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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. Thc maximum bond lcngth is found bctwccn C-C whilc 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 azolc. Namcs of azolcs maintain thc prcfix upon rcduction . Thc 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