Сукцинилированный хитозан показывает антиоксидантную активность в 3,4/7,5 раз ниже ГСБ/Трп и в 3,7/5,7 раз ниже комплексов ГСБ-СХТ/Трп-СХТ. Однако, присоединение сукцинилированного хитозана оказывает положительный эффект на АОА комплексов ГСБ-СХТ и Трп-СХТ. Антиоксидантный эффект (IC_{50}) из расчета по белку/триптофану повышается в 1,4–1,5 раз.

Олигохитозан показывает антиоксидантную активность в 1,4/3 раз ниже ГСБ/Трп и в 1,5/2,5 раз ниже комплексов ГСБ-ОХТ/Трп-ОХТ. Однако, присоединение олигохитозана также оказывает положительный эффект на АОА комплексов ГСБ-ОХТ и Трп-ОХТ. Антиоксидантный эффект (IC_{50}) из расчета по белку/триптофану повышается в 1,7–2 раза.

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IN SILICO CALCULATION OF PYRIMIDIN DERIVATIVE (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) METHYL DIHYDROGEN PHOSPHATE

КВАНТОВО-ХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ПРОИЗВОДНОГО ПИРИМИДИНА (2R,3R)-3,3A-ДИГИДРОКСИ-6-ИМИНО-2,3,3A,9A-ТЕТРАГАДРО-6H-4[2,3,4,5] ОКСАЗОЛО[3,2-A]ПИРИМИДИН-2-ИЛ)МЕТИЛ ДИГИДРОФОСФАТА

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This article presents the results of theoretical calculations of the compound (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)methyl dihydrogen phosphate to determine its equilibrium geometry, free energy and the type of molecular orbitals involved in the formation of the absorption spectrum.

В данной статье представлены теоретические расчеты, относящиеся к новому синтезированному соединению: (2R,3R)-3,3a-дигидрокси-6-имино-2,3,3a,9a-тетрагадро-6H-4[2,3,4,5]оксазоло[3,2-a]пиримидин-2-ил)метил дигидрофосфату. Определены его стандартная геометрия, значение свободной энергии и формы молекулярных орбиталей, участвующие в формировании спектра поглощения 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. When calculating the initial geometry of a molecule with 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. calculation parameters depending on the specific problem. 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 the total energy of the systems under study 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 is 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. The equilibrium geometry of the molecule by the HF/STO-3G* method is shown in Figure 1.

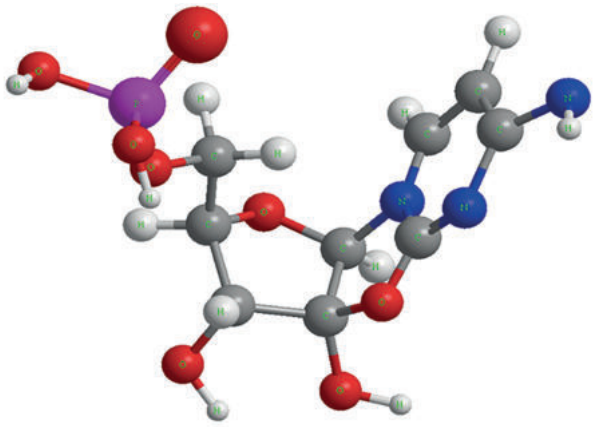


Figure 1 – Optimized molecule by HF/STO-3G method*

Quantum chemical simulation of the equilibrium geometry and electronic structure of (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)methyl dihydrogen phosphate, 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 (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)methyl dihydrogen phosphate. Electronic spectrum was calculated for 10 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 = 232.67 nm and f = 0.0906 (Table 1, Fig. 2, 3). 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.

Table 1

Calculated electron absorption spectrum of the molecule

Excited State	**Wave-length (nm)**	**Configurations Composition (corresponding transition orbitals)**	**Oscilla-tor Strength (f)**
$S_0 \rightarrow S_1$	246.20	0.70(58→59)-0.16(59→58)	0.0040
$S_0 \rightarrow S_2$	456.43	0.39(58→60)-0.36(58→61)+0.35(58→62)-0.15(58→64)	0.0262
$S_0 \rightarrow S_3$	425.43	-0.16(57→59)+0.12(57→63)+0.27(58→62)+0.55(58→63)	0.0053
$S_0 \rightarrow S_4$	353.38	0.13(50→59)-0.15(55→59)+0.26(56→59)+0.34(57→59)+0.14(58→60) +0.30(58→61)+0.16(58→62)-0.13(58→71)-0.12(58→76)	0.0020
$S_0 \rightarrow S_5$	333.41	-0.13(55→59)+0.13(56→59)+0.30(57→59)-0.19(58→60)-0.38(58→61) +0.18(58→63)+0.13(58→72)-0.10(58→75)+0.11(58→76)	0.0380
$S_0 \rightarrow S_6$	314.66	-0.15(50→59)-0.38(56→59)+0.11(57→59)+0.10(58→61)- 0.33(58→71)+0.23(58→72)	0.0104
$S_0 \rightarrow S_7$	302.72	0.15(57→60)-0.16(57→61)-0.40(57→63)-0.11(57→ 64)+0.29(57→71)- 0.21(57→72)	0.0055
$S_0 \rightarrow S_8$	294.27	0.10(55→59)+0.27(56→59)-0.24(57→59)-0.13(58→63)-0.17(58→71) -0.13(58→73)+0.10(58→76)-0.10(58->78)+0.14(58→80)-0.11(58→81) -0.13(58→82)+0.11(58→83)+0.21(58→59)	0.0060
$S_0 \rightarrow S_9$	285.24	-0.16(49→61)-49(56→61)+0.10(56→63)-0.17(57→61)-0.11(58→71)	0.0191
$S_0 \rightarrow S_{10}$	278.36	-0.22(57→59)-0.23(56→61)+0.17(57→59)+0.12(57→63)+0.10(58→62) -0.13(58→65)+0.18(58→71)-0.22(58→72)-0.14(58→73) -0.11(58→78)+0.19(58→80)-0.12(58→92)	0.0219
$S_0 \rightarrow S_{11}$	276.24	-0.10(48→60)-0.32(55→60)-0.10(55 →60)+0.16(56→60)+0.18(56→62)+0 .19(57→60) -0.19(58→60)-0.10(58→60)	0.0171

Excited State	Wave-length (nm)	Configurations Composition (corresponding transition orbitals)	Oscilla-tor Strength (f)
$S_0 \rightarrow S_{12}$	272.05	-0.13(50→59)+0.12(55→54)+0.11(55→61)+0.14(55→62)+0.10(55→63)+ 0.12(56→60) -0.21(56→63)+0.12(57→61)-0.19(57→62)-0.14(57→63)-0.12(58→60)- 0.13(58→84)	0.0071
$S_0 \rightarrow S_{13}$	267.25	0.20(55→60)+0.30(56→60)-0.13(56→61)+0.15(56→62) -0.24(56→63)-0.10(57→66)-0.10(58→65)	0.0395
$S_0 \rightarrow S_{14}$	256.29	0.11)52→60)+0.15(54→60)-0.18)55→59)+0.11)55→63)+0.16)56→60(+0.18)56→64)-0.14)57→59(-0.25)58→60+(0.11)58→62) -0.14)58→64(-0.11) 58→65(-0.13(58→76(	0.0078
$S_0 \rightarrow S_{15}$	251.03	-0.25(50→59)+0.16(54→59)+0.28(55→59)+0.16(56→59)+0.11(56→63) +0.19 (57→59)+0.24(58→80)-0.21(58→84)	0.0054
$S_0 \rightarrow S_{16}$	249.18	0.13(50→59)-0.10(54→59)-0.21(55→59)-0.19(57→59)-0.14(57→61) +0.10(57→76)+0.14(58→61)+0.11(58→73)+0.28(58→80)-0.22(58→84)	0.0198
$S_0 \rightarrow S_{17}$	245.59	0.12(50→59)+0.10(52→63)-0.14(54→63)+0.12(55→60)-0.13(55→61) -0.26(55→63)+0.10(57→61)+0.12(57→63)+0.17(57→71)-0.13(57→72)- 0.17(58→63)	0.0247
$S_0 \rightarrow S_{18}$	242.26	0.11(53→61)- 0.16(55→61)+0.12(56→62)+0.14(56→63)+0.22(57→61)+0.15(58→60) -0.15(58→62)+0.16(58→64)-0.10(58→69)-0.24(58→84)	0.0036
$S_0 \rightarrow S_{19}$	238.00	0.15(55→61)-0.18(57→61)+0.16(58→60)-0.25(58→65)+0.21(58→66) -0.17(58→73)+0.16(58→67)-0.14(58→80)	0.0454
$S_0 \rightarrow S_{20}$	232.67	0.12(53→64)+0.10(54→60)+0.14(54→63)+0.18(55→62)+0.10(55→63) +0.14(56→62)+0.11(57→61)+0.13(58→66)+0.11(58→71)+0.11(58→73)+ 0.14(58→76) -0.11(58→77)+0.11(58-78)-0.10(58→80)0.12(58→84)	0.0906

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).

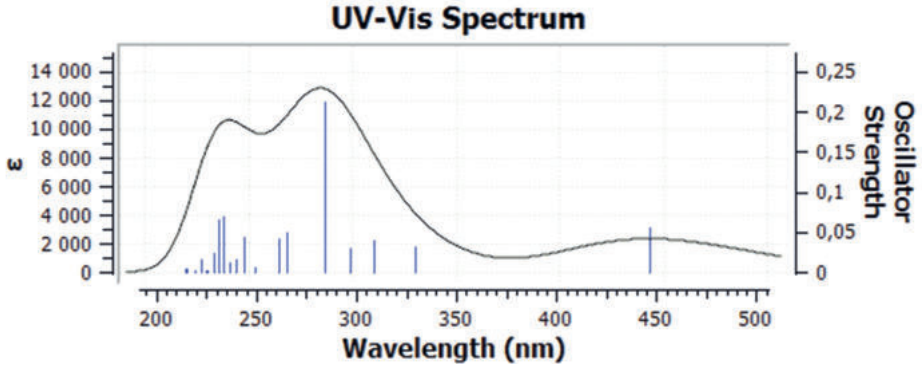
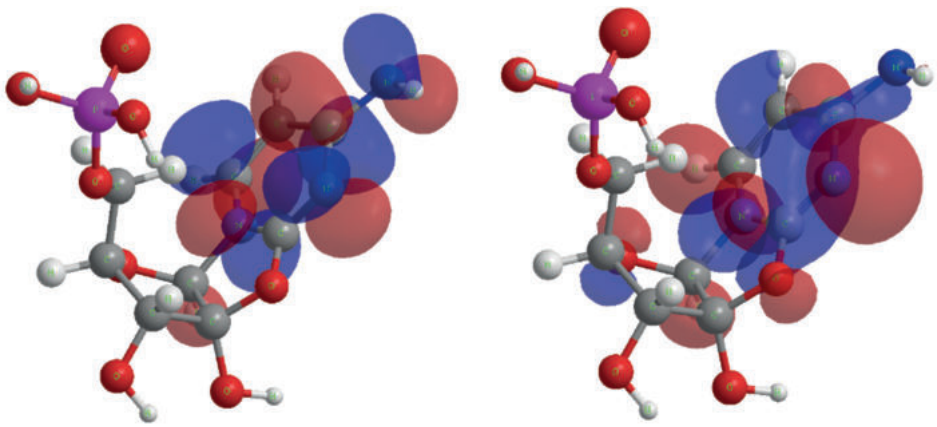


Figure 2 – Absorption spectrum of the title molecule



LUMO (N=59) E=-2.258 eV HOMO (N=58) E=-8.655 eV

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of a molecule (A) at λ = 232.67 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. 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