

Thermal and near-IR photochemical generation of polarons in m-nitroaniline crystals. Application of 2D correlation FT-NIR spectroscopy.

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Streszczenie

Polarized FT-NIR spectra of m-nitroaniline single crystals in the 4200-10500 cm⁻¹ region, non-irradiated and irradiated at 9700 cm⁻¹, corresponding to the -NH₂ stretching second overtone (3 NH s²), were recorded from 300 to 380 K. Direct heating from 325 K to 365 K (phase transition) caused an elevation of the relative background absorbance (A) near 10500 cm⁻¹. The irradiation by low intensity NIR and a subsequent heating resulted in a different increase of A than in the case of non-irradiated sample. The background elevation is supposed to origin from low-lying electronic transitions of radical ions (polarons) generated by irradiation and heating. Our results indicate that the polarons produced photochemically and thermally are different. The 2D correlation analysis was applied to facilitate the band assignment in the NIR region and to throw more light on thermally induced instabilities in the crystal.