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## DFT STUDY OF 1-VINYL- AND 1-(1,2-DICHLOROETHYL)CYANURIC ACID DERIVATIVES

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## DFT STUDY OF 1-VINYL- AND 1-(1,2-DICHLOROETHYL)CYANURIC ACID DERIVATIVES

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Based on the industrial interest in cyanuric acid derivatives, the aim of the study is to perform a theoretical analysis of cyanuric acid trivinyl esters (2a-4a) and trivinyl cyanurate (2b-4b) using the DFT/defs-TZVP method. The frontier MO analysis, electrostatic potential and analysis of non-covalent interactions in these molecules have been used for consideration of electronic structures of all the compounds. The replacement of H atoms on hydroxyl and imino-groups by a vinyl group of cyanuric acid or its tri-keto form leads to a decrease the n-type MO (subsequently increasing  $\pi$ -type MO) of the starting compounds and the HOMO becomes a  $\pi$ -type MO. However, the introducing of a dichloroethyl group to NH group of the tri-keto form led to enhancing of contribution of unbound electron pairs of chlorine atoms in the HOMO, and the HOMO becomes an n-type MO. The results of the ESP analysis showed the formation of positive  $\pi$ -hole potentials in the case of tri-keto derivatives. The presence of strong attractive and repulsive forces and also weak interactions in the case of tri-vinyl and tri-1,2-dichloroethyl derivatives of tri-keto form have been shown by NCI and RDG plots of investigated compounds. The presence of strong attractive and repulsive forces and also weak interactions in the case of tri-vinyl and tri-1,2-dichloroethyl derivatives of tri-keto form have been shown by NCI and RDG plots of investigated compounds.

**Keywords:** cyanuric acid, electronic structure, DFT, FMO, electrostatic potential, non-covalent interactions

## ИССЛЕДОВАНИЕ DFT ПРОИЗВОДНЫХ 1-ВИНИЛ- И 1-(1,2-ДИХЛОРЭТИЛ)ЦИАНУРОВОЙ КИСЛОТЫ

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Основываясь на промышленном интересе к производным циануровой кислоте, целью исследования является осуществление с помощью метода DFT/defs-TZVP теоретического анализа тривиниловых эфиров циануровой кислоты (2a-4a) и тривинилцианурата (2b-4b). Для рассмотрения электронной структуры соединений использованы граничный анализ MO, электростатический потенциал и анализ нековалентных взаимодействий в этих молекулах. Замена атомов H на гидроксильных и иминогруппах на винильную группу циануровой кислоты или ее трикетотормы приводит к уменьшению MO n-типа (впоследствии увеличению MO  $\pi$ -типа) исходных соединений и HOMO становится MO  $\pi$ -типа. Однако введение дихлорэтильной группы в группу NH трикетотормы приводит к увеличению вклада несвязанных электронных пар атомов хлора в HOMO, и HOMO становится MO n-типа. Результаты анализа ESP показали образование положительных потенциалов  $\pi$ -дырок в случае трикетоторм производных. Наличие сильных сил притяжения и отталкивания, а также слабых взаимодействий в случае тривиниловых и три-1,2-дихлорэтилпроизводных трикетотормы показано графиками NCI и RDG исследуемых соединений. Наличие сильных сил притяжения и отталкивания, а также слабых взаимодействий в случае тривиниловых и три-1,2-дихлорэтилпроизводных трикетотормы показано графиками NCI и RDG исследуемых соединений.

**Ключевые слова:** циануровая кислота, электронное строение, ТФП, ФМО, электростатический потенциал, нековалентные взаимодействия

## 1-VINIL VA 1-(1,2-DIXLORETEL)SIYANUR KISLOTA HOSILALARINI DFT ASOSIDA O'RGANISH

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Sianurik kislota hosilalariga sanoat qiziqishidan kelib chiqqan holda, tadqiqotning maqsadi DFT/defs-TZVP usuli yordamida siyanurik kislota trivinil esterlari (2a-4a) va trivinil siyanurat (2b-4b) ning nazariy tahlilini o'tkazishdir. Barcha birikmalarning elektron tuzilishini ko'rib chiqish uchun MO elektrostatik potentsial tahlili va ushbu molekulardagi kovalent bo'lmagan o'zaro ta'sirlarni tahlil qilishda foydalanilgan. Gidroksil va imino guruhlaridagi H atomlarini siyanur kislotaning vinil guruhi yoki uning triketo shakli bilan almashirish boshlang'ich birikmalar va HOMO ning n-turi MO ning pasayishiga (keyinchalik p-tipli MO ning oshishi) olib keladi. p-tipli MO ga aylanadi. Biroq, triketo shaklining NH guruhiga dikloroetil guruhining kiritilishi xlor atomlarining bog'lanmagan elektron juftlarining HOMO ga ta'sirini oshirishga olib keladi va HOMO n-tipli MO ga aylanadi. ESP tahlilining natijalariga asosan triketo hosilalari holatida ijobiy p-bog' potentsiallarining shakllanishini ko'rsatdi. Triketo shaklining trivinil va tri-1,2-dikloroetil hosilalari holatida kuchli va itaruvchi kuchlarning mavjudligi, shuningdek zaif o'zaro ta'sirlar o'rganilgan birikmalarning NCI va RDG chizmalarida ko'rsatilgan. Triketo shaklining trivinil va tri-1,2-dikloroetil hosilalari holatida kuchli jozibali va itaruvchi kuchlarning mavjudligi, shuningdek zaif o'zaro ta'sirlar o'rganilgan birikmalarning NCI va RDG chizmalarida ko'rsatilgan.

**Kalit so'zlar:** siyanur kislota, elektron struktura, TFP, PMO, elektrostatik potentsial, kovalent bo'lmagan o'zaro ta'sirlar

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### Introduction

Cyanuric acid (CA, 1,3,5-triazine-2,4,6-triol) is being a heterocyclic compound can exists in tri-enol (**1a**, fig.1) and tri-keto (**1b**, 1,3,5-triazinane-2,4,6-trione) tautomeric forms [1]. There-

fore, these tautomeric forms and proton transfer between them have been studied by different DFT methods [1-3]. Moreover, supramolecular complex formation abilities of tri-keto form of CA by hydrogen bonds have also been studied by using series of

DFT methods [4, 5]. A slightly aromatic character of CA was determined by Pérez-Manríquez and co-workers [6] through theoretical studies by means of DFT/6-31G(d,p) method. CA have wide application in chemistry and industry by its unique properties and water solubility. As an instance, it is used in chemical synthesis as an intermediate compound for obtaining epoxy resins, chlorinated derivatives, detergents, antioxidants, dyes, pesticides, and antitumour agents [7]. Furthermore, the triallyl and tris(2-hydroxyethyl) derivatives of CA are used as a crosslinking agent in the production of polymeric materials [8-10]. Based on the industrial interest in cyanuric acid derivatives, the aim of the study is to perform a theoretical analysis of cyanuric acid trivinyl esters (2a-4a) and trivinyl cyanurate (2b-4b) using the DFT/def2-TZVP method.

### Materials and methods

The geometries of studied **1a-7a** and **1b-7b** (scheme) compounds have been built using Avogadro program package [11]. Then obtained geometries are fully optimized by B3LYP/def2-TZVP method. The difference in enthalpy of formation ( $\Delta H_f$ ) for all the compounds, Gibbs free energy ( $\Delta G$ ) and entropy ( $\Delta S$ ) of the corresponding pairs (**1a-1b**, **2a-2b**, **3a-3b**, **4a-4b**, **5a-5b**, **6a-6b** and **7a-7b**) are determined by FTIR calculations. The absence of imaginary frequencies has been checked in frequency calculations. ORCA 5.0 program package is used for all calculations [12, 13]. Electrostatic potential surface analyses of all compounds have

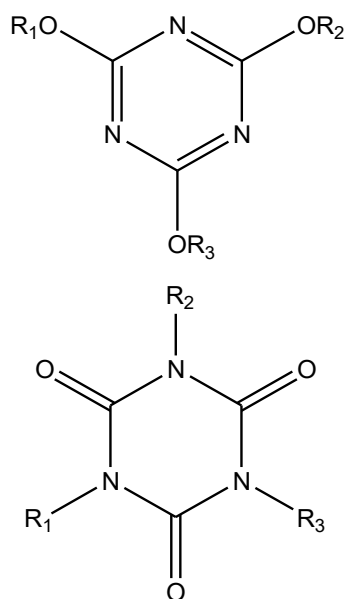
been performed by Multiwfn program package [14] using calculation results file of ORCA program package. ESP surface is visualized by the application of VMD program package [15].

### Results and discussion

CA and its derivatives were the object of theoretical research due to the presence of tautomeric forms and it has been predicted a stability of keto tautomeric form [4, 5]. In present study, gas phase enthalpy differences ( $\Delta H_f = \Delta H_f(a) - \Delta H_f(b)$ ) show relative stability of **1b-7b** tautomeric forms comparing to **1a-7a** (Table 1). In addition, using the equation  $\Delta G = RT \ln K_{eq}$ , the percentage of tautomeric forms in vacuum was estimated (Table 1). It is known that the presence of compounds in one tautomeric form or another and conversion between them depends on the type of solvents, pH of the medium etc. Perhaps conversion between **2a-7a** and **2b-7b** are impossible. However, during the reaction, the corresponding **a** (**2a-7a**) and **b** (**2b-7b**) products can be formed simultaneously.

The goal of the current work is to study the electronic structure of both tautomer forms and the corresponding structures using some quantum-chemical parameters. Therefore, below we consider the quantum-chemical parameters calculated using B3LYP / def2-TZVP for all **1a-7a** and **1b-7b**.

By the parameters of the electronic structure, it can be determined the reaction centers of the molecule, along which the molecule engaged into intermolecular interaction. The main parameters of the electronic structure are the frontier orbitals' energy and their electron density [16-18]. According to the HOMO-LUMO concept [16-18],



- 1a.  $R_1, R_2, R_3 = H$ ;  
 2a.  $R_1 = -CHCH_2, R_2, R_3 = H$ ;  
 3a.  $R_1, R_2 = -CHCH_2, R_3 = H$ ;  
 4a.  $R_1, R_2, R_3 = -CHCH_2$ ;  
 5a.  $R_1 = -CHClCH_2Cl, R_2, R_3 = H$ ;  
 6a.  $R_1, R_2 = -CHClCH_2Cl, R_3 = H$ ;  
 7a.  $R_1, R_2, R_3 = -CHClCH_2Cl$
- 1b.  $R_1, R_2, R_3 = H$ ;  
 2b.  $R_1 = -CHCH_2, R_2, R_3 = H$ ;  
 3b.  $R_1, R_2 = -CHCH_2, R_3 = H$ ;  
 4b.  $R_1, R_2, R_3 = -CHCH_2$ ;  
 5b.  $R_1 = -CHClCH_2Cl, R_2, R_3 = H$ ;  
 6b.  $R_1, R_2 = -CHClCH_2Cl, R_3 = H$ ;  
 7b.  $R_1, R_2, R_3 = -CHClCH_2Cl$

Structures of studied compounds.

**Table 1**  
**Enthalpy, Gibbs free energy and entropy differences**  
**for a-b pairs**

Pair of com- pounds	$\Delta H_f$ , kcal/ mol	$\Delta G$ , kcal/ mol	$\Delta S$ , kcal/ mol	$K_{eq}$ , % (a)*
1a↔1b	-29.14	0.15	-0.5	49.46
2a↔2b	-34.52	-0.79	0.17	57.90
3a↔3b	-37.82	-0.42	-1.69	54.13
4a↔4b	-40.35	-0.30	-2.66	53.05
5a↔5b	-28.81	-0.64	0.05	56.33
6a↔6b	-27.86	-1.35	0.58	63.10
7a↔7b	-8.85	-2.08	1.05	30.21

\* The equilibrium constant ( $K_{eq}$ , in %) determined through  $\Delta G = RT \ln K_{eq}$

the electron-donating and electron-withdrawing ability of a molecule is associated precisely with the level of HOMO and LUMO in the series of related compounds. The electrophilic center in orbital-controlled reactions goes over to the atom, where the greater contribution of the atom to the HOMO while the nucleophilic center where the greater contribution of the atom to the LUMO [16]. According to Kupmans theorem [16, 19], the HOMO and LUMO energies correlate with ionization potential (I, eV) and electron affinity (A, eV). Besides, the difference between these orbitals (energy gap-  $\Delta E$ ) is an important parameter showing the stability of the molecule in the series of related compounds [16-18]. Additionally, some parameters (table 1) are developed based on the energy of HOMO and LUMO, which are called "global indices" [18]. The HOMO, LUMO energy and other global indices such as the chemical hardness ( $\eta$ ) and softness ( $\sigma$ ), electronegativity ( $\chi$ ),

chemical potential ( $\mu$ ) and electrophilicity index ( $\omega$ ) were calculated and listed in the tables 2 and 3.

As demonstrated in Table 2, the +M effect of oxygen atoms of CA is enhanced in the case of compounds **2a-4a**, which is reflected in the energies of HOMO, LUMO and energy gap. However, a decreasing the HOMO level and simultaneously a decreasing the electron-donating ability of **5a-7a** compounds could be noted. The electron-withdrawing ability of these compounds increases due to a decrease in the level of LUMO. The largest energy gap (higher  $\eta$ ) of **5a-7a** compounds shows high kinetic stability and the lowest reactivity of these compounds. The electrophilicity index of CA (**1a**) is equal to 2.69 eV and smaller than tri-keto form (**1b**, 2.71eV). The introducing of a vinyl group to **1a** or **1b** leads to a slight increase in the  $\omega$  values in the series of **2a-4a/2b-4b**. Furthermore, the introducing of a dichloroethyl group in **1a/1b** significantly decreases/increases the electrophilicity index **5a-7a/5b-7b** compounds (Tab. 2 and 3). It is known that compounds with a large value of  $\omega$  are strong electrophiles (weak nucleophiles), and compounds with a small  $\omega$  value are weak electrophiles (strong nucleophiles) [20, 21].

Notably, that the HOMO of initial two pairs (**1a**, **1b**) is n-type MO with high contribution of N and O atom's lone pair, respectively (Fig.1). When a vinyl group is introduced instead of the H atoms of the OH or NH group, a significant change occurs in the HOMO of **4a** and **4b**, i.e., the n-type MO goes down and the HOMO becomes  $\pi$ -type MO (Fig.1). However, when a dichloroethyl group is introduced, instead of the H atoms of the OH and

**Table 2**  
**Quantum-chemical parameters for 1a-7a compounds**

QCP	1a	2a	3a	4a	5a	6a	7a
$E_{HOMO}$ , eV	-8.16	-7.07	-7.06	-7.07	-11.61	-11.70	-11.80
$E_{LUMO}$ , eV	-0.76	-1.12	-1.23	-1.21	3.37	3.12	2.99
$\Delta E$ , eV	7.40	5.95	5.83	5.86	14.98	14.82	14.79
$I = -E_{HOMO}$ , eV	8.16	7.07	7.06	7.07	11.61	11.70	11.80
$A = -E_{LUMO}$ , eV	0.76	1.12	1.23	1.21	-3.37	-3.12	-2.99
$\chi = (I + A)/2$ , eV	4.46	4.09	4.14	4.14	4.12	4.29	4.40
$\eta = (I - A)/2$ , eV	3.7	2.97	2.91	2.93	7.48	7.41	7.39
$\mu_p = -(I + A)/2$ , eV	-4.46	-4.09	-4.14	-4.14	-4.12	-4.29	-4.40
$\sigma = 1/(2\eta)$ , eV	0.13	0.17	0.17	0.17	0.07	0.07	0.07
$\omega = \mu_p^2/2\eta$ , eV	2.69	2.82	2.94	2.92	1.13	1.24	1.31

Table 3

Quantum-chemical parameters of 1b-7b

QCP	1b	2b	3b	4b	5b	6b	7b
$E_{\text{HOMO}}$ , eV	-8.11	-7.26	-7.13	-7.04	-8.29	-8.37	-8.43
$E_{\text{LUMO}}$ , eV	-0.80	-1.18	-1.22	-1.25	-1.25	-1.41	-1.51
$\Delta E$ , eV	7.31	6.08	5.91	5.79	7.04	6.96	6.92
$I = -E_{\text{HOMO}}$ , eV	8.11	7.26	7.13	7.04	8.29	8.37	8.43
$A = -E_{\text{LUMO}}$ , eV	0.80	1.18	1.22	1.25	1.25	1.41	1.51
$\chi = (I + A)/2$ , eV	4.45	4.22	4.17	4.14	4.77	4.89	4.97
$\eta = (I - A)/2$ , eV	3.65	3.04	2.95	2.89	3.52	3.48	3.46
$\mu_p = -(I + A)/2$ , eV	-4.45	-4.22	-4.17	-4.14	-4.77	-4.89	-4.97
$\sigma = 1/(2\eta)$ , eV	0.14	0.16	0.17	0.17	0.14	0.14	0.14
$\omega = \mu_p^2/2\eta$ , eV	2.71	2.93	2.94	2.96	3.23	3.43	3.57

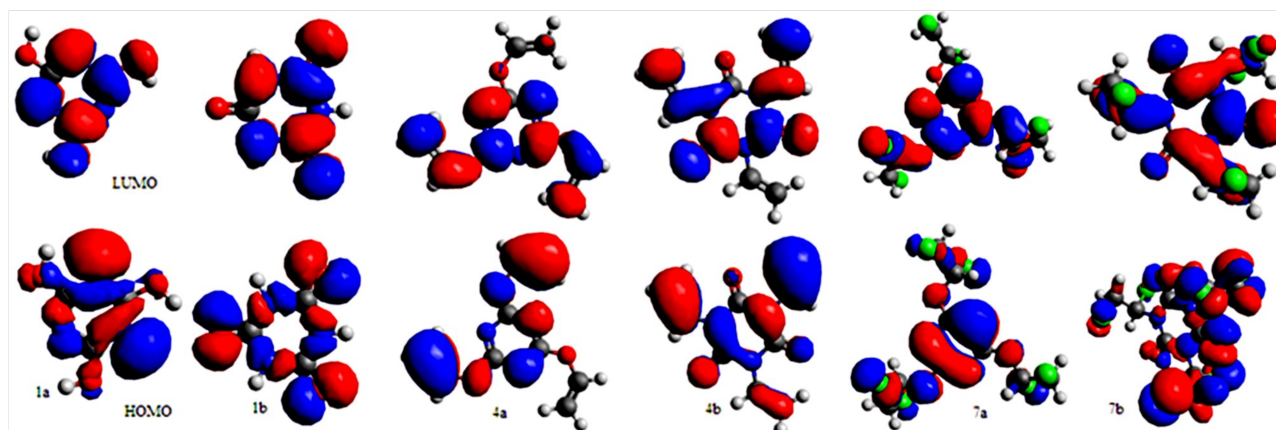


Figure 1. Electron densities on HOMO and LUMO of species 1a/b, 4a/b, and 7a/b.

NH groups, different types of HOMOs are formed. The HOMO of **7a** is a  $\pi$ -type MO, while HOMO of **7b** is an n-type MO with a high contribution of lone pairs of four chlorine (41%) and one oxygen atoms (24%). (Fig. 1). The electrostatic potential (ESP) surface analysis is powerful parameter that describes electron-rich and electron-deficit centers of molecule [22-24]. The ESP surfaces of studied compounds are illustrated in Figure 2 and 3. In the ESP surface, red parts (blue circles and positive numbers) are maxima and they indicate electron-deficit centers, which prone to attack by nucleophiles. Blue parts (red circles and negative numbers) are minima and these centers are rich in electrons. Digits in the figures 2 and 3 show the values of significant centers. For example, five maxima (17.24, 17.24, 50.74, 50.74 and 50.74 kcal/mol) and six minima (23.11, 23.11, 23.11, 25.13 and

25.13 kcal/mol) were determined in the ESP surface of CA (Fig. 2). The largest maximum (50.74 kcal/mol) is located near the H atoms of the OH groups. The other two maxima are located above and below the center of the ring. The lowest minima (-25.13 kcal/mol) are located in vicinities of nitrogen atoms. The next lowest minima (-23.11 kcal/mol) are located near to oxygen atoms. The introductions of a vinyl group instead of H atoms of cyanuric acid are reducing of values electron-rich and electron-deficit centers (Fig. 2). In the ESP surface of **4a**, the maxima (19.58 kcal/mol) are near to  $\alpha$ H atoms of vinyl group. The minima (-19.14 kcal/mol) are located near to N and O atoms (Fig. 2). In the case of **7a**, the ESP surface maxima and minima also reduced relative to **1a**, e.g. the maximum and minimum are equal to 29.76 and -20.53 kcal/mol, respectively.



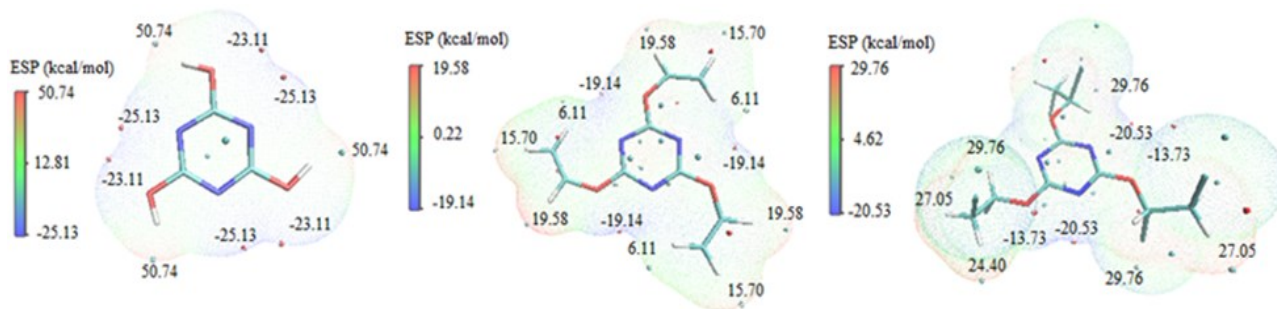


Figure 2. ESP surface maxima and minima for compounds 1a, 4a and 7a.

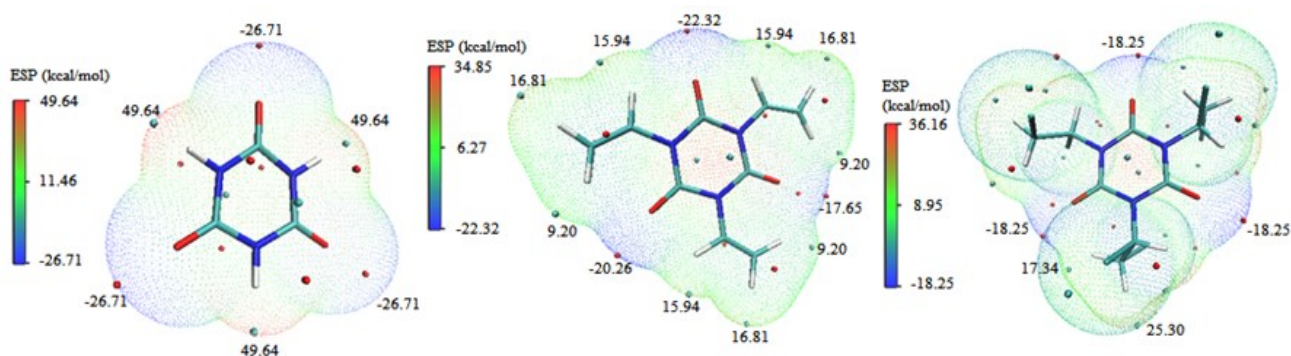


Figure 3. ESP surface maxima and minima for compounds 1b, 4b and 7b.

Very similar ESP surface maxima and minima have been found for tri-keto tautomeric form of cyanuric acid, where minima (-26.71 kcal/mol) are located in vicinity of oxygen atoms and the maxima (49.64) are located near to H atoms of NH group (1b, Fig. 3.). The introductions of a vinyl group instead of H atoms of NH in the case of tri-keto form of cyanuric acid are reducing of values electron-rich and electron-deficit centers in 2b-4b compounds (Fig.3). The largest ESP surface maxima are located above and below the center of the ring in the case of 4b and 7b, which called “positive  $\pi$ -hole potentials” [25]. The ring becomes  $\pi$ -basic

ring due to the less  $\pi$ -electron density above and below the ring of 4b and 7b. The ring could be interacting with negative  $\pi$ -hole potentials [25]. Non-covalent interactions (NCI) play important role in chemistry [24-28]. NCI analysis of 1a, 1b, 4a, 4b, 7a and 7b (Fig. 4) were carried out by Multiwfn program [14] and visualized by VMD program [15]. The reduced density gradients (RDG) versus the electron density multiplied by the sign of the second Hessian eigenvalue [26-28] are given in Figure 5. The nature of specific interactions is highlighted in red-blue-green colors on the color-filled RDG map (Fig. 5). The strong attractive force (H-

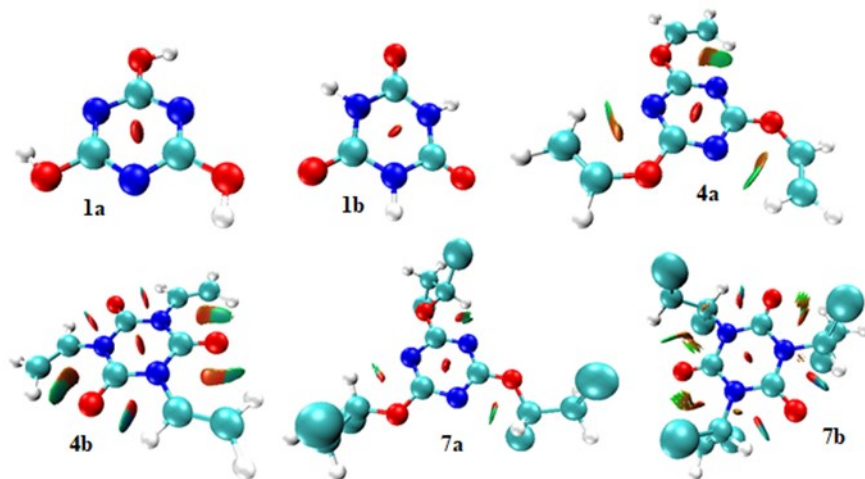


Figure 4. Visualized non-covalent interactions for 1a, 1b, 4a, 4b, 7a and 7b.

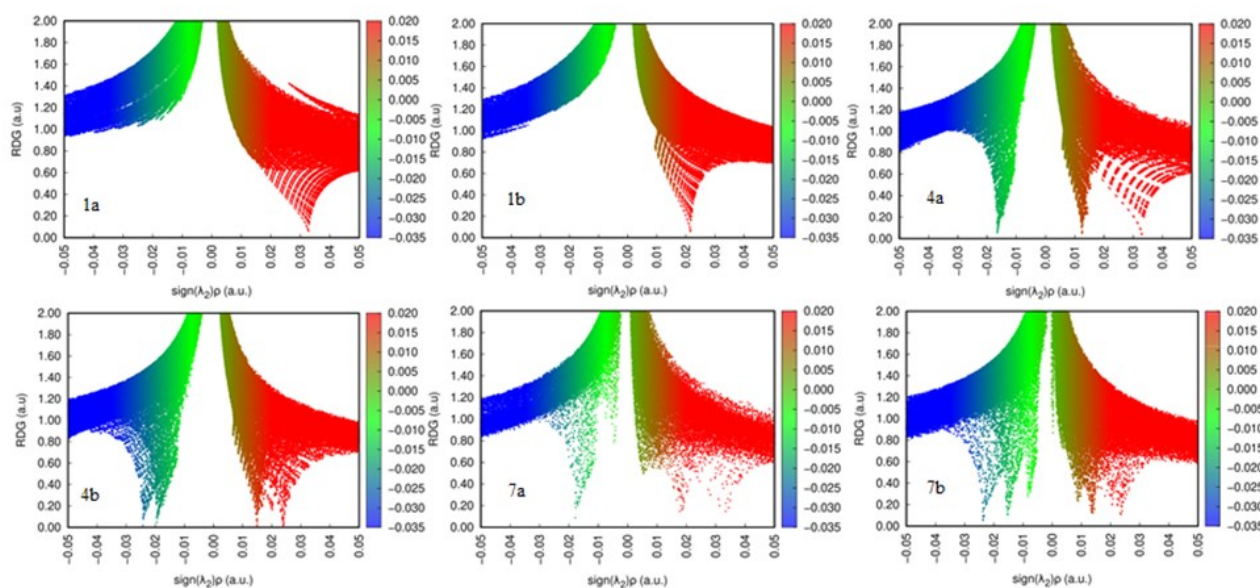


Figure 5. The color-filled RDG map for 1a, 1b, 4a, 4b, 7a and 7b.

bond) is shown in blue and the strong repulsive force (steric effect) is shown in red. Weak interactions (Van der Waals interactions) are highlighted with a green isosurface [26-28]. The presence of a strong steric effect and VdW interactions is evident from the RDG map of compounds **7a/b**.

### Conclusion

The electronic structures of cyanuric acid derivatives are described by the B3LYP/def2-TZVP method. Mono-, di- and tri-vinyl substituted cyanuric acid derivatives as well as trivinylycyanurate and tris(1,2-dichloroethyl) cyanurate have been studied due to the presence of a great interest tri-keto tautomer forms. The frontier MO analysis, electrostatic potential and analysis of non-covalent interactions in these molecules have been used for consideration of

electronic structures of all the compounds. The obtained results indicated that the replacement of H atoms on hydroxyl and imino-groups by a vinyl group of CA or its tri-keto form leads to a decrease the n-type MO (subsequently increasing  $\pi$ -type MO) of the starting compounds and the HOMO becomes a  $\pi$ -type MO. However, the introducing of a dichloroethyl group to NH- group of the tri-keto form led to enhancing of contribution of unbound electron pairs of chlorine atoms in the HOMO, and the HOMO becomes an n-type MO. The results of the ESP analysis showed the formation of positive  $\pi$ -hole potentials in the case of tri-keto derivatives. The presence of strong attractive and repulsive forces and also weak interactions in the case of tri-vinyl and tri-1,2-dichloroethyl derivatives of tri-keto form have been shown by NCI and RDG plots of investigated compounds.

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