

Supporting Information

A New IR Nonlinear Optical Material with 2D 3-Fold Interpenetrated Topology

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1. Materials and Methods:

Materials and methods: All the reagents and solvents were obtained from commercial sources and were used without further purification. Elemental analyses of carbon, hydrogen and nitrogen were carried out with an Elementar Vario EL. Infrared Spectra were obtained with a PE Spectrum-One FT-IR spectrometer using KBr discs. Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer under an N₂ atmosphere (30-1200 °C) at a heating rate of 10 °C min⁻¹. Solid-state optical diffuse reflectance spectrum and the UV-visible absorption spectrum were measured at room temperature with a PE Lambda 900 UV-Visible spectrophotometer in the range of 190-2000 nm. BaSO₄ plate was used as a standard (100% reflectance) for the measurement of the solid-state optical diffuse reflectance spectrum. The measurement of the powder frequency-doubling effect was carried out by using the Kurtz and Perry method^{SI} with a 2.05 μm Q-switch laser. The samples were ground and sieved by using a series of mesh sizes in the range of 25-210 μm. A sample of KTP was prepared as a reference material in an identical fashion.

2. Supporting Figures

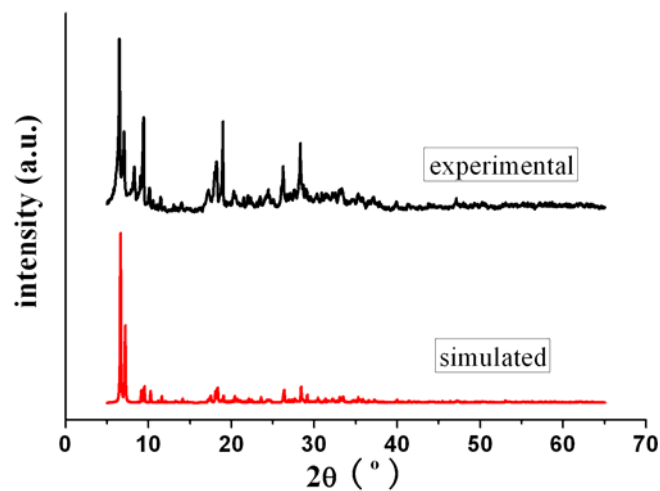


Figure S1 Experimental and simulated X-ray powder diffraction patterns of compound **1**.

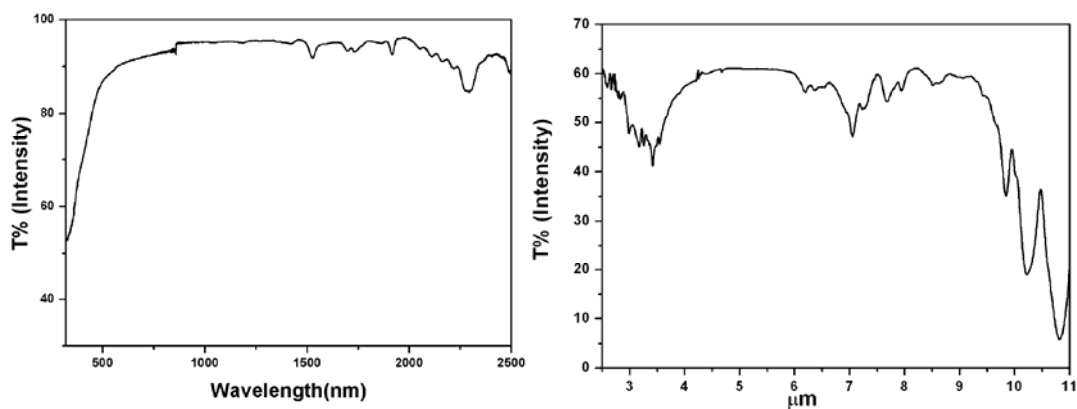


Figure S2 Transmittance curves of **1** in the UV (l) and IR (r) regions.

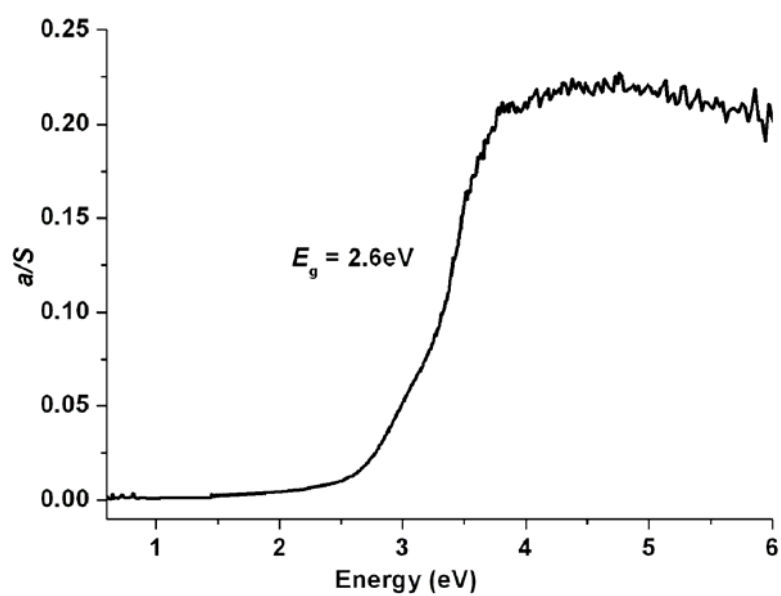


Figure S3 Diffuse reflectance spectrum of compound 1.

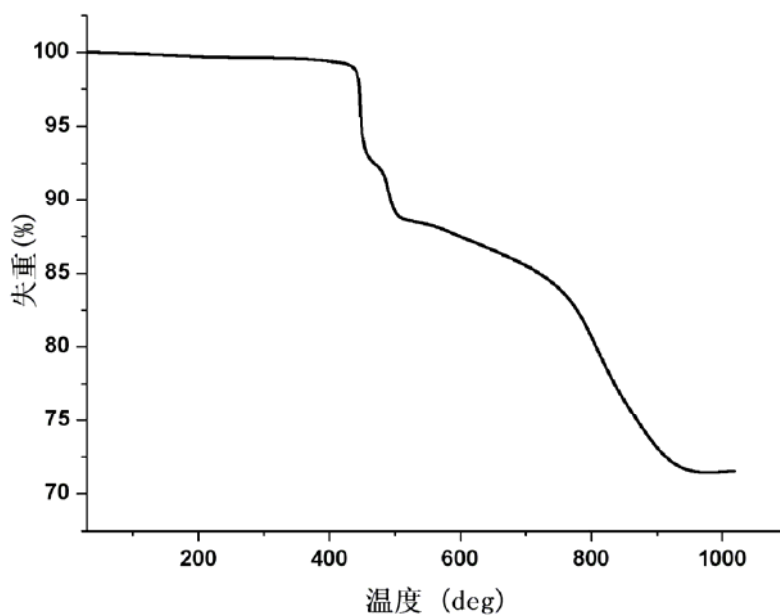


Figure S4 TG diagram of 1.

References:

(s1) Kurtz, S. W.; Perry, T. T. *J. Appl. Phys.*, **1968**, *39*, 3798-3813.