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Investigation by IR Spectroscopy and Quantum Chemical Methods 2-(4,6-Dioxo-1,3,5-Triazinan-2-Ylidene) Hydrazinecarboxyamide

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Annotation: This article describes the synthesis and IR spectroscopy of 2-(4,6-dioxo-1,3,5-triazinane-2-ylidene)hydrazine carboxamide. The synthesized compound was investigated using the methods of elemental analysis and quantum chemical calculations performed in the ChemCraft 1.8 and Gaussian programs.

The semicarbazone of isocyanuric acid was studied using IR spectroscopy methods and quantum chemical parameters compared with the theoretical data on experimental parameters using the Avogadro, ChemCraft 1.8. and Gaussian programs.

Keywords: isocyanuric acid, semicarbazide, IR spectroscopy, structure, quantum chemical calculations.

INTRODUCTION

Triazine compounds represent an important class of heterocyclic chemistry and are 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 production of mono-, di- and three substituted derivatives of 1,3,5-triazine under controlled temperature conditions [3, 4].

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

The reactivity of functional groups of substituents attached to the 1,3,5-triazine ring system also have drawn considerable interest. Recently, the reactivity of peripheral functional groups on aryl substituents added to the structural units of the s-triazine AB2 monomer type has been used in the synthesis of hyperbranched polymers [10, 11]. Although some quantum chemical paramers of hydrazone and semicarbazone have been studied and calculated [8,9], isocyanuric acid, but the reactivity of its peripheral functional groups has not been studied.

THE EXPERIMENTAL PART

SYNTHESIS OF ISOCYANURIC ACID SEMICARBAZONE

0.516 g (0.004 mol) of isocyanuric acid in 100 ml of water was added to 0.446 g (0.004 mol) of hydrochloric acid in 50 ml of water with stirring, drop by drop, 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-triazinane-2-ylidene) hydrazine carboxamide (H_2L^1) with T_{sol} 177-183 ^oC, which was filtered out, was washed with a small amount of benzene and hexane [10-12]. Recrystallization of H_2L^1 from a mixture of ethanol and

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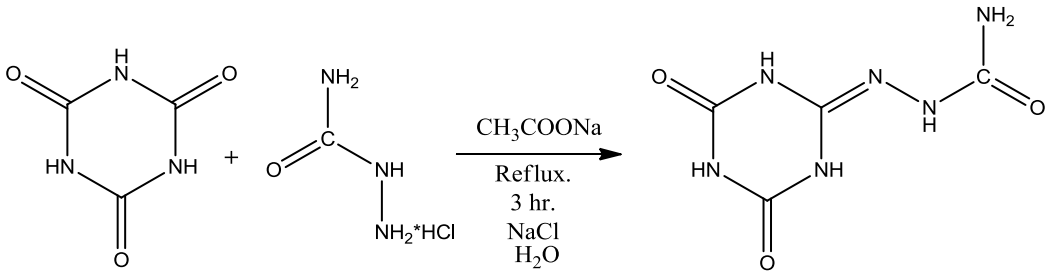
benzene in a ratio of 1:1.5 produced brown monoclinic crystals. Found, %: C, 25.81; H, 3.25; N, 45.15; O, 25.79. For $C_4H_6N_6O_3$ calculated, %: C 25.77; H 3.22; N 45.17; O 25.84 [9.15].



RESULTS AND DISCUSSION

The IR spectroscopic study was carried out on the basis of the Institute of Bioorganic Chemistry of the Academy of Sciences of the Republic of Uzbekistan (IBCh of the Academy of Sciences of the Republic of Uzbekistan). Fourier transform infrared spectra (FTIR) for dried substances were recorded using a Shimadzu IR spectrophotometer (Model 8300) in the range from 400 to 4000 cm^{-1} in the form of KBr tablets [3-5].

In the IR spectrum of the semicarbazone of isocyanuric acid H_2L^1 (Fig. 1,3), the vibrational frequency ν(C=N) (1610.92 $cm^{-}1$) compared with the IR spectrum of the calculation in the Avogadro software package (the absorption band ν(C=N) (1594.53$cm^{-}1$) is shifted to the low frequency region by 6.39 $cm^{-}1$ [6-8,16].

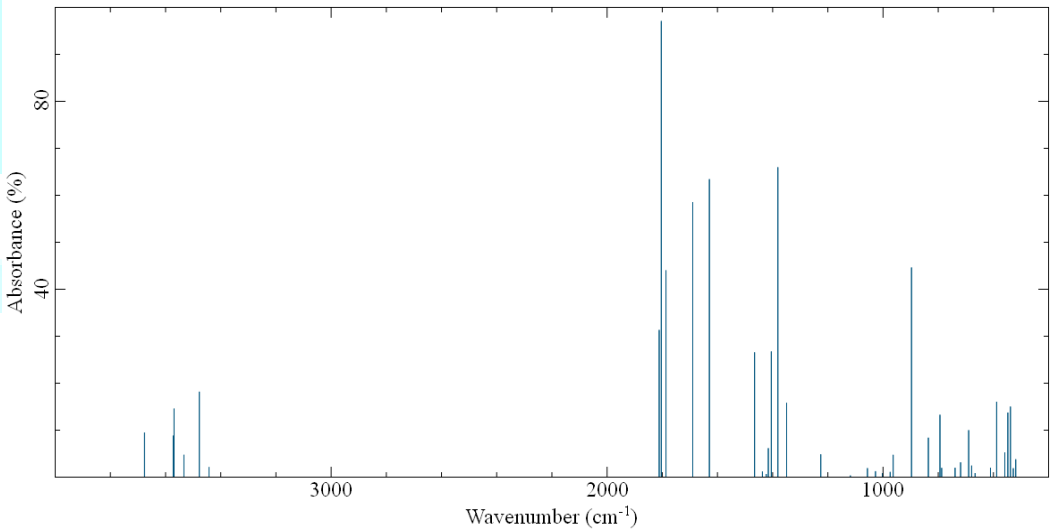


Fig.1. IR spectrum of organic compound 2-(4,6-dioxo-1,3,5-triazine-2-ylidene)hydrazine carboxamide (H_2L^1), calculated using the AVOGADRO program

Studying the C-N spectra: the frequency of stretching C-N is quite a difficult task, since there is mixing of several bands in this area. Sundaraganesan et al. [13] assigned a group of 1689 sm^{-1} to C=N and C-N, respectively, valence vibration for the benzimidazole compound.

IR spectroscopy of the intense absorption band of the NCO group in the region of 2300 sm^{-1} in the reaction mixture. Prbavatiy et al. [14] reported that the band at 1575 sm^{-1} in the FTIR spectrum and 1540 sm^{-1} in both the FTIR and the Raman spectrum is up to C=N valence oscillations.

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Stretching C-N usually lies in the region of 1400-1200 sm^{-1}. In this study, very strong C-N stretching oscillations of the isocyanuric acid semicarbazone were detected between 1778, 1752 and 1463 sm^{-1} in the IR range and a very strong band at 1727 sm^{-1}, a very weak band at 1469 sm^{-1} and 1418 sm^{-1} in the FT-IR spectrum.

If we compare the IR spectra obtained experimentally with the data of theoretical calculations performed in the Gaussian program, it can be noted that some spectra have the same or similar parameters, while others differ greatly.

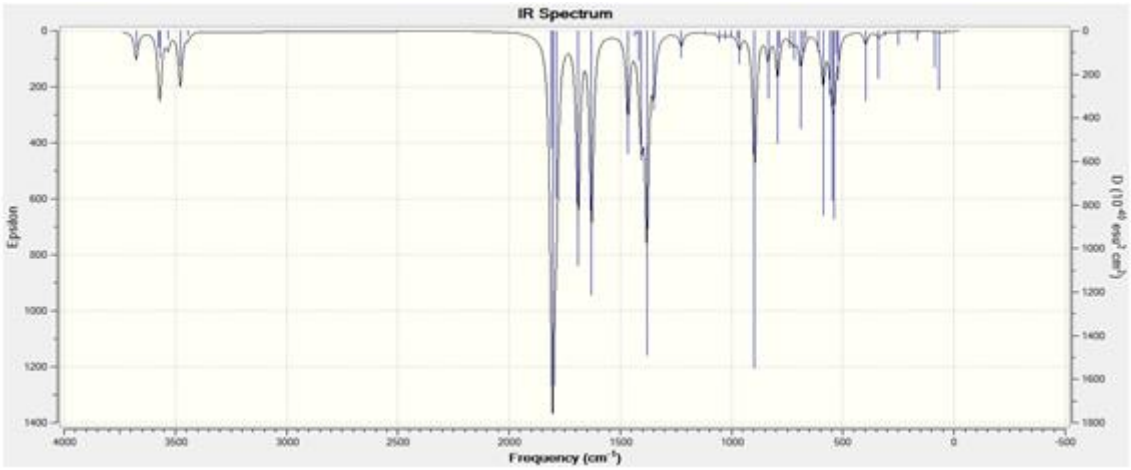

Fig.2. IR spectrum of organic compound 2-(4,6-dioxo-1,3,5-triazine-2-ylidene)hydrazine carboxamide (H_2L^1), calculated using the GAUSSIAN program

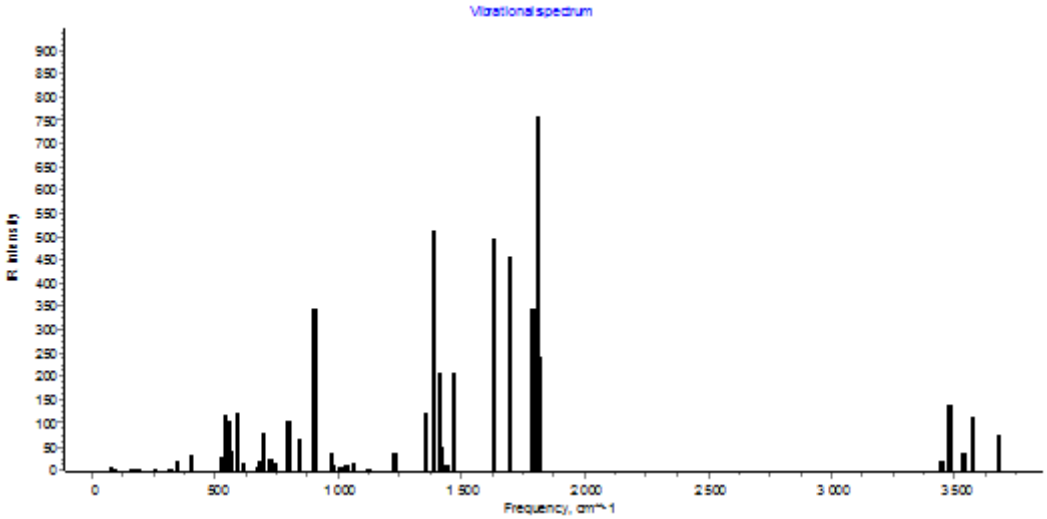

Fig.3. IR spectrum of organic compound 2-(4,6-dioxo-1,3,5-triazine-2-ylidene)hydrazine carboxamide (H_2L^1), calculated using the Chem Craft 1.8 program

CONCLUSION

Thus, the quantum chemical calculations carried out are 2-(4,6-dioxo-1,3,5-triazinane-2-ylidene)hydrazine carboxamide shows the activity of the structure of the molecule and the possibility of obtaining substances with antibacterial and antifungal activity. Also, the resulting substance is very promising for their use in the synthesis of new complex compounds.

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