

**Bond length of Azoles calculated by using density functional theory
(DFT) implemented in the cache software**

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Abstract: This paper we discuss about bond length is a transferable property of a bond between atoms of fixed types, relatively independent of the rest of the molecule. The actual bond length between two atoms in a molecule depends on such factors as the orbital hybridization and the electronic and steric nature of the substituents. The bond length between C4-C5 in 1,2,3-triazole is 1.39 which is maximum. It means the electron negativity difference between these atoms will be minimum. The maximum bond length is found between C-C while minimum bond length is found N-H. Since bond length between N-H minimum therefore the electro negativity difference between atoms N-H will be maximum. The above trend of bond length has been also found in semi-empirical MINDO/3 calculation.

Keywords: azoles, bond length, density functional theory, cache software.

1. Introduction:

An azole is a class of five-membered nitrogen heterocyclic ring compounds containing at least one other non-carbon atom of either nitrogen, sulfur, or oxygen. The parent compounds are aromatic and have two double bonds; there are successively reduced analogs (azolines and azolidines) with fewer. One, and only one, lone pair of electrons from each heteroatom in the ring is part of the aromatic bonding in an azole. Names of azoles maintain the prefix upon reduction. The numbering of ring atoms in azoles starts with the heteroatom that is not part of a double bond, and then proceeds towards the other heteroatom. In molecular geometry, bond length or bond distance is the average distance between nuclei of two bonded atoms in a molecule. It is a transferable property of a bond between atoms of fixed types, relatively independent of the rest of the molecule. Bond length is related to bond order, when more electrons participate in bond formation the bond will get shorter. Bond length is also inversely related to bond strength and the bond dissociation energy, as (all other things being equal) a stronger bond will be shorter. In a bond between two identical atoms half the bond distance is equal to the covalent radius. The actual bond length between two atoms in a molecule

depends on such factors as the orbital hybridization and the electronic and steric nature of the substituents.

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. Now a days, 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. Nor is it a method of aromatizing empirical results. 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 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,

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

lead to an Euler-Lagrange Equation of the for

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

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 electronegativity as the negative of chemical potential,

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

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.

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 :

$$\left\{ \frac{1}{2} \sum_{i=1,2} \nabla_i^2 + \frac{1}{|r_1 - r_2|} + \sum_{i=1,2} v_{ext}(r_i) \right\} \Psi(r_1, r_2) = E\Psi(r_1, r_2),$$

3. Results and Discussion:

3.1. Bond Length: It is the average distance between the nuclei of two atoms bonded together by covalent bond. Since atoms in a molecule are always vibrating with respect to each other and hence it is not possible to determine the exact-distance between the nuclei to atom.

According to MO theory a covalent bond between two atoms is formed by the overlap of their atomic orbital. The over lapping of their atomic orbital bring the two atoms closer to each other. During overlapping when the force of attraction between the two atoms is balanced by the force of repulsion between the nuclei of two atoms then equilibrium. Distance between the two atomic nuclei is called the bond length. Bond length of azoles have been presented table 1

The following point are observed from results.

1. The bond length between C4-C5 in 1,2,3-triazole is 1.39 which is maximum. It means the electron negativity difference between these atoms will be minimum.
2. The bond length between atoms in 1,2,3-triazole has been found in following order :

$$C - C > N - C > N - H > C - H > N - H$$

The maximum bond length is found between C-C while minimum bond length is found N-H. Since bond length between N-H minimum therefore the electro negativity difference between atoms N-H will be maximum. The above trend of bond length has been also found in semi-empirical MINDO/3 calculation.

3. In 1,2,4-triazole the bond length between C2-N3 and N5-N1 is nearly same. Similarly the bond length between C3-N3 and N5-N1 is approximately same.

4. In imidazole, the bond length between atoms are found in following order

$$N - C > C - C > C - H > N - H$$

5. In pyrazole, the bond length between different atoms of found similar trend as in 1,2,3-triazole.

6. In pyrrole, the bond length between C3-C4 is highest therefore electro negatively difference between these two atoms will be smallest while the bond length between N1-H6 is smallest therefore electro-negativity difference between N1-H6 will be highest.

The N-N distance in the triazole ring is very close to the estimated N-N distance for double bond. This result is other member of azoles which are non-aromatic species.

Table 1 : Bond Length

Molecule	Bond	Bond Length	Molecule	Bond	Bond Length	Molecule	Bond	Bond Length
1,2,3-Triazole	N1-N2	1.378	Pyrazole	N1-N2	1.372	Pentazole	N1-N2	1.349
	N2-N3	1.326		N2-C3	1.351		N2-N3	1.32
	N3-C4	1.38		C3-C4	1.425		N3-N4	1.381
	C4-C5	1.39		C4-C5	1.396		N4-N5	1.32
	C5-N1	1.371		C5-N1	1.374		N5-N1	1.349
	N1-H6	1.023		N1-H6	1.02		N1-N6	1.025
	C4-H7	1.09		C3-H7	1.092			
	C5-H8	1.09		C4-H8	1.091			
1,2,4-Triazole				C5-H9	1.091			
	N1-C2	1.344	Pyrrole	N1-C2	1.391			
	C2-N3	1.379		C2-C3	1.394			
	N3-C4	1.338		C3-C4	1.437			
	C4-N5	1.367		C4-C5	1.394			
	N5-N1	1.381		C5-N1	1.391			
	C2-H6	1.091		N1-H6	1.018			
	C4-H7	1.092		C2-H7	1.089			
	N5-H8	1.022		C3-H8	1.092			
Imidazole				C4-H9	1.092			
	N1-C2	1.333	Trtrazole	C5-H10	1.089			
	N1-C3	1.384		N1-N2	1.378			
	C3-N4	1.396		N2-N3	1.314			
	C5-C2	1.388		N3-N4	1.391			
	C2-H6	1.091		N4-N5	1.333			
	C3-H7	1.091		C5-N1	1.361			
	N4-H8	1.021		N1-H6	1.022			
	C5-H9	1.09		C5-H7	1.091			

Conclusion: atoms in a molecule are always vibrating with respect to each other and hence it is not possible to determine the exact- distance between the nuclei to atom. The maximum bond length is found between C-C while minimum bond length is found N-H. Since bond length between N-H minimum therefore the electro negativity difference between atoms N-H will be maximum.

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