

Gas-phase Absorption Spectrum of 2, 4 DNT Explosive from 0.05 to 1.5 THz Using THz Time-Domain Spectroscopy

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Motivation—Terahertz (THz) spectroscopy is emerging as a powerful technique to identify and characterize molecular species. Due to recent advances in femtosecond lasers and optical materials, the THz radiation band from 0.1 to 10 THz is now routinely accessible. Spectroscopically, this is a new and unexplored portion of the spectrum that is rich in unique molecular information. In addition, the propagation properties of THz radiation through the atmosphere are potentially attractive for remote sensing of explosives.

From our previous studies on the propagation of THz radiation through the atmosphere, we have learned that the atmosphere is not as opaque as once thought. There are many THz transmission windows within the atmosphere. However, to capitalize on the THz transmission properties of the atmosphere for explosive vapor sensing, it is important to determine if spectra exist for these molecules within these windows. Therefore, our interests lie in characterizing gas-phase explosive materials to guide the development of novel THz devices for remote sensing of explosives.

Accomplishment—Recently, we have measured the first known gas-phase absorption spectrum of the explosive 2, 4 dinitrotoluene (DNT) from 0.05 to 1.5 THz using time-domain spectroscopy. Figure 1 shows the characteristic signature of 2, 4 DNT with a spectral resolution of 3 GHz. The broad absorption profile from 50 GHz to 600 GHz is the pure rotational spectrum of 2, 4 DNT. Due to the large moments of inertia for the DNT molecule, the density of lines in the rotational spectrum is large, which consequently produces broad absorption. The broad absorption profile in the DNT spectrum

was validated by calculating the pure rotational spectrum using an asymmetric rotor model. The result from the calculation is shown in Fig. 2. The calculation reproduced the measured spectral width of the broad absorption, and it peaked at 275 GHz compared to 240 GHz from the measured spectrum.

The DNT spectrum displayed unexpected fine structure that was superimposed on the broad absorption profile. This structure could be due to the interaction between the internal rotation of the substituent groups and the torsional modes of vibration in the molecule. The presence of these features may provide an opportunity to uniquely identify explosives based upon their absorptions in the THz region of the spectrum.

The explosive material used in the experiments was pure crystalline solid which was converted into the gas phase by heating a unique temperature-controlled gas cell to 145° C. At this temperature, most of the explosive material was converted into the gas phase, and the static pressure measurements were made utilizing 250 to 610 mtorr of DNT.

Significance—Our gas phase absorption measurements of 2, 4 DNT are the first of their kind in the spectral region 0.05 to 1.5 THz. In the terahertz community, many have proclaimed terahertz spectroscopy as the tool to detect and identify explosive material, but no gas phase work has been done. Our results demonstrate the potential of using terahertz spectroscopy for explosive detection and identification. This work will guide the development of novel THz sensors and detectors capable of detecting explosive vapors.

Sponsors for various phases of this work include: Nuclear Weapons, Laboratory Directed Research & Development, and Work for Others/Transportation Security Administration & Technical Support Work Group

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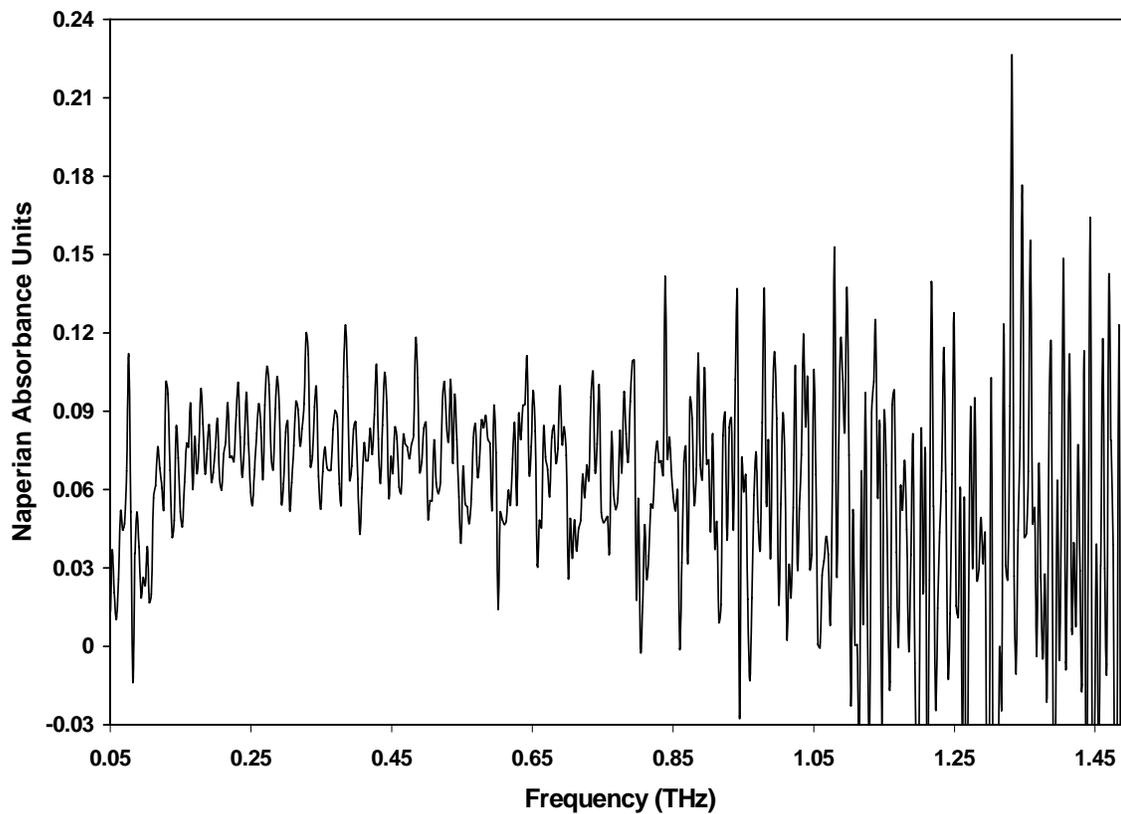


Figure 1. Measured absorption spectrum of gas-phase 2,4 DNT from 0.05 to 1.5 THz.

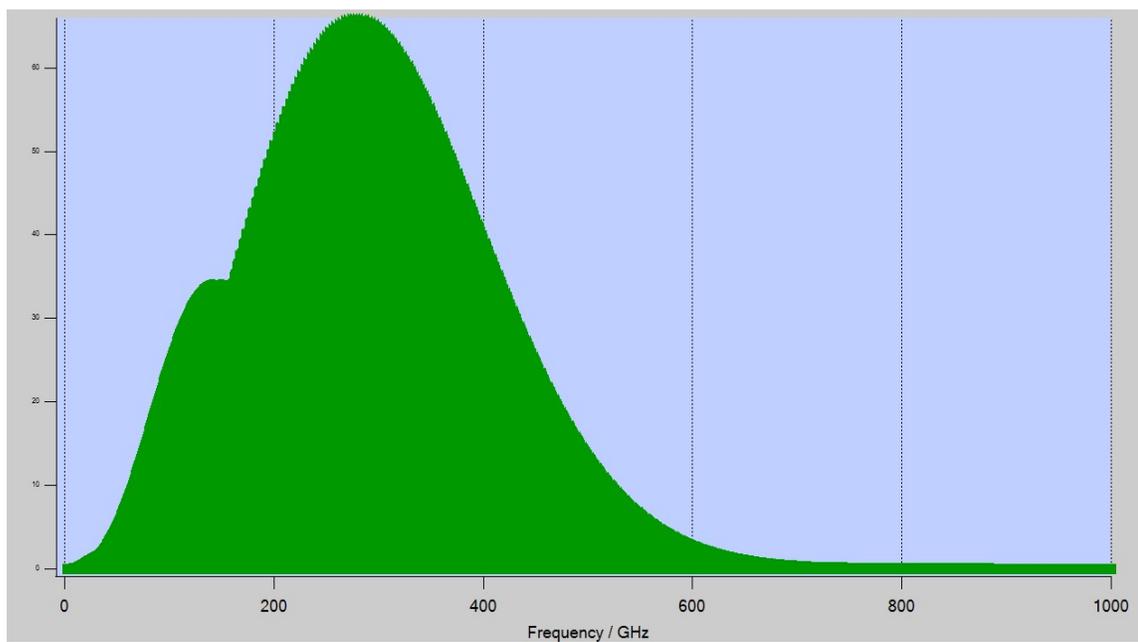


Figure 2. Calculated pure rotational spectrum of gas-phase 2,4 DNT from 0.05 to 1.5 THz utilizing an asymmetric top model.