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Tautomerism and Minimum Polarizability Principle

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Abstract

Computational chemistry is a branch of quantum chemistry which is related to analyzing, reviewing and measuring some systems properties that they can't be measured directly, so it uses math and statistics and it branches in two: Molecular Mechanics Theory and Electronic Structure Theory. In this research, we tried to review some of the molecules which are tautomered for each other and according to the acquired energy (zero point energy), select their stability from and review the Minimum Polarizability Principle. This principle states that the system goes along a status in order to reach the minimum polarizability. So, according to this principle, any molecule which has the least polarizability, it would have the maximum stability.

Keywords: Tautomer, Stability, Computational Chemistry, Minimum Polarizability Principle

Materials and Methods:

In computational chemistry the following four different methods are manipulated:

1- Molecular mechanics method
2- 2- Semi- empirical method
3- Ab initio method
4- Density Function theory (DFT) method

In this research, calculations were followed through several methods and they were compared to each other.

In this research in order to review the information, CNDO method, semi-empirical methods, HF (Hartree-Fock) method from Ab initio approaches and B3LYP from density function theory methods were followed.

It's necessary to mention that the various basis sets were also changed in order to specify the best method and the basis set. 6-31G** and 6-311++G** from the basis sets were used in B3LYP and HF methods.
Polarizability is defined as measuring electronic density changes in an electronic field, e.g.:

$$\propto = -\left(\frac{\partial^2 E}{\partial F_a \partial F_b}\right) \qquad a, b = x, y, z$$

To calculate that, the following relation is used: $\propto = \frac{1}{3}(\propto_{xx} + \propto_{yy} + \propto_{zz})$

Apparatuses:

In order to achieve the required result, Hyper Chem. and Gaussian softwares were used. The first software draws the molecule and optimizes that and then that molecule coordinates enter Gaussian software to draw its precise structure bond length and its several minimums.

Results and discussion:

The achieved results in HF method didn't have great changes through a change in the basis set and this approach has very little mismatch with the minimum polarizability principle.
In the B3LYP method the number of breechings the principle was too much but there wasn't too much change in the results when the basis set changed.

Conclusion:

In determining the stability of the tautomers through calculating zero point energy (ZPE), there is too much discrepancy among the methods. Yet, in one of the method with various basis set the discrepancy would be very low (4%).
In reviewing the Minimum Polarization Principle, CNDO method has no workability because it doesn't calculate polarizability matrix elements.
HF method was very proper and it had the minimum error. B3LYP method also has an acceptable error. The change in the basis set does have any important influence in accordance with MPP principle.
Despite of the fact that the accuracy increases through shifting from CNDO to B3LYP, because all the quantomic functions are not considered and specific approximations are used, then, there's still error possibility.

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