Gas-phase Absorption Spectrum of 2, 4 DNT Using THz Time-domain Spectroscopy

by **R. J. Foltynowicz**

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 explosives sensing applications.

From our previous studies on the propagation of THz radiation through the atmosphere, we learned that the atmosphere is not as opaque as we 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 in these windows. Therefore, our research interests lie in characterizing gas-phase explosive materials to guide the development of novel THz devices for remote explosives sensing applications.

Accomplishment—Recently, we have measured the first known gas-phase absorption spectrum of the explosive 2, 4 dinitrotoluene (DNT) from 0.4 to 2.7 THz using THz time-domain spectroscopy. Figure 1 shows the characteristic signature of 2, 4 DNT. The absorption lines in the 2, 4 DNT spectrum are rotational states of the molecule. The high density of lines can be attributed to the large moments of inertia of DNT which lead to a reduction in the frequency spacings between transitions.

The experimental setup used to make this measurement is shown in Fig. 2. The THz generation is performed by optical rectification of an 800 nm femtosecond laser pulse in a <110> ZnTe crystal. This process generates a broadband THz pulse with a ~1ps period. The THz beam is detected via electro-optic sampling, which exploits induced polarization changes of the probe beam due to the THz interaction within a ZnTe crystal sensor. The polarization changes are proportional to the strength of the THz electric field and hence we measure the electric field strength of the THz radiation as a function of delay time. Currently, the detector bandwidth is 0.40 to 2.7 THz with an instrument spectral resolution of 1 GHz (0.03 cm^{-1}).

The explosive material used was initially a solid that was heated to 150° C in a vacuum cell. At this temperature, most of the explosive material is converted into the gas phase. The equilibrium, static pressure for the experiment was 253 mTorr and the spectral resolution of our measurement was 8 GHz.

Significance—From our previous measurements of atmospheric water, we established a map of the background absorptions from the atmosphere as well as transmission windows. Having this information allowed us to concentrate our molecular identification in these transmission windows. We measured the spectral signature of 2, 4 DNT and found resonances in the transmission windows of the atmosphere. In addition, these lines are unique compared to the water transitions. These data will guide the development of THz sensors and detectors to develop a system that can detect explosive vapors remotely.

Sponsors for various phases of this work include: Nuclear Weapons/Science & Technology, Laboratory Directed Research & Development, and Work for Others/Transportation Security Adminsitration

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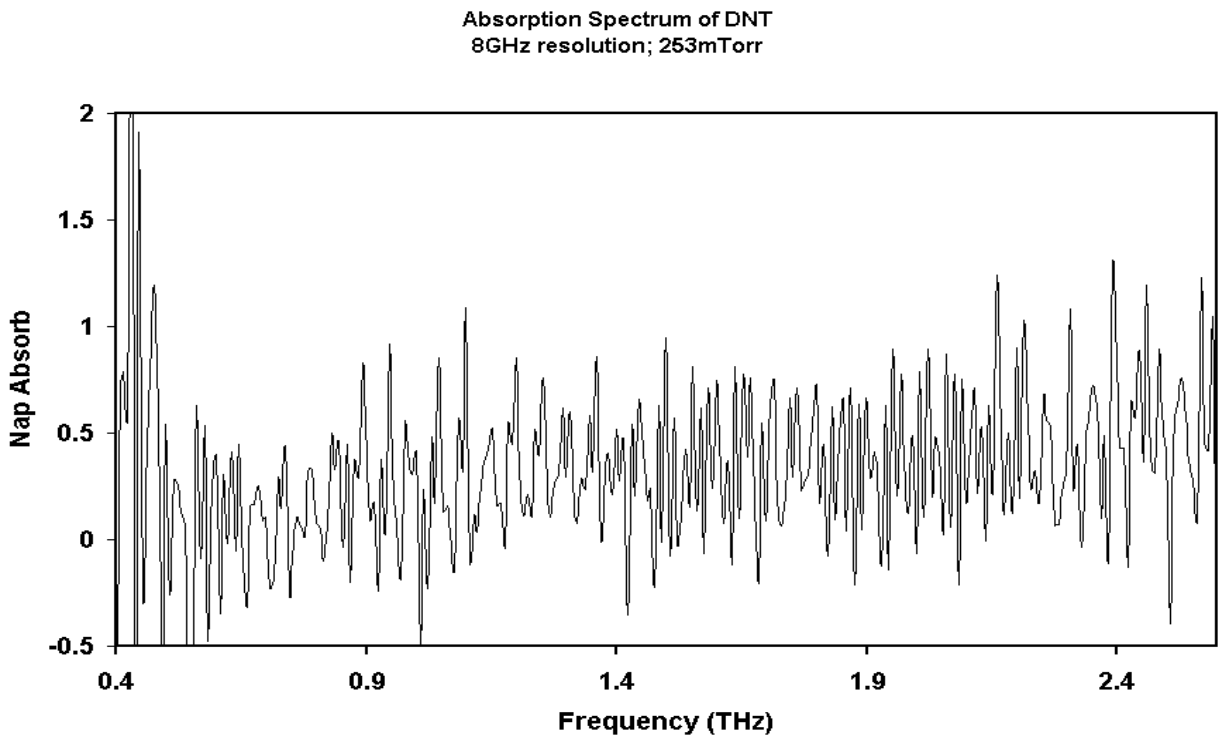

Figure 1. Absorption spectrum of gas-phase 2, 4 DNT from 0.4 to 2.7 THz.

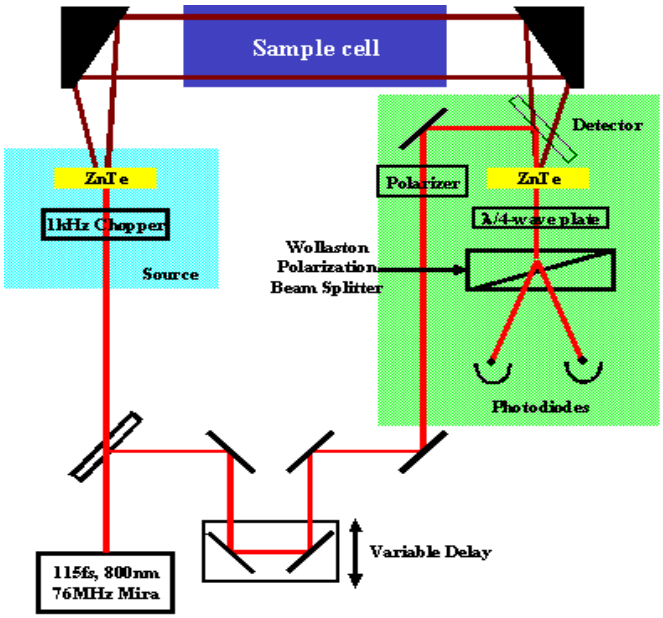

Figure 2. Diagram of the THz time-domain spectrometer. Femtosecond laser pulses chopped at 1KHz pump a <110> ZnTe crystal to produce THz radiation. The THz beam travels through the sample cell and collinearly propagates with an 800nm probe beam with horizontal polarization through a ZnTe sensor. The THz electric field strength is detected via polarization changes induced in the probe beam by the THz beam inducing a change in the birefringence of the ZnTe sensor.