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Polymorphism and cold crystallization in optically nonlinear N-benzyl-2-methyl-4-nitroaniline crystal studied by X-ray diffraction, calorimetry and Raman spectroscopy Source

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Abstract

Polymorphism of N-benzyl-2-methyl-4-nitroaniline (BNA), a terahertz emitter and frequency doubler, was detected and the crystal structures of orthorhombic and monoclinic polymorphs have been determined at room temperature. The differential scanning calorimetry (DSC) studies revealed monotropic phase transition of the monoclinic BNA crystal system at 362K and during re-heating, after the molten BNA cooling, the cold crystallization of the both polymorphs. The variable-temperature Raman spectra in the 700-1700cm⁻¹ range also evidenced the polymorphic transformation from the monoclinic to the orthorhombic, the latter stable in the wide temperature range, crystal system. The comparison of structures, DSC curves, FT-IR and Raman spectra of two forms enabled to recognize the NHO hydrogen bond in the orthorhombic and CHO hydrogen bond in the monoclinic one as well as other intermolecular interactions. The role of dynamic disorder, intra- and intermolecular charge transfers in the molecular mechanism of optical nonlinearity has been discussed. [All rights reserved Elsevier]. (42 References).

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