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RAMAN SPECTRA AND *ab-initio* CALCULATION ANALYSIS OF INTERMOLECULAR INTERACTIONS IN ETHYLACETATE

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Abstract. In this work the C=O vibrational band of ethylacetate was studied using Raman scattering spectra and *ab-initio* calculations. The obtained experiment and *ab-initio* calculations show that the band corresponding to the C=O stretching vibration of ethylacetate is complex and consists of several bands. *ab-initio* calculations were performed in the B3LYP 6-311++G (d,p) basis set, and electro-optical parameters, molecular electrostatic potential (MEP) surface, charge distribution and bond lengths of monomers and dimers of ethylacetate were determined.

Keywords: ethylacetate; Raman spectroscopy; hydrogen bonding; *ab-initio* calculations; electrostatic potential surface.

Etilasetatda molekulalararo ta'sirlarni raman spektlari va noempirik hisoblash tahlillari

Annotatsiya. Ishda etilasetatning C=O tebranish polosa Raman sochilish spektrlari va noempirik hisoblashlar yordamida o'rganilgan. Olingan tajriba va noemperik hisoblashlar ko'rsatadiki, etilasetatning C=O valent tebranishiga tegishli polosa murakkab bo'lib, bir nechta chiziqdan iborat ekan. Noemperik hisoblashlar B3LYP 6-311++G (d,p) bazislar to'plamida amalga oshirildi va etilasetatning elektro-optik parametrlari, monomer va dimerlarining molekulyar elektrostatik potensial sirti, zaryad taqsimoti va bog' uzunliklari aniqlandi.

Kalit so'zlar: etilasetat; Raman sochilish spektri, vodorod bog'lanish, noemperik hisoblashlar, elektrostatik potensial sirti.

Спектры кр и *ab-initio* расчетный анализ межмолекулярных взаимодействий в этилацетате

Аннотация. В данной работе колебательная полоса C=O этилацетата исследована с использованием спектров комбинационного рассеяния и *ab-initio* расчетов. Полученный эксперимент и *ab-initio* расчеты показывают, что полоса, соответствующая валентному колебанию C=O этилацетата, является сложной и состоит из нескольких полос. *ab-initio* расчеты проводилось в базисе B3LYP 6-311++G (d,p), а электрооптические параметры, поверхность молекулярного электростатического потенциала, распределение заряда и длины связей мономеров и димеров этилацетата определенный.

Ключевые слова: этилацетат; рамановская спектроскопия; водородная связь; первоначальные расчеты; поверхность электростатического потенциала.

Intermolecular interactions play a key role in the study of physical, biological and chemical processes [1-2]. In the study of intermolecular interaction forces and intermolecular hydrogen bonds the mixed research of vibrational spectroscopy and theoretical calculations allows to fully justify the obtained experimental results [3-7]. Ethylacetate is widely used in the food industry as a flavoring agent. In production the solvent is widely used in the industry especially in the production of artificial leather [8]. Esters from organic substances are of great interest in the study of hydrogen-bonded complexes in various molecular systems [9-13]. Because esters have two proton-acceptor centers and participate in weak intermolecular hydrogen bonds. Currently one of the main reasons for the deterioration of the environment is the release of harmful gases when fuel is burned. Therefore finding environmentally friendly alternative fuel sources is the main task. In addition, of ethylacetate such fuels are highly effective. The characteristic of burning of ethylacetate at high temperatures was studied on the basis of experiments and calculations. Such researches are based on the study of biofuel production [14]. In [15] the IR spectrum of ethylacetate in the gas phase was studied, and it was said that the maxima of the spectral band were shifted. In [16] ethylacetate and methylcellulose substances were analyzed by FTIR spectra. It is said that hydrogen bonds of the form $C-H\cdots O$ and $O-H\cdots O$ can be formed, and CH_3 is symmetric and asymmetric stretching, C=O stretching, C-C-O stretching

and O-CH_2-C stretching vibrational frequencies were analyzed by F.H. Tukhvatullin and his colleagues. Parallel ($I_{//}(\nu)$) and perpendicular ($I_{\perp}(\nu)$) polarized constituents of ethylacetate were studied using Raman spectra of the C=O refraction band. It was determined that the maxima of the components $I_{//}$ and $I_{\perp}$ differ by 5.3 cm^{-1}. Spectral band is a complex compound consisting of aggregates of monomers and dimers [17].

Raman spectra of ethylacetate were recorded on a Renishaw Invia Raman spectrometer in range of 100-4000 cm^{-1}. A laser with a wavelength of 532 nm and a diffraction grating with a period of 1200 lines/mm were used as an excitation light source. A standard Renishaw CCD Camera detector was used to record the scattered light. All calculations were performed using the Density Functional Theory (DFT) method in Gaussian 09W software. DFT method B3LYP hybrid functional method is convenient for calculating ethylacetate monomer, dimer trimers and various physical parameters [18]. For these reasons, we performed calculations using the B3LYP functional, which includes diffusion and polarization functionals and the 6-311++G(d,p) basis set.

Raman scattering spectra of ethylacetate were recorded in range of 100 cm^{-1} and 4000 cm^{-1} and the spectral band has several vibrational maximum. Since we were interested in the spectral representation of the C=O vibrational band of ethylacetate we considered the spectral analysis of this specific band. In the Raman spectra, the maximum vibration of the band corresponding to C=O of ethylacetate corresponds to 1736 cm^{-1} (Fig. 1a), which resembels to the data presented in the literature [19]. Figure 1b shows the results of *ab-initio* calculations of ethylacetate, where the band at 1792 cm^{-1} corresponds to the C=O stretching vibration. As can be seen from Fig.1 the experimental and ab initio calculation results agree with each other.

Fig.2 shows the ethylacetate spectrum corresponding to the C=O stretching vibration obtained from the total Raman scattering spectrum. The maximum of this vibrational band corresponds to 1736 cm^{-1} and the half-width of the spectral band is 17.7 cm^{-1}. As can be seen from the figure the band has an asymmetry on the high frequency side which indicates the complexity of the band. The main reason for this is the presence of various aggregates in the liquid. We believe that these aggregates are due to the overlapping of spectral bands corresponding to hydrogen-bonded and non-hydrogen-bonded molecules in the liquid.

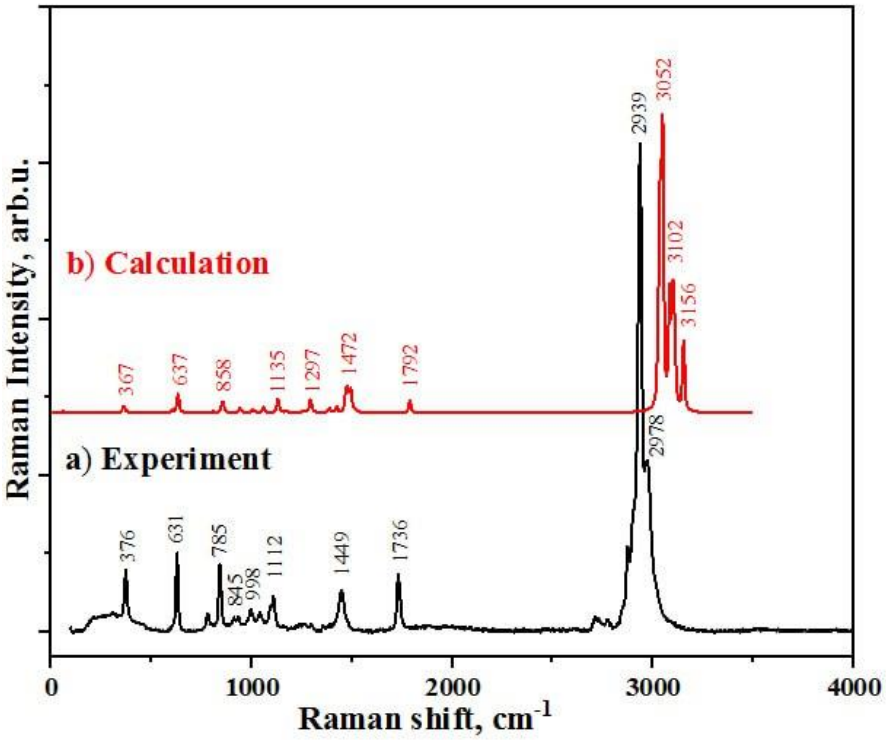


Figure 1. *Raman spectra of neat ethylacetate molecule; a) experiment and b) calculation*

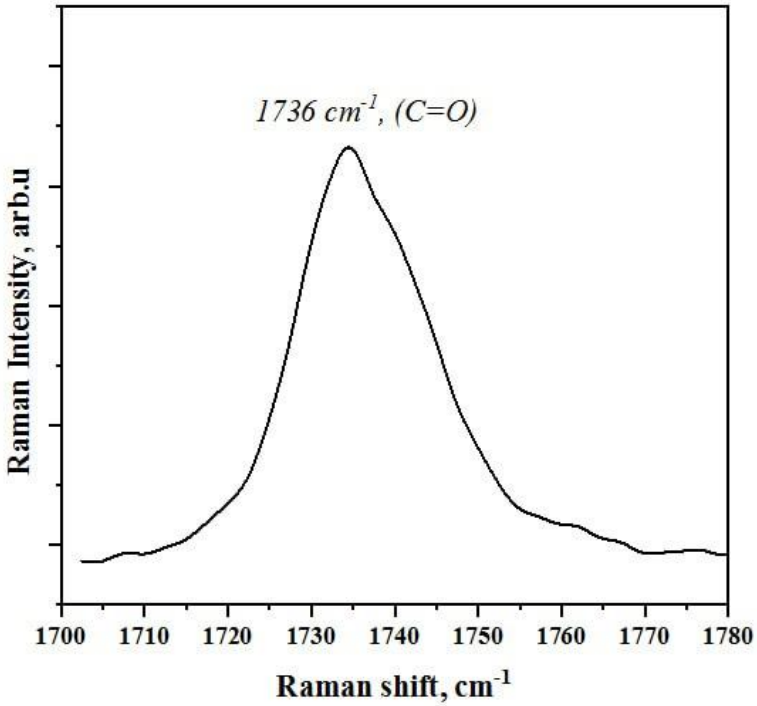


Figure 2. *Raman scattering spectrum related to the C=O stretching vibration of ethylacetate.*

Nowadays *ab-initio* calculations can supplement experimental data or create opportunities to study data that are difficult to obtain in experimentally [20]. A *ab-initio* calculation was performed to explain the complexity of this spectral band

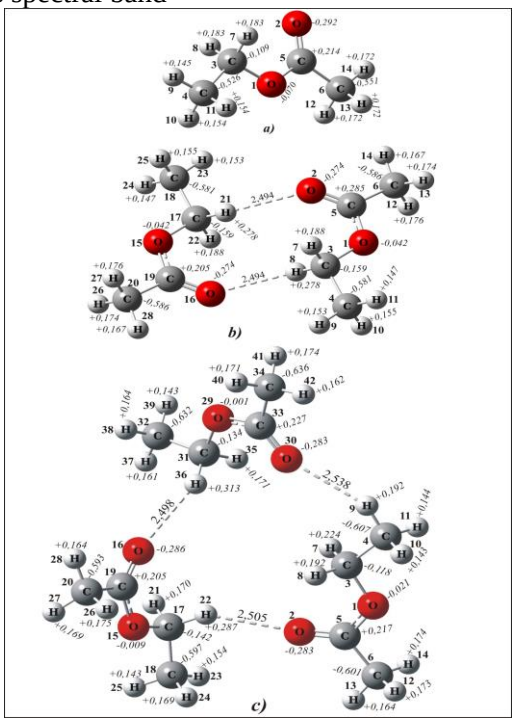


Figure 3. *Molecular clusters of ethylacetate molecule a) monomer, b) dimer and c) trimer*

and to fully justify it. Through *ab-initio* calculations, the mutual orientation of molecules, bond lengths, vibrational frequencies, charge distribution, dimer and trimer formation energies were determined.

Fig.3a shows the ethylacetate monomer. According to calculations, the band at 1792 cm^{-1} corresponds to the C=O vibration in the monomer. The dipole moment of the molecule is 2.08 D (Table 1). Fig.3b shows the ethylacetate dimer. In dimer formation, the O_2 atom of the C=O group of

the first molecule, the H_{21} atom of the CH_2 group of the neighboring molecule, the O_{16} atom of the C=O group of the second molecule have the same bond length of 2.494 Å with the H_8 atoms of the CH_2 group of the first molecule and cyclic closed dimer is formed as a result of the formation of a hydrogen bond. Dimer formation energy is 2.55 kcal/mol. Here the charge of H-atoms involved in hydrogen bonding is different from the charge of other H-atoms. Two spectral bands at 1773 cm^{-1} and 1780 cm^{-1} correspond to the C=O stretching vibration in the dimer. The 1780 cm^{-1} spectral band is not visible because the Raman activity is zero but, the 1773 cm^{-1} spectral band is active. Compared to the monomer it is shifted to a lower frequency by 19 cm^{-1}.

Table 1. *Calculation results for ethylacetate clusters*

Structure	Bond lengths (Å)	Frequency C=O cm^{-1}	Raman activity A^4/AMU	Depolar-P C=O (ρ)	Dipole Moment (Debay)	Hydrogen bond energy (kcal/mol)
Monomer		1792	7.3784	0.2926	2.08	-
Dimer	r(O_2…H_{21})= 2.494 r(H_8…O_{16})= 2.494	1773 1780	20.7215 0.00	0.2576 0.2419	0.00	2.55
Trimer	r(O_2…H_{22})= 2.505 r(O_{16}…H_{36})= 2.498 r(H_9…O_{30})= 2.538	1771 1776 1777	24.68 7.7217 7.3029	0.1027 0.7426 0.7498	0.50	4.47

Fig.3c shows the trimeric molecular cluster of ethylacetate. In the formation of a trimer, the O atom of the C=O group of the first and second ethylacetate molecules participates in hydrogen bonding with one H atom of the CH_2 group. The bond lengths are 2.505 and 2.498 Å. The third bond connects the O atom of the C=O group of the second ethylacetate molecule with one H atom of the CH_3 group of the first molecule. Form cyclic closed clusters with a bond length of 2.538 Å. The energy of formation of such a cluster is 4.47 kcal/mol. The dipole moment is 0.50 D. In the calculations three spectral bands correspond to trimer molecular clusters are 1771; 1776 and 1777 cm^{-1}. The Raman activity of the 1771 cm^{-1} spectral band is high, and the rest are lower. These bands shifted by 21 cm^{-1} and lower than that of the monomer (Fig. 4).

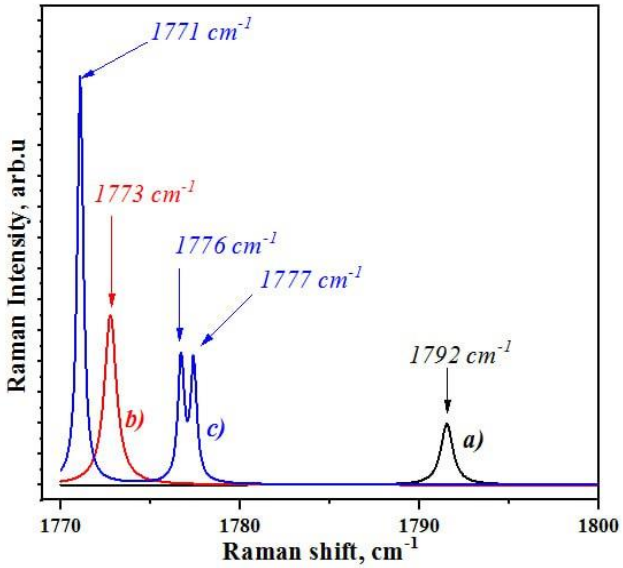


Figure 4. *Raman spectra of ethylacetate molecule (a-monomer; b-dimer; c-trimer)*

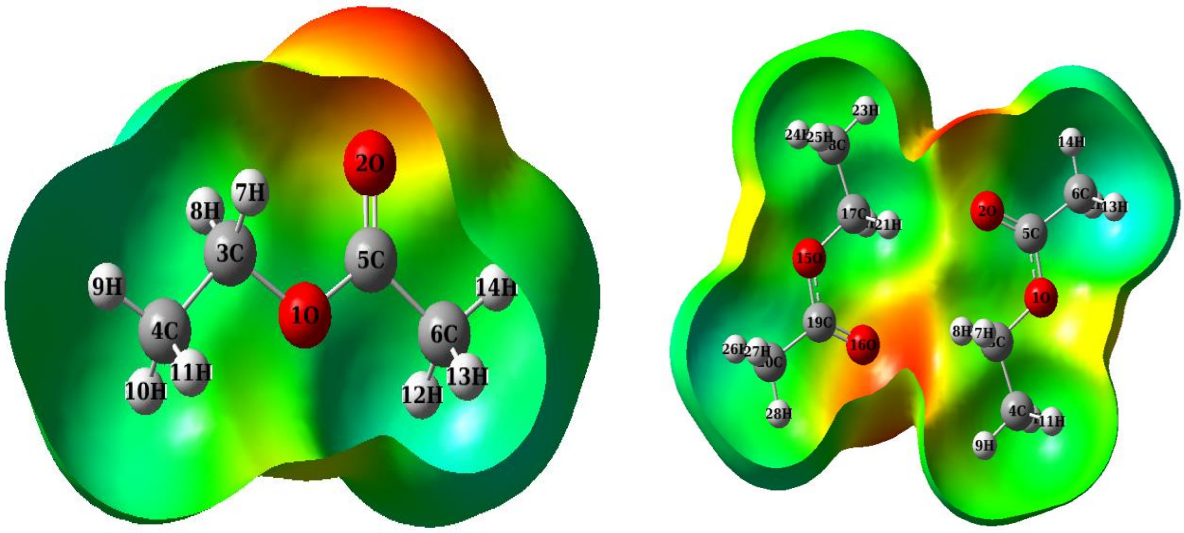


Figure 5. *Molecular electrostatic potential (MEP) surface of ethylacetate monomers and dimers*

Figure 5 shows the electrostatic potential surface obtained as a result of the electron density distribution of atoms in the ethylacetate molecule. Electrostatic potential surfaces describe the size shape and charge density of a molecule. Depending on the level of electrostatic potential it is represented in different colors. The increase in electrostatic potential is shown in the order red<yellow<green<blue. As you can see from the picture the surface around the C=O bond is red, which means it has the least electrostatic potential.

Raman scattering spectra related to the C=O vibration of pure ethylacetate are complex. This complexity is due to the presence of aggregates with different depolarization ratios in the liquid. This leads to the study of the shape of the spectral bands.

Formation mechanisms of isolated monomer, dimer and trimer molecular clusters of ethylacetate were studied with density functional theory (DFT) based on B3LYP 6-311++G (d,p) functional set.

Calculations show that in the formation of ethylacetate dimers and trimers, cyclic closed molecular clusters are formed as a result of the participation of an O atom in the C=O group of the molecule and one H atom in the CH_2 group of the neighboring molecule.

In pure ethylacetate, the C=O vibrational band in dimers and trimers is shifted to a lower frequency compared to the monomer. Dimer and trimer formation energy is 2.55 and 4.47 kcal/mol.

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