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STUDY OF FORMATION MECHANISMS OF COMPLEXES FORMED WITH GLYOXAL SOLUTIONS USING QUANTUM CHEMICAL CALCULATIONS

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Abstract. In this work, interactions of glyoxal in ethyl alcohol, water and dimethylsulfoxide (DMSO) complexes and their spectral manifestations were studied using *ab-initio* calculations. The molecular forces, bond structure and interactions present in the molecule were analyzed. When complex formation energies are calculated, this energy increases as the number of molecules increases. Mulliken charge distributions were also analyzed through the optimal geometry of the molecules. Calculations showed that the complexes are formed through atoms in the C=O and C-H groups of glyoxal. It was shown that the charge distribution in the atoms of this group changed a lot and that complexes were formed through hydrogen bonds in the form of C=O...H and C-H...O. It was also observed that the C=O stretching vibrational bands of glyoxal were shifted to a lower frequency in the complexes formed with ethanol/water/DMSO. Frontier molecular orbitals such as Highest occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO) of glyoxal molecule were analyzed.

Keywords: Raman, ab-initio calculations, hydrogen bond, ethanol, DMSO, water, Mulleken charge distribution, HOMO, LUMO.

Glioksalning eritmalar bilan hosil qilgan kompleslarining shakllanish mexanizmlarini noemperik hisoblash yordamida o‘rganish

Annotatsiya. Ushbu ishda biologik faol glyoxalning etil spirt, suv va dimetilsulfoksid (DMSO) komplekslaridagi o‘zaro ta’sirlar va ularning spektral namoyon bo‘lishi noemperik hisoblashlar yordamida o‘rganildi. Molekulada mavjud bo'lgan molekulyar kuchlar, bog'lanish tuzilishi va o'zaro ta'sirlar tahlil qilindi. Kompleks hosil bo‘lish energiyalari hisoblanganda, molekulalar soni ortishi bilan bu energiya ortib boradi lekin, har bir bog‘lanishga to‘g‘ri keluvchi o‘rtacha vodorod bog‘lanish energiyasi o‘zgarmaydi. Molekulalarning optimal geometriyasi orqali Mulliken zaryad taqsimotlari ham tahlil qilindi. Hisoblashlar shuni ko‘rsatdiki, komplekslar glyoxalning C=O va C-H guruhlaridagi atomlar orqali yuzaga kelib, zaryad taqsimoti aynan shu gruppa atomlarida ko‘p o‘zgarganligi hamda C=O…H, C-H…O ko‘rinishdagi vodorod bog‘lanishlar orqali komplekslar hosil bo‘lishi ko‘rsatib o‘tildi. Shuningdek, glyoxalning C=O valent tebranish polosalari (ethanol/suv/DMSO/) bilan hosil qilgan komplekslarida past chastota tomonga siljiganligi kuzatildi. **Glyoxal molekulasining** Highest occupied molecular orbital (HOMO) va Lowest unoccupied molecular orbital (LUMO) kabi chegaraviy molekulyar orbitallari tahlil qilindi.

Kalit so‘zlar: Raman, ab initio calculations, hydrogen,

diagram, ethanol, DMSO, suv, Mulleken charge distribution, HOMO, LUMO.

Изучение механизмов образования комплексов с растворами глиоксаля с помощью квантово-химических расчетов

Аннотация. В этой работе были изучены взаимодействия глиоксаля в комплексах этиловом спирте, воде и диметилсульфоксиде (ДМСО) и их спектральные проявления с использованием ab-initio расчетов. Были проанализированы молекулярные силы, структура связей и взаимодействия, присутствующие в молекуле. При расчете энергий образования комплексов эта энергия увеличивается с увеличением числа молекул. Распределения заряда Малликена также были проанализированы через оптимальную геометрию молекул. Расчеты показали, что комплексы образуются через атомы в группах C=O и C-H глиоксаля. Было показано, что распределение заряда в атомах этой группы сильно изменилось, и что комплексы образуются через водородные связи в виде C=O...H и C-H...O.Было также замечено, что полосы валентных колебаний C=O глиоксаля были смещены в сторону более низкой частоты в комплексах, образованных с этанолом/водой/ДМСО. Были проанализированы пограничные молекулярные орбитали, такие как высшая занятая молекулярная орбиталь (HOMO) и низшая свободная молекулярная орбиталь (LUMO) молекулы глиоксаля. Ключевые слова: Рамановское рассеяние, ab-initio расчеты, водородная связь, этанол, ДМСО, вода, распределение заряда по Мюллекену, HOMO, LUMO.

Ключевые слова: комбинационное рассеяние света, расчеты ab-initio, водородная связь, этанол, ДМСО, вода, распределение заряда по Малликену, HOMO, LUMO.

1. Introduction. Hydrogen bonding is one of the most important modern research methods in chemistry, biochemistry, biophysics and other sciences, as it is of fundamental importance in protein and DNA binding [1-3]. In fact, hydrogen bonding (HB) is important in the study of microscopic systems in molecular and supramolecular systems such as water or alcohol systems, organic compounds in solution, polymers and proteins [4-7].

Ketones from organic substances are of great interest in the study of hydrogen-bonded complexes in various molecular systems [8-11]. Until now, HB has been widely studied by various experimental and theoretical methods [12-18]. However, due to the very short lifetime of the excited state electron, little information is obtained about hydrogen bonding [19]. Exact theoretical calculations of electronic excited states in complex hydrogen-bonded systems contributed to the difficulty of implementation and lack of knowledge [20-22]. However, photoexcitation can cause changes in hydrogen bonding; such an excited electronic state is called hydrogen bonding dynamics [23-26]. Zhao et al. showed that intermolecular HBs formed between carbonyl chromophores and polar protic solvents can be significantly strengthened in the electronic excited states of carbonyl chromophores. In addition, it has been observed that some nonradiative deactivation processes of photoexcited carbonyl-chromophores can be strongly assisted by the enhancement of intermolecular HB in the excited state [27, 28].

Various experimental and theoretical methods have been developed to better understand the dynamics of hydrogen bonding in excited states for electrons of various molecules in solution [23-26]. The study of water complexes with organic and inorganic compounds is of particular interest. Water is

considered the most common chemical compound on earth and plays an important role in the maintenance of living organisms. When studying biologically active compounds, it is very important to know the process of their interaction with water. Previous spectroscopic studies focused on infrared (IR) spectroscopy of glyoxal oligomers in aqueous solutions [29, 30], in this case, determining the spectral properties of glyoxal is complicated by the addition of specific vibrational frequencies of water, which is a strong absorber in the IR. Due to the low Raman activity of water, Raman spectroscopy can be well suited for investigating the equilibrium in aqueous solutions of glyoxal. The measured concentration of glyoxal in the solution exceeds the concentration predicted by Henry's law [31; 32]. Discrepancy may be partially due to the presence of water, as glyoxal forms hydrated species in solution, making glyoxal more soluble than expected [31]. In addition, water may play an important role in the formation of amorphous solids, where increased HB and increased viscosity reduce crystallization [33]. Understanding the equilibrium of aldehydes, ketones, and other organic compounds with water is important for evaluating the chemical and physical properties of atmospheric aerosol [34; 35]. Small monocarboxylic acids that can form two strong HBs are good compounds for studying complexes between water and organic matter. Currently, molecular complexes formed by biologically active substances with water and other organic compounds are being studied by vibrational spectra by many scientists [36-42].

From the review of the above-mentioned literature, it can be seen that the manifestation of the $C_2H_2O_2$ molecule in the vibrational spectra has been poorly studied by experiments and calculations, and there are problems that have not been solved. Pure glyoxal is rarely found in nature, as glyoxal is usually used as a 40% aqueous solution. Spectroscopic study of glyoxal helps to reveal the properties of this complex water. For this reason, we studied glyoxal and its interactions with various proton-donor and proton-acceptor substances using *ab-initio* calculations. Also, the reactivity of the $C_2H_2O_2$ molecule was evaluated using frontier molecular orbital (FMO) analysis.

2. Theoretical methods. Calculations were made for glyoxal ethanol/water/DMSO complexes using the Gaussian 09 program and the DFT method and the 6-311+G(d,p) basis set [43].

3. Results and discussion.

3.1. Computational results for glyoxal complexes. Through *ab-initio* calculations, the formation mechanism of glyoxal monomer and its various types of dimers was carried out in the Gaussian 09 program using the density functional theory (DFT) method on the basis of the B3LYP 6-311++G(d,p) basis set. Figure 1(a) shows the monomer of glyoxal. It can be seen that the monomer has two C=O and C-H functional groups that are actively involved in intermolecular interaction, and it is a symmetrical molecule with zero dipole moment

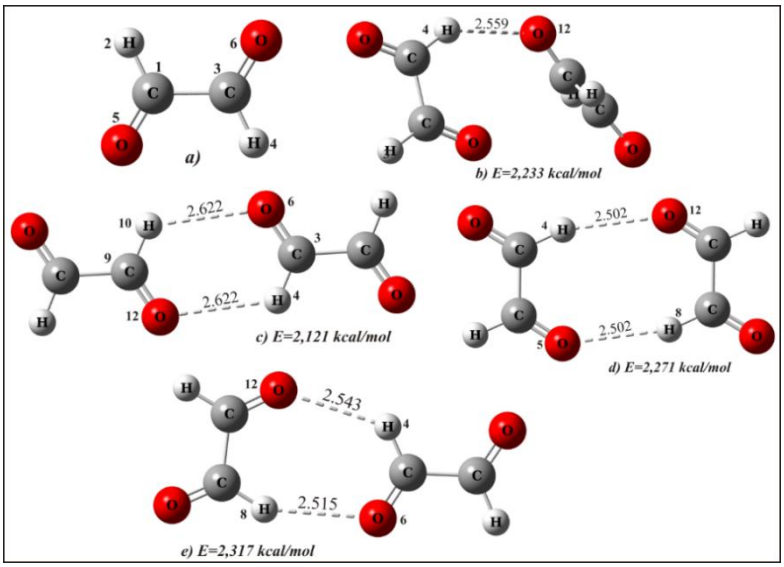


Figure 1. Optimal geometry of glyoxal complexes: a) monomer; b) open dimer; c,d,e) closed dimers.

Figure 1(b) shows the open type dimer of glyoxal. Hydrogen bond lengths are 2.559 Å. Figures 1(c,d,e) show different closed-type dimers of glyoxal [44]. Of the three types of closed dimers, the cyclic closed dimer in Figure 1(e) has the highest energy. The dipole moment of such a dimer is 0.07 D and has changed compared to the state of the monomer, which is related to the symmetry of the molecules. The dimer formation energy is 2.317 kcal/mol, and the complex is formed through two C=O...H hydrogen bonds (bond lengths equal to 2.543 and 2.515 Å). It can be seen from Fig. 1(e) that the energy of the closed dimer is large compared to the rest of the dimers and is energetically stable, therefore, the amount of dimers of this type can be large in the liquid.

3.2. Frontier molecular orbital (FMO) analysis. With the help of theoretical calculations, it is possible to obtain information about the orbitals of a molecule and the transitions between them. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are also called frontier molecular orbitals (FMO). FMO plays an important role in optics, electricity, and quantum chemistry. The energy difference between the HOMO and LUMO is called the "HOMO-LUMO energy gap" and is important for their chemical stability. Also, this energy gap (HOMO-LUMO) is used to display the internal molecular charge transfer (MCT), kinetic polarization, and electronic spectra of a molecule or molecular system [45-46]. Quantum chemical parameters such as global electrophilicity index, hardness, softness, electron affinity and ionization energy can be calculated using Koopmans theorem [48]. Frontier molecular orbitals of glyoxal are shown in Fig. 6. Using HOMO and LUMO energies, various quantum chemical parameters (Table 1) such as ionization energy (IE), chemical potential (μ), hardness (ε), electron affinity (EA), global electrophilicity index (ω) were calculated using the following relations:

- Hardness: $\eta=(E_{HOMO}-E_{LUMO})/2$
- Chemical potential: $\mu=(E_{HOMO}+E_{LUMO})/2$
- Global electrophilic index: $\omega=\mu^2/2\eta$
- Ionization energy: $IE= -E_{HOMO}$
- Electronic affinity: $EA= -E_{LUMO}$

Molecules with a large HOMO-LUMO energy gap are stable and less reactive, while molecules with a low HOMO-LUMO energy gap are reactive. The HOMO-LUMO energy gap of glyoxal is equal to 0.155 eV, which indicates that it is a reactive molecule (Table 1). Table 2 shows the HOMO and LUMO and other orbital energies and the shape of the orbital. The electron molecular orbital becomes full in the HOMO orbital, and the next unfilled orbital becomes the LUMO.

Table 1. Some quantum-chemical parameters of glyoxal

E_{HOMO}	-0.285 eV
E_{LUMO}	-0.130 eV
$E_{HOMO} - E_{LUMO}$	0.155 eV
Hardness	0.077 eV
Chemical potential	-0.207 eV
Global electrophilic index	0.279
$IE= -E_{HOMO}$	0.285 eV
$EA= - E_{LUMO}$	0.130 eV

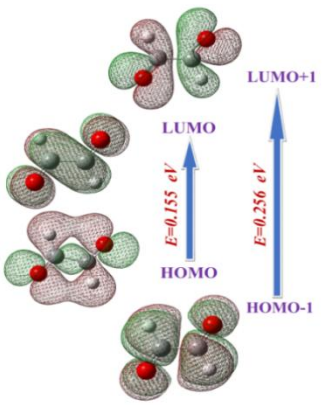
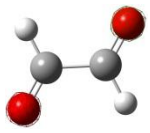
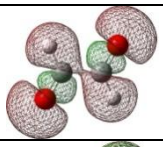
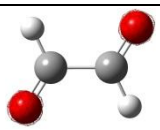
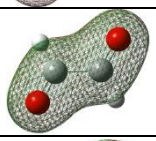
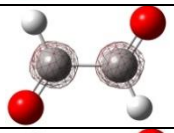
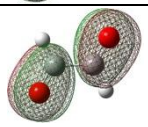
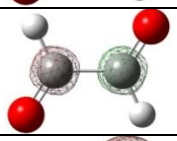
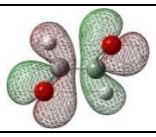
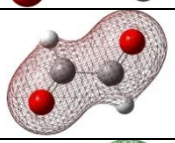
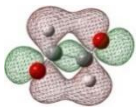
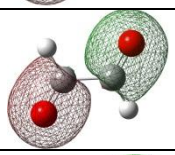
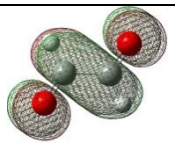
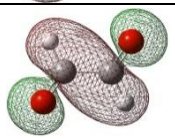
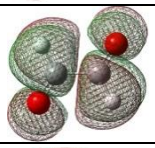
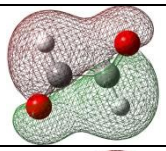
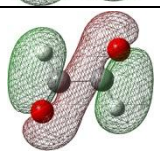
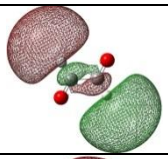
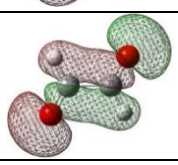
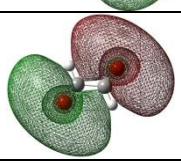


Figure 2. Frontier molecular orbital diagram of glyoxal.

It also determines the threshold of transition of the electron to the excited state and the energy in the orbitals. Glycol has a total of 30 electrons, and these electrons with opposite spin occupy 15 orbitals. The last 15th HOMO has energy of -0.285 eV, and LUMO energy of -0.130 eV, and the difference between them is -0.155 eV, which represents the energy required for an electron to move from the highest filled orbital to the next unfilled orbital. It can be seen from the table that the lowest orbital of glyoxal corresponds to HOMO-14, and the energy corresponding to this state is -19.176 eV and differs from the HOMO energy by 18.891 eV.

Table 2. HOMO, LUMO and other orbital energies and orbital shape of glyoxal.

State	Name of orbital	Energy (ev)	Shape of orbital	State	Name of orbital	Energy (ev)	Shape of orbital
1	HOMO-14	-19.176		11	HOMO-4	-0.475	
2	HOMO-13	-19.169		12	HOMO-3	-0.466	
3	HOMO-12	-10.301		13	HOMO-2	-0.415	
4	HOMO-11	-10.299		14	HOMO-1	-0.346	
5	HOMO-10	-1.109		15	HOMO	-0.285	
6	HOMO-9	-1.096		16	LUMO	-0.130	
7	HOMO-8	-0.723		17	LUMO+1	-0.009	
8	HOMO-7	-0.615		18	LUMO+2	0.001	
9	HOMO-6	-0.517		19	LUMO+3	0.005	
10	HOMO-5	-0.508		20	LUMO+4	0.035	

3.3. The glyoxal and ethanol complexes. Through quantum chemical calculations, the possible bonds of the intermolecular interactions of glyoxal and ethanol of one/two/three/four ethanol

and one glyoxal complexes were calculated. Glycol and Ethanol complexes can form O-H...O=C hydrogen bonds in interaction.

Figure 3 shows the optimal geometry of Glyoxal-ethanol complexes. In Fig. 3(a) it forms closed-type hydrodimer complexes with glyoxal-ethanol. Its dipole moment is 1.7075 D and increased compared to glyoxal monomer. This is because glyoxal and ethanol molecules are not symmetrical with each other. The complex formation energy is 4.457 kcal/mol, through two hydrogen bonds, the first between O^5, H^{15} atoms (bond length 2.112 Å and O-H…C=O) and O^7, H^4 atoms between (bond length 2.353 Å and relatively weak C-H…O form) is formed. Calculations were carried out by increasing the number of ethanol to four. When the number of ethanol increases by two, a cyclic complex with energy is 9.188 kcal/mol formed through four hydrogen bonds (Fig. 3(b)). When the number of ethanol increases by two, a cyclic complex with energy is 9.188 kcal/mol formed through four hydrogen bonds (Fig. 3(b)). Both of these bonds are C=O…H with bond lengths of 2.096 Å.

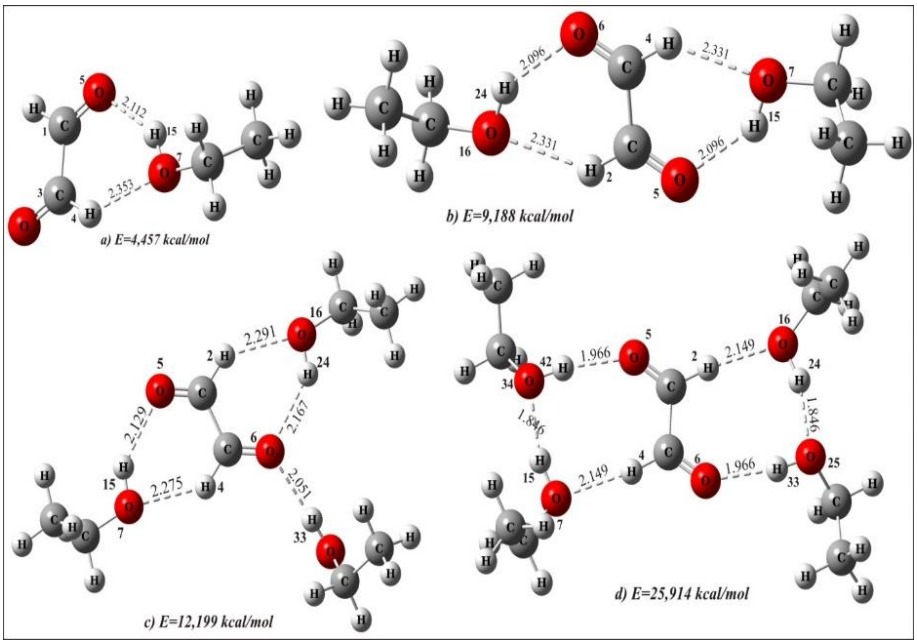


Figure 3. Optimal geometry of glyoxal + ethanol complexes.

The H atoms of the C-H group of glyoxal form a weak hydrogen bond with the O oxygen atoms of ethanol in the form of C-H...O, and the bond lengths are the same 2.331 Å. In the case of a cluster formed by glyoxal with three ethanols (Fig. 3c), the O^6 oxygen atom of the first C=O group of glyoxal participates in H-bonding with two ethanol molecules (bond lengths O^6...H^{24}-2.167 Å, O6... H^{33}-2.051 Å. The O atoms of the second C=O group of glyoxal and the H atoms of the C-H group connect with the third ethanol molecule (O^5...H^{15}-2.129 Å and H^4...O^7-2.275 Å) and form a cluster with an energy of 12.199 kcal/mol. In this case, the C=O vibrational band is shifted down by 18 cm^{-1} compared to the monomer (Fig. 5). In this way, the value of ethanol was increased to four and the calculations were carried out (Fig. 3d), and in the cluster formed by glyoxal + 4 ethanol, the O^5 atom in the first C=O group of glyoxal and the H^4 atom in the C-H group are H- bonded with two ethanol molecules, participates in bonding and bond lengths O^5...H^{42}- .966 Å and H^4...O^7-2.149 Å. The O^6 atom of the second C=O group and the H^2 atoms of the C-H group of glyoxy are connected with the third and fourth ethanol molecules (O^6...H^{33}-1.966 Å and H^2...O^{10}-2.149 Å) with an energy of 25.914 kcal/mol forms a closed structured cluster. As the amount of ethanol increases, the bond energies also increase.

Mulliken atomic charge analysis plays an important role in using quantum chemical calculations to explain the molecular behavior of a system. This is because atomic charges affect a number of molecular properties, including electronic structure, reactivity, dipole moment, polarizability, and vibrational spectrum. Calculating atomic charges involves directly assigning a molecular wave function to the atomic contributions according to some arbitrary, orbital-based scheme

proposed by Mulliken. The Mulliken charge distribution of glyoxal and its association states with ethanol solvent are presented in Table 3.

Table 3: Mulliken charge distribution of glyoxal

Atomic number	Mulliken charge distribution (in electron units)				
	glyoxal (monomer)	glyoxal +1ethanol	glyoxal +2ethanol	glyoxal +3ethanol	glyoxal +4ethanol
C^1	0.068729	0.037013	-0.043703	-0.149529	-0.071001
H^2	0.136984	0.167258	0.291257	0.303047	0.356069
C^3	0.068729	0.005749	-0.044959	0.029492	-0.071674
H^4	0.136984	0.257270	0.291158	0.313598	0.355870
O^5	-0.205713	-0.232993	-0.218666	-0.211171	-0.267568
O^6	-0.205713	-0.200610	-0.218151	-0.252470	-0.267466

In Figure 4, Mulliken charge distributions were also calculated for these complexes. Mulliken's analysis of atomic charge showed that charge exchange between interacting fragments of molecules can affect it. It was found that all hydrogen atoms in glyoxal and glyoxal+$(ethanol)_n$ (n=1,2,3,4) complexes are positively charged, and oxygen atoms are negatively charged. Due to the exchange of charge between hydrogen and oxygen during the formation of the complex, the electron density of C^1 atoms of C=O groups increases dramatically. The charge of the carbon atom in the monomer varies from 0.069e to 0.037e [glyoxal+1 ethanol], -0.044e[glyoxal+2ethanol], -0.149e[glyoxal+3ethanol] and -0.071e[glyoxal +4 ethanol]. Similarly, the charge value of the oxygen atom (O^5) in the monomer is -0.206e to -0.298e, -0.233e [glyoxal +1ethanol], -0.218e [glyoxal +2ethanol], -0.211e [glyoxal +3ethanol] and -0.267e[changes as glyoxal +4ethanol] (Table 1). And that of H^{15} atom in ethanol increased to 0.249e [glyoxal+1ethanol] and 0.374e [glyoxal+4ethanol]. Such changes in charge distribution contribute to the elongation of C=O groups, which leads to changes in frequencies at different solvent concentrations. If we look at the charge of the atoms involved in the interaction for glyoxal + ethanol, the charge value of C^1 and C^3 atoms changed to the opposite charge as the number of bonds increased. The charge modulus of H^2 and O^5 atoms has increased. Figure 4 shows that the charge distribution has changed for the Glyoxal+ethanol complex, and this change is significantly larger for the atoms involved in the interaction.

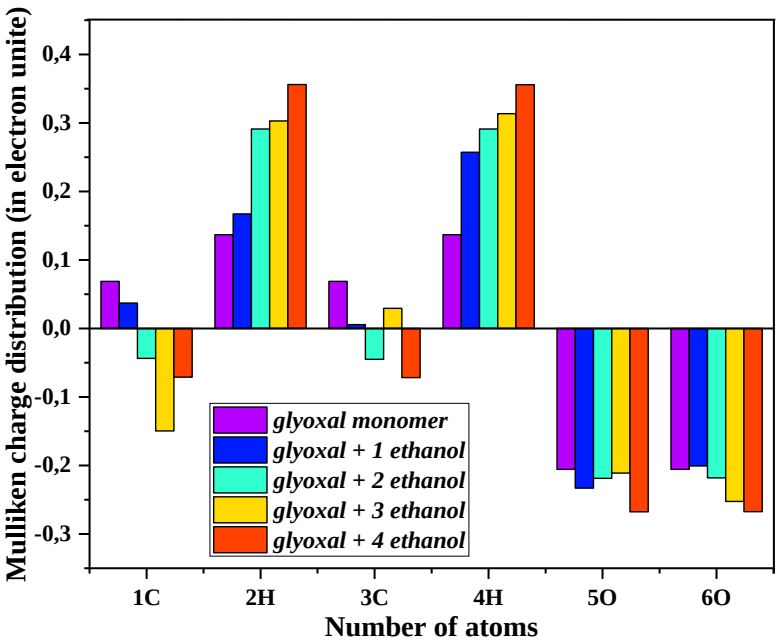


Figure 4. Mulliken charge distribution of glyoxal + ethanol complexes.

Figure 5 shows the Raman spectrum of C=O stretching vibrations for glyoxal and its complex with ethanol. In Fig. 5(b), for the glyoxal+1 ethanol dimer, this vibration corresponds to 1792 cm^{-1} and is shifted to a lower frequency by 9 cm^{-1} compared to the monomer. Figure 5(c) shows the Raman spectrum of the C=O stretching vibrational bands of the glyoxal+2ethanol complex. This band corresponds to 1785 cm^{-1} and is shifted to a lower frequency by 16 cm^{-1} compared to the monomer.

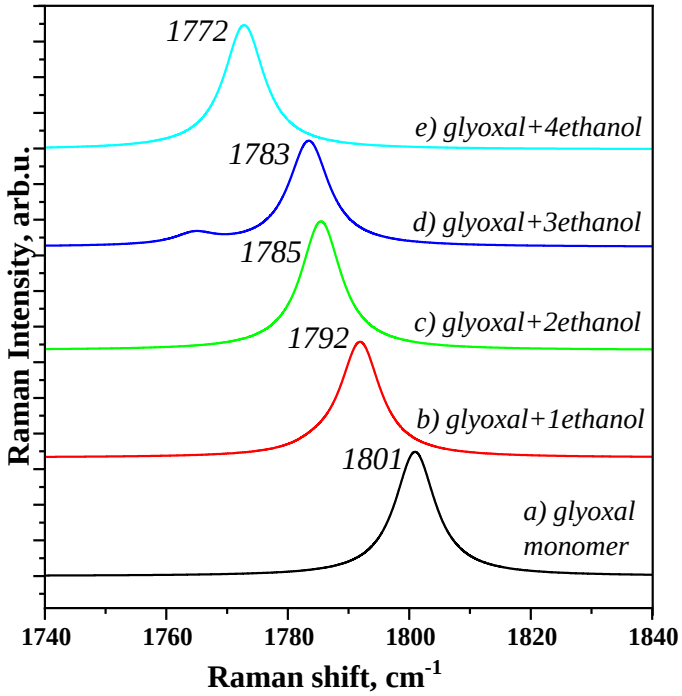


Figure 5. Raman spectra of the C=O stretching vibration band for glyoxal + ethanol complexes obtained in the calculations.

In the glyoxal+4 ethanol complex, this vibrational band is 1772 cm^{-1} and shifted to a lower frequency of 29 cm^{-1} compared to the monomer. So, as the number of ethanol molecules in the glyoxal+ethanol complex increases, the vibration frequencies of C=O decrease and shift to a lower frequency. This corresponds to the shift of the stretching vibration bands in the hydrogen bond theory to the low frequency side. Such a change in the band maxima can be estimated as follows:

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

According to the formula, the frequency is inversely proportional to the square root of the mass, therefore, the increase in the number (mass) of the atoms participating in the hydrogen bond and the redistribution of the charges of the atoms of the molecule leads to a shift in the maxima of the spectral lines.

3.4. Calculation results for glyoxal + water complexes. The interaction between glyoxal complexes with proton donor and proton acceptor water molecules was calculated using *ab-initio* calculations.

Figure 6(a) shows the dimer formed by (Glyoxal+(H_2O)) with a water molecule. In dimer formation, H-bonding between O5 atom of glyoxal and H^9 atoms of water molecule (bond length 2.068 Å) and O^7 atom of water molecule with H^4 atom of C-H group of glyoxal (bond length 2.374 Å) due to H-bonding, a dimer with a closed structure is formed. Dimer formation energy is 4.739 kcal/mol, dipole moment is 1.823 D. The 1792 cm^{-1} band corresponds to the vibration of C=O bound in the dimer and is shifted down by 9 cm^{-1} compared to the monomer (Fig. 6b).

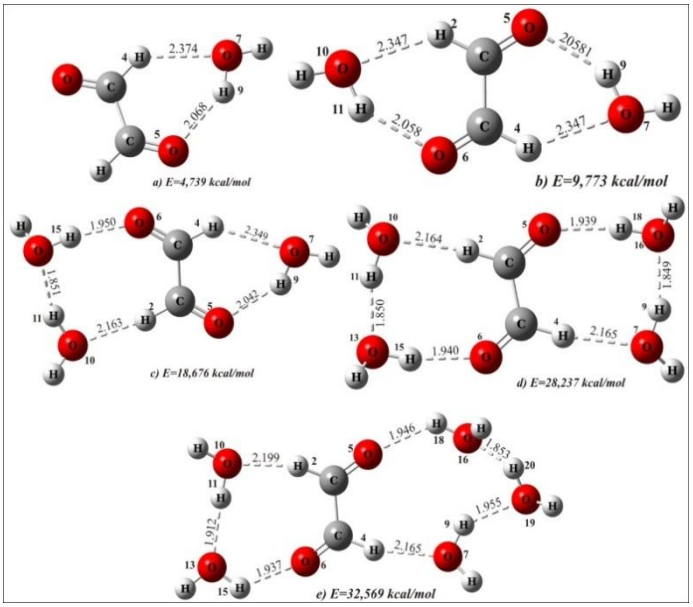


Figure 6. Optimal geometry of complexes formed by glyoxal with water molecules.

Figure 6(b) shows molecular clusters of Glyoxal+$(H_2O)_2$, where the H-bond between the O^5 atom of glyoxal and H^9 atoms of the water molecule is 2.581 Å, and the O^7 atom of the water molecule is 2.581 Å. H^4 is connected to a hydrogen atom by an H-bond with a bond length of 2.347 Å. The O^6 oxygen atom of the second C=O group of glyoxal forms a bond with the H^{11} atom of the water molecule with a bond length of 2.058 Å, and the O^{10} atom of the water molecule forms a bond with the H^2 atom of glyoxal with a bond length of 2.347 Å, and due to hydrogen bonding with two water molecules of glyoxal, a closed structure trimer is formed. The bound C=O vibrational maximum in the trimer corresponds to 1786 cm^{-1} and is shifted down by 15 cm^{-1} relative to the monomer (Fig. 12c). In the clustered state of glyoxal+$(H_2O)_3$ (Fig. 10c), the O^5 atom of the first C=O group of glyoxal participates in H-bonding with one water molecule (bond lengths O^5...H^9-2.042 Å, O^7...H^4 -2.349 Å). The O^6 atom of the second C=O group and the H^2 atom of the C-H group of glyoxy are connected with the second and third water molecules (O^6...H^{15}-1.950 Å and H^2...O^{10}-2.163 Å) and have a closed structure with an energy of 18.676 kcal/mol form a cluster. In the cluster formed by Glyoxal+$(H_2O)_4$ in Figure 6(d), the O^5 oxygen atom of the first C=O group of glyoxal and the H^4 hydrogen atom of the C-H group participate in H-bonding with two water molecules, and the bond lengths are O^5...H^{18} - 1.939 Å, H4...O7-2.165 Å. The O^6 atom of the second C=O group and the H^2 atoms of the C-H group of glyoxy are connected with the third and fourth water molecules (O^6...H^{15}-1.940 Å and H^2...O^{10}-2.164 Å) and the energy was 28.237 kcal/mol forms a closed structured cluster. In this case, the C=O vibrational band is shifted down by 27 cm^{-1} relative to the monomer (Fig. 8e). When we look at the clusters formed by glyoxal with 5 water molecules, glyoxal binds up to four water molecules, while the fifth and subsequent water molecules continue to form a chain bond with water molecules without participating in binding to the glyoxal molecule. It was also observed that oxygen atoms O^5 and O^6 of both C=O groups of glyoxal participate in H-bonding with two water molecules, and hydrogen atoms H^2 and H^4 of the C-H group participate in H-bonding with a water molecule. The cluster formation energy is 32.569 kcal/mol (Fig. 6e). From here, it can be said that glyoxal molecule participates in intermolecular interaction with water molecules, and as the amount of water molecules increases, the energy of complex formation increases, which means that the complex is stabilized. Mulliken charge distribution of glyoxal and its association states with proton-donor and proton-acceptor solvents are presented in Table 4.

Table 4: Mulliken charge distribution of glyoxal

Atomic number	Mulliken charge distribution (in electron units)				
	glyoxal (monomer)	glyoxal +1water	glyoxal +2water	glyoxal +3water	glyoxal +4water
C^1	0.068729	0.050120	0.001371	-0.039241	-0.004060
H^2	0.136984	0.155340	0.249936	0.299610	0.302211

C^3	0.068729	0.029166	0.001679	0.029858	-0.004455
H^4	0.136984	0.224438	0.250069	0.253270	0.301191
O^5	-0.205713	-0.231368	-0.229956	-0.235486	-0.281132
O^6	-0.205713	-0.207073	-0.230043	-0.269219	-0.280219

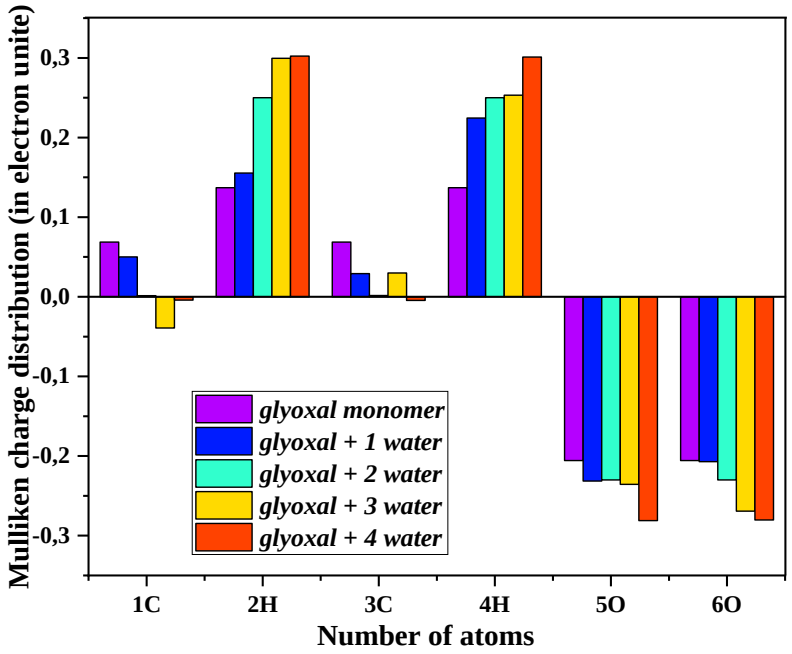


Figure 7. Mulliken charge distribution of glyoxal + water complexes.

It can be seen from Figure 7 that the charge distribution for glyoxal + water complexes has also partially changed, and this change is significantly larger for the atoms involved in the interaction. Also, as the value of water in the complex increased, the charge distribution changed more in the atoms participating in the interaction, as mentioned above. From the calculation results, it can be seen that glyoxal forms hydrogen bonds in the form of C=O...H with water molecules, and due to these bonds, shifts in the bands towards low frequency are observed. Figure 8 shows the calculated Raman scattering spectra of the C=O stretching vibrational bands in the complexes formed by glyoxal with water.

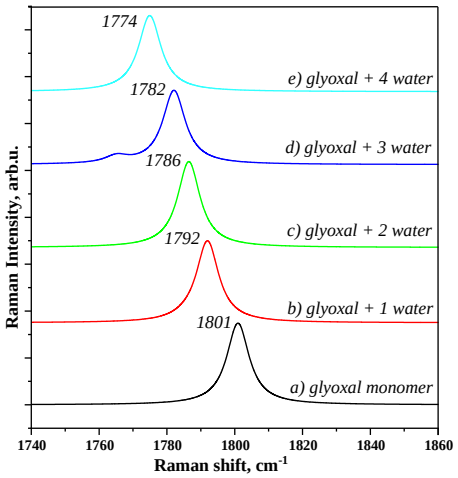


Figure 8. Raman spectra of C=O stretching vibrational bands of glyoxal+water complexes.

3.5. Calculation results for glyoxal + DMSO complexes. Figure 9 shows the optimal geometry of glyoxal+DMSO complexes. Figure 9(a) shows the closed-type hydrodimer of glyoxal+1DMSO. The dipole moment of such a dimer is 4.8715 D. The complex formation energy is 4.876 kcal/mol, and it is connected by two hydrogen bonds. The first of these bonds is between H^2, O^8

atoms (bond length 2.177 Å and C-H…O) and O^5, H^{11} between atoms (bond length 2.608 Å and C=O…H or C-H…O relatively weak) is formed

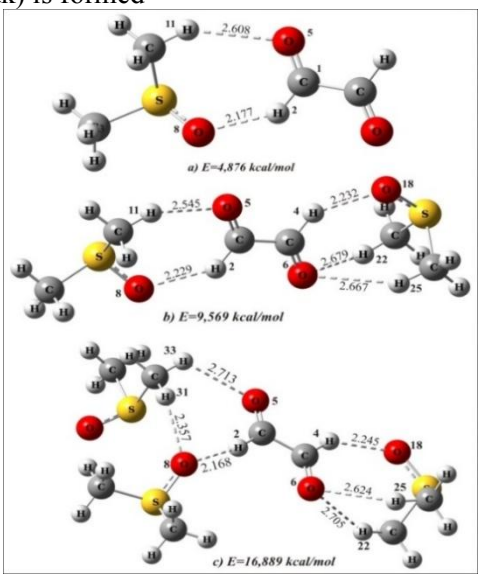


Figure 9. Optimal geometry of glyoxal+DMSO complexes: a) Glyoxal + 1 DMSO, b) Glyoxal + 2 DMSO and c) Glyoxal + 3 DMSO

Figure 9(b) shows the glyoxal + 2DMSO complex. The dipole moment for this complex is 2.1499 D, which is sharply reduced compared to the dimer state, and the energy of complex formation is 9.569 kcal/mol, and it is connected by five hydrogen bonds. Three of the hydrogen bonds are weak hydrogen bonds of the form C=O…H, with bond lengths of 2.545 Å (C^1=O^5…H^{11}), 2.679 Å (C^3=O^6…H^{22}), and 2.667 Å (C^3=O^6…H^{25}). Our fourth and fifth hydrogen bonds are C-H…O hydrogen bonds with hydrogen bond lengths of 2.229 Å (C^1-H^2…O^8) and 2.232 Å (C^3-H^4…O^{18}). For glyoxal + DMSO, the charges of the atoms involved in the interaction also change. The dipole moment of this complex is 4.7364 D, which is increased compared to the glyoxal+2DMSO complex. This means that the symmetry of the molecule has partially changed. The complex formation energy is 16.889 kcal/mol, and it is connected by six hydrogen bonds. Three of these hydrogen bonds are weak hydrogen bonds of the form C=O…H, with bond lengths of 2.713 Å (C^1=O^5…H^{11}), 2.705 Å (C^3=O^6…H^{22}), and 2.624 Å (C^3=O^6…H^{25}), respectively. The fourth and fifth hydrogen bonds are C-H...O hydrogen bonds with hydrogen bond lengths of 2.168 Å (C^1-H^2...O^8) and 2.245 Å (C^3-H^4...O^{18}). Sixth hydrogen bonds were observed between two DMSOs with a bond length of 2.357 Å (S^7-O^8…H^{31}) (Fig. 9c).

Mulliken charge distribution of glyoxal and its association with DMSO (Table 5).

Table 5: Mulliken charge distribution of glyoxal

Atomic number	Mulliken charge distribution (in electron units)			
	glyoxal (monomer)	glyoxal +1DMSO	glyoxal +2DMSO	glyoxal +3DMSO
C^1	0.068729	0.095422	-0.025114	-0.147650
H^2	0.136984	0.257126	0.251370	0.274544
C^3	0.068729	-0.045518	-0.107915	0.042773
H^4	0.136984	0.125889	0.263782	0.282871
O^5	-0.205713	-0.246738	-0.241527	-0.208626
O^6	-0.205713	-0.209273	-0.227507	-0.238306

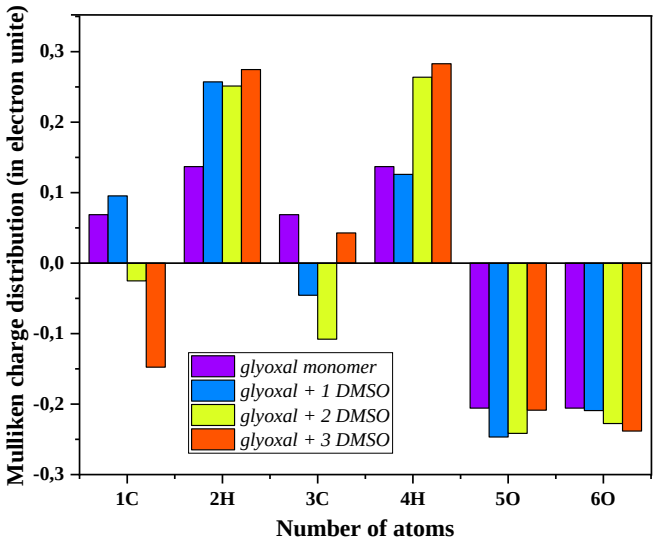


Figure 10. Mulliken charge distribution of glyoxal+DMSO complexes.

If we look at the charge of carbon atoms in glyoxal of glyoxal + DMSO complexes, we can see that the modulus of charge values of C^2 and C^3 atoms has changed dramatically (Fig. 10). If we look at the charge of the atoms involved in the interaction, the modulus of the charge values of O^6 and H^2 atoms has increased. The charge modulus of the O^5 atom first increased and decreased as the amount of DMSO increased. It can be seen from Figure 10 that the charge distribution has changed for the glyoxal + DMSO complex, and this change is significantly larger for the atoms involved in the interaction.

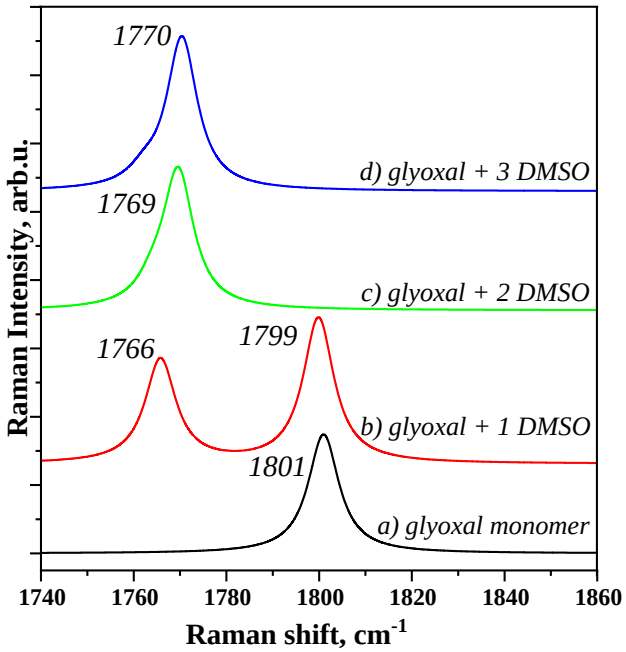


Figure 11. Raman spectra of C=O stretching vibration band for glyoxal + DMSO complexes.

Figure 11 shows the Raman spectrum of C=O stretching vibrations for glyoxal and its complex with DMSO. In Fig. 11(b), for the glyoxal+1DMSO dimer, these vibrations correspond to the 1766 and 1799 cm^{-1} spectral bands and are shifted by 35 cm^{-1} relative to the monomer. In Fig. 11(c), the spectral band at 1769 cm^{-1} corresponds to the C=O stretching vibration for the glyoxal+2DMSO complex and is shifted by 32 cm^{-1} relative to the monomer.

Conclusions. Formation mechanisms of isolated dimers of glyoxal and its molecular complexes with proton-donor and proton-acceptor molecules (ethanol/water/DMSO) were determined by density functional theory (DFT) method and B3LYP/6-311++G(d, p). The interaction forces, bond structure and interactions present in the molecule are explained. Computational analysis suggests that

cyclically closed dimers are energetically stable. When the Mulliken charge distributions are depicted graphically, the charges of the C-H, C=O group and C atoms participating in the interaction of glyoxal are greatly changed. Glyoxal complexes are formed as form C=O...H (strong) and C-H...O (weak). Complex formation energies increase with the number of molecules, and the average hydrogen bond energy corresponding to each bond does not changed. C=O stretching vibration bands in glyoxal+ethanol/water/DMSO complexes shift to low frequency as the number of molecules increases, which confirms the presence of intermolecular H-bonding. Glycol has a total of 30 electrons, and these electrons with opposite spin occupy 15 orbitals. The last 15 orbitals have HOMO energy of -0.285 eV and LUMO energy of -0.130 eV, and the difference between them is -0.155 eV.

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