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CONFORMATIONAL ANALYSIS AND INTRAMOLECULAR HYDROGEN BONDING IN HEPTANE-3-AMINO-5-ONE

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Introduction

β-Ketoamines are a class of chemical compounds which form an intramolecular hydrogen bonded system assisted by resonance [1]. These compounds are capable of forming complexes with metal ions [2]. To identify the structure and stability of these complexes, the structure and intramolecular hydrogen bond strength of the ligands should be investigated.

In this study, all theoretically possible conformers of heptane-3-amino-5-one, a *β*-ketoamine compound, are optimized using density functional theory (DFT) to identify the stable conformers. The strength of hydrogen bond in all stable conformers is estimated not only by considering the geometrical parameters obtained from the theoretical calculations, but also by calculating the hydrogen bond energies using Bader's atoms in molecules (AIM) theory and natural bond orbital (NBO) analysis.

Methods

All calculations have been performed at the B3LYP/6-311++G** level of theory, using Gaussian 09 program [3]. To obtain the stable conformers of the titled molecule, the C_2H_5 groups at both sides of the molecule, were rotated around C2-C3 and C5-C6 bonds (Fig. 1). The electron densities, Laplacian of the critical point of NH···O bond, and the hydrogen bond energies were calculated by AIM2000 program [4].

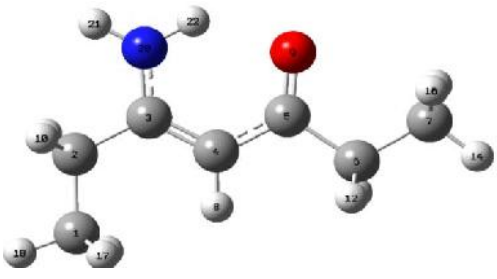

Fig.1. Atom numbering of heptane-3-amino-5-one.

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Results and Discussion

Theoretically, 10 conformers were possible for heptane-3-amino-5-one. However, according to our calculations, 4 stable conformers were obtained, which their N···O distances are in the range of 2.649-2.678 Å. It confirms that the hydrogen bond in this molecule is considerably stronger than 4-amino-3-penten-2-one (APO) [5]. The difference between the studied compound and APO is the substitution of the $–CH_3$ groups by the $–C_2H_5$ groups in the chelated ring of APO. According to our study, two factors are responsible for this interesting bond strength, i.e., steric effect and inductive effect. The results obtained from AIM and NBO calculations also confirm the above conclusion.

Conclusions

The structure and intramolecular hydrogen bond strength of heptane-3-amino-5-one has been investigated using B3LYP/6-311++G** level of theory. The results indicate that 4 out of 10 conformers are stable and the strengths of the intramolecular hydrogen bonds in these conformers are considerably higher than the simplest similar molecule (APO).

References

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