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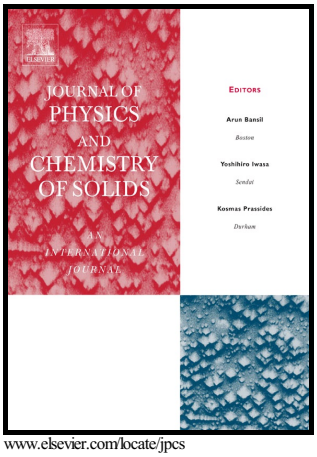

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Synthesis, X-Ray crystal structure and highly non-linear optical properties of inorganic-organic hybrid compound: 1,4-Diazbicyclo-octane oxonium tri- nitrates single crystal.

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Abstract

A new nonlinear optical hybrid crystal 1,4-Diazbicyclo[222]octane oxonium tri-nitrates (DOTN), of the dimension $4 \times 12 \times 1$ mm^3. The crystal was grown using water as solvent at room temperature and crystal structure was determined by X-Ray diffraction respectively, this title compound was shown to crystallize in non-centrosymmetric trigonal system with space group P31c. The recorded FTIR spectrum has proven the presence of various functional groups in the grown crystal as well as the formation of DOTN. Besides, the thermal stability and melting temperature of the DOTN crystal were identified from the TG/DSC analysis. The suitability of this material for optical application was studied by non-linear optical (NLO) and UV-Visible absorption techniques. Furthermore, the nonlinear optical property was analyzed by Kurtz-Perry powder technique and was 3.4 times than that of KDP (potassium dihydrogen phosphate) single crystals. The first hyperpolarizability of nitrate was determined by Second Harmonic light Scattering.

***Keywords**:* Crystal structure, X-ray diffraction, Optical materials, High nonlinearity, Infrared Spectroscopy; Thermal Behavior.

1.Introduction