

The IR temperature studies of phase transition of 4-aminopyridinium-hydrogen maleate-maleic acid: isotopic effect and nonlinear optical properties.

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Streszczenie

[4-NH₂C₅H₄NH][C₄H₃O₄][C₄H₄O₄] (abbreviated as APM) and its N,O-deuterated analogue have been synthesized. The single-crystal X-ray diffraction studies for N,O-deuterated analogue are reported. The Kurtz and Perry powder SHG technique confirms the second order nonlinear optical properties of APM. The structural phase transition of APM occurring at 312 K has been examined by infrared spectroscopy. The infrared temperature studies on the polycrystalline APM showed that the modes arising from NH $\cdots$ O and OH $\cdots$ O intermolecular hydrogen bonds vibrations appear to be very sensitive to the structural phase transition. The molecular mechanism of the phase transition is explained in terms of significant changes in the hydrogen bond configuration.

Słowa kluczowe

infrared, phase transition, 4-aminopyridine, Maleic acid, Second harmonic generation

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