

Research Article

Terahertz Absorption Spectroscopy of Benzamide, Acrylamide, Caprolactam, Salicylamide, and Sulfanilamide in the Solid State

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Received 6 September 2013; Accepted 14 December 2013; Published 16 February 2014

Academic Editor: Yizhuang Xu

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Terahertz (THz) absorption spectra of the similarly structured molecules with amide groups including benzamide, acrylamide, caprolactam, salicylamide, and sulfanilamide in the solid phase at room temperature and 7.8 K for salicylamide are reported and compared to infrared vibrational spectral calculations using density functional theory. The results of THz absorption spectra show that the molecules have characteristic bands in the region of 0.2–2.6 THz ($\sim 7\text{--}87\text{ cm}^{-1}$). THz technique can be used to distinguish different molecules with amide groups. In the THz region benzamide has three bands at 0.83, 1.63, and 1.73 THz; the bands are located at 1.44 and 2.00 THz for acrylamide; the bands at 1.24, 1.66 and 2.12 THz are observed for caprolactam. The absorption bands are located at 1.44, 1.63, and 2.39 THz at room temperature, and at 1.22, 1.46, 1.66, and 2.41 THz at low temperature for salicylamide. The bands at 1.63, 1.78, 2.00, and 2.20 THz appear for sulfanilamide. These bands in the THz region may be related to torsion, rocking, wagging, and other modes of different groups in the molecules.

1. Introduction

Spectroscopy is a powerful technique for measuring, analyzing, and identifying various molecules. Frequencies in the far-infrared (FIR, $650\text{--}50\text{ cm}^{-1}$) and terahertz (THz) ($0.1\text{--}10\text{ THz}$, or $3.3\text{--}333.6\text{ cm}^{-1}$) ranges correspond to motions of the entire molecular structure, involving relatively large masses and relatively shallow potentials [1, 2]. THz spectroscopy is being used for a number of important analytical applications in such areas as threat detection [3–5] and pharmaceutical characterization [6–8]. Its utility stems from solid-state compounds and molecules containing low-energy vibrations that, taken as a whole in this region, serve as spectral “fingerprints” usable for their detection and characterization. THz spectroscopy of condensed-phase biological

samples are investigated ranging from the simple crystalline forms of amino acids, carbohydrates, and polypeptides to the more complex aqueous forms of small proteins, DNA, and RNA [9–14]. THz hydration studies uncovered that the dynamical hydration shell of saccharides consists of several hundred water molecules and up to thousand water molecules for proteins [15–17]. THz spectroscopy is regarded as the renaissance of far-infrared spectroscopy [18].

Amide groups contribute significantly to the protein structure. A variety of techniques such as IR, NMR, Raman, ultrasonic absorption, and UV/Vis spectroscopies have been used to characterize both the intermolecular and intramolecular bonding in amide compounds [19–22]. Salicylamide is a nonsteroidal anti-inflammatory agent with analgesic and antipyretic properties. Its therapeutic action and potential

toxicity are still the subject of research, which makes it necessary to control its presence in biological fluids [23]. For acrylamide, it is found that its administration to laboratory animals caused tumor formation in various organs, the exact mechanism involved still being unclear [24, 25]. Sulfanilamides are successfully employed as effective chemotherapeutic agents for the prevention and cure of bacterial infections in human biological systems. Determination of molecules with amide groups is essential in many analyses of biological and clinical applications.

Here we have investigated the low-frequency vibrational motions of salicylamide, benzamide, acrylamide, caprolactam, and sulfanilamide in the solid state by concentrating on the spectral region between 7 and 650 cm^{-1} where crystal lattice vibrations, hydrogen bond bending modes and collective modes, and so forth may occur [26]. The experimental results indicate that FIR and THz time-domain technique can be effective tools to detect different molecules with amide groups and the bands in the region may be related to torsion, rocking, wagging, and other modes of different groups of the molecules.

2. Experimental

2.1. Materials. Salicylamide, benzamide, acrylamide, caprolactam, and sulfanilamide were obtained from commercial sources and used without further purification.

2.2. Physical Measurements. The THz absorption spectra were recorded on the THz time-domain device of Capital Normal University of China, based on photoconductive switches for generation and electrooptical crystal detection of the far-infrared light. The experimental apparatus for terahertz transmission measurements has been discussed in detail elsewhere [27]. The preparation of the samples was by pressing mixed pellets with polyethylene powder (pure sample for benzamide); the diameter of the samples is 13 mm and the thickness of the samples is about 0.8 mm. The detection of THz absorption spectra was carried out at N_2 atmosphere to avoid the influence of water vapor. The resolution of the spectra is 40 GHz. The THz frequency-domain spectra were obtained from the corresponding THz time-domain spectra via Fast Fourier Transform. Through comparison of THz frequency-domain spectra of the samples and corresponding references, the THz absorption spectra of the samples were obtained. Effective spectrum range is 0.2–2.6 THz, respectively.

The FIR spectra of benzamide, acrylamide, caprolactam, and salicylamide were measured using common used Nujol mull method, because mineral oil has no absorption in the far-IR region and the method can protect sample in solid state against wet and avoid distortion of bands or happening of ion exchange. Samples were suspended in the Nujol mull and then were daubed on a thin polyethylene window and another thin polyethylene window as background for comparison. Far infrared spectra in the range of $650\text{--}50\text{ cm}^{-1}$ were taken on a Nicolet Magna-IR 750-II Spectrometer at room temperature and at 8 cm^{-1} resolution, 128 scans. The optical bench was

purged with dried air. The FIR spectrum of sulfanilamide was measured on a Bruker VERTEX 80v FTIR spectrometer at 4 cm^{-1} resolution and 32 scans. The preparation of the sample was by pressing mixed pellets with polyethylene powder.

All theoretical calculations were performed with the Gaussian 03 software package [28]. Density functional theory (DFT) calculations were used to determine the equilibrium structures and harmonic vibrational frequencies of the molecules. The B3LYP [29] hybrid density functional was used with the 6-311++G (3df, 2pd), Gaussian-type basis set [30]. Full geometry optimizations were conducted in each case and harmonic frequency analyses performed on these optimized structures.

3. Results and Discussion

The molecular structures of benzamide, acrylamide, caprolactam, salicylamide, and sulfanilamide are shown in Figure 1. The THz and FIR spectra of benzamide, acrylamide, caprolactam, salicylamide, and sulfanilamide are shown in Figures 2 and 3, respectively. The corresponding band positions in the FIR and THz absorption spectra of the samples and possible assignments are listed in Table 1.

3.1. The THz Absorption Spectra of the Molecules. All of the structures of benzamide, acrylamide, caprolactam, salicylamide and sulfanilamide have amide groups. The difference of benzamide, and salicylamide is that there is one more OH group in the structure of salicylamide, and both of the two molecules have benzene ring (ph). The THz absorption spectra of benzamide, acrylamide, caprolactam, salicylamide and sulfanilamide in Figure 2 show that in the THz region benzamide has three bands: 0.83, 1.63, and 1.73 THz ($38, 54, 58\text{ cm}^{-1}$); acrylamide has two bands located at 1.44 and 2.00 THz ($48\text{ and }67\text{ cm}^{-1}$); caprolactam has three bands at 1.24, 1.66 and 2.12 THz ($41, 55\text{ and }71\text{ cm}^{-1}$). The absorption bands of salicylamide are located at 1.44, 1.63, and 2.39 THz ($48, 54, 80\text{ cm}^{-1}$) at room temperature, and its bands have shifted to 1.46, 1.66, and 2.41 THz ($49, 55\text{ and }80\text{ cm}^{-1}$), and 1.22 THz (41 cm^{-1}) band becomes clear at low temperature. For sulfanilamide, the bands are located at 1.63, 1.78, 2.00 and 2.20 THz ($54, 59, 67, \text{ and }73\text{ cm}^{-1}$). For these molecules, some of the peak positions are similar, for example, 1.63 THz for benzamide, salicylamide, and sulfanilamide, 1.66 THz for caprolactam; 1.22 and 1.24 THz for salicylamide and caprolactam; 2.00 THz for benzamide and sulfanilamide; 1.44 and 1.46 THz for caprolactam and salicylamide, respectively. However, most of the bands are different in peak positions and relative intensities, which show that THz method is sensitive to different molecular structures.

To clarify the bands in the THz region, second derivatives have been performed using Omnic 5.0 software for the THz spectra of the samples, and the results show that main bands and some relatively minor bands are observed in the second derivatives results (shown in Figure 4). The main bands are observed for each sample, which has a good agreement with the corresponding THz absorption spectrum. For benzamide, only three main bands are observed, it is the same as

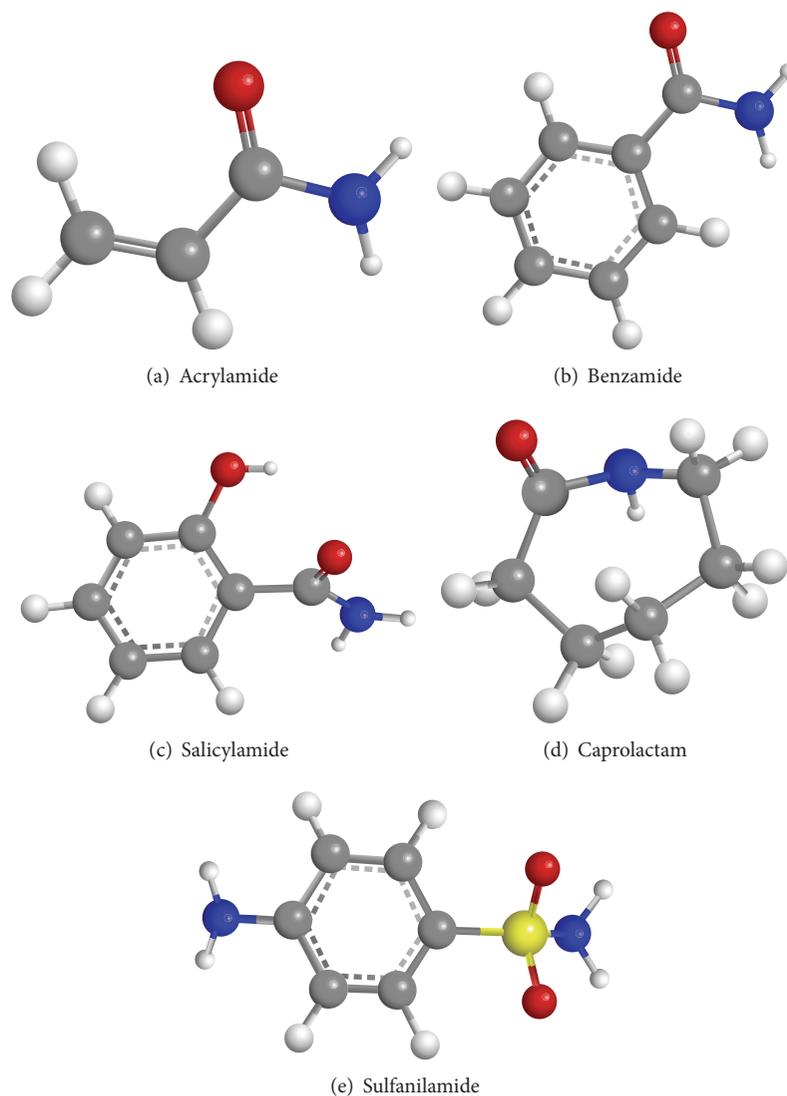


FIGURE 1: The molecular structures of acrylamide, benzamide, salicylamide, caprolactam, and sulfanilamide. (a) Acrylamide; (b) benzamide; (c) salicylamide; (d) caprolactam; (e) sulfanilamide.

the THz spectrum. For sulfanilamide, in the second derivatives results, 54, 60, 66, 72, 74, 81 cm^{-1} are observed (54, 59, 67, and 73 cm^{-1} in the absorption spectrum), so 73 cm^{-1} band is formed by 72 and 74 cm^{-1} bands; for caprolactam, 71 cm^{-1} band is formed by 66, 69, and 71 cm^{-1} child-bands; for acrylamide, weak band at 48 cm^{-1} is emphasized in the second derivatives results, 67 cm^{-1} band mainly has several child-bands: 64, 67, 70, 74, and 82 cm^{-1} ; for salicylamide, 40, 48, 54, 64, 69, 79 cm^{-1} bands are observed compared to 48, 54, and 80 cm^{-1} in the absorption spectrum. 40 cm^{-1} band is observed at low temperature. It seems that there is a band at 64 cm^{-1} for salicylamide. The results show that second derivatives methods help observing the THz bands.

3.2. The FIR Spectra of the Five Molecules with Amide Group.

The FIR spectra of benzamide, acrylamide, caprolactam,

salicylamide and sulfanilamide, after automatic baseline correction shown in Figure 3 indicate that the five molecules have different band positions and relative band intensities.

For salicylamide, it has many bands in the region: 608, 564, 526, 515, 456, 421, 385, 296, 160, 146, 108, and 93 cm^{-1} . For benzamide, its bands are as follows: 635, 529, 412, 382, 251, 177, 151, 110, 89, and 54 cm^{-1} ; for acrylamide, it has several bands in the region: 619, 508, 314, 185, 122, and 67 cm^{-1} ; for caprolactam, it has relatively more bands in the region: 581, 503, 488, 398, 337, 323, 258, 195, 129, 87, 69, and 56 cm^{-1} . Sulfanilamide has the bands located at 641, 626, 563, 541, 497, 450, 414, 365, 302, 224, 132, 88, 72, and 58 cm^{-1} in its FIR spectrum. The FIR and THz results are consistent for the samples in the 100–50 cm^{-1} region as shown in Table 1.

For benzamide and salicylamide, there is one OH difference. Their FIR spectra have various peak positions and relative intensities; only several peak positions are close,

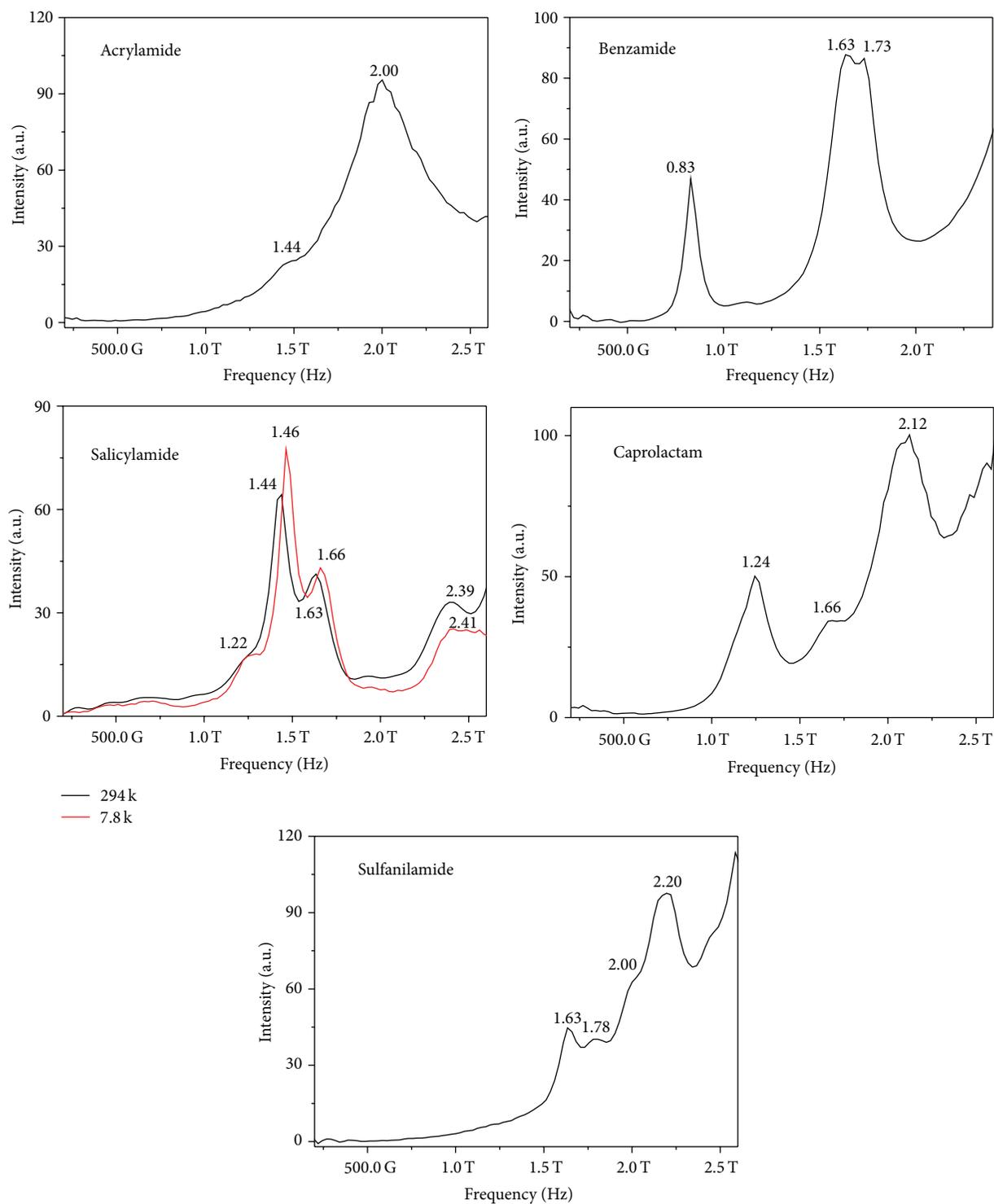


FIGURE 2: THz absorption spectra of acrylamide, benzamide, salicylamide, caprolactam, and sulfanilamide.

such as 529(benzamide)/526(salicylamide); 382/385; 151/146; 110/108; 89/93 cm^{-1} . Other bands are located at different positions. For acrylamide and caprolactam, the bands at 508/503, 314/323, 185/195, 122/129, and 67/69 cm^{-1} are similar in some extent. Caprolactam has relatively more bands in the FIR region. Sulfanilamide has two strong bands located at 563

and 541 cm^{-1} , and the band at 365 cm^{-1} is relatively strong, and other bands are weak. The five molecules have different characteristic bands in the FIR region.

3.3. DFT Calculation and Analyses for the FIR and THz Spectra of the Molecules. The assignment of the spectra in the FIR and

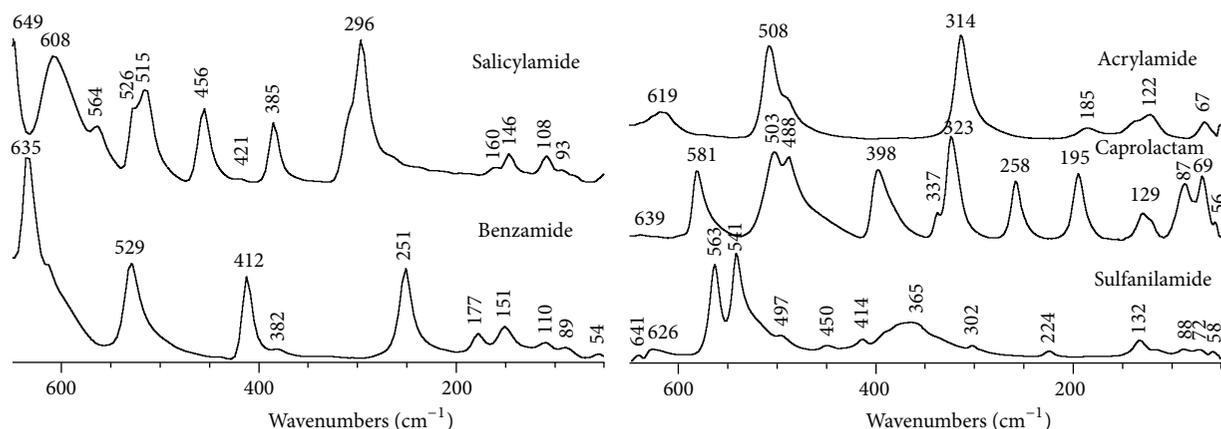


FIGURE 3: FIR spectra of acrylamide, benzamide, salicylamide, caprolactam, and sulfanilamide in the 650–50 cm^{-1} region.

THz region is difficult. Fortunately, there are some calculation results for benzamide, salicylamide, and sulfanilamide [31–36]. Using similar method shown in the references, based on the calculated results of RB3LYP/6-311++G (3df, 2pd), and with the aid of visualization software of Gaussian View 4.1, the observed vibrational modes in the far-infrared and THz region can be assigned as shown in Table 1. The assignment is dependent on the result of calculation from molecular structure and patterns of vibrational modes. Some calculation results for the bands below 100 cm^{-1} are shown in Figure 5. The calculated band positions are similar to experimental results in some extent as the calculations in [31–36], but the relative intensities of the bands compared to experimental results are not good as the calculation results for four vitamin molecules [37].

According to the DFT calculation results (shown in Table 1), the bands in the FIR and THz region mainly consist of movement of whole molecular skeleton. The absorption bands in the THz region are related to torsion, rocking, wagging, twisting, and other modes of different groups in the molecules. For example, in the calculation results, the main absorption bands of sulfanilamide below 100 cm^{-1} are centered at 15 and 85 cm^{-1} . The 15 cm^{-1} band corresponds to out-of-plane wagging of ph ring and twisting of NH_2 (the one in S(=O)-NH_2); 85 cm^{-1} band is related to out-of-plane wagging of ph ring and wagging of two NH_2 ; 113 cm^{-1} band is related to rocking of NH_2 ; 167 cm^{-1} band is related to deformation of S(=O)-NH_2 and in-plane wagging of ph. For benzamide, 554 cm^{-1} band is assigned to twisting of NH_2 and wagging of ph; 503 cm^{-1} band is assigned to in-plane wagging of ph and amide; 415 cm^{-1} band is assigned to out-of-plane folding of ph ring; 375 cm^{-1} band is assigned to in-plane rocking of amide, wagging of ph, and stretching of CC. 341 cm^{-1} band is assigned to wagging of NH_2 ; 217 cm^{-1} band is assigned to in-plane rocking of the ring, and rocking of C=O-NH_2 ; 152 cm^{-1} band is assigned to out-of-plane vibration of ph ring and rocking of NH_2 ; 57 cm^{-1} band

is assigned to out-of-plane vibration of ph-CONH_2 and wagging of NH_2 .

For salicylamide, 30 cm^{-1} band is assigned to twisting of ph-CONH_2 ; 141 cm^{-1} band is assigned to out-of-plane vibration of whole molecule; 184 cm^{-1} band is assigned to wagging of NH_2 ; 247 cm^{-1} band is assigned to out-of-plane wagging of whole molecule, especially ph ring; 275 cm^{-1} band is assigned to rocking of NH_2 , rocking of ph; 383 cm^{-1} band is assigned to in-plane vibration of ph and torsion of (C=O-NH_2 and COH); 419 cm^{-1} band is assigned to out-of-plane folding of ph and stretching of NH ; 439 cm^{-1} band is assigned to in-plane wagging of ph; twisting of (C=O-NH_2 and COH); 509 cm^{-1} band is assigned to rocking of NH_2 , rocking of (C=O and OH), in-plane wagging of ph, and so forth. For acrylamide, 114 cm^{-1} band is assigned to wagging of NH_2 and wagging of CH=CH_2 ; 190 cm^{-1} band is assigned to wagging of NH_2 ; 277 cm^{-1} band is assigned to rocking of (CH=CH_2) and rocking of (C=O-NH_2); 468 cm^{-1} band is assigned to rocking of NH_2 and wagging of (CH=CH_2); 470 cm^{-1} band is assigned to twisting of (CH=CH_2) and twisting of NH_2 ; 613 cm^{-1} band is assigned to twisting of NH_2 and twisting of CH_2 , and so forth. For caprolactam, 107 cm^{-1} band is assigned to wagging of CH_2 , stretching of C=O , and out-of-plane vibration of the ring; 158 cm^{-1} band is assigned to rocking of CH_2 and in-plane vibration of the ring; 258 cm^{-1} band is assigned to rocking of CH_2 , wagging of CH_2 , stretching of NH , stretching of C=O , and so forth; 301 cm^{-1} band is assigned to stretching of NH and in-plane vibration of the ring; 323 cm^{-1} band is assigned to rocking of CH_2 ; 402 cm^{-1} band is assigned to in-plane vibration of the ring, and so forth. In most of the cases whole molecule is involved in the vibration modes. The calculation results are similar in some extent to the results in [31–37]. The calculations in Table 1 are only preliminary results, because only single molecule and in gas phase have been considered here, so it is reasonable that the calculation and experimental results have some differences.

TABLE 1: Calculated and experimental vibrational frequencies for salicylamide, benzamide, acrylamide, caprolactam, and sulfanilamide (cm^{-1})^a.

Compounds	Experiment		Calculation	Vibrational assignments
	FIR	THz-TDS	6-311++G(3df, 2pd)	
Salicylamide	526		538	τ_{ph}
	515		509	ρ_{NH_2} , $\rho(\text{C}=\text{O}$ and $\text{OH})$, in-plane wagging of ph
	456		439	In-plane wagging of ph, $t(\text{C}=\text{O}-\text{NH}_2$ and $\text{COH})$
			419	Out-of-plane folding of ph, ν_{NH}
	385		383	β_{ph} , $\tau(\text{C}=\text{O}-\text{NH}_2$ and $\text{COH})$
	296		275	ρ_{NH_2} , $\rho(\text{ph})$
			247	Out-of-plane wagging of whole molecule, especially ph ring
	161		184	ω_{NH_2}
	146			
	108		141	$\gamma(\text{whole molecule})$
	94			
		80		
		54 (55*)		
	48 (49*)			
	41*	30	$t(\text{ph}-\text{C}=\text{O}-\text{NH}_2)$	
Benzamide			503	In-plane wagging of ph and amide
			415	Out-of-plane folding of ph ring
	412		414	Out-of-plane folding of ph ring, ρ_{NH_2}
	383		375	In-plane rocking of amide group, ω_{ph} , ν_{CC}
			341	ω_{NH_2}
	251		217	In-plane rocking of ph ring, $\rho(\text{C}=\text{O}-\text{NH}_2)$
	178			
	151		152	γ_{ph} ; ρ_{NH_2}
	110			
	90			
	58			
	54	57	$\gamma(\text{ph}-\text{CONH}_2)$, ω_{NH_2}	
	38			
Acrylamide	508		470	$t(\text{CH}=\text{CH}_2)$, t_{NH_2}
			468	ρ_{NH_2} , $\omega(\text{CH}=\text{CH}_2)$
	314		277	$\rho(\text{CH}=\text{CH}_2)$, $\rho(\text{C}=\text{O}-\text{NH}_2)$
	185		190	ω_{NH_2}
	122		114	ω_{NH_2} , $\omega(\text{CH}=\text{CH}_2)$
	67			
	48			
Caprolactam	503		508	ν_{NH} ; ρ_{CH_2}
	488		437	$\nu_{\text{C}=\text{O}}$; ν_{NH} ; ω_{CH_2} ;
	398		402	β_{ring}
	337		323	ρ_{CH_2}
	323		301	ν_{NH} ; β_{ring}
	258		258	ρ_{CH_2} ; ω_{CH_2} ; ν_{NH} ; $\nu_{\text{C}=\text{O}}$;
	195		158	ρ_{CH_2} , β_{ring}
	129		107	ω_{CH_2} ; $\nu_{\text{C}=\text{O}}$; γ_{ring}
	87			
	69	71		
56	55			
	41			

TABLE I: Continued.

Compounds	Experiment		Calculation	Vibrational assignments
	FIR	THz-TDS	6-311++G(3df, 2pd)	
Sulfanilamide		73	85	Out-of-plane wagging of ph, ωNH_2
		67		
		59		
		54	15	Out-of-plane wagging of ph, tNH_2

^a β : in-plane vibration; τ : torsion; γ : out-of-plane vibration; ν : stretching; ω : wagging; ρ : rocking; t : twisting, ph: benzene ring.

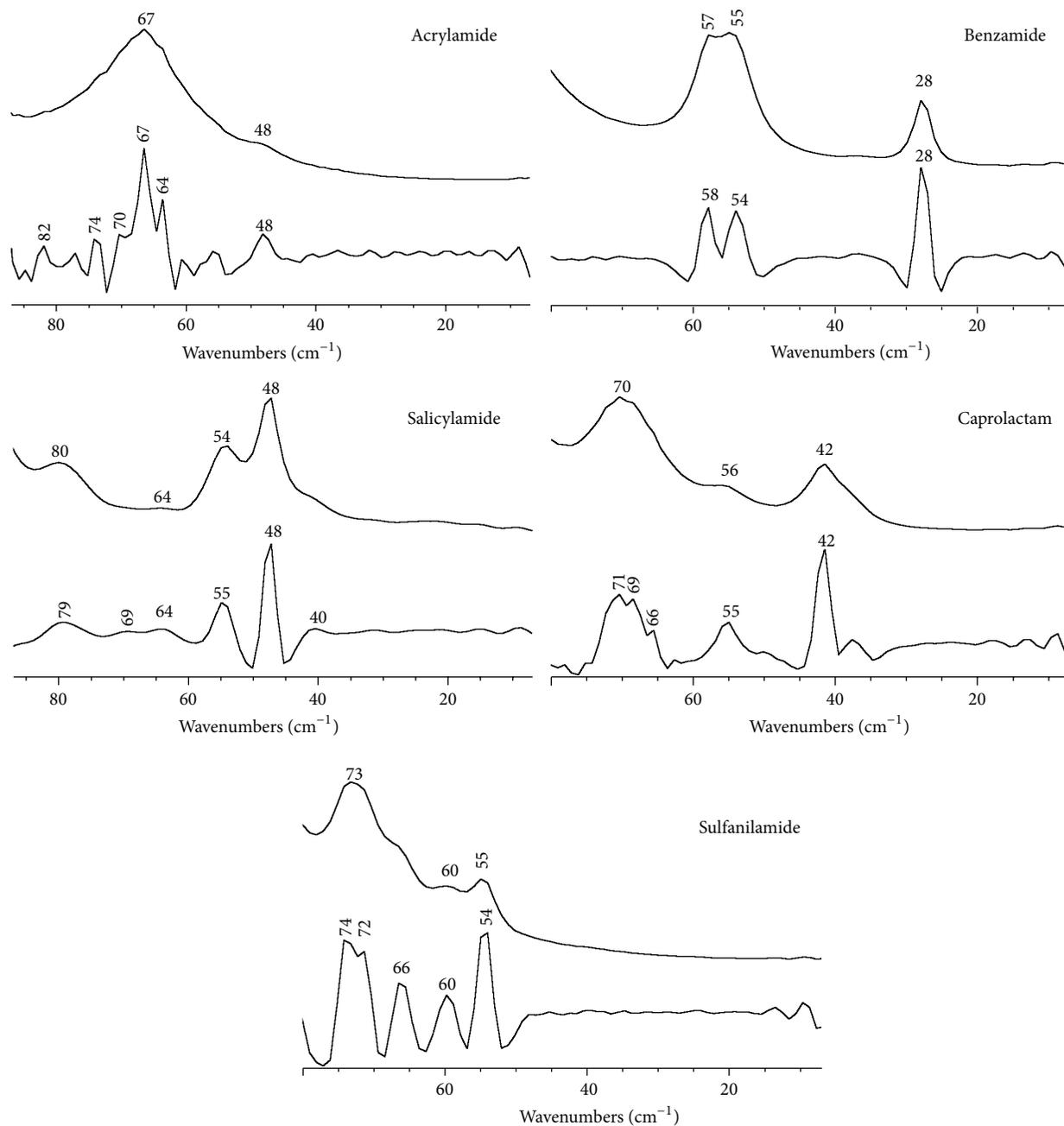


FIGURE 4: The second derivatives results for the THz spectra of the samples using Omnic 5.0 software.

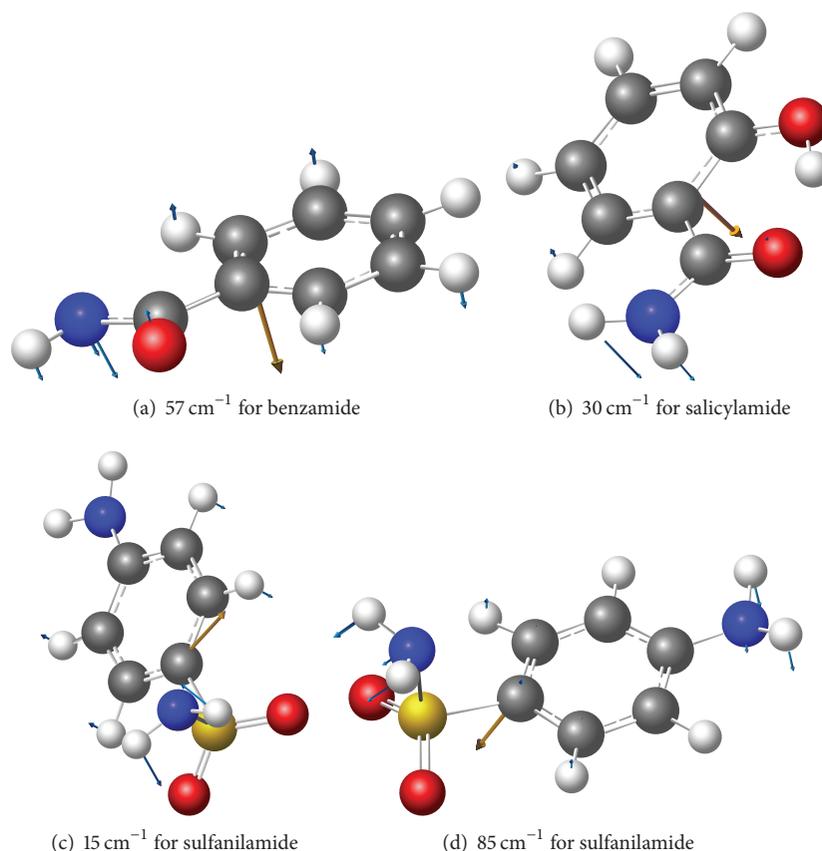


FIGURE 5: Low-frequency vibrational modes of the molecules below 100 cm^{-1} . (a) 57 cm^{-1} for benzamide; (b) 30 cm^{-1} for salicylamide; (c) 15 cm^{-1} for sulfanilamide; (d) 85 cm^{-1} for sulfanilamide.

4. Conclusions

The FIR and THz characteristic bands of five molecules with amide groups are observed using FIR and terahertz time-domain spectroscopy. The five molecules exhibit several bands in the THz region, which may be related to torsion, rocking, wagging, and other modes of different groups in the molecules according to calculation and the assignments in the references. THz spectra are effective method to distinguish different molecules with amide groups. In addition, it is also the basis for investigation on hydration of amide group, and so forth.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

The authors gratefully acknowledge the financial support by National Natural Science Foundation of China for the Grants (21001009 and 50973003), the State Key Project for Fundamental Research of MOST (2011CB808304), National High-tech R&D Program of China (863 Program) of MOST

(2010AA03A406), and the Scientific Research Project of Beijing Municipal Commission of Education and Beijing Natural Science Foundation (Grant no. KZ201310028032). Limin Yang is one of the corresponding authors.

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