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Bond length calculation of aniline and its reaction products by semi-empirical method

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Abstract

A semi-empirical molecular orbital method MINOD/3 is used to evaluate the bond length of aniline, and its reaction product like diphenyl urea, acetanilide and benzanilide. The results obtained are in good agreement with experimental result.

Keywords: MINDO/3, FORCE, GEO-OK.

Introduction

The molecular orbital studies of molecules describes the classical chemical bond in terms of quantum chemical parameters. The concept of bond length and bond angle are of direct chemical significance to get an immediate insight into the bounding situation in different molecules. A continued interest has been show by the quantum chemists in the above classical chemical concepts for the molecular system because these parameters can be put well into correspondence with the corresponding chemical notions. In general these parameters may be useful in correlating the quantum mechanics and ordinary chemistry and can be useful in giving better results and getting deeper understanding of the results of the actual quantum chemical calculations for particular system.

The bond length have been computed from the total bond orders using Coulson’s bond order-bond length relationship. The relationship has been used with a fair amount of success in both-electron and all valence electron semi-empirical theories. Mulliken in his work on population analysis used two quantities namely, the bond order and overlap population in order to define the strength of chemical bond. Although both the quantities have different forms and magnitude but essentially they have same meaning.

In molecular orbital theory, the molecular orbital coefficients of AO’s define the density matrix and are a basis to determine the probability of electron distribution among the atoms. The density matrix contains information about the system and can be defined in ab-initio as well as semi-empirical molecular orbital formalism. We have evaluated the bond length of aniline and its reaction products like diphency1 urea, acetanilide and benzanilide using the MINDO/3 method.

Method of Calculation

A semi-empirical method MINDO/3 is used to calculate bond length of aniline, diphenyl urea, acetanilide and benzanilide by MOPAC software, MINOD/3 is the improved version of MINDO (modified intermediate neglect of differential overlap). It is a method for the quantum calculations of molecular electronic structure in computational chemistry.

Results and Discussion

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 of the atoms.

According to MO theory, a covalent bond between two atoms is formed by the overlap of their atomic orbitals. The overlapping of their atomic orbitals 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. The calculated bond length of aniline and its reaction product are presented in Table.

The following points are observed from these results:

1. In aniline the bond length between C_5-C_6 is 1.431 which is maximum it means the electro negativity difference between these atoms will be minimum.
2. The bond lengths between atoms in aniline has been found in following order:
   C-C > C-N > C-H > N-H
   The maximum bond length is found between C-C while minimum bond length is found between N-H. Since bond length between N-H is minimum therefore the electronegativity difference between atoms N-H will be maximum.
3. It is also found that the presence of-NH_2 group of C_5 in aniline, increases the bond length between C_5-C_6. So that in all ring carbon bond length between C_5-C_6 is maximum.
4. The bond length between C_1-C_2 and C_2-C_3 is approximately same, similarly the bond length between C_4-C_5 and C_5-C_6 in nearly equal in aniline.
5. In diphency1 urea the bond length between different atoms is generally found in following order:
   C-C > C-N > C-O > C-H > N-H
6. The bond length between C-C is maximum while bond length between N-H is minimum. So that electronegativity difference between C-C will be least while electronegativity difference between N-H will be highest.
7. In diphenyle urea one-NH group is attached with C_{10} and bond length between C_{10}-C_{11} us higher than other C-C bond length in first ring carbon while other-NH group is attached with C_4 and bond length between C_4-C_5 is higher than the other C-C bond in second ring carbon. Thus we conclude that the presence of-NH group increases the bond length. This trend is exactly similar as in the case of aniline.
8. The bond length between C-O is less than the bond length between C-N because the bond order between C=0 is greater than that of C-N. Thus, if bond order increases then bond length decreases.
9. In acetanilide, the highest bond length is found between C_2-C_3. The presence of-CH_3 group at C_2, increases the bond length. Therefore the electronegativity differences between atoms C_2-C_3 will be least.
10. In ring carbon, the bond length between C_4-C_5 is greater than other C-C bond length. The presence of-NH group at C_4 increases the bond length.
11. In acetanilide, the bond length between different atoms is found in the following order:
    C-C > C-N > C-O > C-H
12. The bond length between N_1-H_{15} is smallest. Therefore electronegativity difference between N_1-H_{15} will be highest.
13. It has also been seen that the bond length between C-H which is attached to the ring carbon is slightly less than that attached with the carbon of-CH_3 group.
14. In benzanilide, the bond length between different atoms is found in the following order:
    C-C > C-N > C-O > C-H > N-H
    This trend is exactly similar as in case of acetanilide.
15. In the acetanilide and benzanilide, the-CO group is attached at carbon C_3. Therefore the bond length between C_2-C_3 is maximum. The presence of-CO group at C_3, increases the bond length between C_2-C_3. So electronegativity difference between C_2-C_3 will be least.

15\. The presence of-CO group at C_3 increases the bond length between C_3-C_4 and presence of-NH group at C_9 also increases the bond length between C_9-C_{11}.

16\. Since bond length between C-O is greater than that of N-H, therefore electronegativity difference between C-O is less than that of N-H.

Thus, from above discussion we see that the similar trend is obtained in aniline as well as its reaction products.

Table: Bond length (A^0)

Molecule	Bond	Bond length
Aniline	C_1-C_2	1.407
	C_2-C_3	1.405
	C_3-C_4	1.402
	C_5-C_6	1.431
	C_5-N_7	1.350
	C_6-H_8	1.105
	C_1-H_9	1.106
	C_2-H_{10}	1.103
	C_3-H_{11}	1.106
	C_4-H_{12}	1.106
	N_7-H_{13}	1.011
	N_7-C_{14}	1.011
Di-phynyl urea	N_1-C_2	1.376
	C_2-N_3	1.373
	N_3-C_4	1.400
	C_4-C_5	1.427
	C_5-C_6	1.402
	C_6-C_7	1.416
	C_7-C_8	1.404
	C_8-C_9	1.405
	N_1-C_{10}	1.398
	C_{10}-C_{11}	1.429
	C_{11}-C_{12}	1.424
	C_{12}-C_{13}	1.405
	C_{13}-C_{14}	1.402

	C_{14}-C_{15}	1.399
	C_{14}-H_{16}	1.104
	C_{15}-H_{17}	1.105
	C_{11}-H_{18}	1.110
	C_{12}-H_{19}	1.102
	C_{13}-H_{20}	1.107
	N_{1}-H_{21}	1.033
	C_{2}-O_{22}	1.222
	N_{3}-H_{23}	1.032
	C_{5}-H_{24}	1.106
Molecule	Bond	Bond length
	C_{6}-H_{25}	1.105
	C_{7}-H_{26}	1.101
	C_{8}-H_{27}	1.106
	C_{9}-H_{28}	1.105
Acetanilide	N_{1}-C_{2}	1.679
	C_{2}-C_{3}	1.765
	N_{1}-C_{4}	1.442
	C_{4}-C_{5}	1.540
	C_{6}-C_{7}	1.464
	C_{7}-C_{8}	1.387
	C_{8}-C_{9}	1.607
	C_{8}-H_{10}	1.100
	C_{9}-H_{11}	1.100
	C_{5}-H_{12}	1.100
	C_{6}-H_{13}	1.100
	C_{7}-H_{14}	1.100
	N_{1}-H_{15}	1.100
	C_{2}-O_{16}	1.614
	C_{3}-H_{17}	1.109
	C_{3}-H_{19}	1.109
Benzanilide	N_{1}-C_{2}	1.373
	C_{2}-C_{3}	1.503
	C_{3}-C_{4}	1.425
	C_{3}-C_{5}	1.423
	C_{4}-C_{6}	1.404
	C_{6}-C_{7}	1.408
	C_{7}-C_{8}	1.403
	N_{1}-C_{9}	1.400
	C_{9}-C_{10}	1.422
	C_{9}-C_{11}	1.432
	C_{11}-C_{12}	1.402
	C_{12}-C_{13}	1.405
	C_{13}-C_{14}	1.403
	C_{13}-H_{15}	1.103
	C_{14}-H_{16}	1.106
	C_{10}-H_{17}	1.106
	C_{11}-H_{18}	1.106
	C_{12}-H_{19}	1.106
	N_{1}-H_{20}	1.036
	N_{1}-H_{20}	1.036
	C_{2}-O_{21}	1.218
	C_{4}-H_{22}	1.107
	C_{6}-H_{23}	1.104
	C_{7}-H_{24}	1.105
	C_{8}-H_{25}	1.105
	C_{5}-H_{26}	1.107

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