Asian Journal of Chemistry; Vol. 25, No. 13 (2013), 7635-7636

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2013.14473

*NOTE*

# Theoretical Studies of the Glycoluril Molecular Clips Using Quantum Calculations

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(*Received*: 24 August 2012; *Accepted*: 5 July 2013) AJC-13771

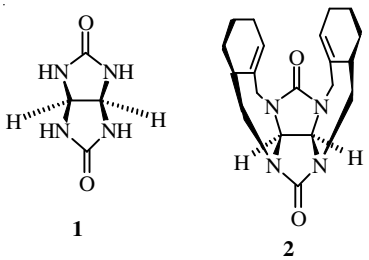
Theoretical calculations were performed to determine the structure of a simple glycoluril (**1**) and its derivative (**2**). Full geometry optimizations were carried out by MP2 method using 6-311++G** basis set of the GAUSSIAN 98 program. The geometrical parameters including bond lengths (R) and bond angles (A) were estimated at the same level.

**Key Words: Glycoluril, Quantum calculations, Molecular clip.**

The glycolurils have been received a great deal of attention due to their practical applications, such as fertilizers[1] polymer crosslinking[2], explosives[3], stabilizers of organic compounds[4], combinatorial chemistry[5], bleaching activators[6] and in supramolecular chemistry[7].

Follow up of our work[8], the MP2 calculations were carried out on the simple glycoluril (**1**) and its derivative which have two benzene walls, **2**.

Full geometry optimizations were carried out for a simple glycoluril (**1**) and its derivative with two benzene walls, **2**, by the MP2 method using 6-311++G** basis set of the GAUSSIAN 98 program[9-11] (**Scheme-I**). To find a global minimum on a specific surface, all possible conformations of the given species were examined through scanning the specific dihedral angles at B3LYP/6-311++G** level. All calculations were carried out for gas phase at 298 K temperature and **1** atm pressure.



**1** **2**

**Scheme-I:** Molecular structure of glycoluril (**1**) and its derivative (**2**)

Thermal energies (E), enthalpies (H) and Gibbs free energies (G) were calculated for a simple glycoluril, **1** and its derivative (**2**) with two benzene walls at MP2/6-311++G**// B3LYP/6-311++G** level of theory (**Scheme-I**). Geometrical parameters including bond lengths (R) and bond angles (A) were estimated at the same level.

The C=O bond lengths in **1** and **2** are 1.209 and 1.215 Å, respectively which indicate the C=O bond is stronger for **1** with respect to **2**. Moreover, the N-C (amide) bond lengths in **1** and **2** are 1.391 and 1.386 Å, respectively. Therefore, the C=O bond length in **1** and **2** changed in contrast to the N-C (amide) bond length which indicate that the conjugation of the lone pair electrons of nitrogen atoms with the C=O bond in **2** is more than **1**.

The N-CH bond lengths in **1** and **2** are 1.454 and 1.449 Å, respectively. The CH-CH bond length in **1** and **2** are 1.567 and 1.558 Å, respectively. Two carbon atoms of two benzene rings selected to compute the distance between the two benzene rings in **2**. The distance of two carbon atoms of two benzene rings in **2** is 6.587.

The N-C-N bond angles in **1** and **2** are 116.26º and 84.97º, respectively. It seems that two benzene rings lead to decrease the bond lengths of the N-C-N **2**.

The highest occupied orbital molecular HOMO and lowest unoccupied molecular orbital LUMO of **1** and **2** were calculated. It appears that the HOMO and LUMO of **1** are -11.53 and 1.23 eV, respectively. The HOMO and LUMO of **2** are -8.97 and 1.29 eV, respectively. The energy of the HOMO in **2** is higher with respect to **1** which indicates the nucleophilic character of **2**. The LUMO of **1** is similar to **2** that indicate identical electrophilic character of **1** and **2**.

## Conclusion

Full geometry optimizations were carried out for a simple glycoluril (**1**) and its derivative (**2**) with two benzene walls, by DFT method using 6-311++G** basis set of the GAUSSIAN 98 program. The C=O bond length in **1** and **2** changed in contrast to the N-C (amide) bond length which indicate that the conjugation of the lone pair electrons of nitrogen atoms with the C=O bond in **2** is more than **1**. The HOMO and LUMO studies indicated that the nucleophilic character of **2** is more than **1**.

## ACKNOWLEDGEMENTS

Islamic Azad University, Miyaneh Branch is gratefully acknowledged for financial support of this research.

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