Arora, J Theor Comput Sci 2017, 4:2
DOI: 10.4172/2376-130X.1000158

Journal of
Theoretical & Computational Science

Review Article Open Access

Spectral Simulation Studies of Some Simple Organic Compounds

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Abstract

It is a demand in the modern era of chemical sciences to develop and design new and useful compounds for the service of mankind without the use of methods which are traditional one. Workers were trying to develop and synthesize series of new compounds since past in the laboratories using traditional synthetic methods and they used to check their properties thereafter. This process is time consuming and this lead to synthesis of a large number of compounds. Some recent trends have emerged and developed in the field of designing of compounds which may include microwave synthesis, computer aided designing etc. Out of these methods this presentation/article will focus on computer aided simulation of spectra of compounds on the PC. These computational methods are less time consuming, involve less chances of error, helpful in controlling and causing less pollution and may prove to be helpful in designing compounds with desired properties, in the studies like this. This presentation includes introduction to the computational methods, especially semi-empirical methods. A little bit theory behind these methods and their applications and use of software/ s methods in simulation of spectra of simple organic compounds.

Keywords: Computational chemistry; Molecular modeling; IR spectra; Spectral simulation

Introduction

Chemistry today: A different view

Now-a-days use of molecular modeling in chemical sciences with the help of software is the field of interest of various workers. Theoretical or computational chemistry research includes studies like geometrical studies including computation of geometrical parameters for a new molecule, simulation of spectra related to this molecule with computation of some or more properties for these molecules [1]. One can have a vision of a different view of Chemistry as shown in Figure 1.

Science is defined as the study of how nature behaves. Modern scientists agree that there are four methods in science:

1. Observational science

2. Experimental science

3. Theoretical science

4. Computational science

Among these, theoretical science is primarily mathematical. Theoretical scientists often attempt to mathematically represent some observable or non-observable phenomenon. By applying a variety of mathematical techniques, theoreticians look to "prove" the validity of some hypothesis or conjecture and so far as computational science is concern:

• Computational science is the application of computer science and mathematical techniques to the solution of large and complex problems.

• Computational science allows scientists to do things that were previously too difficult to do due to the complexity of the mathematics, the large number of calculations involved, or a combination of the two.

• Computational science allows scientists to build models that allow predictions of what might happen in the lab.

Computational science is often defined as being that science that is at the intersection of science, computer science, and mathematics. Alternatively known as modeling and simulation, as shown in Figure 2.

In Chemistry, it is found that chemists are increasingly identifying themselves as molecular modelers and/or computational chemists.

Molecular modeling is rapidly becoming one of the important tools, along with basic lab skills and the use of specialized chemistry tools such as infrared spectrophotometers and spectroscopy instruments. Keeping this in mind, this paper has been presented which includes the studies of simulation of spectra of simple organic compounds which are carried out by our research group [1,2].

Computational Details

Intel based Pentium core-2 Duo machine with configuration Intel (R) core TM 2 Duo CPU, T5450@1.66 GHZ, 2 GB RAM, 250 GB HDD was used to run all the calculations.

Semi-empirical AM1, PM3, MNDO and ZINDO1 quantum chemical calculations were carried out by the computer software HYPERCHEM 8.0 version and calculated parameters such as normal modes frequencies of vibration [1-6].

Results and Discussion

Normal modes analysis and spectral simulation studies for the compounds

Normal modes analysis of some of the organic compounds can be performed using specific keywords with the help of these computer packages mentioned above using AM1, PM3, MNDO and ZINDO methods with the help of semi-empirical packages. On the basis of normal mode analysis computer simulation of IR spectra can be done [7-14].

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Received July 24, 2017; **Accepted** August 16, 2017; **Published** August 22, 2017

Citation: Arora K (2017) Spectral Simulation Studies of Some Simple Organic Compounds. J Theor Comput Sci 4: 158. doi:10.4172/2376-130X.1000158

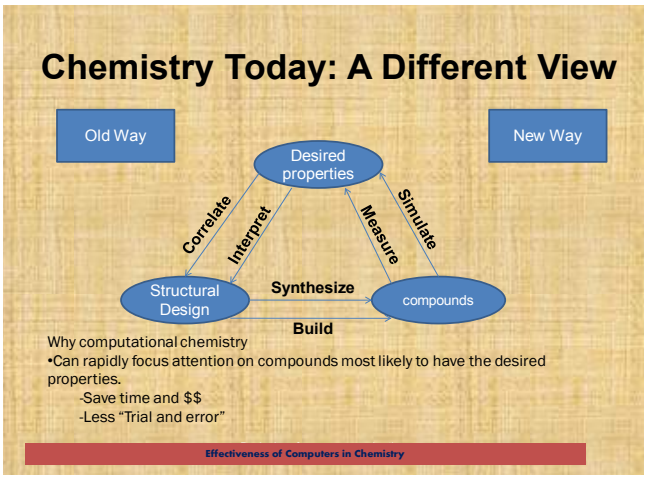


Figure 1: Vision of a different view of Chemistry.

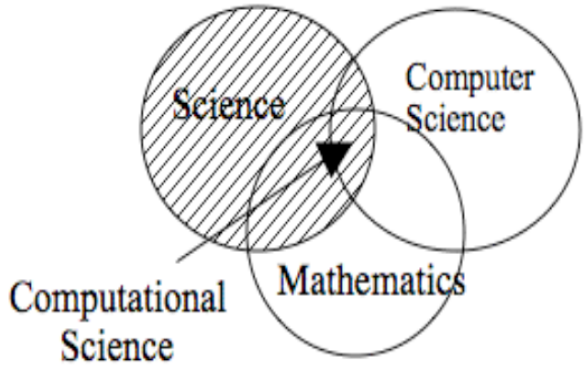


Figure 2: Computational Science: Amalgamation of Science, Computer Science and Mathematics.

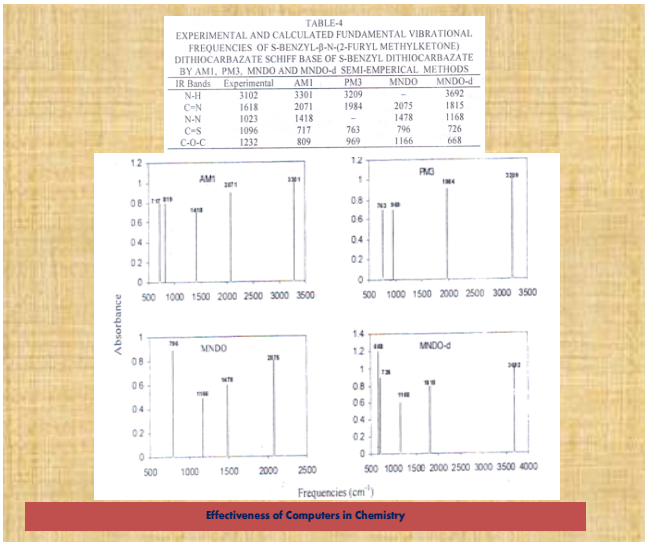


Figure 3: Computer simulated IR for for S-Benzyl 1-β-M-(2-furyl methyl ketone) dithio carbazate.

One such study for S-Benzyl 1--M-(2-furyl methyl ketone) dithio carbazate Schiff base has been carried out with AM1, PM3 MNDO and MNDO-d methods. These computer simulated IR spectra are shown in Figure 3.

Assignment of peaks with computed peaks for this compound shows that the results obtained are in good agreement with experimental spectral data obtained for this compound. Major peaks assigned are shown in Figure 3 above with simulated spectra on the basis of computed peaks.

Simulation of spectra of various compounds was done by our research group based on semi-empirical methods of study. Studies of some of these are given in this presentation. Spectra of 4-N-[(2-Nitro) benzalidene] amino antipyrine (2NBAAPy) was simulated and studied. Structure of the compound mentioned above is shown in Figure 4.

Experimental and Computed (AM1, PM3, MNDO, ZINDO1) Group frequencies of vibration (cm^{-1}) for 4-N-[(2-Nitro)benzalidene] aminoantipyrine (2NBAAPy) are shown in Tables 1 and 2 below with their simulated (AM1, PM3, MNDO and ZINDO1) spectra in the Figure 5 along with the correlation/regression graphs between experimentally observed and computed spectral peaks data (Figure 6).

Structure of one another Schiff base compound viz. 4-N-[(4Hydroxy-3-methoxy)benzalidene] amino antipyrine(4MBAAPy) is shown in Figure 7. Studies related to Simulation of spectra of 4-N-[(4Hydroxy-3-methoxy)benzalidene] amino antipyrine(4MBAAPy) along with their simulated spectral data and spectra are given in Figure 8.

Spectral peaks appear in simulated spectra of compounds match well with the experimentally observed peaks in their real spectra, of course within permissible limits. The results so obtained using these packages reveals that computations done on the basis of AM1 are well and reasonably good as compared to other methods i.e., PM3, MNDO AND ZINDO.

Correlation between experimental and computed spectral data is perfect as it is clear from Figure 9. It is almost 0.99999 which shows that this type of studies involving these semi-empirical packages is significant and may be used to teach and train students without having real life spectra of any compound.

This simulation is useful for the purpose of research also to establish and study the spectra of compounds, in the absence of arrangements for real life spectra.

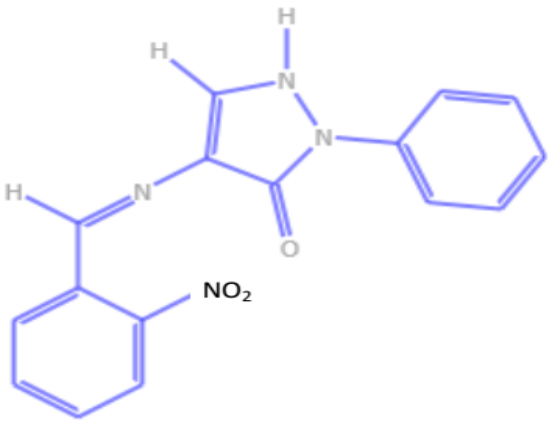
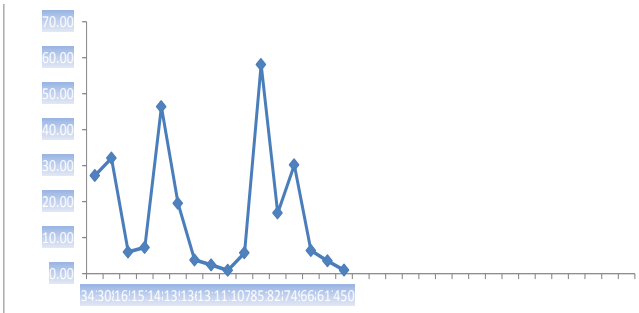
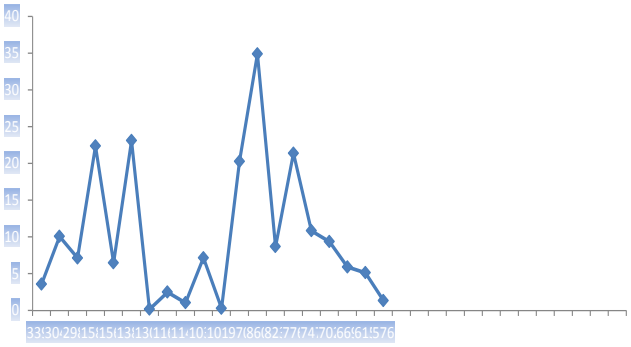


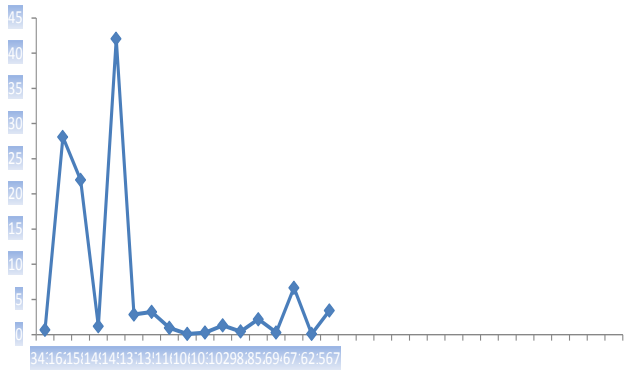
Figure 4: Structure of 4-N-[(2-Nitro)benzalidene]aminoantipyrine(2NBAAPy).



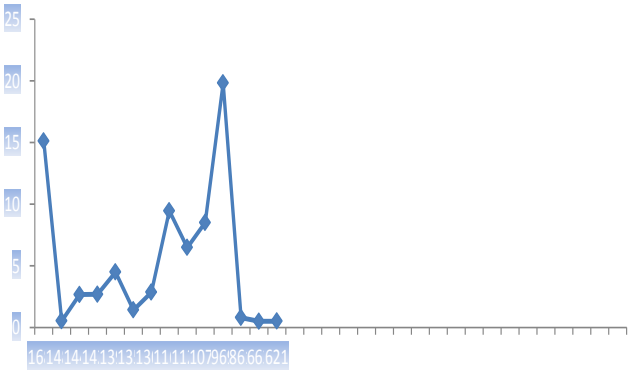
AM1 computed spectra (Vibration Frequency in cm^{-1} Vs. Transmittance).



PM3 computed spectra (Vibration Frequency in cm^{-1} Vs. Transmittance).

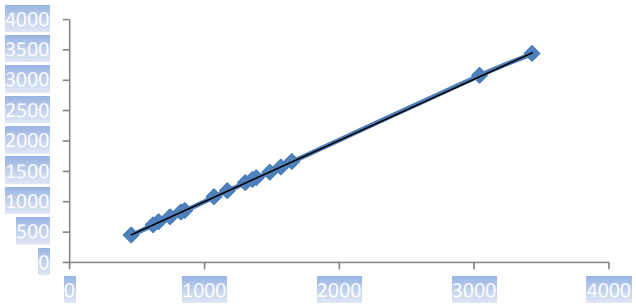


MNDO computed spectra (Vibration Frequency in cm^{-1} Vs. Transmittance).

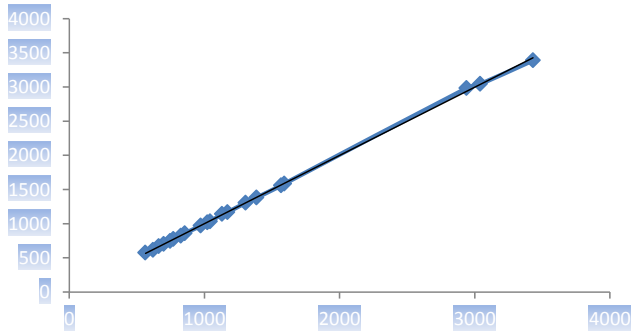


ZINDO1 computed spectra (Vibration Frequency in cm^{-1} Vs. Transmittance).

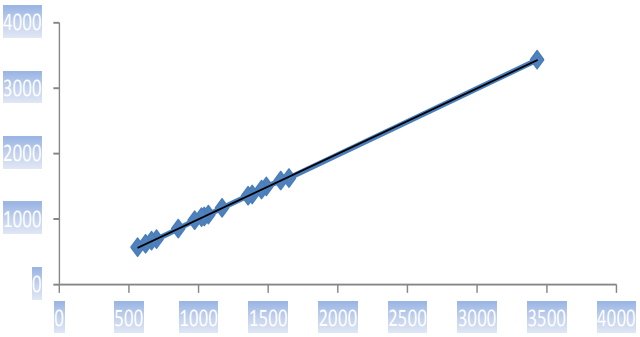
Figure 5: Simulated spectra of the compound 4-N-[(2-Nitro)benzalidene] aminoantipyrine(2NBAAPy) under study.



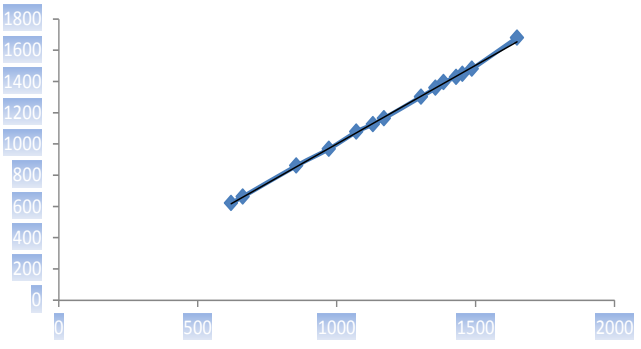
Correlation diagram between AM1 computed spectral data Vs. experimental spectral data.



Correlation diagram between PM3 computed spectral data Vs, experimental spectral data.



Correlation diagram between MNDO computed spectral data Vs. experimental spectral data.



Correlation diagram between ZINDO computed spectral data Vs. experimental spectral data.

Figure 6: Correlation diagrams between computed spectral data and experimental spectral data of the compound 4-N-[(2-Nitro)benzalidene] aminoantipyrine (2NBAAPy) under study.

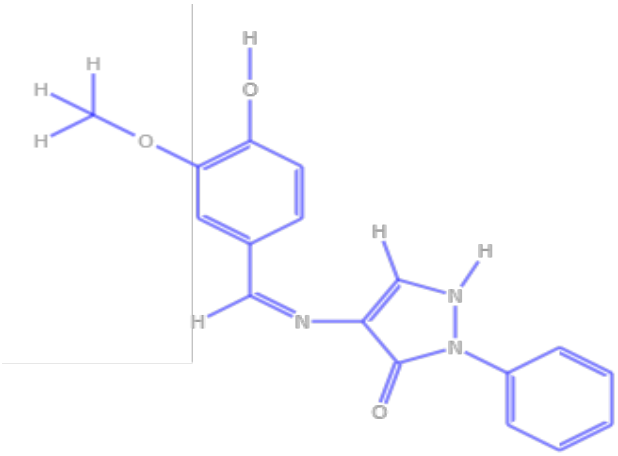
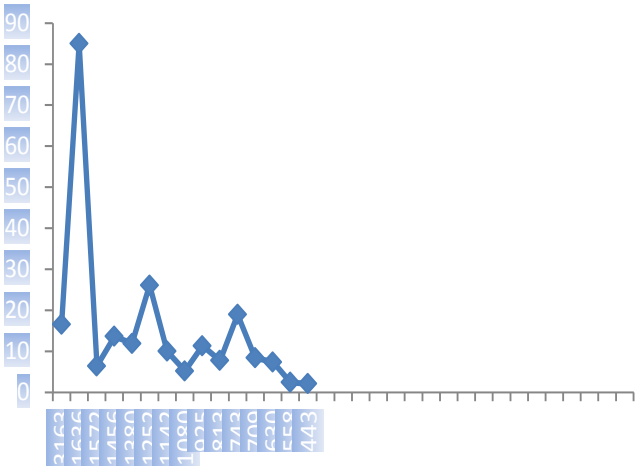
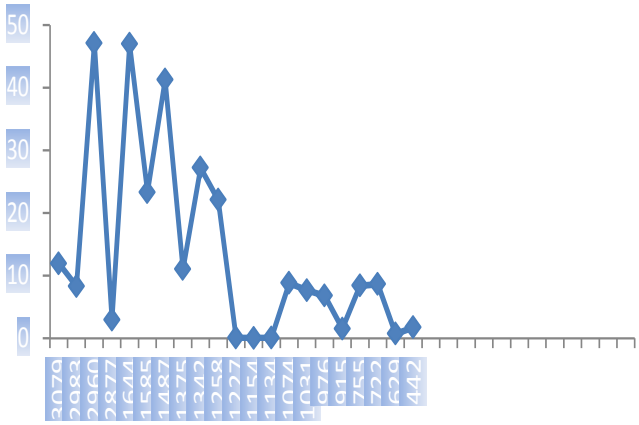


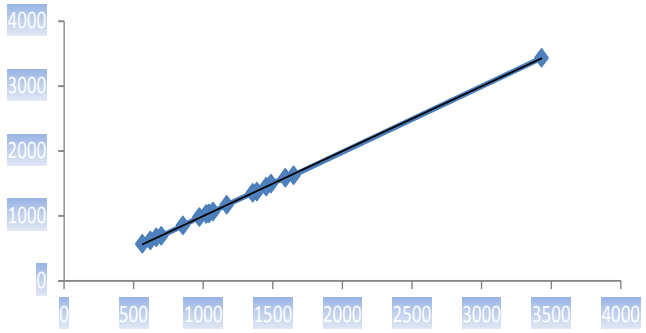
Figure 7: Structure of 4-N-[(4Hydroxy-3-methoxy) benzalidene] aminoantipyrine(4MBAAPy).



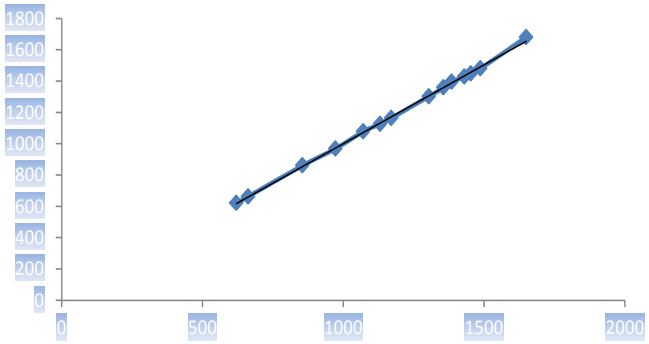
AM1 computed spectra of the compound (Vibration Frequency in cm^{-1} Vs. Transmittance).



PM3 computed spectra of the compound (Vibration Frequency in cm^{-1} Vs. Transmittance).

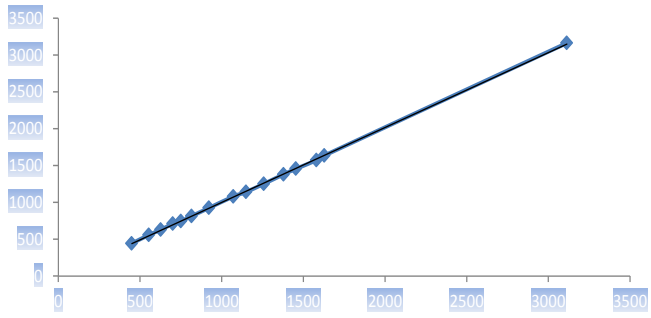


MNDO computed spectra of the compound (Vibration Frequency in cm^{-1} Vs. Transmittance).

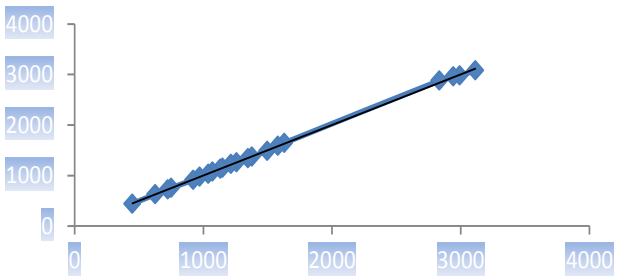


ZINDO computed spectra of the compound (Vibration Frequency in cm^{-1} Vs. Transmittance).

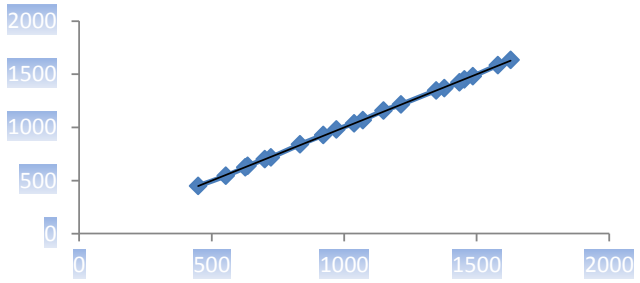
Figure 8: Simulated spectra of the compound 4-N-[(4Hydroxy-3-methoxy) benzalidene] aminoantipyrine (4MBAAPy) under study.



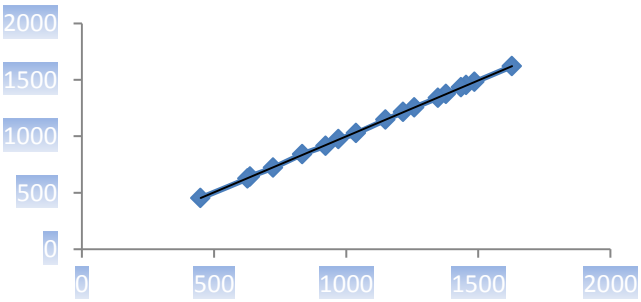
Correlation diagram between AM1 computed spectral data Vs. experimental spectral data.



Correlation diagram between PM3 computed spectral data Vs. experimental spectral data.



Correlation diagram between MNDO computed spectral data Vs. experimental spectral data.



Correlation diagram between ZINDO computed spectral data Vs. experimental spectral data.

Figure 9: Correlation diagrams between computed spectral data and experimental spectral data of the compound 4-N-[(4Hydroxy-3-methoxy) benzalidene] amino antipyrine(4MBAAPy) under study.

Conclusion

Semi-empirical computational methods are the best tools for this type simulation study of various organic compounds. These methods may prove to be useful tolls not only for teaching but for research purpose also. These methods are less time consuming. AM1 methods are most reasonably good results oriented and more accurate among all these discussed semi-empirical methods.

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S. No.	Experimental Group Frequency (cm^{-1})	AM1 Computed Group Frequency (cm^{-1})	PM3 Computed Group Frequency (cm^{-1})	MNDO Computed Group Frequency (cm^{-1})	ZINDO1 Computed Group Frequency (cm^{-1})	Assignment
1.	3431	3437	3390	3431	-	υ_{as} (N-H) in NH_2
2.	3041	3080	3044	-	-	υ (C-H)
3.	2939	-	2983	-	-	υ (C-H)
4.	2864	-	-	-	-	υ (=C-H) Aldehyde
5.	1649	1657	-	1627	1681	υ (C=O)
6.	1591	-	1586	1585	-	(NH_2) Sci
7.	1568	1570	1560	-	-	NO_2 Grp. (Aromatic)
8.	1487	1484	-	1496	1481	υ (C=C)
9.	1453	-	-	1451	1448	υ (C=C)

Table 1: Partial IR spectral, experimental as well as simulated data with assignment of the compound under study.

S. No.	Experimental Group Frequency (cm^{-1})	AM1 Computed Group Frequency (cm^{-1})	PM3 Computed Group Frequency (cm^{-1})	MNDO Computed Group Frequency (cm^{-1})	ZINDO1 Computed Group Frequency (cm^{-1})	Assignment
1.	3113	3163	3079	-	-	υ (C-H)
2.	2993	-	2983	-	-	υ (C-H)
3.	2942	-	2960	-	-	υ_{as}(C-H) in CH_3
4.	2834	-	2877	-	-	(=C-H) Aldehyde
5.	1628	1636	1644	1634	1621	υ(C=O)
6.	1603	-	-	-	-	υ(C=C)
7.	1580	1572	1585	1585	-	(NH_2) Sci
8.	1497	-	-	-	-	υ(C=C)
9.	1486	-	1487	1480	1481	υ (C=C)
10.	1454	1456	-	1450	1454	υ (C=C)

Table 2: Partial IR spectral, experimental as well as simulated data with assignment of the compound under study.

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