Conclusion: We used a personal computer with an intel core i7 processor (3.6 GHz CPU) with the Ubuntu 18.04 operating system installed. When calculating the initial geometry of a molecule with an (2R,3R)-3,3a-dihydroxy-6-imino-2,3,3a,9a-tetrahadro-6H-four[2,3,4,5]oxazolo[3.2-a]pyrimidin-2-yl)methyldihydrogen phosphate compound base, the method of molecular mechanics (MM+) of the Chem Draw 20.0 software package was chosen. The maximum wavelength with a high oscillator strength was observed 2R,3R)-3,3a-dihydroxy-6-imino-2,3,3a,9a-tetrahadro-6H-4[2,3,4,5] oxazolo[3,2-a]pyrimidin-2-yl)methyl dihydrogen phosphate λ= 232.67 nm and f = 0.0906. The calculation showed that the strongest electron transition is observed at the absorption maximum of 232.67 nm, which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_{20}$ the remaining transitions have a small value of f and are forbidden by symmetry.

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IN SILICO INVESTIGATION OF 5-(4-AMINO-2-OXOPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL)METHYL DIHYDROGEN PHOSPHATE

КВАНТОВО-ХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ 5-(4-АМИНО-2-ОКСОПИРИМИДИН-1(2H)-ИЛ]-3,4-ДИГИДРОКСИТЕТРАГИДРОФУРАН-2-ИЛ) МЕТИЛДИГИДРОФОСФАТА

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This paper represents theoretical calculations related to newly synthetized oxopyrimidin compound 5-(4-amino-2-oxopyrimidin-1(2h)-yl)-3,4- dihydroxytetrahydrofuran-2-yl)methyl dihydrogen phosphate in order to define its optimized geometry, free energy and form of molecular orbitals participated in formation of UV/Vis spectrum.

В данной статье представлены теоретические расчеты, относящиеся к новому синтезированному оксопиримидиновому соединению: 5-(4-амино-2-оксопиримидин-1(2h)-ил)-3,4-дигидрокситетрагидрофуран-2-ил)метилдигидрофосфату. Определены его стандартная геометрия, значение свободной энергии и формы молекулярных орбиталей, участвующие в формировании спектра поглощения изучаемой молекулы.

Keywords: computational chemistry, HF/STO-3G*, UV/Vis spectrum.

Ключевые слова: компьютерная химия, HF/STO-3G*, УФ спектр.

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For calculations, we used a personal computer with an intel core i7 processor (3.6 GHz CPU) with the Ubuntu 18.04 operating system installed. For calculation of initial geometry of the molecule 5-(4-amino-2-oxopyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl dihydrogen phosphate compound, the method of molecular mechanics (MM+) of the ChemDraw 20.0 software package was chosen. The starting geometry of the molecule was additionally optimized in the solvent medium of Water by the HF/STO-3G method of the Gaussian 09W software package until the global minimum of total energy of systems was reached. To find the global energy minimum and the most stable conformers, we analyzed all stationary points on the potential energy surface of molecules. The HF/STO-3G* method was

used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances [2]. The Gauss View 06 program was used to visualize the results of the calculations. The equilibrium geometry of the molecule by the HF/STO-3G* method is shown in Figure 1.

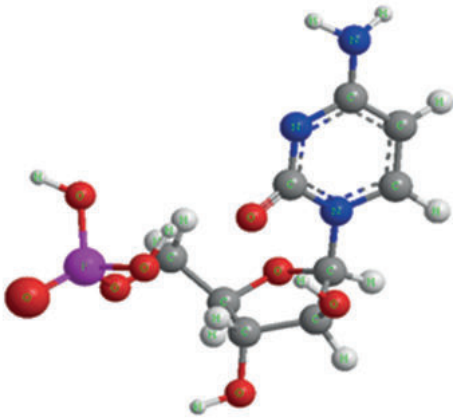


Figure 1 – Optimized structure by HF/STO-3G method*

Quantum chemical simulation of the equilibrium geometry and electronic structure of 5-(4-amino-2-oxopyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyldihydrogenphosphate, full optimization and calculation of the electronic structure were carried out by HF/STO-3G* method. This method is used to calculate the optimized geometries, electronic absorption spectra, total energy and heat of formation, and was used by us to calculate the electronic absorption spectrum of 5-(4-amino-2-oxopyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyldihydrogenphosphate. Electronic spectrum of the 5-(4-amino-2-oxopyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyldihydrogenphosphateis calculated for 20 one-electron excitations in the region 164.72-5191.14 nm. The results of calculation of the absorption spectrum are given in the table.

The maximum wavelength with a high oscillator strength was observed at λ = 253.11 nm and f = 0.1415 (Table 1, Fig. 2, 3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 253.11 nm, which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_8$. The remaining transitions have a small value of f and are forbidden by symmetry.

Table 1

Calculated electron absorption spectrum of the molecule

Excited State	Wavelength (nm)	Configurations Composition (corresponding transition orbitals)	Oscillator Strength (f)
$S_0 \rightarrow S_1$	366.59	-0.23 (56→60)-0.61 (59→60)	0.0485
$S_0 \rightarrow S_2$	318.98	-0.17 (55→60)-0.29 (56→60)-0.13 (56→61)-0.14(56→62) -0.14 (56→63)-0.38 (57→60)-0.17 (58→60)-0.17(59→61) -0.15 (59→62)	0.0229
$S_0 \rightarrow S_3$	295.84	-0.10 (52→63)-0.10 (52→65)-0.14 (56→61)-0.15 (56→63) -0.17 (56→65)-0.18 (57→61)-0.21 (57→63)-0.18 (57→65) -0.30 (59→61)-0.26 (59→63)	0.0028
$S_0 \rightarrow S_4$	284.06	-0.10 (55→60)-0.18 (56→60)-0.19 (56→61)-0.21 (57→60) -0.12 (57→63)-0.10 (57→65)-0.34 (59→61)-0.28 (59→62) -0.12 (59→65)	0.0167
$S_0 \rightarrow S_5$	272.59	-0.14 (56→61)-0.15 (56→62)-0.10 (56→63)-0.23 (57→61) -0.19 (57→62)-0.11 (57→63)-0.47 (58→60)-0.13 (59→60)	0.1151
$S_0 \rightarrow S_6$	269.63	-0.12 (56→62)-0.11 (56→63)-0.24 (57→60)-0.22 (57→61) -0.27 (58→60)-0.17 (59→61)-0.340 (59→63)-0.14 (59→65)	0.0920
$S_0 \rightarrow S_7$	256.11	-0.11 (53→60)-0.17 (53→61)-0.15 (53→62)-0.15 (54→61) -0.14 (54→62)-0.19 (55→61)-0.18 (55→62)-0.12 (55→63) -0.20 (57→60)-0.12 (57→63)-0.13 (58→61)-0.10(58→62) -0.16 (59→63)	0.0065
$S_0 \rightarrow S_8$	253.11	-0.12 (57→61)-0.15 (57→62)-0.11 (57→63)-0.28 (58→61) -0.29 (58→62)-0.20 (58→63)-0.11 (59→61)-0.18 (59→62) -0.25 (59→63)	0.1415

Excited State	Wavelength (nm)	Configurations Composition (corresponding transition orbitals)	Oscillator Strength (f)
$S_0 \rightarrow S_9$	241.62	-0.24 (51→61)-0.37 (51→62)-0.16 (51→63)-0.10(51→67) -0.10 (54→62)-0.12 (56→60)-0.13 (57→60)-0.12 (57→61) -0.13 (58→63)-0.10 (58→65)	0.0373
$S_0 \rightarrow S_{10}$	241.30	-0.19 (51→61)-0.28 (51→62)-0.11 (51→63)-0.10 (54→62) -0.16 (56→60)-0.18 (57→60)-0.13 (57→61)-0.11 (57→62) -0.12 (57→65)-0.10 (58→60)-0.20 (58→63)-0.13 (58→65) -0.13 (59→65)	0.0582
$S_0 \rightarrow S_{11}$	238.39	-0.10 (56→60)-0.26 (57→63)-0.18 (57→65)-0.15 (57→66) -0.11 (58→62)-0.18 (58→63)-0.14 (58→65)-0.26 (58→66) -0.20 (58→67)	0.0138
$S_0 \rightarrow S_{12}$	236.25	-0.10 (56→63)-0.10 (57→61)-0.14 (57→62)-0.17 (57→63) -0.10 (57→66)-0.22 (58→60)-0.26 (58→61)-0.14 (58→62) -0.14 (58→65)-0.22 (58→66)-0.16 (58→67)-0.10 (59→62) -0.11 (59→63)	0.0163
$S_0 \rightarrow S_{13}$	234.64	-0.10 (55→60)-0.20 (56→60)-0.12 (56→61)-0.14 (56→63) -0.12 (56→64)-0.11 (56→65)-0.17 (56→68)-0.12 (57→63) -0.14 (58→63)-0.10 (59→60)-0.17 (59→68)-0.10 (59→70) -0.11 (59→73)	0.0284
$S_0 \rightarrow S_{14}$	229.34	-0.10 (55→60)-0.20 (56→60)-0.12 (56→61)-0.14 (56→63) -0.12 (56→64)-0.11 (56→65)-0.17(56→68)-0.12 (57→63) -0.14 (58→63)-0.10 (59→60)-0.17(59→68)-0.10 (59→70) -0.11(59→73(	0.0717
$S_0 \rightarrow S_{15}$	225.16	-0.10(47→62)-0.10(48→62)-0.10(50→64)-0.16(56→62) -0.19(56→63)-0.12(56→68)-0.11(56→73)-0.12(57→61) -0.19(57→62)-0.10(57→63)-0.11(59→62)-0.14(59→68)	0.0443
$S_0 \rightarrow S_{16}$	222.36	-0.10(50→64)-0.20(56→61)-0.10(56→62)-0.14(56→63) -0.10(56→64)-0.12(56→65)-0.15(56→68)-0.13(57→62) -0.12171(57→68) -0.22(59→68)-0.10(59→70)	0.0501
$S_0 \rightarrow S_{17}$	219.61	-0.10(50→63)-0.30(50->64)-0.13(52→69)-0.10(52→70) -0.12(55->68)-0.14(55→69)-0.13(55→70)-0.15(56→68) -0.15(56→69)-0.13(56→70)-0.14(59→68)-0.13(59→69)	0.0072
$S_0 \rightarrow S_{18}$	217.75	-0.16(52→60)-0.27(53→60)-0.23(54→60)-0.28(55→60) -0.12(57→60)-0.12(58→63) -0.11(59→60)	0.0370
$S_0 \rightarrow S_{19}$	217.04	-0.11(56→66)-0.11(56→67)-0.18(58→61)-0.16(58→63) -0.10(58→67)-0.12(58→75)-0.15(59→65)-0.19(59→66) -0.12(59→67)-0.11366(59→68)	0.0113
$S_0 \rightarrow S_{20}$	212.82	-0.10)52→60(-0.12(55→61)-0.15(55→63)-0.10(56→65) -0.10(56→66)-0.11(56→74)-0.15(56→75)-0.11(57→61) -0.10(57→63)-0.13(57→66-0.10(58→63)-0.13(59→65)	0.0212

The theoretical absorption spectrum of the optimized molecule in a solvent medium was calculated using the Gaussian16 software package using HF/STO-3G* method. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2.

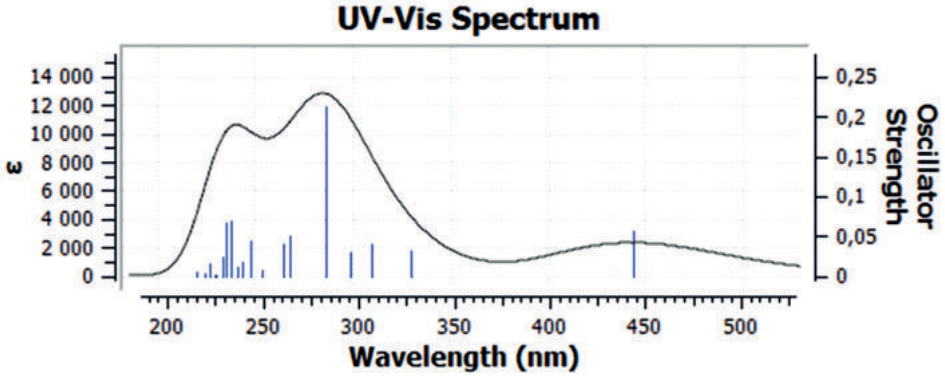
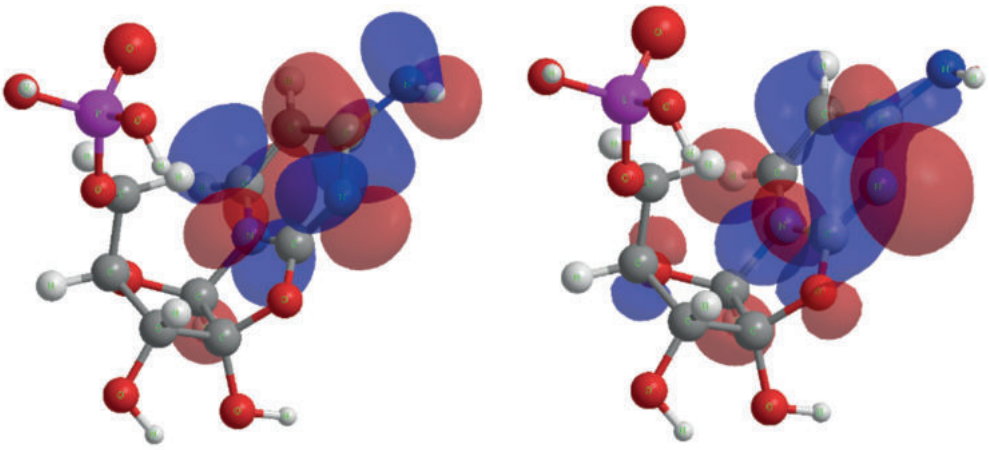


Figure 2 – Absorption spectrum of the title molecule



LUMO (N=60) E = 1.979 eV HOMO (N=59) E = -8.802 eV

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of a molecule (A) at λ = 253.11 nm

Conclusion: We used a personal computer with an intel core i7 processor (3.6 GHz CPU) with the Ubuntu 18.04 operating system installed. For calculation of initial geometry of the molecule 5-(4-amino-2-oxopyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl dihydrogen phosphate compound, the method of molecular mechanics (MM+) of the Chem Draw 20.0 software package was chosen. The maximum wavelength with a high oscillator strength was observed at λ = 253.11 nm and f = 0.1415 (Table, Fig. 2,3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 253.11 nm, which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_8$. The remaining transitions have a small value of f and are forbidden by symmetry.

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КОМПЬЮТЕРНЫЙ СКРИНИНГ НОВЫХ ПОТЕНЦИАЛЬНЫХ ИНГИБИТОРОВ ФИБРИЛЛООБРАЗОВАНИЯ МОЛЕКУЛЫ ИНСУЛИНА

COMPUTER SCREENING OF NEW POTENTIAL INHIBITORS OF INSULIN FIBRIL FORMATION

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Проведен молекулярный докинг инсулина с потенциальными ингибиторами агрегации цАМФ и Ap_4A с целью прогнозирования формирования возможных комплексов между ними. Низкомолекулярные соединения оптимизированы методом DFT с функционалом B3LYP/6-31G(d,p). Произведены молекулярно-динамические расчеты для полученных комплексов и определены значения свободных энергий изучаемых комплексов. Проанализированы типы межмолекулярных взаимодействий в комплексах.