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Review

Theoretical investigation of 4-amino triazolylpentazole: A breakthrough to nitrogen-rich heterocycles

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ABSTRACT

The novel investigation of 4-amino triazolylpentazole has been studied when triazolylpentazole was substituted with amino group, this could be investigated by the computational methods. Since the generation of molecular nitrogen as an end-product is highly designed in order to avoid environment pollution and health risks, as well as to reduce detective plume signatures, compounds containing a backbone of directly linked nitrogen (catenated nitrogen) are of great interest. The theoretical evidence of the possibility to synthesize of triazolylpentazole is a major challenge for nitrogen-rich chemistry.

Contents

1. Introduction

The present scenario of nitrogen-rich compounds is highly promising. The energetic materials with high energy densities are environmentally favorable since the decomposition of these materials would ideally produce only the molecular nitrogen (N_2), which is environmentally acceptable as per the study of several literature procedures. Recently, the new remarkable polynitrogen species like $N5^-$, $N5^+$, $N5^+N5^-$, $N3^-$, $N11^+$, $N11^-$, $N6^-$, radical anion were investigated [1,2] and computational studies have been identified several polynitrogen compounds as suitable candidates for synthesis purpose. Perhaps apart from dinitrogen, azidopentazole is believed to be the most promising candidate for synthesis of a compound consisting only of nitrogen atoms in its parentheses. But some of the substituted pentazoles was synthesized by some eminent scientist such as phenyl pentazole by Huisgen and Ugi [3] and Polyazapentalenes have been investigated by Elguero, Claramunte et al. [4,5]. But no new pentazole derivatives of 4-amino triazolylpentazole (**2**) have been investigated since the first reports on pentazole compounds is available in the literature in the late 1950's.The main objective of this study is to find out theoretical evidence for a pentazole compound with the highest possible nitrogen content [6,7], because in spite of

Abbreviations: ΔHf^O, Standard heat of formation (kcal/mol); ρ (rho), Density (g/cm^3); N–N, Nitrogen nitrogen single bond; N=N, Nitrogen nitrogen double bond; N_2, Dinitrogen; ΔE, Change in energy; ΔG^O, Change in free energy; R_1, Substituent's (R_1 = H, NH_2); NH_2, Amino group; C2, Space group; *a* (Å), Bond length (Å); *b* (Å), Bond length (Å); *c* (Å), Bond length (Å); β (deg), Bond angle (°C).

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all research only four solids with nitrogen contents greater than 90% i.e. NH_4N_3, $N_2H_5N_3$, $N_2H_5N_3$, N_2H_4 and $LiBN_{12}$ are available in the literature [8,9]. Since polynitrogen compounds are very difficult to synthesize in the academic laboratory. To avoid this situation a well equipped laboratory is very essential to carry out research because of its high energy and density [10]. So the author is completely interested to pursue a theoretical study regarding this new molecule, and a sincere effort continues to convert the same ideology into an experimental orientation in our laboratory. Again, the author expects, it will be possible to achieve the target from experiment in our laboratory conditions in near future. In this context, the author has been interested to predict the spectral characteristic and some computational study of triazolylpentazole species exclusively in this communication [11,12].

2. Results and discussion

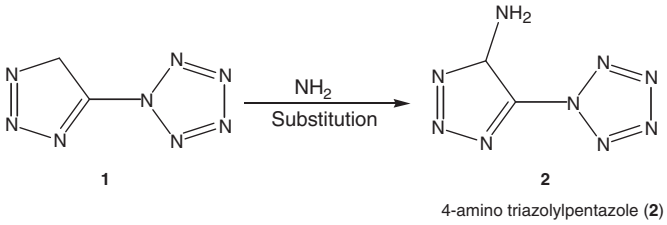
The synthesis of the predicated molecule is a single step substitution reaction, but it is very difficult to synthesize in academic laboratory. The author proposed the synthesis process in theoretically since there is no literature available regarding this novel molecule till now. The author is wondering to find out the synthesis methods/conditions in the next part of his work because it is difficult to find out in the present investigation. So it may be easy to synthesize the same in high energy research laboratory. Still then, the research is going on smoothly at your centre. The results are shown in Scheme 1.

Triazolylpentazole
Chemical formula: $C_2H_2N_8$
Exact mass: 138.0402
Elemental analysis: C, 17.42; H, 1.46; N, 81.14

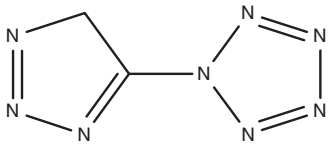
From the study of elemental analysis, it suggests that the starting material is a nitrogen-rich compound as it contains very good percentage of nitrogen in its parentheses. So the author hopes that it is a very good starting material to synthesize the target molecule. The results are shown in Scheme 2. The selected studies of bond length (Å) and bond angle (°C) of triazolylpentazole (**1**) were determined by a computational method. The results are shown in Table 1.

5-(2H-pentazol-2-yl)-4H-1, 2, 3-triazol-4-amine
Chemical formula: $C_2H_3N_9$
Exact mass: 153.05
Molecular weight: 153.11
M/z: 153.05 (100.0%), 154.05 (5.5%)
Elemental analysis: C, 15.69; H, 1.97; N, 82.34

From the study of elemental analysis, it suggests that the predicated molecule is a nitrogen-rich compound as it contains very good percentage of nitrogen in its parentheses. It will produce more heat of formation and it may be useful in future defence sciences. So it is quite encouragable to investigate this molecule in a greater expects in your laboratory. The results are shown in Scheme 3.



Scheme 1. The synthesis of the predicated molecule in a single step reaction.



Scheme 2. Molecular mass and elementary analysis of triazolylpentazole (1).

3. Spectral characterization of 4-amino triazolylpentazole

The characteristic study of predicated polynitrogen compound could be determined as shown in the MS(%), C,H,N analysis, molecular weight, molecular formula, ^{1}H NMR and ^{13}C NMR spectroscopy.

3.1. ^{1}H and ^{13}C NMR spectra of 4-amino triazolylpentazole

The ^{13}C NMR spectral data's of the molecule are discussed and the results are given in Fig. 1.

Protocol of the ^{13}C NMR predictions:

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
C	164	162.8	1-imine
		0.9	1-C
		?	1unknown substituent(s)
		0.0	1-R from N-imine
			−>1 increment(s) not found
CH	61.8	−2.3	Aliphatic
		14.9	1 alpha −C=N
		56.6	2 alpha −N
		22.6	2 beta −N
		−10.2	2 gamma −N
		0.0	2 delta −N
		−19.8	General corrections

Herein, the author was stated that some of the substituent's of amino group containing heterocyclic ionic salts as per the literature process.

Substituent's	α	β	γ	δ
NH_2	−29.0	−11.4	+4.6	−0.6
NH_3^+	−26.0	−7.5	4.6	0

The ^{1}H NMR spectroscopic data's are quite dependable and represented in Fig. 2.

Protocol of the ^{1}H NMR predictions:

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
NH_2	2.0	2.00	Amine
CH	2.6	1.50	Methine
		1.13	1 alpha −N
		?	2 unknown alpha substituent(s)
			−>2 increment(s) not found

Example 1, substituent's parameters of NH_2

Substituent's	α	β	γ	δ
NH_2	−29.0	−11.4	+4.6	−0.6

From the study of literature, it was confirmed that the ^{13}C–^{1}H coupling constant range (~110–320 Hz)

Interaction	Terminal and internal				Terminal and internal
Substituent's	α		β		γ
NH_2	+29	+24	+11	+10	−5
CH_3	+9	+6	+10	+8	2