single-crystal infrared, Raman and terahertz measurements have been carried out for the molecular charge transfer material 2-(-methylbenzylamino)-5-nitropyridine. This information, together with experimental frequency doubling data and theoretical calculations of the electro-optic coefficient, was used to deduce the optical phonon contribution to the linear electro-optic coefficient. The optical phonon spectra are dominated by three intense bands attributed to vibrations of the ring, NO₂ substituent and N-H bond. The most intense scattering arose from the _{bb} component of the polarisability tensor. This implied that the most significant contribution to the transition polarisability arises from the electronic transition near 435 nm, polarised along the b-axis of the crystal. The strongest bands in the infrared spectra are also associated with the same three bands. This implies that efficient electron-phonon coupling (or electronic delocalization) in the conjugated system. DFT calculations of optical phonon frequencies and eigenvectors were used to help assign relevant vibrational features and to derive useful information about the molecular structure. The information obtained from this study is important for assessing the suitability of this material for generating terahertz frequencies by optical rectification. (31 References).