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Toxic chemical compound detection by terahertz spectroscopy: a review

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Abstract:

Terahertz (THz) spectroscopy is a rapidly emerging technology in the field of analytical chemistry. THz spectroscopy shows substantial scientific potential given that numerous absorption and emission molecular lines of interest in the chemical sciences belong to this spectral region. This article focuses on the current research progress on the detection of harmful gases, pesticides, antibiotics, toxic chemical compounds, and drugs of abuse by THz spectroscopy. The article also analyzes the key factors used for the detection of toxic chemical compounds by THz spectroscopy.

Keywords: rapid detection, terahertz spectroscopy, toxic chemical compound

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Introduction

Terahertz (THz) molecular spectroscopy provides considerable scientific potential because numerous absorption and emission molecular lines of interest in the chemical sciences belong to this spectral region, where numerous chemical species exhibit strong characteristic rotational and ro-vibrational transitions. Electromagnetic waves with frequencies between 0.3 and 10 THz or millimeter-wavelength ($3\text{--}300\text{ cm}^{-1}$) are described as THz radiation. They are assigned in the electromagnetic spectrum between the microwave/millimeter and the far-infrared regions. Molecular rotations in the gas phase, crystalline phonon vibrations, low-frequency vibrations, and intermolecular vibrations in the solid state have been proven by spectroscopic procedures in the THz range (Figure 1) (Walther et al., 2010; Son, 2014). In this range, numerous biological and chemical compounds exhibit characteristic absorptions and dispersions because of vibrational transitions, mostly collective and intermolecular vibrational modes. These THz vibrational modes provide fingerprint information for THz detection and identification given that THz vibrational modes provide fingerprint information of organic molecules for identification. THz molecular spectroscopy has been widely used in chemistry and related fields. In this minireview, we will concentrate on the research progress on the detection of harmful gases, pesticides, antibiotics, toxic chemical compounds, and illicit drugs by THz systems. The article also analyzes the key factors used for the detection of toxic chemical compounds by THz spectroscopy.

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Figure 1: Characteristic absorption frequencies of chemical compounds in the THz region.

Characterization of THz spectroscopy

THz time-domain spectroscopy (THz-TDS) has been widely used for chemical detection and identification (Pereira & Shulika, 2013; Saeedkia, 2013; Song & Nagatsuma, 2015). A typical THz-TDS system is shown schematically in Figure 2 (Qin, Ying & Xie, 2013). The system is composed of an ultrafast pulsed laser, THz emitter, THz detector, and a time-delay stage. The ultrafast laser beam is split into pump and probe beams. The pump beam is incident on the THz emitter to generate THz pulses, and the THz pulses are collimated and focused on the sample by parabolic mirrors. After transmission through the sample, the THz pulses are collimated and refocused on the THz detector. The probe beam is used to gate the detector and measure the instantaneous THz electric field. A delay stage is used to offset the pump and probe beams, and allows the THz temporal profile to be iteratively sampled. Coming from the same source, the pump and probe pulses show a defined temporal relationship. Propagating along an optical delay line, the probe beam samples the THz pulses and records their electric field as a function of time delay. The THz pulses passing through a sample show amplitude attenuation and time delay. A Fourier transform is then used to convert this TDS to a frequency domain spectrum.

Figure 2: Schematic of the THz-TDS system.

Different pulse-wave THz radiation methods were used, such as THz-TDS. Continuous-wave (CW) THz radiation instrument was also used for THz experiment (Mittleman, 2003; Thompson, 2008). The simplicity and potential low cost of CW sources can be advantageous for certain applications, such as far-infrared region spectrometers.

Many polar gases show narrowband absorption features in the THz range caused by rotational transitions (Exter, Fattinger & Grischkowsky, 1989; Theuer et al., 2011). Generally, liquids do not have narrowband absorption features. Nonpolar liquids show a weak broadband absorption. Polar liquids have strong absorption in the entire THz range. Many solid crystalline molecules show vibrational phonon modes in the THz range. Crystalline solid samples have distinguishable absorption lines due to the low-frequency vibrational modes (Hangyo, Tani & Nagashima, 2005; Theuer et al., 2011).

Pollutant gas detection

The detection of gas-phase samples is a major application of THz-TDS and plays a role in diverse fields. The characterization is used for gas detection because numerous polar gases exhibit unique spectral signatures from probing transitions between rotational quantum levels.

Medvedev, Behnke, and Lucia (2005) applied a THz-TDS experiment system to acquire the spectra of CS_2 , CH_2F_2 , CHF_3 , and CHI_3 . The mixture of these gas species was detected, and gas mixture analysis is possible using THz-TDS in combination with powerful signal processing algorithms. Assefzadeh, Jamali, and Aleksander (2016) introduced an electronic source with an on-chip antenna that can generate picosecond pulses to perform broadband THz gas spectroscopy for trace gas detection. The result showed NH_3 exhibits the strongest absorption peak at 572 GHz, and SO_2 and H_2S can be detected as well. Hsieh et al. (2016a, 2016b) developed a method to decrease the influence of unwanted aerosols through gas detection using a fiber-based, asynchronous optical-sampling THz-TDS with the ability to obtain the CH_3CN spectral fingerprints of rotational transition and a method to provide immunity against aerosol scattering CH_3CN influence. Hsieh et al. (2016a, 2016b) developed a photomixing THz synthesizer phase-locked to dual optical frequency comb CW THz radiation THz-TDS experiment apparatus for gas detection. THz frequency-domain spectroscopy of CH_3CN gas and its

isotope $\text{CH}_3^{13}\text{CN}$ was tested by a THz-TDS apparatus in the frequency range of 0.600–0.720 THz. The result shows that the THz synthesizer is highly promising for high-precision THz-TDS of low-pressure molecular gases and will facilitate the qualitative and quantitative analyses of multiple gases. Smith and Arnold (2015) measured the THz spectra of water, ammonia, acetonitrile, methanol, ethanol, acetaldehyde, propionaldehyde, and propionitrile by commercial THz-TDS (see Figure 3). Selectivity coefficients for THz spectra are higher than those derived from the fingerprint region of the IR spectrum. Superior selectivity was further developed in THz spectroscopy for gas analytical measurements and identification. Kilcullen et al. (2015) applied a commercial THz-TDS system for the detection of carbon monoxide detection. The sample gas cell is 13.6 cm in length with high-resistivity Si windows on each end. RMS (root mean square) noise floor method was used for the apparatus. The limit of detection (LOD) for THz-TDS systems and methods was 40 ppm of carbon monoxide. Liang (2015) developed a THz technique for the identification and determination of the principal gas components, including methane (CH_4), ethane (C_2H_6), carbon monoxide (CO), and carbon dioxide (CO_2) distilled from oil shale. C_2H_6 represented the largest refraction property. The results indicated that THz technique combined with mathematical method is an effective tool for gas detection in the unconventional natural gas industry. Mouret et al. (2013) set up a THz sensor system based on a commercially available multiplier chain applied to the analysis of trace gases. The pollutant SO_2 gas was generated in a 1.25-m-long stainless steel gas cell with Teflon windows, and the test frequency ranged from 630 to 930 GHz. The estimated LOD for SO_2 was 1 ppm.

Figure 3: Expanded view of absorbance for THz spectra of acetaldehyde (black), acetonitrile (red), ethanol (green), water (yellow), methanol (blue), ammonia (magenta), propionaldehyde, propionaldehyde (cyan), and propionitrile propionitrile (gray).

Azzam et al. (2013) reported the pure rotational transition spectrum of hydrogen sulfide (H_2S) detection by a THz instrument. A total of 320 pure rotational transitions of H_2^{32}S in its first excited bending vibrational state are recorded and analyzed for the first time, and 86 transitions were analyzed for H_2^{34}S . Neese et al. (2012) acquired the submillimeter/THz spectrum of a mixture of 14 gases, including HCN, ClCN, CO, NO, C_2H_2 , NH_3 , HCl, and others, in the 210–270 GHz region. Different gases show complex redundancy of the rotational fingerprint. The gas cell was coupled with preconcentration to increase sensitivity. The detection limit of deuterated acetonitrile by THz apparatus was 69 ppt. Cai, Wang, and Shen (2013) collected the spectral characteristics of the air pollution gases SO_2 and H_2S . Spectra were measured by THz-TDS technique within a range of 0.2–2.6 THz. Shimizu et al. (2009, 2011) measured N_2O gas by the THz-TDS instrument. They developed an experimental system for remotely detecting dangerous gases. The gas cell was 1 m in length, and detection experiments were conducted at long distances of 3.6 m and low N_2O concentration of 25%. The result shows that gases can be remotely detected using active THz wave detection (Figure 4). Demers and Garet (2018) reported on a portable THz spectrometer mounted to a consumer drone UAV for gas monitor. Tanno et al. (2017) investigated on butane and ethane gases absorbed on ZIF-8 detection by THz spectrometer. Mihin et al. (2018) reported that $(\text{HCN})_2$ was tested by high-resolution synchrotron THz.

Figure 4: Operating principle of remote gas-sensing system based on THz spectroscopy.

Lu, Karpowicz, and Zhang (2009) established a field-induced second-harmonic generation pulsed THz apparatus for gas detection. More than 10 gaseous samples were measured, and the selected gas samples included nitrogen, xenon, sulfur hexafluoride (SF_6), carbon disulfide (CS_2), cyclopentene (C_5H_8), and alkane gases (CH_4 , C_2H_6 , C_3H_8 , $n\text{-C}_4\text{H}_{10}$, $n\text{-C}_5\text{H}_{12}$, and C_6H_{14}). Fused quartz was used for gas cell windows. A figure of merit method was introduced to characterize the sensitivity of gases. Harmon and Cheville (2004) reported on THz-TDS based on a gas cell-detecting gas species in the low part-per-million range in near real time. Gas cell path length can be changed, and the number of passes (4, 8, or 12 single passes) was controlled by the angles of mirrors A and C, corresponding to path lengths of 2.5, 5.0, or 7.5 m, respectively. Methyl chloride vapor can be detected at low pressures to 1 Pa in gas cells. Lin et al. (2008) introduced a method that involves extracting line positions from gas species without a reference pulse and classifying the positions by means of the minimum Euclidean distance method using the THz-TDS spectral line catalog. Hindle et al. (2008) reported a monochromatic CW THz source THz system for gas detection. THz spectrum characterization was used for the collection and analysis of H_2S pollution gas. Almoayed, Piyade, and Afsar (2007) reported the THz spectra of SO_2 gas and CO gas by dispersive Fourier transform spectroscopy (DFTS). The frequency range of DFTS was 60 GHz to 6 THz. The THz spectra of CO and SO_2 at different pressure were acquired, and the result showed that gas pressure is related to absorption spectra and refractive index. Medvedev, Behnke, and Lucia (2005) applied the THz-TDS instrument for gas monitoring and quantification. The spectral resolution approach can quantify the complex rotational spectrum of gases at a rate of 10 elements per second at high signal-to-noise ratio. The result shows that THz-TDS spectra provide “absolute” specificity and “zero” false-alarm rates even in complex mixtures.

As discussed above, high chemical selectivity for pollutant gas measurements is observed at THz frequencies. The application of THz gas measurement technology may perform important roles in online gas detection and remote gas sensing.

The list of toxic chemical compounds detected by THz spectroscopy are shown in Table 1.

Table 1: List of toxic chemical compounds detected by THz spectroscopy.

Type of THz spectroscopy	Target compound	Range of THz	Reference
THz-TDS	Difluoromethane, methenyl iodide, etc.	254.6–256.2 GHz	Medvedev, Behnke, and Lucia (2005)
THz-TDS	Sulfur dioxide, ammonia, etc.	572 GHz	Assefzadeh, Jamali, and Aleksander (2016)
CW THz-TDS	Acetonitrile	0.60–0.72 THz	Hsieh et al. (2016a)
CW THz-TDS	$\text{CH}_3^{13}\text{CN}$	0.60–0.72 THz	Hsieh et al. (2016b)
THz-TDS	Ammonia, propionaldehyde, propionitrile, etc.	$2\text{--}125\text{ cm}^{-1}$	Smith and Arnold (2015)
THz-TDS	Carbon monoxide	0–3 THz	Kilcullen et al. (2015)
THz-TDS	Methane, ethane	0.2–1.5 THz	Liang (2015)
Sub-THz	Sulfur dioxide	630–930 GHz	Mouret et al. (2013)
FTS	Hydrogen sulfide	1.4–10.5 THz	Azzam et al. (2013)

SMM/THz THz-TDS	Hydrocyanic acid, acetonitrile, etc. Sulfur dioxide, hydrogen sulfide	210–270 GHz 0.2–2.6 THz	Neese et al. (2012) Cai, Wang, and Shen (2013)
THz standoff detection	Nitrogen monoxide	440–490 GHz	Shimizu et al. (2009)
THz standoff detection	Nitrogen monoxide	440–490 GHz	Shimizu et al. (2011)
Pulsed THz waves	Sulfur hexafluoride, carbon disulfide, etc.	0.3–10 THz	Lu, Karpowicz, and Zhang (2009)
THz-TDS	Trichloromethane	0.1–1.8 THz	Harmon and Cheville (2004)
THz-TDS CW THz DFTS	Carbon monoxide, nitrogen monoxide, etc. $H_2^{32}S$; $H_2^{33}S$ Sulfur dioxide, carbon monoxide	0.1–2.0 THz 1016–1028 GHz $10\text{--}30\text{ cm}^{-1}$	Lin et al. (2008) Hindle et al. (2008) Almoayed, Piyade, and Afsar (2007)
THz-TDS	Fluoromethane, carbon disulfide, etc.	246.8–261.2 GHz	Medvedev, Behnke, and Lucia (2005)
THz-TDS	Carbon dioxide	2 THz	Demers and Garet (2018)
THz-TDS THz-TDS Reflectance THz-TDS Reflectance THz-TDS THz-TDS	Butane, ethane, etc. (HCN) ₂ Chlorpyrifos-methyl methomyl Carbendazim	0.5–6.2 THz $119.1\text{--}119.5\text{ cm}^{-1}$ 0.3–2.3 THz 0.5–2 THz 0.1–2 THz	Tanno et al. (2017) Mihrin et al. (2018) Xu et al. (2017) Lee et al. (2016) Qin et al. (2017a) and Qin, Xie, and Ying (2017b)
THz-TDS THz-TDS THz-TDS THz-TDS THz-TDS THz-TDS	Methomyl, carbamate, etc. Carbaryl Difenoconazole Imidacloprid Dicofol, chlorpyrifos, daminozide, etc. Sulfapyridine, sulfathiazole, and tetracycline	0.1–3 THz 1.8–6.3 THz 0.66–1.57 THz 0.3–1.7 THz 0.3–3 THz 0.5–6.0 THz	Baek et al. (2016) Sun et al. (2016) Zhou et al. (2015) Chen (2015) Maeng et al. (2014) Massaouti et al. (2013)
THz-TDS	AMS	0.6–1.3 THz	Wang, Ma, and Wang (2012)
THz-TDS THz-TDS FTS THz-TDS THz-TDS	α -Endosulfan Quintozene <i>cis</i> -Permethrin Dimethylurea Tetracycline hydrochloride	1.68–1.91 THz 0.1–1.05 THz $20\text{--}400\text{ cm}^{-1}$ 0.6–1.8 THz 0.3–2.0 THz	Hou et al. (2012) Wang et al. (2011) Suzuki (2011) Zhao et al. (2018) Qin et al. (2017a) and Qin, Xie, and Ying (2017b)
THz-TDS THz-TDS THz-TDS	Glyphosate Benzoyl peroxide Potassium sorbate	0.15–3 THz 0.2–2.0 THz 0.2–2.0 THz	Wang et al. (2017) Zou et al. (2017) Li, Zhang, and Ge (2017)
THz-TDS THz-TDS FTS	Aldrin, dieldrin, and endrin Dibutyl phthalate	0.2–1.8 THz 0.2–2.6 THz (THz-TDSs), 1.8–10 THz (FTS)	Song and Li (2012) Zhao et al. (2015)
THz-TDS THz-TDS THz-TDS	DBP, DINP, DEHP Melamine Copper sulfate, zinc sulfate	0.2–2.0 THz 1.99–2.99 THz 0.2–1.6 THz	Liu et al. (2016) Cui et al. (2009) Li, Zhao, and Li (2009)
THz-TDS THz-TDS THz-TDS THz-TDS	Pb cation Pb cation Sodium nitrate, aluminum nitrate Cocaine free base, cocaine hydrochloride, ephedrine hydrochloride, etc.	0.1–1.2 THz 0.1–1.2 THz 0.2–2.5 THz 0.1–6 THz	Li and Chen (2016) Li and Zhao (2016) Li et al. (2015) Davies, Burnett, and Fan (2008)
THz-TDS	Ketamine, methylephedrine, cocaine, ephedrine, etc.	0.1–2.5 THz	Pan (2010)
THz-TDS	Ephedrine, hydrochloride, papaverine hydrochloride	0.2–2.6 THz	Deng et al. (2009)
THz-TDS	Acetaldehyde, methanol, isopropyl alcohol, etc.	238–252 GHz	Neumaier et al. (2015)

Pesticides and antibiotics

The THz technology offers extensive applications in the research fields of pesticide and antibiotic identification and residual pesticide detection. Xu et al. (2017) set up a THz-TDS combined with metamaterials experiment apparatus used to detect the organophosphorus pesticide chlorpyrifos-methyl. Metamaterials were composed of square metal patch arrays (see Figure 5). The reflectance of the metamaterials was measured by a commercial THz-TDS and converted from time domain data to frequency domain data through fast Fourier transform method. The LOD of chlorpyrifos-methyl was 0.204 mg L^{-1} . Lee et al. (2016) developed a THz-TDS system with nanoslot antenna array apparatus to detect residual pesticide methomyl. A THz spectrum in a reflection configuration was used to detect low-concentration methomyl absorbed at the fruit surface only with sample contact (see Figure 6). Qin et al. (2017a) and Qin, Xie, and Ying (2017b) combined THz-TDS with principal component analysis (PCA) and clustering by fast search and finding of density peaks (CFSFDP) method for pesticide detection. PCA-CFSFDP is a potential identification method for pesticide identification and detection. Baek et al. (2016) tested methomyl and carbamate insecticide by using THz-TDS. The characteristic THz absorption peaks of methomyl were 1, 1.64, and 1.89 THz. The test sample matrices were wheat and rice flour. Sun et al. (2016) determined carbaryl in rice powder by using THz-TDS. The characteristic THz absorption peak of carbaryl was in the frequency range of 1.8–6.3 THz. The partial least squares regression chemometric method was used to establish two quantitative analysis models. Wang et al. (2017) reported that glyphosate pollution in soil was detected by THz spectrometer.

Figure 5: (A) Schematic diagram of THz metamaterials detection of CM. (B) A scanning electron microscope (SEM) image of the THz metamaterials; the metal patch length is $105 \mu\text{m}$ and the period of the metamaterials is $140 \mu\text{m}$. (C) Reflectance curves of simulation and experimental results of THz metamaterials detection.

Figure 6: (A) A schematic image of a sensing chip contacting to the apple peel sample that was partially contaminated by a dropping of pesticide. (B) A schematic of THz reflection configuration for multilayered samples and measured reflected.

Zhou et al. (2015) studied the THz spectra of the solid pesticide difenoconazole. The absorption spectra of difenoconazole were in the frequencies of 0.66, 0.80, 1.03, 1.31, and 1.57 THz, and the experiment results fit well with the simulated results by density functional theory (DFT) method. Chen (2015) reported the quantitative analysis of imidacloprid in rice powder samples by using a THz-TDS instrument. The absorption coefficient spectra of imidacloprid in the frequency range of 0.3–1.7 THz were obtained. Different chemometric methods were compared and used to quantitatively determine imidacloprid. Maeng et al. (2014) tested the THz spectra of dicofol, chlorpyrifos, chlorpyrifos-methyl, daminozide, imidacloprid, diethyldithiocarbamate, and dimethyldithiocarbamate in wheat flour mixtures. The THz absorption peaks were tested in the frequency range of 0.1–3 THz. Seven pesticides exhibited different frequency-dependent refractive indices, although five of the seven pesticides showed no specific absorption peaks in this frequency range. Massaouti et al. (2013) characterized the THz spectra of three antibiotics (sulfapyridine, sulfathiazole, and tetracycline), and two acaricides (coumaphos and amitraz). Multiple antibiotics were identified in their mixture with honey THz fingerprints. Wang, Ma, and Wang (2012) quantitatively detected the components of mixtures of the herbicide ammonium sulfamate (AMS) in agricultural products by using the THz instrument. The method was established by collection of the absorption coefficient spectra of pure AMS and quantitative analysis by partial least squares (PLS) technology.

Hou et al. (2012) investigated the absorption coefficient spectrum and refractive index spectrum of the pesticide α -endosulfan by THz instrument. The absorption peaks of α -endosulfan were at 1.7 and 1.88 THz in the experiment, partially matching with 1.68 and 1.91 THz obtained in the DFT calculation. The matching peaks are attributed to the intramolecular vibrational modes of α -endosulfan. Wang et al. (2011) studied the absorbance spectrum of bactericide quintozone in the THz range. Quantitative analysis was carried out on quintozone MtBE solutions in the concentration range of 30–100 $\mu\text{g/mL}$. Suzuki (2011) tested the THz spectra of *cis*-permethrin by FTIR at the THz region within an experimental frequency range of 20–400 cm^{-1} . The absorption spectra interfered with the clay and emulsifier experiments that were also being conducted.

Toxic chemical compounds

Li, Zhang, and Ge (2017) applied the THz-TDS system for the detection of potassium sorbate in milk powder. The experiment results show that potassium sorbate exhibits a characteristic absorption peak at 0.98 THz. Song and Li (2012) measured the THz transmission spectra of three different persistent organic pollutants (POPs) (aldrin, dieldrin, and endrin) by using THz-TDS. Test frequencies were in the range of 0.2–1.8 THz. The absorption peak is in reasonably good agreement with the theoretical simulation by B3LYP DFT and experiment. The THz detection method may be used to study POPs in soil quality evaluation or safety inspection further. Zhao et al. (2015) proposed a method for detection of the known industrial plasticizer dibutyl phthalate by THz-TDS system. Liu et al. (2016) studied the THz transmission spectrum of phthalic acid esters. Test frequencies were in the range of 0.2–2.0 THz for three PAEs: di-*n*-butyl phthalate (DBP), di-isononyl phthalate (DINP), and di-2-ethylhexyl phthalate ester (DEHP). The refractive indices were 1.524, 1.535, and 1.563 for DINP, DEHP, and DBP, respectively.

Cui et al. (2009) applied the THz-TDS system to detect melamine. The THz transmission spectra of pure melamine and two kinds of its mixtures with polyethylene and milk powder were collected. The THz transmission spectrum of melamine present two absorption peaks at 1.99 and 2.29 THz. Li, Zhao, and Li (2009) tested the THz spectrum of copper sulfate and zinc sulfate in soil by THz-TDS. The absorption coefficient and refractive index were tested in the frequency range of 0.2–1.6 THz. The methods can be used to measure the metal residues in the soil. Li and Chen (2016) and Li and Zhao (2016) studied the quantitative analyses of the Pb cation in soil by THz-TDS. Li et al. (2015) investigated the absorption coefficient and the refractive index of four types of nitrate solution (sodium nitrate, aluminum nitrate, calcium nitrate, and magnesium nitrate) using the THz-TDS system. A PLS model was used to establish quantitative analysis methods. Zhao et al. (2018) investigated the dimethylurea isomer spectrum detection by THz spectrometer. Qin et al. (2017a) and Qin, Xie, and Ying (2017b) developed a method to analyze tetracycline hydrochloride solution by attenuated total reflection THz-TDS. Zhou et al. (2015) investigated benzoyl peroxide in flour analyzed by THz spectrometer.

Drugs of abuse

Numerous studies have used THz spectroscopy in the detection of illicit drugs. THz waves are transparent to most dry dielectric materials, such as cloth, paper, wood, and plastic. Based on this property, THz waves can be used for the qualitative valuation of items in packaging or bags for security checking.

Davies, Burnett, and Fan (2008) reported the application of THz-TDS system for seven illicit drugs or drug precursor detection. The THz transmission spectrum of cocaine free base, cocaine hydrochloride, 3,4-methylenedioxy-*N*-methamphetamine (MDMA), ephedrine hydrochloride, amphetamine sulfate, diamorphine (heroin), and morphine sulfate pentahydrate (morphine) was collected by polytetrafluoroethylene (PTFE) compressed into pellet sample. The THz-TDS spectra of cocaine free base and cocaine hydrochloride have absorption peak at 1.54 THz. MDMA and 4,5-methylenedioxy amphetamine have absorption peak at 1.24, 1.71, and 1.90 THz. THz transmission spectrum of different packages were also collected in that study.

Pan (2010) collected THz spectra for seven pure illicit drugs. Support vector machine (SVM) was used to classify the THz absorption spectra and determine the main contents proportion of mixtures. Deng et al. (2009) measured and reported the THz spectra of ephedrine hydrochloride and papaverine hydrochloride. The experiment result matched more with theoretical calculation in gas-phase simulation by semi-empirical theory than by DFT for some chemical compounds. Neumaier et al. (2015) applied the THz spectra in illicit drugs and security detection. He and Shen (2013) established a THz database containing 38 kinds of pure illicit drugs. The database includes absorption coefficient and refractive index spectra of illicit drugs. SVM, back propagation (BP), radial basis function (RBF) artificial neural network algorithm methods were suited for identification analysis. Self-organizing feature map (SOM) algorithm methods were suited for quantitative analysis.

Conclusions and outlook

During the last decade, various THz technologies have undergone rapid development and there has been an increasing interest in their use for chemical sensing. THz technologies had been widely used for toxic chemical compound detection for its many merits such as fingerprint character, transmission property, and other uses. With continuous progress, THz spectroscopy will play important role in toxic chemical compound on-site detection and nondestructive examination.

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