

Theoretical Study of Polarizability of Azoles

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Abstract- I Calculated polarizability of azoles (1,2,3 – Triazole 1,2,4 – Triazole, Imidazole, Pentazole, Pyrazole, Pyrrole, Tetrazole) under the frame work of D.F.T., 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 is 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.

Indexed Terms- Molecular structure, Cache Software., DFT, Azole. Polarizability.

I. INTRODUCTION

Density functional theory is a quantum mechanical modelling method used in physics and chemistry to investigate the electronic structure of many body systems in particular atoms molecules and the condensed phase with this theory. The properties of a many electrons system can be determined by using functional, so as functions of: -another function which in this case is the spatially dependent electron density. Hence the name density functional theory comes from the use of functional of the electron density. DFT is among the most popular & versatile methods available in condensed matter physics computational physics and chemistry. DFT has over the past decade emerged as a tangible and versatile computational method. It has been employed to obtain thermo chemical data, molecule structure as well as activation barriers; dipole moments and other one electron properties.

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

methods 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 has not been used to the same degree as HF method in geometry optimization. On the other hand, the HF programs 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.

II. 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 $\rho(\mathbf{r})$, and the external potential $v(\mathbf{r})$ in the form

$$E(\rho) = F(\rho) + \int d\mathbf{r} \rho(\mathbf{r}) v(\mathbf{r}),$$

where $F(\rho) = T(\rho) + V_{ee}(\rho)$, $T(\rho)$ is the electronic kinetic energy functional, and $V_{ee}(\rho)$ 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, $N = \int d\mathbf{r} \rho(\mathbf{r})$

lead to a Euler-Lagrange Equation of the form

$$\mu = (\partial E / \partial \rho(\mathbf{r})) v = v(\mathbf{r}) + \partial F / \partial \rho(\mathbf{r}),$$

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 $n(\mathbf{r})$ as the physical system. This is the Kohn-Sham system, and using density functional method, one can derive its potential $v_s(\mathbf{r})$ 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. In the Born-Oppenheimer approximation, we treat the heavy nuclei as fixed points, and we want only to solve the ground-state quantum mechanical problem for the electrons. In regular quantum mechanics, we much solve the Schrodinger equation:

$$\left\{ \frac{1}{2} \sum_{i=1,2} \nabla_i^2 + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \sum_{i=1,2} v_{\text{ext}}(\mathbf{r}_i) \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2) = E \Psi(\mathbf{r}_1, \mathbf{r}_2),$$

Where the index i runs over the two electrons, and the external potential, the potential experienced by the electrons due to the nuclei, is

$$v_{\text{ext}}(\mathbf{r}) = -Z/r - Z'/r - R \cdot \hat{z} / l,$$

Where Z is the charge on each nucleus, \hat{z} is a unit vector along the bond axis, and R is a chosen internuclear separation. For larger systems with N electrons, the wave function depends on all $3N$ co-ordinates of those electrons.

We note at this point that, with an exact ground-state wave function, it is easy to calculate the probability density of the system:

The probability density tells that the probability of finding an electron in d^3r around \mathbf{r} is $n(\mathbf{r}) d^3r$. For a system of two *non-interacting* electrons in some potential, $v_s(\mathbf{r})$, chosen somehow to mimic the true electronic system. Because the electrons are non-interacting, their co-ordinates decouple, and their wave function is a simple product of one-electron wave functions, called *orbitals*, satisfying:

$$\left\{ -\frac{1}{2} \nabla^2 + v_s(\mathbf{r}) \right\} \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}),$$

where $\Phi(\mathbf{r}_1, \mathbf{r}_2) = \hat{O}_0(\mathbf{r}_1) \hat{O}_0(\mathbf{r}_2)$. This is a much simple set of equations to solve, since it only has 3 coordinates. Even with many electrons, say N , one would still need to solve only a 3-D equation, and then occupy the first $N/2$ levels, as opposed to solving a $3N$ -coordinate Schrodinger equation. If we can get our non-interacting system to accurately 'mimic' the true system, then we will have a computationally much more tractable problem to solve.

III. RESULTS AND DISCUSSION

The polarizability of azoles calculated by D.F.T. program has been presented in table 1. If the electrons in a molecule are easily moved as the result of a stimulus, then the molecule is easily polarizable. 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 result is a net stabilization due to only induced dipole we used molecular modeling Cache Software to calculate 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 the calculated Polarizability of azoles by D.F.T. program is found in good agreement with the experiment the change 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 provide a remarkable sample and effective way of estimating average molecular polarizability the two much shorts molecular uses are in the orthogonal directions

TABLE - 1 POLARIZABILITY

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

CONCLUSION

A net stabilization due to only induced dipole we used molecular modeling Cache Software to calculate 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.

ACKNOWLEDGEMENT

The authors are highly thankful to the Principal, M.L.K. (P.G.) college, Balrampur, for providing necessary facilities during this work.

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