THEORETICAL STUDY OF STRUCTURAL PROPERTIES OF AZOLES

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Abstract:- We Calculated dipole moment and polarizability of azoles(1,2,3 – Triazole 1,2,4 – Triazole, Imidazole, Pentazole, Pyrazole, Pyrrole, Tetrazole) under the frame work of D.F.T. The calculated dipole moment by density functional theory is remarkably in sensitive to the size of basis sets, once polarization functions have been included. The inclusion exist ex-charge improves the performance and provide results very close to the experimental value, even with relatively small basis sets. The calculated Polarizability of azoles by D.F.T. program are found in good agreement with the experiment the charge in average polarizability of an atom brought about by bonding must be virtual independent of nature of the bonds termed, even when the atom takes part in π system.

KEYWORDS:- molecular structure, Cache Software., DFT, dipole moment, azole. Polarizability.

1-INTRODUCTION

In recent year it has been possible to determine molecular structure by theoretical methods with increasing accuracy. of particular importance in this development has been the implementation of automated Procedures based on analytical expressions for the energy gradient. It is now routine to carry out geometry optimizations of organic molecules based on HF or correlated ab initio methods with an accuracy of ±0.02Å, or better, for bond distances. The application of ab initio methods, in particular on the HF level, has been less successful in the area of transition metal chemistry.

The inability of the HF method to supply reliable structural data for transition metal complexes can, as in the case of bond energies, be traced back to the near degeneracy error as discussed by Luthi et al. The deficiency of the HF method can be removed by configuration interaction methods. However, such method are costly and less amenable to automated geometry optimization procedures based on analytical expressions. The method based on approximate D.F.T. might be quite accurate for geometry optimizations. Approximate density functional method have not been used to the same degree as HF method in geometry optimization. On the other hand the HF program have utilized automated procedures based on analytical expressions for the energy gradients for a long time.

This situation has now changed with the derivations of analytical expressions for the energy gradients within the density functional formalism and their implementation and integration into general purpose programs. Numerous calculations on molecular of molecular structure have appeared over the past few years. Very recent calculation by Andzelm and Pederson indicate that geometrical parameters optimized by LDA are of the same quality as parameters optimized by the MP2 ab initio method for organic molecules.

It remains to be seen whether more advanced theories, in which nonlocal corrections are taken into account, will be able to supply more accurate geometrical parameters for transition-metal complexes. The HF method represents conformational energies of saturated systems. The D.F.T. based methods have proven more accurate than standard ab initio technique.
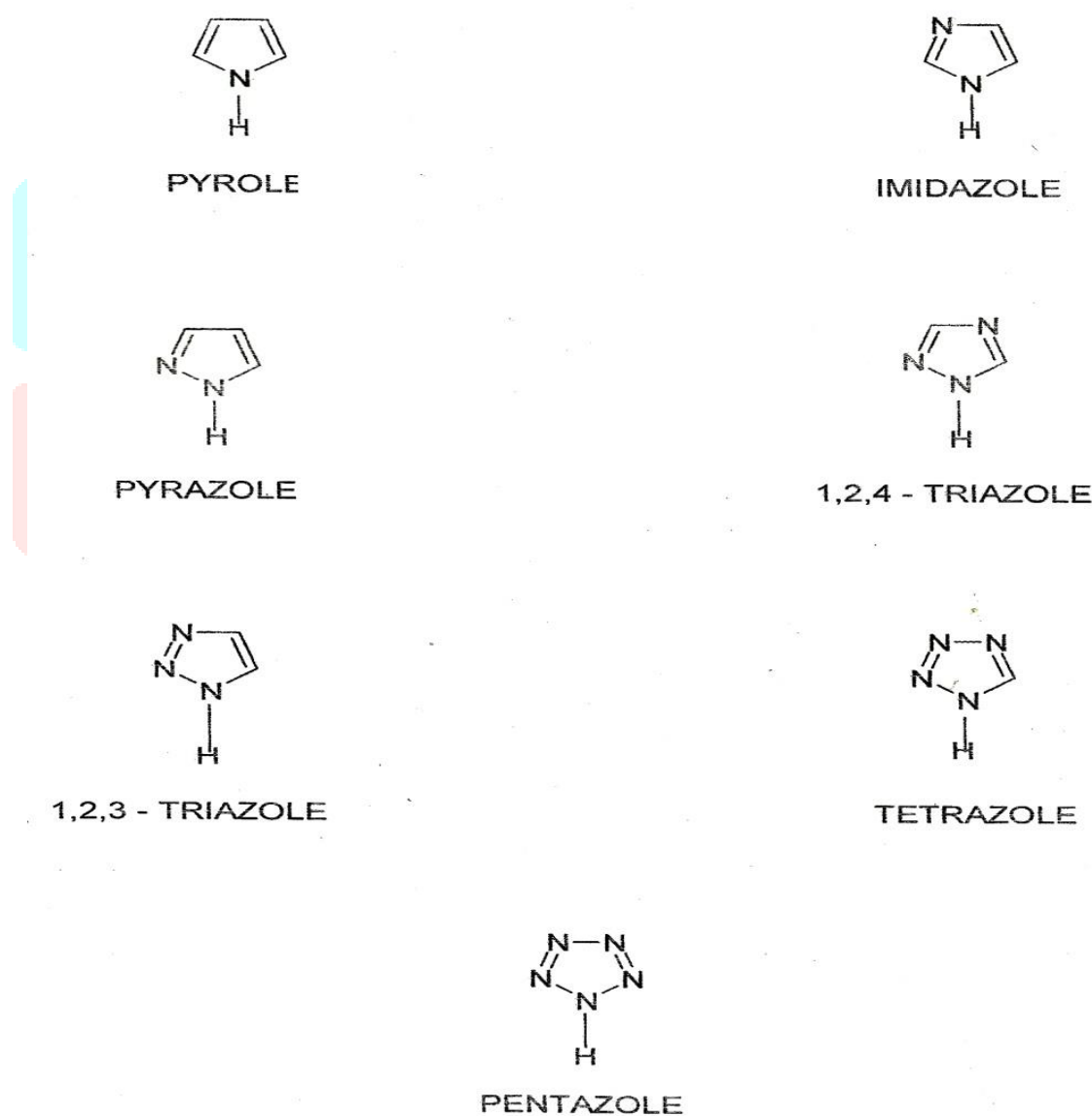

FIG.: AZOLES

2- METHOD OF CALCULATION:-

The detail of functional forms used in present Calculations has been described and discussed below. All the calculation are performed with the help of Cache Software. We have used cache software for calculating the following properties for azoles and its derivatives. Density functional theory (DFT) as long been the mainstay of electronic structure calculations in solid-state physics, and has recently become popular in quantum chemistry. This is because present-day approximate functional provide a useful balance between accuracy and computational cost, allowing much larger system to be treated than traditional *ab initio* method, while retaining much of their accuracy. Nowadays, traditional wave function method, either variational or perturbative, can be applied to find highly accurate results on smaller systems, providing benchmarks for developing density functional, which can then be applied to much larger systems.

But DFT is not just another way of solving the Schrodinger equation. Density functional theory is a completely different, formally rigorous, way of approaching *any* interacting problem, by mapping it *exactly* to a much easier-to-solve non-interacting problem. In DFT the ground state energy of an atom or a molecule is written in terms of electron density $\rho(r)$, and the external potential $v(r)$ in the form

$$E(\rho) = F(\rho) + \int dr\, \rho(r)\, v(r),$$

where $F(\rho) = T(\rho) + V_{ee}(\rho)$, $T(\rho)$ is the electronic kinetic energy functional, and $V_{cc}(\rho)$ is the electron-electron interaction energy functional. The minimization of the total energy, subject to the condition that the total number of electrons is fixed,

$$N = \int dr\, \rho(r)$$

lead to an Euler-Lagrange Equation of the for

$$\mu = (\partial E/\delta\rho(r))_v = v(r) + \partial F/\delta\rho(r),$$

where the Lagrange multiplier μ, is the chemical potential. The solution of this equation leads to the ground state density, from which one can determine the ground state energy. Parr et. al define the electro negativity as the negative of chemical potential,

$$\chi = -\mu = -(\partial E/\partial N)_v$$

In a Kohn-Sham calculation, the basic steps are very much the same, but the logic is entirely different. Imagine a pair of non-interacting electrons which have precisely the same density $n(r)$ as the physical system. This is the Kohn-Sham system, and using density functional method, one can derive its

potential v_s (r) if one knows how the total energy E depends on the density. A single simple approximation for the unknown dependence of the energy on the density can be applied to all electronic system, and predicts both the energy and self-consistent potential for the fictitious non-interacting electrons. In this view, the Kohn-Sham wave function of orbital is not considered an approximation to the exact wave function. Cache computer aided chemistry enables to apply mathematical models from classical and quantum mechanics to calculate experimental results. Cache enables create a chemical sample model and perform calculations to discover molecular properties and energy values using computational applications which apply equations from classical mechanics and quantum mechanics. If we have run an experiment that employed a quantum mechanical procedure previously, this information is already present in the sample file and we do not to re-compute it unless we have changed the geometry of the molecule.

3-RESULTS AND DISCUSSION:

3.1 DIPOLE MOMENT: The Calculated dipole moment of azoles under the frame work of D.F.T. have presented in table 1

The electrical center of positive and negative charges associated with the covalent bond may be regarded as being displaced related to one and other, So as to from a dipole. In general every covalent bond between two atoms will be associated with a dipole moment the value of this moment will be equal to the product of electronic charge and relative displacement of the positive and negative electrical centers. The magnitude of dipole moment or the polarity of bond, to we a general term depends on the relative electron attracting tendencies of the two atom concerned, varies from one element to another.

The dipole moment of the bond a regarded as victories in character that is they have magnitude and direction both. The direction of bond. Shows its direction. The dipole moment of molecules as a whole may be regarded as equal to the vector sum of individual bond moments.

Preferably symmetrical molecules has dipole moment zero they are called non polar while unsymmetrical molecules have a resultant dipole moment and they are called polar. Polar molecules having an appreciable electrostatic field.

The electronic dipole moment is an important molecular properties closely related to the charge distribution in the various orbital of the molecules. This property of molecules is a fundamental important because of two reasons.

1.   A comparison between calculated and experimental values provides a test for reliability of the wave functions and validity of calculated charge distribution.

2.   Since charge in dipole moment means charge in normal coordinates which in turn determined intensity of bands observed in the infrared spectrum of molecules.

The dipole moment may be considered as the response of wave function (energy) electric field, in the limit where the field strength is very small.

The HF dipole moment is two large, which is quite general, as the HF wave function over estimates the ionic contribution. The results to the experimental values.

The calculated dipole moment by density functional theory is remarkably in sensitive to the size of basis sets, once polarization functions have been included. The inclusion exist ex-charge improves the performance and provide results very close to the experimental value, even with relatively small basis sets.

3.2 POLARIZABILITY: The polarizability of azoles calculated by D.F.T. program has been presented in table 2

If the electrons in a molecule are easily moved as the result of a stimulus, then the molecules is easily polarizability. Thus if an applied electric field can easily induce a dipole, then the polarizability is larger. Any induced dipole will lower the energy of the system, but this stabilization might be masked by the presence of a permanent dipole. To avoid this, use is made of an alternating electric field. If the molecule has an intrinsic dipole, then the molecule will be stabilized in one direction. When the field is reversed, the molecule will be destabilized but on averaging the two effects, the results is a net stabilization due to only induced dipole we used molecular modeling Cache Software to calculator the polarizability of azoles. The computed molecular polarizability can be used to find the total tensor of the polarizability. In our molecular system; we assume that the principal molecular axis is along the axis and the two much shorts molecular uses are in the orthogonal directions.

The calculated Polarizability of azoles by D.F.T. program are found in good agreement with the experiment the charge in average polarizability of an atom brought about by bonding must be virtual independent of nature of the bonds termed, even when the atom takes part in π system. The contribution by bonding can be absorbed in to additional atomic contribution while determine in

bonding leads to large charges in the component of polarizability tensor. They have little effect on average polarizability.

These results provides a remarkable sample and effective way of estimating average molecular polarizability.

TABLE 1 : DIPOLE MOMENT

Molecule	Dipole Moment (debye)
1,2,3 – Triazole	4.459
1,2,4 – Triazole	2.902
Imidazole	3.795
Pentazole	3.93
Pyrazole	2.303
Pyrrole	1.934
Tetrazole	5.373

TABLE -2 POLARIZABILITY

Molecule	Polarizability
1,2,3 – Triazole	5.664
1,2,4 – Triazole	5.547
Imidazole	6.175
Pentazole	4.587
Pyrazole	6.158
Pyrrole	6.76
Tetrazole	5.101

CONCLUSIONS:- Theoretical study of structural properties (dipole moment and polarizability) of azoles. The dipole moment may be considered as the response of wave function (energy) electric field, in the limit where the field strength is very small. A net stabilization due to only induced dipole we used molecular modeling Cache Software to calculator the polarizability of azoles. The computed molecular polarizability can be used to find the total tensor of the polarizability. In our molecular system . we assume that the principal molecular axis is along the axis and the two much shorts molecular uses are in the orthogonal directions.

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