International Journal of Academic Pedagogical Research (IJAPR)
ISSN: 2643-9123
Vol. 5 Issue 5, May - 2021, Pages: 104-106

Synthesis, Structure, Tautomerism And Investigation Of Some Quantum Chemical Parameters Of Compound 2-(4,6-Dioxo-1,3,5-Triazinan-2-Ylidene)Hydrazinecarboxyamide

1Bakhtiyor Shukurullayevich Ganiyev and 2Ferangiz Sadilloyevna Aslonova

1Lecturer of Bukhara State University. M. Ikbol 11, 200117, Bukhara, Uzbekistan
E-mail: b.ganiyev1990@gmail.com
2Student of Bukhara State University. M. Ikbol 11, 200117, Bukhara, Uzbekistan
E-mail:aslonovaferangiz@gmail.com

Abstract: *This article describes the synthesis and tautomerism of 2-(4,6-dioxo-1,3,5-triazinan-2-ylidene) hydrazinecarboxyamide. The synthesized compound was investigated using elemental analysis methods, and quantum chemical calculations performed in ChemCraft 1.8 and Gaussian programs. Composite methods of the Gaussian family (G4) and density functional theory (DFT) methods (BLYP / 6-311 + G (d, p)) were used. The data obtained indicate that the BLYP / 6-311 + G (d, p) well suited for describing such systems in order to save machine resources. Based on the calculated resistance series, it was established that the main form is diketo-enolform.*

Keywords: isocyanuric acid, semicarbazide, tautomerism, molecule, charge, structure, quantum chemical calculations.

Introduction

Triazine compounds are an important class of heterocyclic chemistry and are being intensively studied [1, 2].

Cyanuric acid is an inexpensive, commercially available reagent used to prepare a variety of s-triazine derivatives. The ease of displacement of oxygen atoms in isocyanuric acid by various nucleophiles enhances the usefulness of this reagent for the preparation of mono-, di-, and three substituted 1,3,5-triazine derivatives under controlled temperature conditions [3, 4].

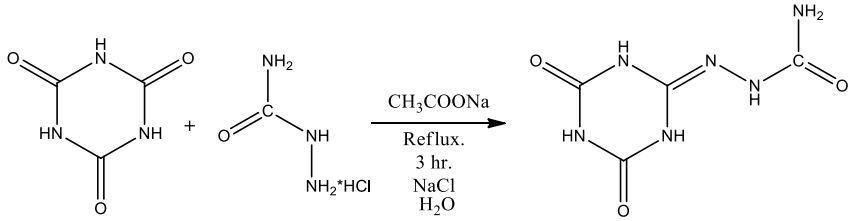
Triazine frameworks served as the basis for the development of compounds with a wide range of properties useful in medicinal and agricultural applications [5-7].

The reactivity of the functional groups of substituents attached to the 1,3,5-triazine ring system also have aroused considerable interest. Recently, the reactivity of peripheral functional groups on aryl substituents added to the structural units of the monomer type s-triazine AB_2 are used in the synthesis of hyperbranched polymers [10, 11]. Although some quantum-chemical parameters of hydrazone and semicarbazone of isocyanuric acid have been studied and calculated at work [8,9], the reactivity of its peripheral functional groups have not been studied.

Experimental part

Synthesis of isocyanuric acid semicarbazone.

To 0.446 g (0.004 mol) of hydrochloric semicarbazide in 50 ml of water, 0.516 g (0.004 mol) of isocyanuric acid in 100 ml of water was added dropwise with stirring, and then 0.41 g of sodium acetate was added. The reaction mixture was left for 3 days at room temperature. Precipitated polycrystalline precipitate 1.02 g (78%) 2-(4,6-dioxo-1,3,5-triazinan-2-ylidene)hydrazinecarboxyamide (H_2L^1), melting point 177-183 ºC, which was filtered out, washed with a small amount of benzene and hexane [10-12]. Recrystallization of H_2L^1 from a mixture of ethanol and benzene in a ratio of 1:1.5 gave brown monoclinic crystals. Found,%: C, 25.81; H, 3.25; N, 45.15; O, 25.79. Calculated for $C_4H_6N_6O_3$,%: C 25.77; H 3.22; N 45.17; O 25.84 [9.15].

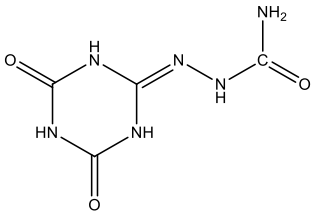


Results and discussion

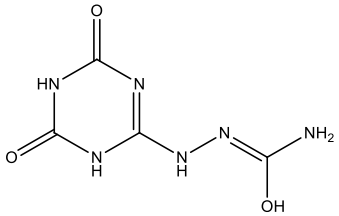
The organic ligands obtained by us studied the keto-enol (4 tautomeric forms) tautomerism of 2-(4,6-dioxo-1,3,5-triazinan-2-ylidene) hydrazinecarboxyamide. The relative stability of tautomers calculated using by quantum-chemical methods in view of condensed phase for the water and dimethyl sulfoxide (DMSO).

The method of quantum chemistry is used to study the photophysical properties of linear and angular semicarbazides and thiosemicarbazides with conjugated external carbonyl compounds. Our theoretical approach is based on the concepts and methods of quantum chemistry and the theory without radiative transitions in polyatomic organic molecules [13-16].

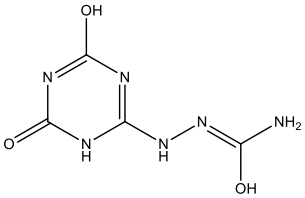
International Journal of Academic Pedagogical Research (IJAPR)
ISSN: 2643-9123
Vol. 5 Issue 5, May - 2021, Pages: 104-106



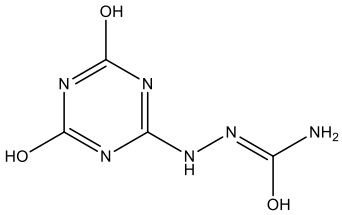
A)2-(4,6-dioxo-1,3,5-triazinan-2-ylidene)hydrazinecarboxamide



Б) (Z)-N'-(4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-yl)carbamohydrazonic acid



C) (Z)-N'-(4-hydroxy-6-oxo-1,6-dihydro-1,3,5-triazin-2-yl)carbamohydrazonic acid



Д) (Z)-N'-(4,6-dihydroxy-1,3,5-triazin-2-yl)carbamohydrazonic acid

Geometry optimization and conformational analysis of H_2L^1, a representative of the group of effective carbonyl and hydroxyl agents in the synthesis of semicarbazone or thiosemicarbazone ligands, were performed in the Chem3D Pro 12.0 program using an extended and modified version of the MM2 force field by the method of molecular mechanics [8,9,17,18].

For calculations by the method of molecular mechanics and molecular dynamics in Chem3D Pro 12.0, there is an MM2 item in the Calculations menu, in which there are the corresponding Minimize Energy items to optimize the geometry of the molecular system and Molecular Dynamics to run the molecular dynamics algorithm. The calculation results are presented in the form of table 1.

Table 1.

Analysis Results of Minimize Energy

Compound	A	Б	C	Д
Stretch:	0.3065	0.4913	0.4343	0.4023
Bend:	5.4504	4.4746	4.2657	3.1684
Stretch-Bend:	0.0438	-0.0022	0.0291	0.0030
Torsion:	9.3529	4.9200	0.8400	0.0160
Non-1,4 VDW:	-1.9163	-2.3810	-2.7916	-3.0005
1,4 VDW:	-6.9144	1.4374	6.1543	9.3533
Dipole/Dipole:	-20.7114	-6.0702	-4.5543	5.2488
Total energy:	-17.3859 kcal/mol	2.8699 kcal/mol	4.3777 kcal/mol	15.1912 kcal/mol

We calculated geometric parameters (bond lengths, bond and torsion angles) and conformational analysis for 2-(4,6-dioxo-1,3,5-triazinan-2-ylidene) hydrazinecarboxyamide in the special application Chem3D Pro 12.0 of the software package ChemOffice Ultra [14] using an extended and modified version of the MM2 force field by molecular mechanics.

Conclusion

In this way, a series of relative stability of the tautomers of 2-(4,6-dioxo-1,3,5-triazinan-2-ylidene) hydrazinecarboxyamide was calculated taking into account nonspecific (water, DMSO) and specific solvation in water (six-water cluster). It follows from quantum chemical calculations that the most stable tautomer of isocyanuric acid semicarbazone in all calculation models is diketo-enolform.

Acknowledgements

The authors are grateful to Doctor of Chemical Sciences, Professor of the Academician Sadykov Institute of Bioorganic Chemistry of the Academy of Sciences of the Republic of Uzbekistan Ashurov Jamshid Mengnorovich and Associate Professor of Samarkand State University of Uzbekistan Abdulla Kuvatov, as well as the Institute staff of Bioorganic Chemistry of the Academy of Sciences of Uzbekistan for their practical assistance in preparing the article.

REFERENCES

1. G. Giacomelli, A. Porcheddu, 1,3,5-Triazines, In Comprehensive Heterocyclic Chemistry III; K. Turnbull (Eds.), Elsevier Science & Technology, **2008**, 197-290.

2. E. M. Smolin, L. Rapoport, s-Triazine and Derivatives in The Chemistry of Heterocyclic Compounds; Interscience: New York, **1959**.

3. V. I. Mur, *Russ. Chem. Rev.*, **1964**, 33, 92–103 and references therein.

4. M. E. Quirke, 1,3,5-Triazines. Comprehensive Heterocyclic Chemistry; Katritzky, A. R., Rees, C. W., Eds.; Pergamon: New York, NY, **1984**, 3, 457–530.

5. D. L.Comins, O′ ’Connor. Advances in Heterocyclic Chemistry; Katritzky, A. R., Ed.; Academic: New York, NY, **1988**, 44, 243.

6. G. Giacomelli, A. Porcheddu, L. De Luca, *Curr. Org. Chem.*, **2004,** 8, 1497–1519.
7. H. M. LeBaron, J. E. McFarland, O. C. Burnside, The Triazine Herbicides; Elsevier, San Diego, USA, **2008**.

8. Ganiyev B., Ostonov F., Kholikova G., Salimov F. Calculations of quantum chemical parameters of the compound of isocyanuric acid with semicarbazide // International Independent Scientific Journal. 2020. Vol.2. №. 16. P. 3-9.

9. Ganiev B.Sh., Kholikova G.K., Salimov F.G. Synthesis and research by methods of IR spectroscopy and quantum chemistry -6–((2,4-dinitrophenyl) hydrazone-1,3,5-triazinane-2,4-dione // Universum: Chemistry and biology: electronic scientific journal. 2020. №. 6 (72). P.

10. Puchkov Sergey Veniaminovich. Computer technologies in science, technology, education. Calculations of physicochemical and thermodynamic characteristics of organic compounds: guidelines for laboratory work and independent work. – Kemerovo: KuzGTU, 2013 .—P. 23

11. A short reference book of physical and chemical quantities / ed. A. A. Ravdel, A. M. Ponomareva. – 9th ed., Rev. and add. – SPb .: Special Literature, 1999 .—P. 232

12. Ganiev B.Sh., Kholikova G.K., Salimov F.G. The use of cyanuric acid as an environmental disinfectant. Materials of the international scientific conference “Innovative solutions to engineering and technological problems of modern production.” 2 VOL. 14-16 nov. Bukhara, -2019. P. 21-23

13. ChemOffice // CambridgeSoft [Electronic resource]. – Mode of access : http://www.cambridgesoft.com/software/details/?ds=1. – Date of access : 22.11.2010.

14. Soloviev, M.E. Computer chemistry / M.E. Soloviev, M.M. Soloviev. – M.: Solon-Press, 2005 .—536 p.

15. Litvak M.M. Calculation of geometric parameters and conformational analysis of 1,2-O-cyanoethylidene derivatives of carbohydrates by the method of molecular mechanics // Scientific Bulletin of Belgorod State University. Series: Natural Sciences. -2012. – T.21. – №.21 (140)

16. Litvak M.M. Computer as a research tool in the study of chemistry and related disciplines // Scientific Bulletin of Belgorod State University. Series: Humanitarian Sciences. -2014. – T.21. – №. 6 (177)

17. Shibayama, A.; Kajiki, R.; Kobayashi, M.; Mitsunari, T.; Nagamatsu, A. 6-Acyl-1,2,4-triazine-3,5-dione derivative and herbicides. Patent WO 2012002096; Chem. Abstr. 2012, 156, 122559.

18. Fesenko, Anastasia A., et al. “N2-Alkylation of semicarbazones. A general and efficient protocol for the synthesis of 2-alkylsemicarbazides from semicarbazide.” Organic Chemistry part ii (2019): 176-189.

19. Abdurakhmonov SF et al. Synthesis and study of binuclear complexes of vanadyl (II) based on bis-5-hydroxypyrazolines // Universum: chemistry and biology. – 2019. – №. 12 (66). -P. 50-55