

Comparison IR spectra of alanine $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$ and alanine $\text{CD}_3\text{CH}(\text{NH}_2)\text{COOH}$

Szczepan Brym

University of Warmia and Mazury, Faculty of Mathematics and Computer Science,
Ścenczna 54, 10 -710 Olsztyn, Poland;
E-mail: szbrym@matman.uwm.edu.pl

Abstract. Comparison of spectra by ATR FTIR technique was made. For comparison the fingerprint region below 1500cm^{-1} was chosen. After replacement of hydrogen with deuterium in side chain the frequency shift of most of the bands to lower values in FTIR spectrum was observed.

1. Introduction

Alanine is one of optically active, unpolar aliphatic amino acids [1]. Lateral chain presented contains methyl group CH_3 . Linear formula has form $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$. Molecular weight $89,09\text{ g/mol}$. Melting temperature 295°C . After replacement of hydrogen with deuterium, the linear formula becomes $\text{CD}_3\text{CH}(\text{NH}_2)\text{COOH}$ with molecular weight $92,11\text{ g/mol}$ and melting temperature $314,5^\circ\text{C}$. Structure of alanine is presented in figure 1 [2].

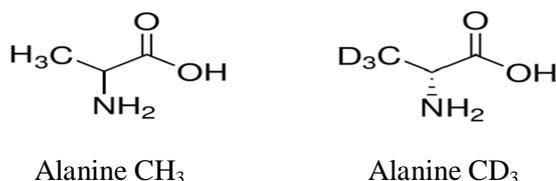


Figure 1: CH_3 and CD_3 forms of alanine molecules.

2. Experimental setup and results

FT-IR spectra of the solid compounds were obtained as attenuated total reflection (ATR), using Nicolet 6700 FT-IR spectrometer, equipped with a diamond crystals, XT-KBr beam splitter and a DLaTGS detector in the range from $500\text{-}4000\text{cm}^{-1}$, with 64 scans and a spectra resolution of 4cm^{-1} , at a room temperature. For comparison the fingerprint region i.e. below 1500cm^{-1} was chosen. Figure 2 displays the $4000\text{-}550\text{ cm}^{-1}$ spectral region of the MIR spectra of the CH_3 and CD_3 alanine.

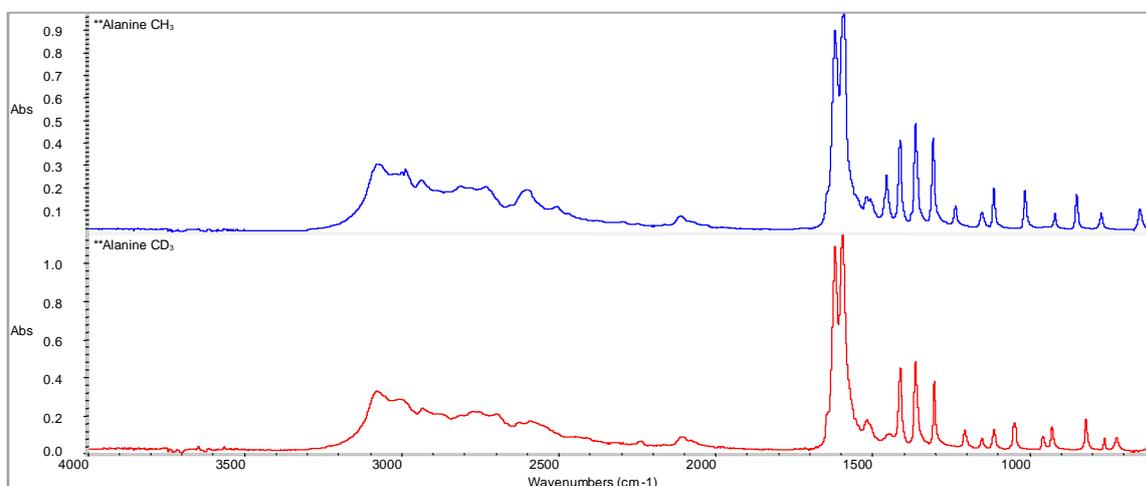


Figure 2: The MIR spectra of the CH_3 and CD_3 alanine.

Figure 3 displays the 1500-550 cm^{-1} spectral region of the MIR spectra of the CH_3 and CD_3 alanine.

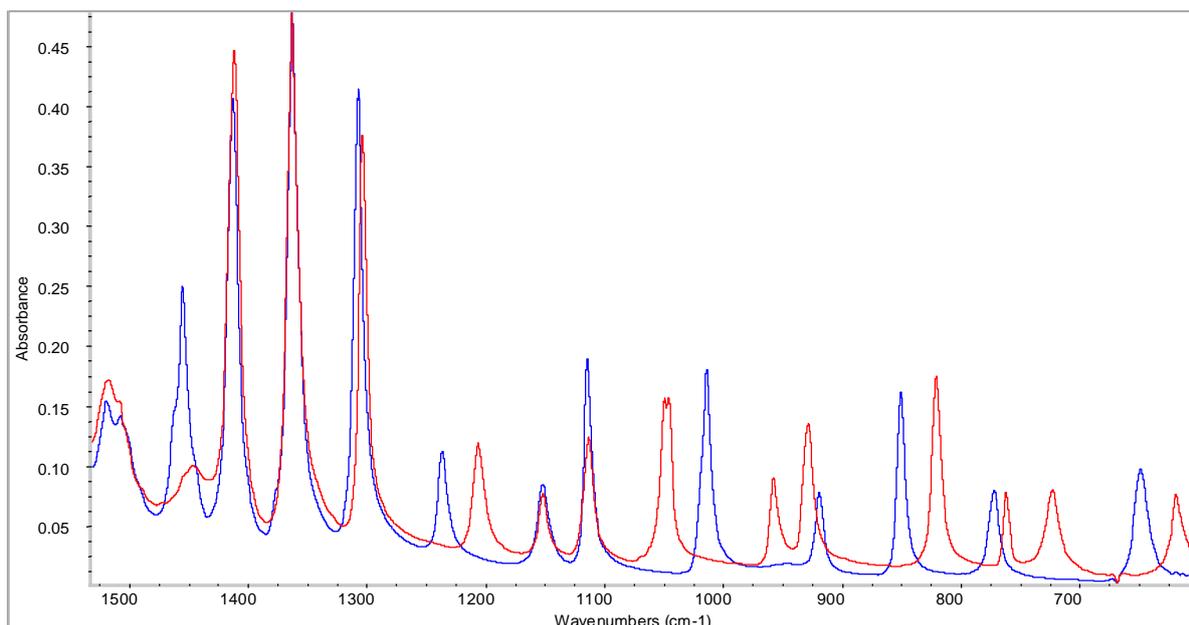


Figure 3: The spectra of the CH_3 and CD_3 alanine in the fingerprint region.

The corresponding frequencies and the band assignments are presented in table 1.

Table 1. Vibrational frequencies of alanine CH_3 and alanine CD_3 in the fingerprint region.

Alanine CH_3		Alanine CD_3	
Assignment	Exp. (MIR)	Assignment	Exp. (MIR)
asCH_3	1455,87	asCD_3	1446,75
sCH_3	1413,12	sCD_3	1412,11
sCOO	1363,15	sCOO	1363,14
sNH_2	1307,77	sNH_2	1304,02
asCH	1236,97	asCH	1206,66
NH_2	1152,39	NH_2	1152,22
C-N	1114,71	C-N	1113,34
CH_3	1014,18	CD_3	1046,08
NH_2	919,32	NH_2 (double)	957,99
C-OO	850,75		928,92
CN	772,25	C-OO	820,87
COO	648,97	CN (double)	762,15
			723,11
		COO	618,75

a) Frequencies in cm^{-1} ; -stretching, -bending, -wagging, -rocking, s-symmetric, as-asymmetric.

b) Bands in bold are presented in figure 4 below.

After replacement of hydrogen to deuterium in side chain in FTIR spectrum frequency shift of most of the bands to lower values was observed. Because the vibrations are complex, the frequency ratio of comparative bands did not exceed 1,1. The spectrum of alanine CH_3 in this field consists of separate single bands. After deuteration complex and double bands of diverse intensity were observed.

The profiles of these bands were examined. The selected bands and approximated Voigt profiles are presented in figure 4.

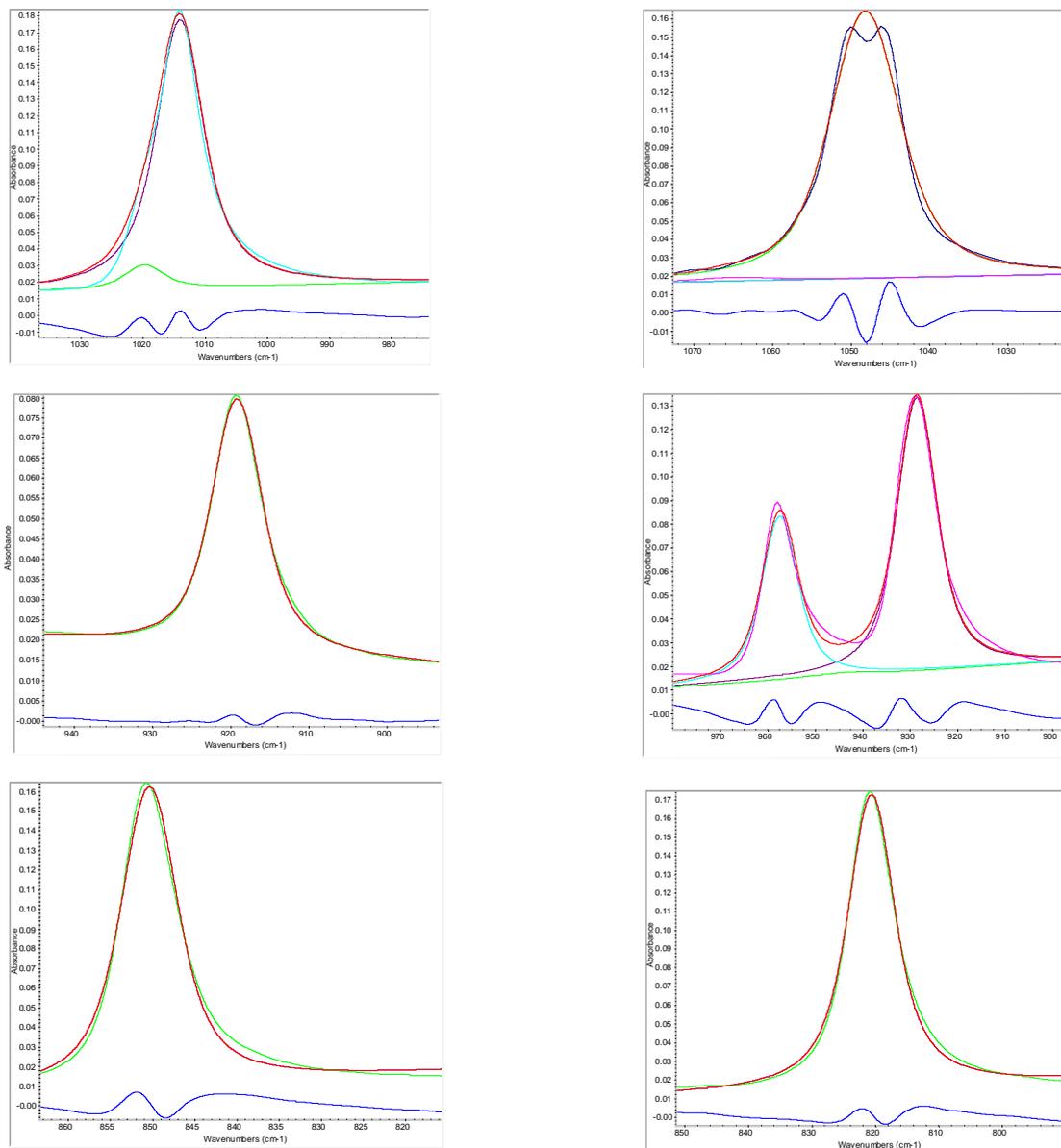


Figure 4: Selected bands of alanine CH₃ on the left with respective bands of alanine CD₃ on the right.

3. Conclusions

In FTIR spectrum the frequency shift was observed for most of the bands to lower values. We found the increase of vibrational frequencies for two bands. We also noticed that two vibrational frequencies turned into doublets in the spectrum after deuteration. Probably, this result is due to the Fermi resonance. In this work we also demonstrated that the shape of the spectral lines can be approximated by one or more of the Voigt profiles.

References

- [1] Rosado M T S, Duarte M L R S and Rui F *Journal of Molecular Structure* 410-411(1997) p 343
- [2] Lenarz W J and Lane M D (red.) *Encyclopedia of Biological Chemistry* 2004 Elsevier