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Д.В.Сокольский атындағы «Жанармай,
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ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН
АО «Институт топлива, катализа и
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NAS RK is pleased to announce that News of NAS RK. Series of chemistry and technologies scientific journal has been accepted for indexing in the Emerging Sources Citation Index, a new edition of Web of Science. Content in this index is under consideration by Clarivate Analytics to be accepted in the Science Citation Index Expanded, the Social Sciences Citation Index, and the Arts & Humanities Citation Index. The quality and depth of content Web of Science offers to researchers, authors, publishers, and institutions sets it apart from other research databases. The inclusion of News of NAS RK. Series of chemistry and technologies in the Emerging Sources Citation Index demonstrates our dedication to providing the most relevant and influential content of chemical sciences to our community.

Қазақстан Республикасы Ұлттық ғылым академиясы "ҚР ҰҒА Хабарлары. Химия және технология сериясы" ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Web of Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Химия және технология сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді химиялық ғылымдар бойынша контентке адалдығымызды білдіреді.

НАН РК сообщает, что научный журнал «Известия НАН РК. Серия химии и технологий» был принят для индексирования в Emerging Sources Citation Index, обновленной версии Web of Science. Содержание в этом индексировании находится в стадии рассмотрения компанией Clarivate Analytics для дальнейшего принятия журнала в the Science Citation Index Expanded, the Social Sciences Citation Index и the Arts & Humanities Citation Index. Web of Science предлагает качество и глубину контента для исследователей, авторов, издателей и учреждений. Включение Известия НАН РК в Emerging Sources Citation Index демонстрирует нашу приверженность к наиболее актуальному и влиятельному контенту по химическим наукам для нашего сообщества.

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MOLECULAR STRUCTURE AND QUANTUM CHEMICAL CALCULATIONS 4-ETHYL-5-(2-HYDROXYPHENYL)-1,2,4-TRIAZOL-3-THIONE

Abstract. The article is devoted to the study of the spatial structure of 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione. The molecular and crystalline structure was determined by x-ray diffraction analysis. Data on the spatial structure and crystal packing of the molecule are presented. It is established that phenyl and triazole rings are flat. Due to hydrogen bonds, the molecules in the crystal form three-dimensional networks. The results of an X-ray diffraction study were deposited at the Cambridge Center for Crystal Structural Data. The structure of the synthesized 1,2,4-triazole was studied by ¹H NMR spectroscopy. When analyzing the ¹H NMR spectrum of the compound, characteristic signals of the protons of the aromatic ring are observed. The value of the chemical shift and the integrated signal intensity are determined. A quantum chemical study of 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione was carried out by the DFT method using the B3LYP exchange-correlation functional in combination with the Dunning basic set cc-pVDZ. The molecular characteristics of the compound, such as total electron energy, rotational constants, dipole moment and contributions, and thermodynamic functions, are predicted. The equilibrium geometric parameters of the 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione molecule were determined. The performed analysis of the spatial configuration and molecular parameters showed a qualitative correspondence between the crystalline and gas-phase structures of the molecule, while it was noted that the main difference is observed in the relative orientation of six- and five-membered cycles.

Keywords: crystal structure, x-ray diffraction, 1,2,4-triazole, 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione, quantum chemical calculations, DFT method, geometric and energy characteristics.

Introduction

Derivatives of 1,2,4-triazole provide great synthetic possibilities for obtaining new effective drugs. A number of 1,2,4-triazole derivatives have been successfully used in medicine as medicines for the treatment of fungal and viral infections, diseases of the cardiovascular system, etc. [1-4]. New derivatives of 1,2,4-triazole are known, which have shown antiviral [5, 6], anti-inflammatory [7, 8], anticonvulsant [9, 10], antitumor [10, 11], antibacterial [12, 13] and other types of activity. Consequently, some of the 1,2,4-triazole derivatives have been approved as drugs, such as anastrozole, letrozole, risatriptan, ribavirin, alprazolam, fluconazole and posaconazole. This leads to intensive studies of both the preparation methods and the properties of the new derivatives of 1,2,4-triazoles.

It is well known that s-triazoles can exist in two tautomeric forms, and most studies have shown that the thion form was dominant in the solid state and in a neutral solution [14–16]. However, there are some studies that describe the presence of a thiol form [17–20].

Nevertheless, it was shown that thiolthionetautomerism plays an important role in several processes related to biological activity, such as proton transfer and hydrogen bonds [21-24].

Currently, X-ray diffraction analysis is one of the most informative, unique and accurate tools for studying the spatial structure of synthesized compounds, which has made a significant and decisive contribution to the study of almost all inorganic and organic classes [25].

Previously, we synthesized a number of 1,2,4-triazoles based on hydrazides of *o*- and *p*-hydroxybenzoic acids, which were obtained by interaction with thiosemicarbazides in an aqueous solution of caustic potassium followed by acidification with acetic acid. X-ray diffraction analysis was used to characterize the crystal structure of 4-allyl-3-(4-hydroxyphenyl)-1H-1,2,4-triazole-5(4H)-thione [26-28]. In continuation of studies in this direction, we present experimental data on the spatial structure and calculated quantum chemical parameters of 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione (1).

Experimental part

The NMR¹H spectrum was recorded on a Bruker DRX500 spectrometer (500 MHz) in a DMSO-*d*₆ solution relative to the internal standard — TMS.

X-ray diffraction analysis of 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione (1). Crystals for X-ray diffraction analysis were obtained by double crystallization of compound 1 from 2-propanol.

Cell parameters and intensities of 3461 reflections (1340 independent, $R_{\text{int}} = 0.0223$) were measured on a «Bruker P4» diffractometer (MoK α , graphite monochromator, ω scanning, $2.96^\circ \leq \theta \leq 22.44^\circ$) at a temperature of 298 K. Monoclinic crystals, $a = 9.8479(6)$, $b = 7.9892(7)$, $c = 13.914(1)$ Å, $\beta = 102.616(3)^\circ$, $V = 1068.3(1)$ Å³, $Z = 4$ C₁₄H₉N₃O₃, space group P2₁/c, $d_{\text{bbsq}} = 1.376$ g/cm³, $\mu = 0.279$ mm⁻¹. The initial array of the measured intensities was processed and absorption was taken into account using the SAINT and SADABS programs (multi-scan, $T_{\text{min}} = 0.7072$, $T_{\text{max}} = 0.7448$) [29].

The structure is deciphered by the direct method. The positions of non-hydrogen atoms are refined in the anisotropic approximation by full-matrix least squares. Hydrogen atoms of the hydroxyl and amino groups were identified from difference synthesis and their positions were refined in the isotropic approximation, the remaining hydrogen atoms were placed in geometrically calculated positions and their positions were refined in the isotropic approximation with fixed positional and thermal parameters (rider model). In the calculations, 1191 reflections of independent reflections with $I \geq 2\sigma(I)$ were used, the number of refined parameters is 145. Final divergence factors: R_1 0.0301, wR_2 0.0786 (for reflections with $I \geq 2\sigma(I)$), R_1 0.0347, wR_2 0.0833 (for all reflections), $\text{GooF} = 1.057$. Peaks of residual density: $\Delta\rho = 0.146$ and -0.219 e/Å³. The structure has been deciphered and refined using the SHELXS [30] and SHELXL-2018/3 [31] programs. PCA data in the form of a CIF file was deposited at the Cambridge Center for Crystal Structural Data (CCDC 1921694).

The quantum chemical calculation for the 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione molecule in the gas phase was carried out using the density functional theory method (DFT/B3LYP) [32] using the Gaussian program [33]. In this case, the correlation-consistent Dunning basis set cc-pVDZ was used, which was specially developed to more fully take into account correlation effects.

Results and discussions

When analyzing the ¹H NMR spectrum of compound 1, characteristic signals of the protons of the aromatic ring are observed. So, the signals of the protons of the aromatic ring are recorded at 7.78 ppm. ($J_{\text{H}\alpha\text{H}\beta} 8.7$ Hz), 6.81 ppm ($J_{\text{H}\alpha\text{H}\beta} 8.7$ Hz), 7.32 ppm (1H, CH⁴_{arom}), 7.02 ppm. (1H, CH¹_{arom}) in the form of doublets, respectively. At 6.95 ppm (1H, CH²_{arom}), 7.42 ppm. (1H, CH³_{arom}) signals appear in the form of triplets. In a weak field, signals of protons of aromatic hydroxyl are recorded at 10.33 ppm. and thioamide N-H proton at 13.8 ppm in the form of two small broadened singlets. Signals of methyl group protons resonate at 1.05 ppm. ($J_{\text{HH}} 7.1$ Hz) as a triplet and methylene group at 3.85 ppm. ($J_{\text{HH}} 7.2$ Hz) as a quartet.

The spatial structure and packaging of the 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione molecule (1) are shown in Figures 1 and 2.

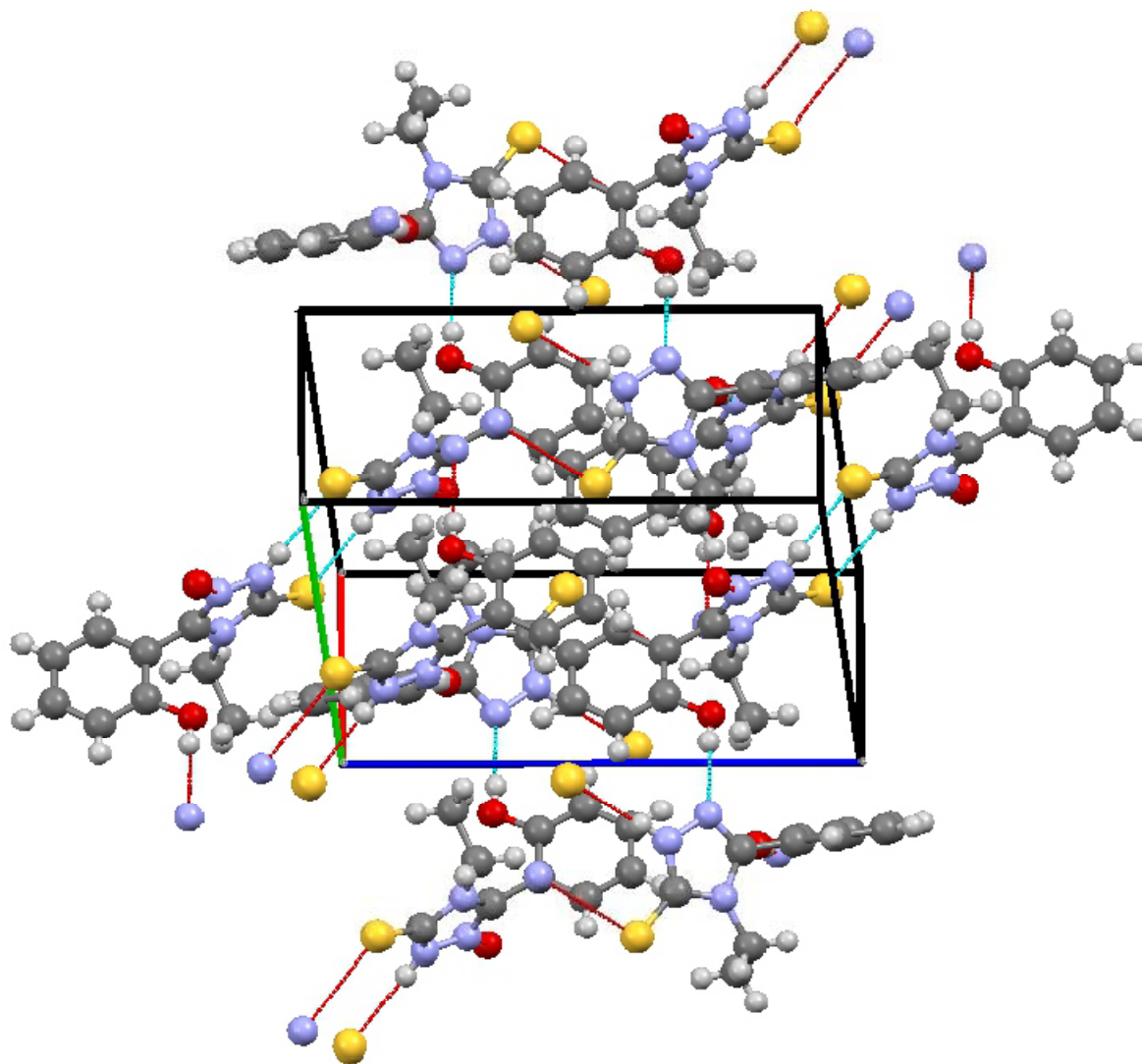
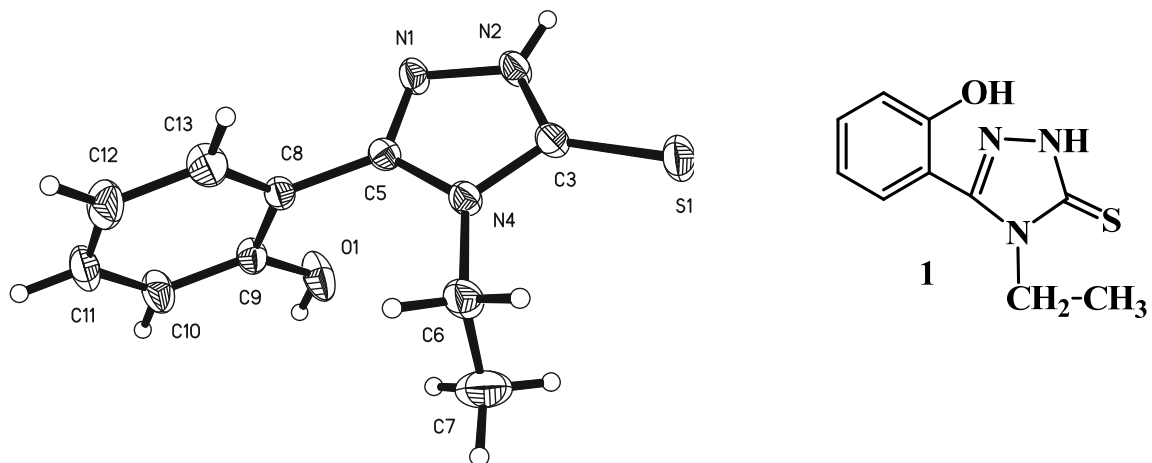


Figure 2 – Packing molecule 1 in the crystal

From the obtained data of X-ray diffraction analysis, it follows that the bond lengths (table 1) and bond angles (table 2) in compounds 1 are close to usual [34]. In molecule 1, the triazole ring is flat; the atoms N1, N2, C3, N4, and C5 are coplanar with an accuracy of ± 0.003 Å. The sulfur atom S1, C6 of the ethyl and C8 phenyl groups slightly leave this plane (by -0.051, 0.053 and -0.035 Å, respectively). The phenyl cycle, flat with an accuracy of ± 0.001 Å, is unfolded relative to the triazole by 85.6°. The O1 atom of the hydroxyl group is practically located in this plane (0.013 Å).

In the crystal, molecules 1 form an intermolecular hydrogen bond N2 \cdots H ... S1 (1-x, -y, 1 - z) (distance N ... S 3.299 (2) Å, H ... S 2.44 (2) Å, angle N-H ... S 176 (2)°), linking the triazole moieties of two molecules into dimers. The hydroxyl group forms a hydrogen bond with the N1 atom of another molecule, O1 \cdots H ... N1 (1-x, 1/2 - y, 1/2 - z) (distance O ... N 2.853(2) Å, H ... N 2.07(2) Å, angle O - H ... N 175(2)°), forming in three-dimensional infinite grids.

A theoretical quantum-chemical approach was used to determine the physicochemical characteristics of 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione. In order to find the minimum energy configuration of the molecule in the ground state, the structure is optimized for all independent coordinates. Figure 3 shows an optimized three-dimensional model of the molecule under study (according to quantum chemical calculations). The calculated quantum-chemical structural parameters of the molecule are given (table 1 and table 2) in comparison with the experimental X-ray diffraction data.

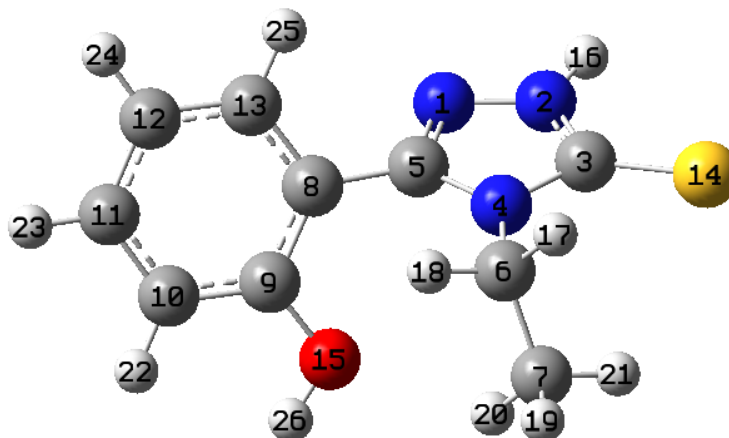


Figure 3 – Optimized Molecule 1 Structure (B3LYP/cc-pVDZ Method)

A comparison of the crystalline and gas-phase structures of the molecule showed a qualitative correspondence between them. The main difference is the relative orientation of the two cycles. In the crystalline structure, the torsion angle is -93.6° , for a molecule in the gas phase it is -54.62° . According to quantum-chemical calculations, valence bonds between atoms in a gas-phase molecule are more stretched (by 0.001-0.106 Å). Only for N(1)-N(2) and N(4)-C(6) are shortened bonds observed. In the case of O-H and C-H bonds, the calculations give values close to standard (0.96 and 1.09 Å, respectively) values (table 1), while PCA bonds are shorter.

Table 1 - Bond lengths in the molecule of 1

Bond	Length, Å		Angle	Value, deg	
	Exp.	Theor. (B3LYP/cc-pVDZ)		Exp.	Theor. (B3LYP/cc-pVDZ)
S(1)-C(3)	1.6746(19)	1.677	C(3)-N(4)-C(6)	125.18(15)	123.26
O(1)-C(9)	1.358(2)	1.364	C(5)-N(4)-C(6)	126.64(15)	128.39
O(1)-H(01)	0.79(2)	0.969	N(1)-C(5)-N(4)	110.83(15)	111.23
N(1)-C(5)	1.302(2)	1.310	N(1)-C(5)-C(8)	125.76(16)	122.29
N(1)-N(2)	1.378(2)	1.364	N(4)-C(5)-C(8)	123.37(16)	126.32
N(2)-C(3)	1.333(3)	1.362	N(4)-C(6)-C(7)	112.31(17)	113.59

Angle	τ , deg		Angle	τ , deg	
	Exp.	Theor. (B3LYP/cc- pVDZ)		Exp.	Theor. (B3LYP/cc- pVDZ)
N(2)-H(2)	0.87(2)	1.012	N(4)-C(6)-H(6A)	109.1	106.78
C(3)-N(4)	1.371(2)	1.388	C(7)-C(6)-H(6A)	109.1	111.52
N(4)-C(5)	1.375(2)	1.390	N(4)-C(6)-H(6B)	109.1	106.32
N(4)-C(6)	1.468(2)	1.466	C(7)-C(6)-H(6B)	109.1	109.92
C(5)-C(8)	1.477(2)	1.478	H(6A)-C(6)-H(6B)	107.9	108.44
C(6)-C(7)	1.502(3)	1.527	C(6)-C(7)-H(7A)	109.5	110.89
C(6)-H(6A)	0.9700	1.099	C(6)-C(7)-H(7B)	109.5	110.22
C(6)-H(6B)	0.9700	1.101	H(7A)-C(7)-H(7B)	109.5	109.46
C(7)-H(7A)	0.9600	1.098	C(6)-C(7)-H(7C)	109.5	109.15
C(7)-H(7B)	0.9600	1.099	H(7A)-C(7)-H(7C)	109.5	108.77
C(7)-H(7C)	0.9600	1.102	H(7B)-C(7)-H(7C)	109.5	108.29
C(8)-C(13)	1.389(3)	1.404	C(13)-C(8)-C(9)	119.56(17)	118.57
C(8)-C(9)	1.390(3)	1.410	C(13)-C(8)-C(5)	120.09(16)	118.88
C(9)-C(10)	1.383(3)	1.400	C(9)-C(8)-C(5)	120.34(16)	122.45
C(10)-C(11)	1.376(3)	1.396	O(1)-C(9)-C(10)	123.47(17)	122.20
C(10)-H(10)	0.9300	1.094	O(1)-C(9)-C(8)	117.03(16)	117.66
C(11)-C(12)	1.367(3)	1.397	C(10)-C(9)-C(8)	119.50(17)	120.14
C(11)-H(11)	0.9300	1.092	C(11)-C(10)-C(9)	120.15(18)	120.28
C(12)-C(13)	1.382(3)	1.395	C(11)-C(10)-H(10)	119.9	120.34
C(12)-H(12)	0.9300	1.091	C(9)-C(10)-H(10)	119.9	119.37
C(13)-H(13)	0.9300	1.091	C(12)-C(11)-C(10)	120.85(18)	120.25
C(9)-O(1)-H(01)	111.1(16)	109.12	C(12)-C(11)-H(11)	119.6	120.35
C(5)-N(1)-N(2)	104.04(15)	103.95	C(10)-C(11)-H(11)	119.6	119.40
C(3)-N(2)-N(1)	113.35(15)	114.55	C(11)-C(12)-C(13)	119.61(19)	119.36
C(3)-N(2)-H(2)	127.6(14)	124.33	C(11)-C(12)-H(12)	120.2	120.51
N(1)-N(2)-H(2)	118.8(14)	121.11	C(13)-C(12)-H(12)	120.2	120.13
N(2)-C(3)-N(4)	103.64(15)	102.33	C(12)-C(13)-C(8)	120.34(18)	121.40
N(2)-C(3)-S(1)	128.90(14)	128.13	C(12)-C(13)-H(13)	119.8	120.46
N(4)-C(3)-S(1)	127.44(15)	129.51	C(8)-C(13)-H(13)	119.8	118.15
C(3)-N(4)-C(5)	108.13(15)	107.93			

Table 2 - Torsion angles in the molecule of 1

C(5)-N(1)-N(2)-C(3)	-1.0(2)	-0.97	N(1)-C(5)-C(8)-C(13)	-93.6(2)	-54.62
N(1)-N(2)-C(3)-N(4)	0.8(2)	1.46	N(4)-C(5)-C(8)-C(13)	83.8(2)	120.31
N(1)-N(2)-C(3)-S(1)	-177.57(14)	-176.67	N(1)-C(5)-C(8)-C(9)	87.9(2)	121.75
N(2)-C(3)-N(4)-C(5)	-0.29(19)	-1.35	N(4)-C(5)-C(8)-C(9)	-94.7(2)	-63.31
S(1)-C(3)-N(4)-C(5)	178.12(14)	176.75	C(13)-C(8)-C(9)-O(1)	-179.38(18)	177.31
N(2)-C(3)-N(4)-C(6)	177.16(16)	-174.46	C(5)-C(8)-C(9)-O(1)	-0.9(3)	0.93
S(1)-C(3)-N(4)-C(6)	-4.4(3)	3.64	C(13)-C(8)-C(9)-C(10)	0.4(3)	-1.68
N(2)-N(1)-C(5)-N(4)	0.78(19)	0.01	C(5)-C(8)-C(9)-C(10)	178.84(18)	-178.07
N(2)-N(1)-C(5)-C(8)	178.45(16)	175.64	O(1)-C(9)-C(10)-C(11)	179.5(2)	-178.02
C(3)-N(4)-C(5)-N(1)	-0.3(2)	0.88	C(8)-C(9)-C(10)-C(11)	-0.2(3)	0.92
C(6)-N(4)-C(5)-N(1)	-177.73(17)	173.53	C(9)-C(10)-C(11)-C(12)	-0.1(3)	0.20
C(3)-N(4)-C(5)-C(8)	-178.07(16)	-174.52	C(10)-C(11)-C(12)-C(13)	0.3(3)	-0.52
C(6)-N(4)-C(5)-C(8)	4.5(3)	-1.88	C(11)-C(12)-C(13)-C(8)	-0.2(3)	-0.27
C(3)-N(4)-C(6)-C(7)	-88.1(2)	-77.10	C(9)-C(8)-C(13)-C(12)	-0.2(3)	1.37
C(5)-N(4)-C(6)-C(7)	88.8(2)	111.27	C(5)-C(8)-C(13)-C(12)	-178.65(19)	177.89

The deviation of the valence angles from similar experimental ranges from 0.04–3.47°, both in the direction of decreasing and increasing values. For dihedral angles, a larger scatter of values is observed when comparing theoretical and experimental data. Differences in the geometric configuration of the 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione molecule in different states of aggregation were expected, because, as you know, the geometry of the molecule in the crystal is determined by packing, in pairs - corresponds to the global minimum of total energy.

Theoretical physico-chemical characteristics, such as total energy, zero-point energy, rotational constants, electric dipole moment and others, are given in table. 3.

Table 3 - Physicochemical parameters of molecule 1 according to calculations by the B3LYP/cc-pVDZ method

Options	B3LYP/ cc-pVDZ
Totalenergy, a.u.	-1025.417093
Rotational Constants, GHz	
A	
B	1.1483336
C	0.3421134
	0.2921099
Dipole moment and its components, D	
μ_{total}	6.265
μ_x	-6.0563
μ_y	1.5974
μ_z	0.1367
E_{B3MO} , a.e.	-0.19583
E_{HOMO} , a.e.	-0.04063
$\Delta E_{B3MO-HOMO}$, eV	4.223
I, eV	5.329
A, eV	1.106
χ , eV	3.218
η , eV	2.112
S, eV	0.473
C_v , cal/mol·K	51.489
S, cal/mol·K	116.640

Due to the different values of the rotational constants, the molecule is an asymmetric top. Such fundamental properties as the dipole moment, ionization potential, electron affinity, etc., are directly dependent on the geometry of the molecule (table 3). The 4-ethyl-5-(2-hydroxyphenyl)-1,2,4-triazole-3-thione molecule is highly polar. The contributions of the X, Y, and Z components to the total dipole moment are different; the vector of the dipole moment is directed mainly along the X axis.

The most significant orbitals in a molecule are the so-called boundary orbitals: the highest occupied molecular orbital (HOMO) and the lowest free molecular orbital (LUMO). The HOMO energy characterizes the ability to donate an electron, LUMO — to accept an electron, the energy gap between them — the chemical stability of the molecule, with $I = -E_{VBMO}$ and $A = -E_{NCMO}$ (table 3) [35]. The molecule has a rather large ionization potential, electronegativity, and positive electron affinity. The width of the HOMO-LUMO energy gap (ΔE) indicates a sufficiently low polarizability of the molecule, which is consistent with the large value of its constant dipole moment. The high value of the dipole moment is due to the presence of electronegative atoms in the molecule.

Using these data, the molecular characteristics presented in table 3 were theoretically calculated, such as electronegativity χ , chemical rigidity η , and chemical softness S [35]. Absolute electronegativity is calculated as the half-sum of the ionization potential and electron affinity, and absolute chemical rigidity as their half-difference. The stiffness of a substance is considered as a measure of resistance to changes in electronic configuration. Chemical softness is the inverse of stiffness. The table also shows the calculated values of the thermodynamic properties of the compound, such as isochoric heat capacity and entropy.

ӨЖ 539.19 +548 +547:541.61

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4-ЭТИЛ-5-(2-ГИДРОКСИФЕНИЛ)-1,2,4-ТРИАЗОЛ-3-ТИОННЫҢ МОЛЕКУЛАЛЫҚ ҚҰРЫЛЫМЫ МЕН КВАНТТЫ-ХИМИЯЛЫҚ ЕСЕПТЕУЛЕРІ

Аннотация. Мақала 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тионның кеңістіктік құрылымын зерттеуге арналған. Қосылыстың молекулалық құрылымы рентген құрылымды әдіс арқылы анықталынды. Молекуланың кристалдық қаптамасы мен құрылымы бойынша мәліметтер келтірілген. Фенилді мен триазолды циклдары жазықтықты екені көрсетілген. Молекуланың сутектік байланысы арқылы кристалда үш өлшемді тордың болатындығы көрсетілген. Рентген құрылымды зерттеу нәтижелері Кембриджтің кристалл құрылымды мәліметтер орталығында тіркелген. Синтезделген 1,2,4-триазолдың құрылымы ЯМР ¹H-спектроскопия әдісімен зерттелінді. Қосылыстың ЯМР ¹H спектрінде ароматтық сақинаға тән келетін протондардың сигналы байқалады. Химиялық ығысудың мәні және интегралды сигнал қарқындылығы анықталынды. 4-Этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тионды кванттық химиялық зерттеу DFT әдісімен ВЗЛҮР алмасу-корреляциялық функциясын қолданып, Даннингтың негізгі жиынтығы cc-pVDZ жиынтығымен жүргізілді. Толық электронды энергия, айналу константалары, диполь моменті мен қосындылар және термодинамикалық функциялар сияқты қосылыстың молекулалық сипаттамалары болжамдалған. 4-Этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тион молекуласының тепе-тең геометриялық параметрлері анықталды. Кеңістіктік конфигурация мен молекулалық параметрлердің талдауы молекуланың кристалды және газды фазалық құрылымдарының арасындағы сапалы сәйкестікті көрсетілді, алайда басты айырмашылық алты және бес мүшелі циклдердің салыстырмалы бағытында байқалатындығы анықталынды.

Түйін сөздер: кристалдық құрылым, рентген құрылымды анализ, 1,2,4-триазол, 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тион, квантты-химиялық есептеу, DFT әдісі, геометриялық және энергетикалық сипаттамалар.

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МОЛЕКУЛЯРНАЯ СТРУКТУРА И КВАНТОВО-ХИМИЧЕСКИЕ РАСЧЕТЫ 4-ЭТИЛ-5-(2-ГИДРОКСИФЕНИЛ)-1,2,4-ТРИАЗОЛ-3-ТИОНА

Аннотация.Статья посвящена исследованию пространственной структуры 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тиона. Молекулярная и кристаллическая структура определена методом рентгеноструктурного анализа. Приведены данные по пространственному строению и кристаллической упаковке молекулы. Установлено, что фенильные и триазольные циклы плоские. За счет водородных связей молекулы в кристалле образуют трехмерные сетки. Результаты рентгеноструктурного исследования депонированы в Кембриджском центре кристаллоструктурных данных. Исследовано строение синтезированного 1,2,4-триазола методом ЯМР ¹H-спектроскопии. При анализе спектра ЯМР ¹H соединения наблюдаются характерные сигналы протонов ароматического кольца. Определено значение химического сдвига и интегральная интенсивность сигналов. Методом DFT с использованием обменно-корреляционного функционала ВЗЛҮР в сочетании с базисным набором Даннинггсс-рVDZ проведено квантово-химическое исследование 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тиона. Предсказаны молекулярные характеристики соединения, такие как полная электронная энергия, вращательные постоянные, дипольный момент и

вклады, термодинамические функции. Определены равновесные геометрические параметры молекулы 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тиона. Выполненный анализ пространственной конфигурации и молекулярных параметров показал качественное соответствие кристаллической и газовой структур молекулы, при этом отмечено, что основное отличие наблюдается в относительной ориентации шести- и пятичленных циклов.

Ключевые слова: кристаллическая структура, рентгеноструктурный анализ, 1,2,4-триазол, 4-этил-5-(2-гидроксифенил)-1,2,4-триазол-3-тион, квантово-химические расчеты, метод DFT, геометрические и энергетические характеристики.

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