American Journal of Advanced Scientific Research (AJASR)
ISSN: 2195-1381
Vol. 2 Issue 9, January – 2025, Pages 427-432

The Effect Of Intermolecular Interactions Of Aromatic Hydrocarbons And Their Representation In Vibration Spectra

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Abstract: In recent years, research conducted worldwide has shown the importance of determining the proton-donor and proton-acceptor properties of hydrocarbons and theoretically studying the nature of intermolecular interactions in them. Studying the role of hydrogen atoms in hydrocarbons in intermolecular interactions makes it possible to determine the proton-donor and proton-acceptor properties of aromatic hydrocarbons in the process of forming molecular complexes.

Keywords: Aromatic hydrocarbons, Raman spectra of molecular complexes, methylbenzene, combinatorial scattering, non-empirical calculations.

The study of molecular interactions is a separate independent branch of condensed matter physics [1]. As we know, liquids and their various solutions are among the most complex systems, while liquids themselves are complex, and scientific research is still being conducted on their structure, anomalous properties, intermolecular hydrogen bonding, and molecular landscape. Liquids and their mixtures play an important role in the food and other industries, as well as in the functioning of organisms. Therefore, the study of liquids is still relevant today.

Toluene is a six-membered ring of six carbon atoms, with one hydrogen atom per carbon and one methyl group (CH_3) bonded to three hydrogen atoms per carbon [2]. In this paper, the molecular geometry, optimized parameters, and vibrational frequencies of methylbenzene are described using the Gaussian density functional method. (DFT) and B3LYP//6/311++G(2d,p) basis sets.

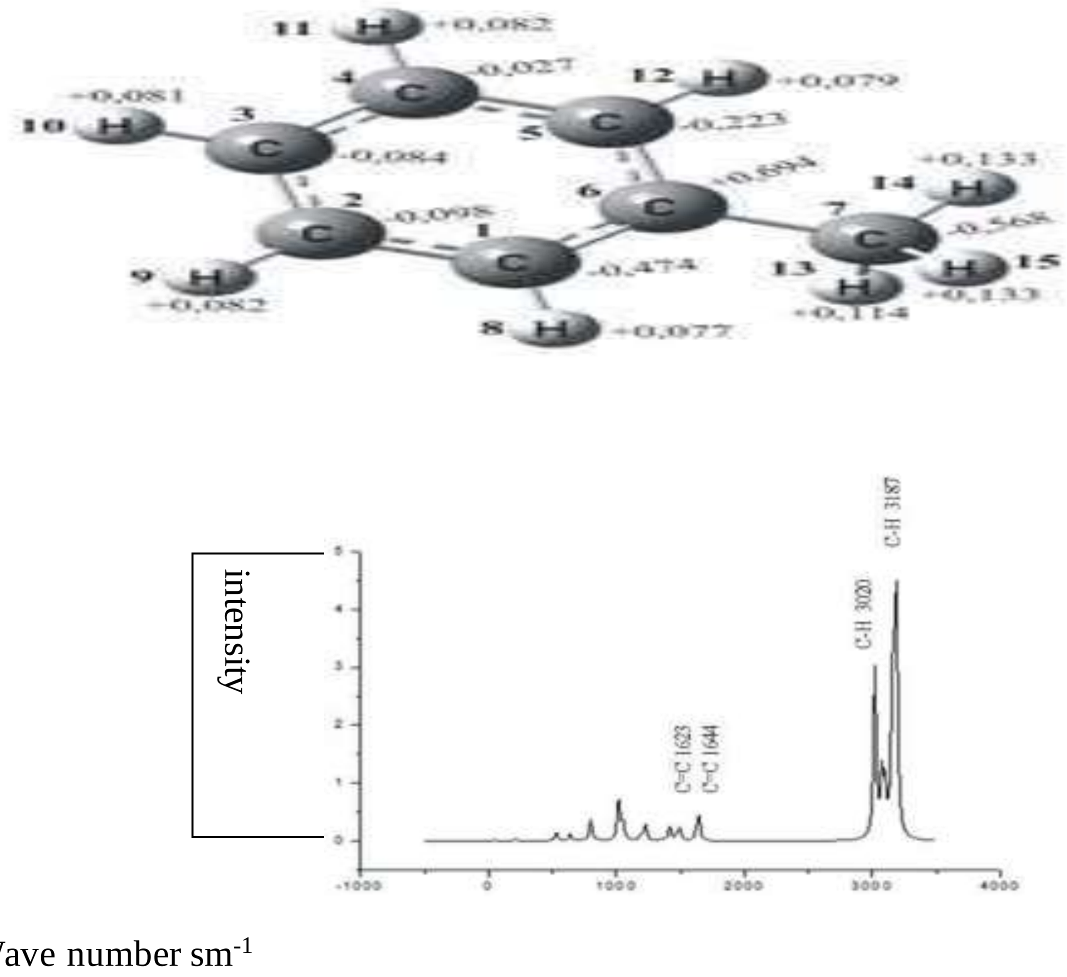


Figure 1. *The geometric structure and combinatorial scattering spectrum of the optimized monomer molecule of methylbenzene are presented.*

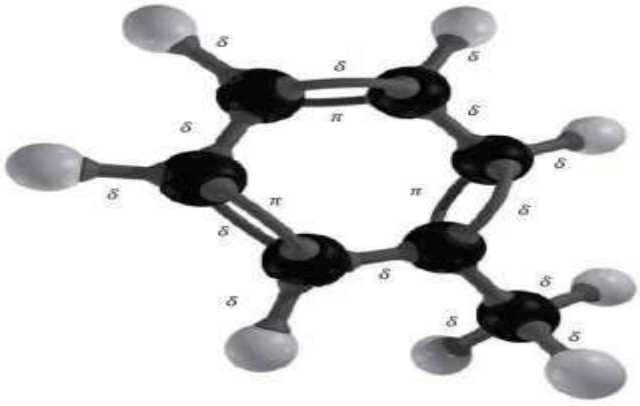


Figure 2 *There are 15 bonds in the methylbenzene molecule, and the remaining 3 are π bonds*

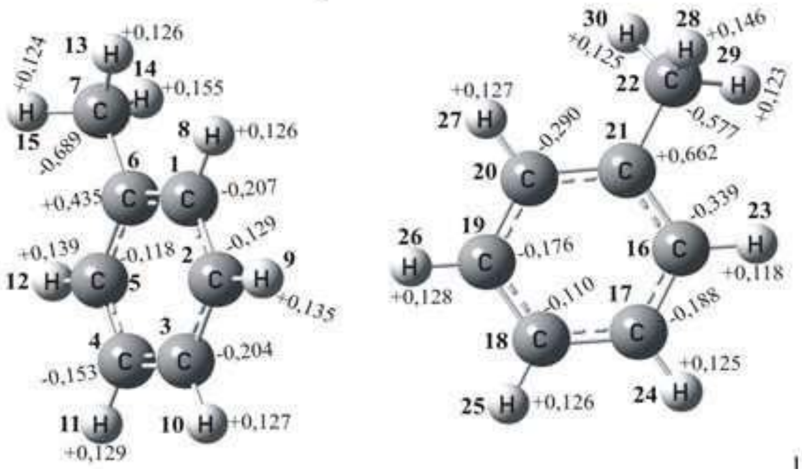
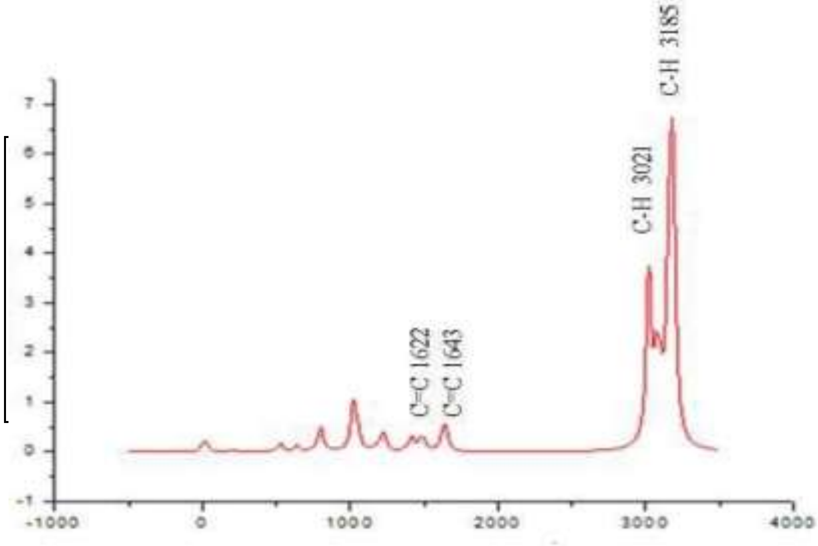


Figure 3. *Geometric structure of optimized dimer molecules of methylbenzene*

Two methylbenzene monomers can orient towards each other and form various aggregations through T-shaped interactions. In this case, the dimer formation energy is ΔE=0.116 (kcal/mol). The dipole moment of the methylbenzene dimer complex is 0.6743D.



Wave number sm^{-1}

Figure 4 Combinatorial scattering spectrum of methylbenzene dimer

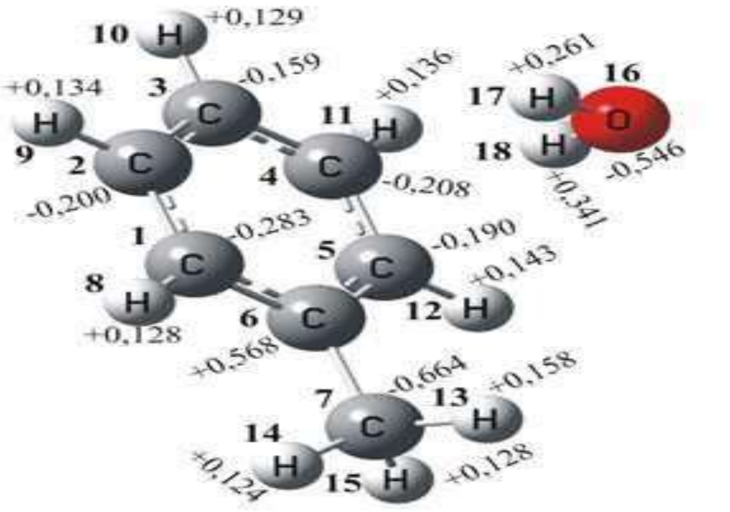


***Figure 5** Optimal geometry of the methylbenzene-water complex determined in the B3LYP/6-311++G(2d,p) functional set*

A complex state of methylbenzene and 1 water is presented, and an O-H·bond is formed with a distance of 2.61 A between the 18H atom and the center of the methylbenzene ring. The O-H·bond energy is 0.241 (kcal/mol) and the dipole moment is 2.29 D.

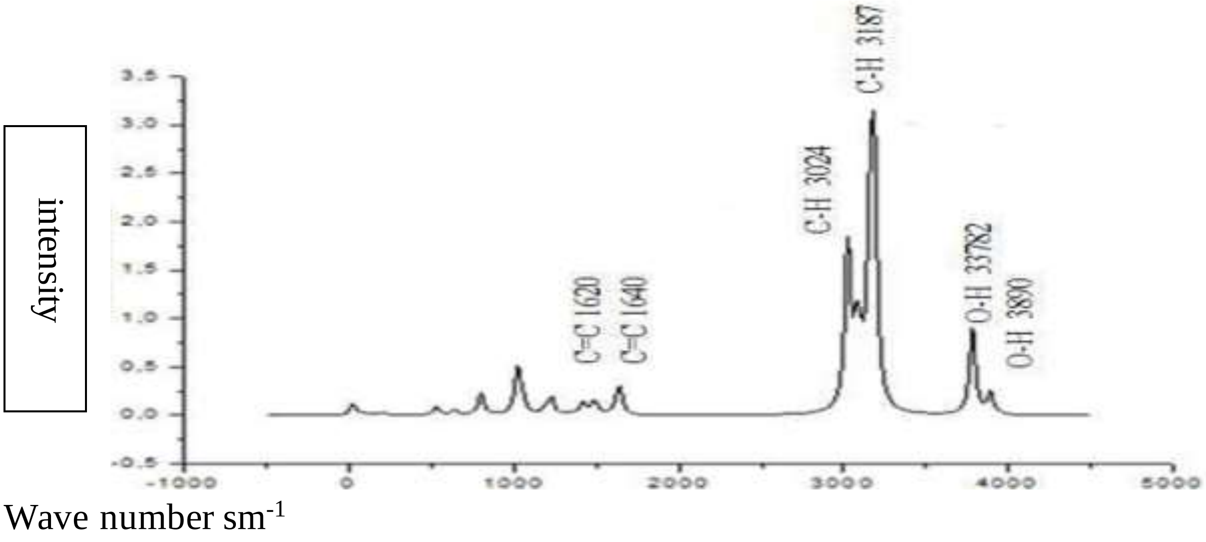
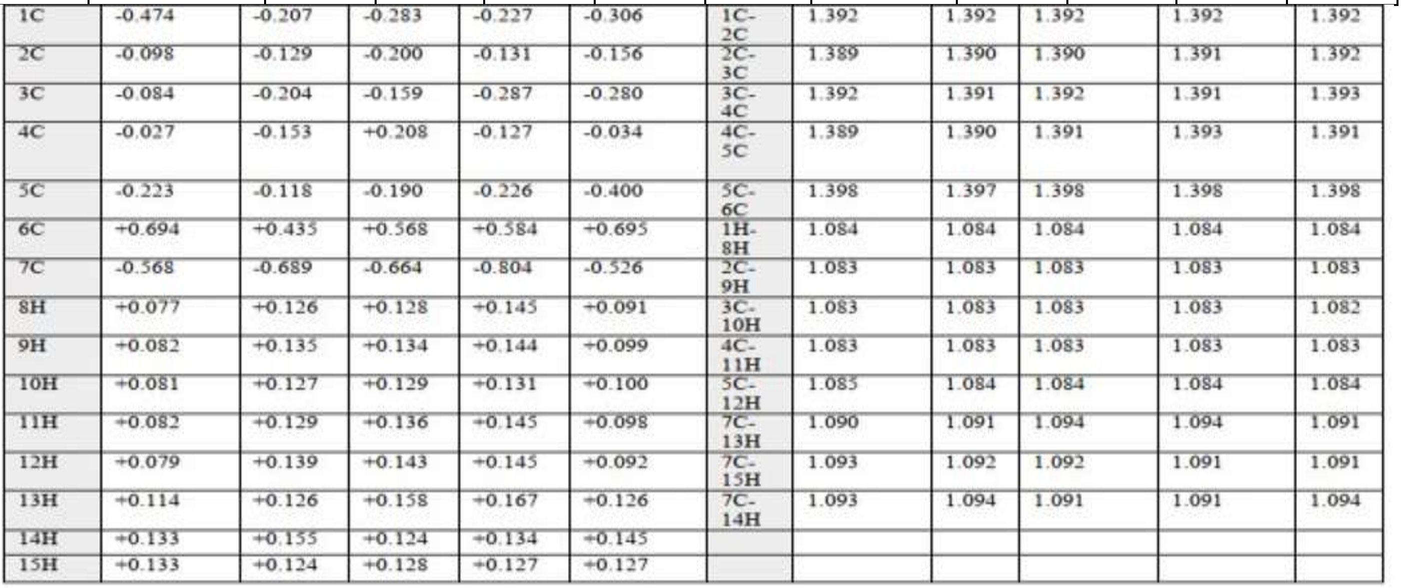


Figure 6 *Combinatorial scattering spectrum of the water complex of 1 with methylbenzene.* When methylbenzene bonds with the water monomer, the bond is directed towards the ring center of the water monomer, and the distance between them is 2.6 Å. We can see that the OH

symmetric vibration belonging to the water monomer has shifted from 3812 cm^{-1} to 3782 cm^{-1}, that is, it has shifted to a lower frequency by 30 cm^{-1}. Also, the OH asymmetric vibration has shifted to a lower frequency from 3916 cm^{-1} to 3890 cm^{-1}.

The table shows the changes in charge distributions and bond lengths in methylbenzene monomer, dimer, and its solutions.



Atom charges	Metilbenzol monomer	Metil benzol dimer	Metil benzol and water	Metil benzol and 2 waters	Metil benzol and 3 waters	Bonds length A	Metil benzol monomer	Metil benzol dimer	Metil benzol and water	Metil benzol and 2 waters	Metil benzol and 3 waters
1C	-0.474	-0.207	-0.283	-0.227	-0.306	1C-2C	1.392	1.392	1.392	1.392	1.392
2C	-0.098	-0.129	-0.200	-0.131	-0.156	2C-3C	1.389	1.390	1.390	1.391	1.392
3C	-0.084	-0.204	-0.159	-0.287	-0.280	3C-4C	1.392	1.391	1.392	1.391	1.393
4C	-0.027	-0.153	+0.208	-0.127	-0.034	4C-5C	1.389	1.390	1.391	1.393	1.391
5C	-0.223	-0.118	-0.190	-0.226	-0.400	5C-6C	1.398	1.397	1.398	1.398	1.398
6C	+0.694	+0.435	+0.568	+0.584	+0.695	1H-8H	1.084	1.084	1.084	1.084	1.084
7C	-0.568	-0.689	-0.664	-0.804	-0.526	2C-9H	1.083	1.083	1.083	1.083	1.083
8H	+0.077	+0.126	+0.128	+0.145	+0.091	3C-10H	1.083	1.083	1.083	1.083	1.082
9H	+0.082	+0.135	+0.134	+0.144	+0.099	4C-11H	1.083	1.083	1.083	1.083	1.083
10H	+0.081	+0.127	+0.129	+0.131	+0.100	5C-12H	1.085	1.084	1.084	1.084	1.084
11H	+0.082	+0.129	+0.136	+0.145	+0.098	7C-13H	1.090	1.091	1.094	1.094	1.091
12H	+0.079	+0.139	+0.143	+0.145	+0.092	7C-15H	1.093	1.092	1.092	1.091	1.091
13H	+0.114	+0.126	+0.158	+0.167	+0.126	7C-14H	1.093	1.094	1.091	1.091	1.094
14H	+0.133	+0.155	+0.124	+0.134	+0.145						
15H	+0.133	+0.124	+0.128	+0.127	+0.127						

Conclusion: *Two methylbenzene monomers can form various aggregations by orienting themselves towards each other and forming a T-shaped interaction. In this case, the dimer formation energy is 0.115 (kcal/mol). A complex state of methylbenzene and 1 water is presented, and an O-H··· bond is formed with a distance of 2.61 Å between the 18H atom and the center of the methylbenzene ring. There are various ways in which a water molecule can interact with the aromatic species under consideration. One type of interaction is a conventional H-bond, in which the proton-donating OH approaches the electron cloud.*

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