# Optical Rectification from Next Generation Organic THz Generation Crystals

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**Abstract:** We recently developed new organic nonlinear optical crystals for THz generation. We report the optical and THz properties of PNPA and MNA and discuss how they pave the way for the future of THz spectroscopy. 

## 1. Introduction

THz frequencies (0.1 to 10 THz) have a wide range of scientific application, from studying phonon modes and mapping out carrier dynamics, to noninvasive hyperspectral imaging [1-2]. Optical rectification of infrared light through nonlinear optical (NLO) crystals is one of the most widely used generation sources of THz frequencies of light, due to high conversion efficiencies, strong single-cycle electric fields, and broad bandwidths from 0.5 to 10 THz. Organic NLO crystals possess higher nonlinear optical coefficients ($\chi^2$) and exhibit stronger molecular hyperpolarizabilities and are therefore often preferred in comparison to their inorganic counterparts. Through data mining of crystallographic databases combined with 1$^{st}$-principles calculations, our group has discovered and characterized a number of new organic THz generation crystals that exceed the performance of industry standards [3].

In this work, we report the optical and THz properties of NLO organic crystals PNPA and MNA and discuss how they pave the way for the future of THz spectroscopy applications [4-5].

## 2. Results

PNPA and MNA crystals were characterized for THz generation using the optical rectification and electro-optic sampling setup described in Ref. [6]. With this setup, we measured the field strengths in PNPA crystals of up to 2.3 MV/cm, which far outperforms measurements taken (using the exact same experimental setup) with commonly used crystals DAST and OH-1. **Figure 1** shows a comparison of the performance of these three crystals.

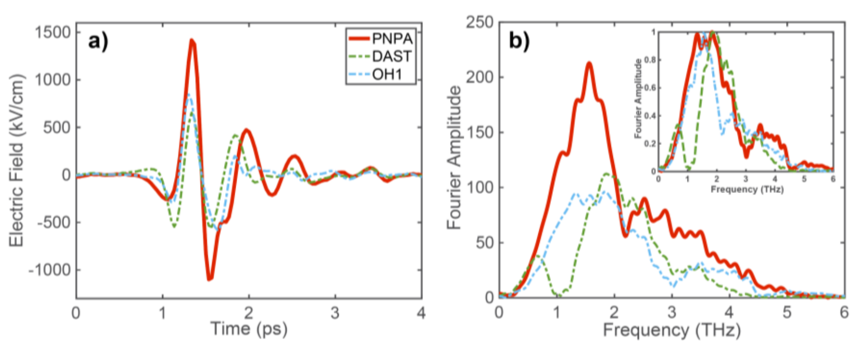


Fig. 1. (a) Electric field of PNPA, DAST, and OH1 measured at the same pump fluence and (b) the Fourier transform spectrum of each crystal. The inset of (b) shows the normalized spectra, detailing the unique absorptions of each crystal.

The pump wavelength of 800 nm is particularly interesting due to the commercial availability of Ti:sapphire lasers. Red NLO crystals such as DAST and OH-1 are not suitable for high-intensity THz generation at 800 nm due to low damage thresholds and two-photon absorption. Yellow crystals, however, absorb at shorter wavelengths, resulting in efficient THz generation when pumped at 800 nm without a high risk of damage. This enables research groups without optical parametric amplifiers to perform THz spectroscopy. **Figure 2a** depicts the time traces of yellow crystals MNA, BNA, and inorganic GaP for reference pumped with the same fluence at 800 nm. The associated spectra are included in **figure 2c**. MNA meets the performance of its widely used derivative, BNA, at this technologically important wavelength. Additionally, MNA has a higher melting point range (128 – 129 ˚C versus 101 ˚C) and therefore a higher laser-induced damage threshold (LIDT) than BNA, allowing it to be pumped with higher laser fluences [6].

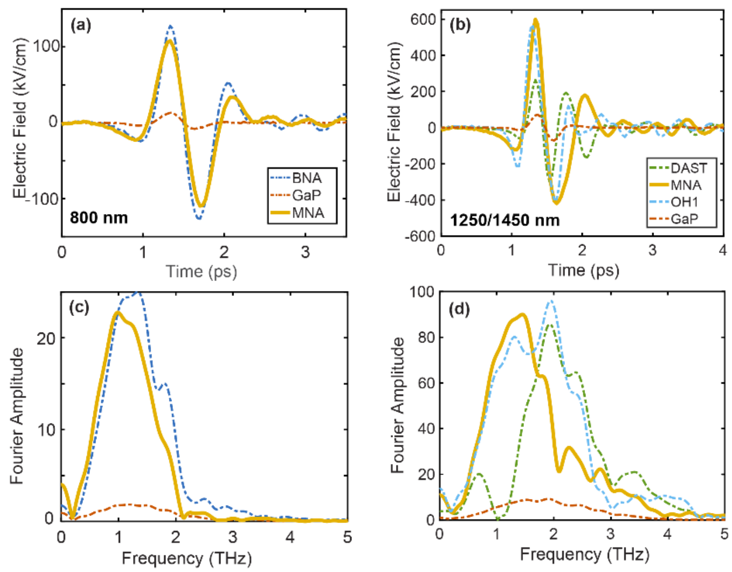


Fig. 2. (a) Time traces of MNA, BNA, and GaP with a pump wavelength of 800 nm. (c) Time traces of MNA at 1250 nm compared with DAST, GaP, and OH1 at 1450 nm. (b) and (d) show the spectrum of each of the traces in (a) and (c), respectively.

**Figure 2b** shows a comparison of the THz electric field produced by MNA with the most widely used THz generation crystals, DAST and OH-1 at longer wavelengths obtained via OPA output. MNA is the only known yellow crystal that rivals the performance of these organic THz generators at longer wavelengths. The spectrum of each is depicted in **figure 2d**.

## 3. Summary

We conclude that PNPA and MNA set a new industry standard for THz generation through optical rectification. The broadband output from PNPA is stronger than any other known THz generator, and the wavelength versatility of MNA distinguish these two NLO crystals from others.

## 4. References

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