ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
MATHEMATICS, PHYSICS, THEORETICAL MECHANICS
FASCICLE II, YEAR XIV (XLV) 2022, No. 1
DOI: https://doi.org/10.35219/ann-ugal-math-phys-mec.2022.1.02

Vibrational analysis of hallucinogenic amphetamines

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Abstract: Vibrational spectroscopy represents a very useful technique that measures the interaction of infrared radiation with materials by absorption, emission, or reflection. It is a very powerful way to investigate and identify chemical compounds or functional groups that exist in solid, liquid, or gaseous forms. It can also be used to characterize and identify chemical compounds. This paper presents the vibrational analysis of some representative 2C-x and DOx hallucinogenic amphetamines.

Keywords: vibrational spectroscopy, hallucinogens, amphetamines.

1. INTRODUCTION

Vibrational spectroscopy is a method of non-destructive identification and characterization with the help of which the specific chemical bonds of atoms can be identified. In general, almost any substance with covalent bonds absorbs electromagnetic radiation from the infrared region of the electromagnetic spectrum at different frequencies. By absorbing infrared radiation by molecules, the vibrational energy of the binders between atoms changes. It is thus possible to identify the functional groups present in the chemical structure of the analyzed substances [1]. There are two important groups of vibration: stretching and bending vibrations [2]. This paper presents the vibrational analysis of a selection of 2C-x and DOx compounds, based on their ATR-FTIR spectra.

Fourier-transform infrared spectroscopy (FTIR) is an important technique used to obtain the infrared spectrum of substances. In order to transform the raw data into the real spectrum, a mathematical transformation, called Fourier transformation is applied. One important advantage of using FTIR spectrometers consists in the fact that the data is collected at the same time for all the wavelengths [3].

Attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) uses an ATR crystal, which produces an evanescent wave in contact with the IR radiation [4]. The ATR-FTIR method has the advantage that only a small amount of sample is needed in order to analyze a substance [5].

Hallucinogenic amphetamines are an important class of drugs that produce changes in perception and mood, being continuously seized over the black market [6]. From the analysis of their spectra, an important series of functional groups contained in the substances belonging to the two classes of drugs can be determined [7].

2. EXPERIMENTAL

The ATR-FTIR spectra of the main hallucinogenic amphetamines of the 2C-x and DOx classes were analyzed for the identification of the main functional groups. The spectral analysis of three of the substances belonging to the two classes of hallucinogenic amphetamines, namely 2-(4-iodo-2,5-dimethoxyphenyl)ethanamine (2C-I), 2-(4-bromo-2,5-dimethoxyphenyl)ethanamine (2C-B), and 1-(4-bromo-2,5-dimethoxyphenyl)propane-2-amine (DOB), will be presented.

3. RESULTS AND DISCUSSIONS

The ATR-FTIR spectra of the compounds presented in Figure 1, Figure 2 and Figure 3 were analyzed.

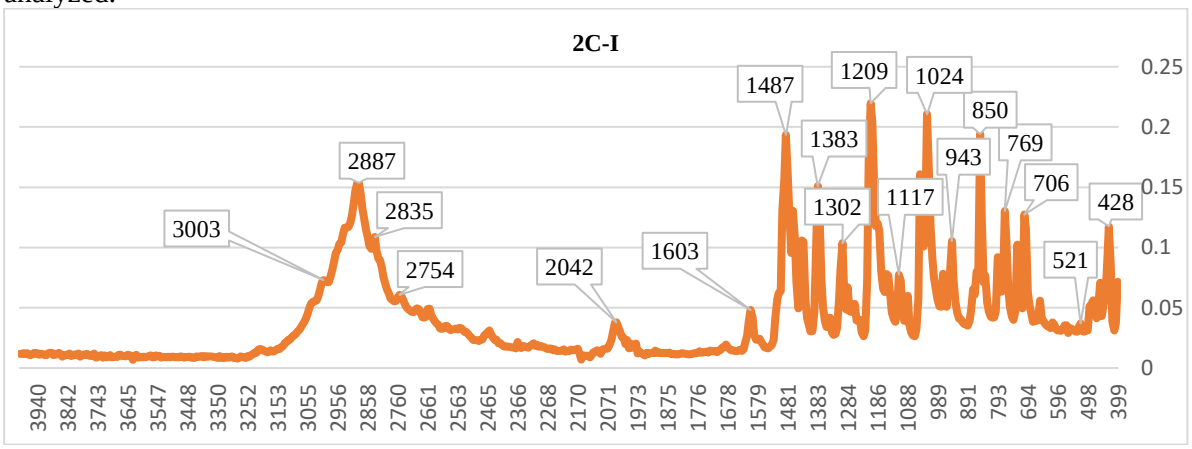

Fig. 1. The ATR-FTIR spectrum of 2-(4-iodo-2,5-dimethoxyphenyl)ethanamine

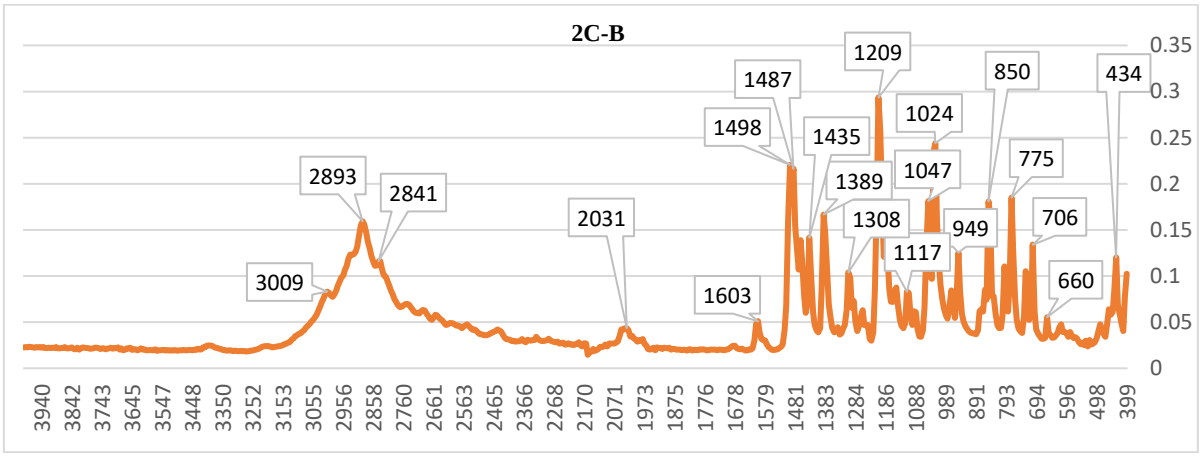

Fig. 2. The ATR-FTIR spectrum of 2-(4-bromo-2,5-dimethoxyphenyl)ethanamine

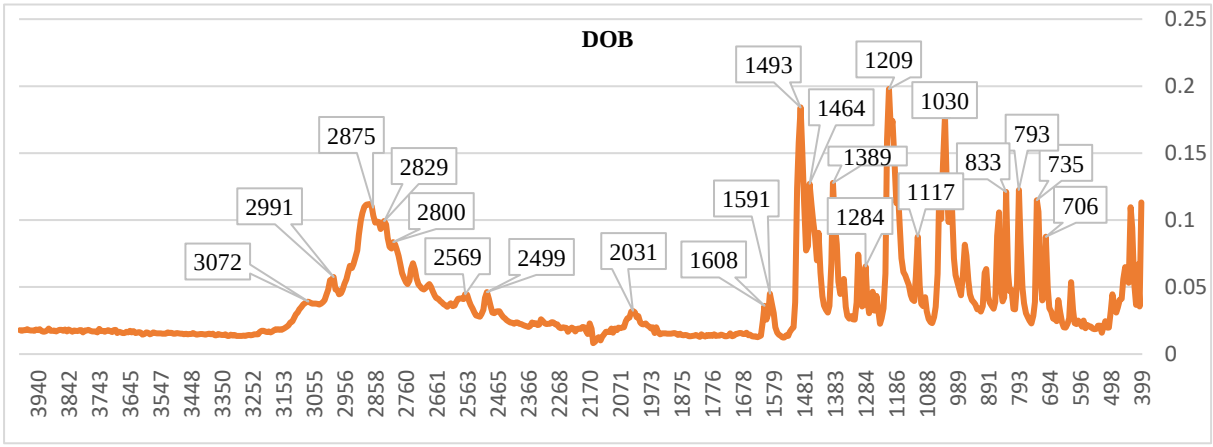

Fig. 3. The ATR-FTIR spectrum of 1-(4-bromo-2,5-dimethoxyphenyl)propane-2-amine

The functional groups and modes of vibration [8-11] identified for the most important peaks present in the spectra of the targeted 2C-x and DOx compounds are presented in Table 1, Table 2 and Table 3.

Table 1. Vibrational analysis of 2-(4-iodo-2,5-dimethoxyphenyl)ethanamine

2C-I	Group	Modes of vibration	Compound class
3003	C-H	stretching	aromatics
2887	C-H	stretching	alkane
	N-H	stretching	amine salt
2835	N-H	stretching	amine salt
2754			
2042			
1603			aromatic hidrocarbons
	N-H	bending	amine
1435	C–C	stretching	in the aromatic ring
	C-H	bending	alkane (methyl group)
	CH_2	bending	methylene
1383	CH_3	bending	methyl
	C-H	bending	alkane
1302			
1209	C-O-C	stretching	
	C-O	stretching	alkyl aryl ether
1117	C-N	stretching	amine
1024	C-N	stretching	amine
943			
850	C–H	bending	
769	C–H	bending	
706			benzene derivative
521	C-I	stretching	halo compound
428			

Table 2. Vibrational analysis of 2-(4-bromo-2,5-dimethoxyphenyl)ethanamine

2C-B	Group	Modes of vibration	Compound class
3009	C-H	stretching	aromatics
2893	C-H	stretching	alkane
	N-H	stretching	amine salt
2841	N-H	stretching	amine salt
2031			
1603			aromatic hidrocarbons
	N-H	bending	amine
1498	C–C	stretching	aromatic ring

1487			aromatic hidrocarbons
1464	CH_3	bending	methyl
	CH_2	bending	methylene
1435	C-H	bending	alkane (methyl group)
1389	CH_3	bending	methyl
	C-H	bending	alkane
1308			
1209	C-O-C	stretching	
	C-O	stretching	alkyl aryl ether
1117	C-N	stretching	amine
1047	C-N	stretching	amine
1024	C-N	stretching	amine
949			
850	C–H	bending	
798	C–H	bending	
775	C–H	bending	
706	C–H	bending	
			benzene derivative
660	C-Br	stretching	halo compound
434			

Table 3. Vibrational analysis of 1-(4-bromo-2,5-dimethoxyphenyl)propane-2-amine

DOB	Group	Modes of vibration	Compound class
3072	C-H	stretching	aromatics
2991	C-H	stretching	alkane
2875	N-H	stretching	amine salt
	C-H	stretching	alkane
2829	N-H	stretching	amine salt
	C-H	stretching	alkane
2800	N-H	stretching	amine salt
2737			
2569			
2499			
2031			
1608	N-H	bending	primary amine
1591	N-H	bending	primary amine
	C–C	stretching	aromatic ring
1493	C–C	stretching	aromatic ring
1464			
	CH_3	bending	methyl
	CH_2	bending	methylene
	C-H	bending	alkane (methyl group)

1435			aromatic hidrocarbons
1389	CH_3	bending	methyl
	C-H	bending	alkane
1354			
1308			
1284			
1209	C-O-C	stretching	
	C-O	stretching	alkyl aryl ether
1198	C-N	stretching	amine
1117	C-N	stretching	amine
1030	C-N	stretching	amine
966			
897	C-H	bending	1,2,4-trisubstituted
856	C–H	bending	
833	C–H	bending	
793	C–H	bending	
735	C–H	bending	
706	C–H	bending	
			benzene derivative
625	C-Br	stretching	halo compound
492			
451			
434			
399			

The vibrational analysis of the spectra indicates that the three substances have the most important peaks in approximately the same regions, i.e. in the spectral regions of 3010-2500 cm^{-1}, 1600-700 and 690-500 cm^{-1}. The main functional group identified are C-H, N-H, CH_2, CH_3, C-C, C-N and the aromatic ring. The vibrations associated with aromatic hydrocarbons were also identified, along with the halo compounds, namely bromine and iodine.

4. CONCLUSIONS

The analysis of the ATR-FTIR spectra of the hallucinogenic selected substances, namely 2-(4-iodo-2,5-dimethoxyphenyl)ethanamine (2C-I), 2-(4-bromo-2,5-dimethoxyphenyl)ethanamine (2C-B), and 1-(4-bromo-2,5-dimethoxyphenyl)propane-2-amine (DOB), reveals the existence of threemain spectral domains. The first spectral range corresponds to 3010-2500 cm^{-1} and reveals the presence of the N-H and C-H groups, being also relevant for the presence of the aromatic ring. The second spectral domain, namely, 1600-700 cm^{-1} includes the highest number of peaks of the spectrum, showing the presence of the N-H, C-H, CH_2, CH_3, C-N, and C-C groups, but also the presence of the aromatic ring. The third spectral region varies from 690 to 500 cm^{-1}, being suggestive for the presence of the halo substituents, in this case bromine and iodine. In conclusion, the analysis of the ATR-FTIR spectra emphasize the similarities existing between the analyzed compounds, being an efficient, selective method of characterization.

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