

# Terahertz Spectroscopic Characterization of Naphthalene and 1-Nitronaphthalene

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**Abstract**—Terahertz absorption spectra of parent polycyclic aromatic hydrocarbon (naphthalene) and its nitropolycyclic aromatic hydrocarbon (1-nitronaphthalene) have been investigated using terahertz time-domain spectroscopy (THz-TDS) technique. The results show large difference in 0.1~2.2 THz region, which probably originated from the difference of molecular structure and lattice vibrational modes. The study indicates that THz-TDS technology can offer a new experimental method to identify and analyse such kinds of environmental pollutants.

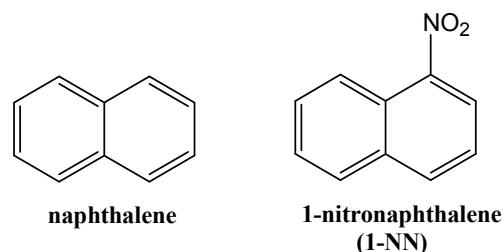
## I. INTRODUCTION

**N**ITROPOLYCYCLIC aromatic hydrocarbons (NPAHs) compounds are one of the most important and wide-spread classes of environmental pollutants that has long been of interest in the fields of physical chemistry, environmental science, toxicology, cancer research, and energy sciences [1-3]. NPAHs are released to the environment as a result of direct emissions from incomplete combustion processes, and are formed in situ in the atmosphere by oxidation and/or active nitrite radical reactions of the corresponding parent PAHs. NPAHs are believed to represent a highly potential human-health risk and most of them are more mutagenic and carcinogenic than their parent PAHs in the bacterial mutagenicity assay [4,5]. It is important to investigate the effects of the substituted nitro group position on the NPAHs vibrational spectra and explore the possible relationships between molecular structural properties and biochemical activities of these NPAHs compounds.

THz radiation covers a wide frequency range from 100 GHz to 10 THz. For quite a long time, this range was referred as the THz gap due to very few available sources and components. Recently, with the fast innovation in ultrafast laser and semiconductor technologies, the THz region has been revived for a wide range of applications[6-8]. Compared with the traditional vibrational (infrared and Raman) technology, the terahertz time-domain spectroscopy (THz-TDS) technology, which is can obtain the information of the sample's absorption and dispersion at the same time. As complementary tools of Raman and infrared, THz spectroscopy can be used for the analysis of weak intermolecular molecular interactions, molecular conformation changes and environmental effects as well as the identification of the molecular structure of constituents[9,10].

In the present work, terahertz absorption spectra of a model parent PAHs and NPAHs compounds (naphthalene and 1-nitronaphthalene, 1-NN shown in Figure 1), have been

investigated using terahertz time-domain spectroscopy (THz-TDS) technique at room temperature. The experimental results show large difference among absorption spectra of 1-NN its parent naphthalene compound in 0.1~2.2 THz region, which probably originated from the difference of NPAHs' molecular structure and lattice vibrational modes.



*Figure 1:* Structures and abbreviated names of 1-NN and the corresponding parent naphthalene.

## II. RESULTS

As shown in Figure 2(a), the THz waveform signal of sample has a time delay compared with reference signal due to the THz refractive index of the samples larger than the refractive index in the air, while the reason for the decrease in amplitude is owe to the absorption of 1-NN and naphthalene compounds. The amplitude of 1-NN (red line) is much less than that of the corresponding naphthalene (green line) and this result is agreement with that the absorption coefficient of NPAHs is much stronger comparing to that of parent PAHs compounds.

Figure 2(b) shows the THz absorption spectra of 1-NN and parent naphthalene. 1-NN has been identified in the THz region by specific absorption features, distinguished at frequencies 0.52, 0.71, 1.05, 1.26, 1.35 and 1.75 THz. But for naphthalene, there are no obvious resonance peaks below 2.0 THz.

It is known that many factors contribute to the low-frequency vibrational spectrum. Intermolecules vibrational modes or lattice vibration are considered as the main components in the THz frequency region. THz measurements give the rich information on both molecular conformation and intermolecular environment. For 1-NN, such weak intermolecular molecular interactions will be changed due to the nitro-group substitution compared with its corresponding parent naphthalene, so the corresponding lattice vibrational modes shown in THz absorption spectrum (Figure 1) will be different from that of parent PAHs. The distinct fingerprint

absorption of 1-NN compound in THz region indicates that THz-TDS technology can absolutely give us a new experimental method to identify and monitor such NPAHs environmental pollutants.

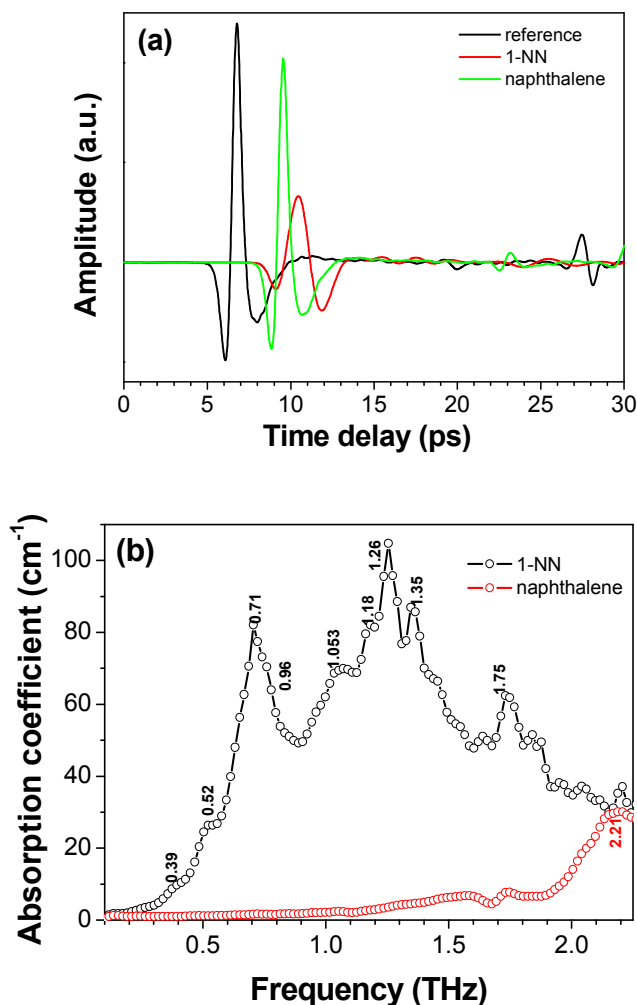


Figure 2: THz waveforms (a) absorption spectra (b) of reference, 1-NN and parent naphthalene.

### III. SUMMARY

THz-TDS vibrational spectroscopy provides rich fingerprint information for discriminating 1-NN and its parent naphthalene. The reported results indicate that THz-TDS technique can become a new further analytical method to identify and analyse such kind of environmental NPAHs pollutants. Further work will be performed to investigate the possible relationship between the different NPAHs vibrational properties and the effects of the substituted nitro- group position to better know their photoreactivity and biochemical activity mechanism.

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