# A Combined Experimental and Theoretical Investigation on The Molecular Structure, Ft-Ir Spectra of 4-((1h-Indol-3-Yl) Methylene Amino) Phenol

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**Abstract:**

This study involves the synthesis of the title molecule 1H-IMAP, characterized by using FT-IR spectrum and theoretical calculation of the optimized geometrical parameters of the most stable structure of the title molecule 1H-IMAP and computation of its vibrational frequencies using Hartree-Fock(HF) method of basis sets 6-31G(d,p), HF/6-311G(d,p) and Density functional theory (DFT) method of basis set B3LYP/6-31G(d,p) has been made by using Gaussion 03 software and compared both theoretical and experimental values. Non-Linear optical (NLO) properties of the 1H-IMAP was studied by determining the electric dipole moment, polarizability, and hyperpolarizability with the aid of the above mentioned basis sets.

**Keywords:** DFT, Geometrical Parameters, basis sets, HF

## Introduction

Indole derivatives as dual-effective medicines for neurodegenerative disease treatment The hydroxyl derivative of indole is important in the central nervous system, and it has been shown to cause long-term serotonin depletion in brain tissues[1-4]. The synthesis technique, experimental and theoretical FT-IR studies of 4-((1H-indol-3yl) methylene amino) phenol are described in this paper.

To the best of our knowledge, a complete theoretical study of 1H-IMAP have not been reported so for. In this study HF and DFT level of theories were utilized to determine the optimized geometry, vibrational wave numbers, molecular parameters viz., dipole moment, polarizability ($\alpha$), hyperpolarizability ($\beta$), chemical potential, hardness ($\eta$), and electrophilicity index ($\omega$).

## Experimental Section

A mixture of Indole-3-Carboldehyde (72g, 1.0mol) is added dropwise and with stirring during 2hrs to p-hydroxy aniline (73g, 1.0mol). During this addition the temperature rises from 25 to $40^0$C and an aqueous layer separates nearer at the end of the addition. The organic layer is treated with anhydrous potassium carbonate (15g), stirred at $25^0$C for 17 hrs, and then decanted onto barium oxide (12g). After the mixture has been stirred for 10 hrs, it is filtered and the organic filterate is distilled to separate the imine as a colourless liquid. The compound 4-((1H-indol-3yl) methylene amino) phenol in the solid form was synthesized. The FT-IR spectrum of this compound was recorded in the range of 400-4000cm⁻¹ on PERKIN-ELMER 360 model IR double beam spectrophotometer using KBr pellet technique with 4

cm-1 resolution over 40 scans. The spectral measurement carried out at Central Instrumentation Faculty (CIF), Pondicherry University, Puducherry (India).

## Computational Details

Geometry optimization and vibrational spectra calculations were carried out on a PC using the Gaussian-03 software package at the Hatree–Fock level of theory with the 6-31 G (d,p) and 6-311G(d,p) basis sets, and DFT computations were carried out at the B3LYP/6-31 G (d,p) level of theory. Hatree–Fock does not include electron correlation; however it considers average affect of electron repulsion but not the explicit electron-electron repulsion [5].

At the optimized structure of 1H-IMAP, no imaginary wave number modes were observed, indicating that a real minima on the potential surface was discovered. The best shape was determined by reducing energy with all geometrical parameters without imposing molecular symmetry requirements. The fundamental modes are overestimated by the HF and DFT hybrid B3LYP functional methods. Density functional theory calculations have been claimed to offer excellent vibrational frequencies of molecular compounds when the measured frequencies are scaled to correct for the expected treatment of electron correlation, basis inadequacies, and anharmonicity [6, 7, 8, 9]. As a result, scaling factors must be applied to achieve a much greater agreement with experimental results.

Thus the scaling factors: 0.8992, 0.9051 and 0.9550 [10] have been uniformly applied to the HF and B3LYP methods respectively. The observed discrepancy between theoretical and experimental frequencies of any particular vibration of the molecule could be a consequence of basis set incompleteness, neglect of anharmonicity and electron correlation. The general tendency of quantum chemical method is overestimated the force constant at the exact equilibrium geometry of the molecule [11]. The assignments of the calculated wave numbers are aided by Gauss view program [12]. Combining the result of Gauss view program and the vibrational frequency assignments were made with a high degree of precision, taking into account symmetry.

## Results and Discussion
## Molecular Geometry

In accordance with the atomic numbering scheme shown in Figure 1, the optimised structural parameters of 1H-1MAP determined by ab inito HF level with 6-31G(d,p), 6-311G(d,p), and DFT/B3LYP level with 6-31G(d,p) basis sets are described in Table 1
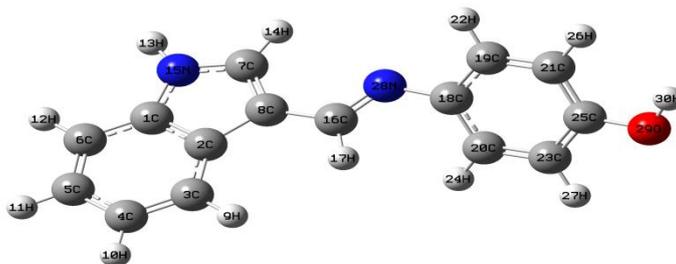


**Figure1.Optimized molecular structure of 1H-1MAP**

Since the exact crystal structure of the title compound is not available till now, the optimized structure can only be compared with other similar systems for which the crystal structures have been solved. Therefore optimized geometrical parameters of 1H-1MAP are compared to those of *N2'-(1H-indol-3ylmethylene) carbonic dihydrazide. The optimized bond distance of all the C-H bands is greater than the experimental value (0.95 Å) of *N2'-(1H-indol-3ylmethylene) carbonic dihydrazide.

For the optimized indole(PhI) ring of the title compound, it has been observed that the optimized C3-H9, C4-H10, C5-H11, C6-H12 and C7-H14 bond distances are larger than the experimental C-H bond distance 0.9500Å of the reference molecule [13].

Computed bond distances of C1-C2, C1-C6, C2-C3, C2-C8, C3-C4, C4-C5, C5-C6 and C7-C8 bond distances in indole ring(PhI) of the title compound by DFT method show closely related to experimental data of reference molecule [13]. But at same time C-C bond distance computed in HF method is found to be basis set sensitive and hence the value computed by HF/6-311G(d,p) coincides very well with experimental C-C bond length of reference molecule[13].

Table1. Geometric bond length of 1H-1MAP by B3LYP/6-31G(d, p), HF/ 6-31G(d,p) and HF/ 6-311G(d,p)

| Bond length (Å) | B3LYP/ 6-31G (d,p) | HF/ 6-31G (d,p) | HF/ 6-311G (d,p) | XRD [12] |
|---|---|---|---|---|
| C1-C2 | 1.4201 | 1.399 | 1.3983 | 1.4125 |
| C1-C6 | 1.3974 | 1.3923 | 1.3918 | 1.3973 |
| C1-N15 | 1.3856 | 1.3753 | 1.3749 | 1.3784 |
| C2-C3 | 1.4048 | 1.399 | 1.3986 | 1.4013 |
| C2-C8 | 1.4485 | 1.4485 | 1.4481 | 1.4431 |
| C3-C4 | 1.3894 | 1.3748 | 1.3742 | 1.3866 |
| C3-H9 | 1.0861 | 1.0758 | 1.0754 | 0.95 |
| C4-C5 | 1.4091 | 1.403 | 1.4025 | 1.4024 |
| C4-H10 | 1.0858 | 1.0755 | 1.0752 | 0.95 |
| C5-C6 | 1.3901 | 1.3749 | 1.3743 | 1.3844 |
| C5-H11 | 1.0857 | 1.0756 | 1.0753 | 0.95 |
| C6-H12 | 1.0862 | 1.076 | 1.0757 | 0.95 |
| C7-C8 | 1.3822 | 1.3578 | 1.3571 | 1.3807 |
| C7-H14 | 1.0796 | 1.0699 | 1.0698 | 0.95 |
| C7-N15 | 1.3704 | 1.3591 | 1.359 | 1.3672 |
| C8-C16 | 1.4484 | 1.4588 | 1.4596 | 1.4424 |
| H13-N15 | 1.0073 | 0.9915 | 0.9911 | 0.88 |
| C16-H17 | 1.0997 | 1.086 | 1.0861 | 0.95 |
| C16-N28 | 1.2866 | 1.2589 | 1.2559 | 1.2862 |
| C18-C19 | 1.4039 | 1.3884 | 1.3871 | 1.3887 |
| C18-C20 | 1.4086 | 1.3932 | 1.3922 | 1.384 |
| C18-N28 | 1.4049 | 1.4078 | 1.4084 | 1.3712 |
| C19-C21 | 1.3914 | 1.3832 | 1.3831 | 1.4007 |
| C19-H22 | 1.0852 | 1.0748 | 1.0745 | 0.95 |
| C20-C23 | 1.3905 | 1.3822 | 1.3813 | 1.3816 |
| C20-H24 | 1.0858 | 1.0754 | 1.0751 | 0.95 |
| C21-C25 | 1.3993 | 1.386 | 1.385 | 1.4111 |
| C21-H26 | 1.0883 | 1.0776 | 1.0774 | 0.95 |
| C23-C25 | 1.3988 | 1.3854 | 1.3845 | 1.3949 |
| C23-H27 | 1.0851 | 1.0745 | 1.0744 | 0.95 |
| C25-O29 | 1.369 | 1.3539 | 1.3533 | 1.3626 |
| O29-H30 | 0.966 | 0.9425 | 0.9402 | 0.84 |

The optimized N15-H13 bond distance for the title compound is 0.9915Å in HF/6-31G (d,p) 0.9110Å in HF/6-31G(d,p) and 1.0073Å in B3LYP/6-31G(d,p). The latter one shows much deviation from the experimental N-H bond distance 0.8800Å of the reference molecule [13].

The experimental bond distance of C=N is 1.2862 Å and the computed C16=N28 bond distance is 1.2866 Å in B3LYP/6-31G(d,p), 1.2589 Å in HF/6-31G(d,p) 1.2559 Å in HF/6-311G(d,p). The B3LYP/6-31G(d,p) method renders values that are very much coincide with the experimental values of reference molecule and better than other two methods.

The optimized (PhI) C1-N15 and C7-N15 bond distances of five membered ring of indole moiety are computed. The B3LYP/6-31G(d,p) method shows good agreement with the experimental value of reference compound 1.3784 Å.

Table2. Geometric bond angle of 1H-1MAP by B3LYP/6-31G(d, p), HF/ 6-31G(d,p) and HF/ 6-311G(d,p)

| Bond Angle (°) | B3LYP/ 6-31G(d,p) | HF/ 6-31G(d,p) | HF/ 6-311G(d,p) | XRD [12] |
|---|---|---|---|---|
| C2-C1-C6 | 122.65 | 122.49 | 122.45 | 122.54 |
| C2-C1-N15 | 107.1 | 107.5 | 107.5 | 107.85 |
| C6-C1-N15 | 130.23 | 129.99 | 130.04 | 129.59 |
| C1-C2-C3 | 118.61 | 118.83 | 118.86 | 118.98 |
| C1-C2-C8 | 106.96 | 106.62 | 106.62 | 106.55 |
| C3-C2-C8 | 134.42 | 134.54 | 134.58 | 134.45 |
| C2-C3-C4 | 119.05 | 119.05 | 119.06 | 118.75 |
| C2-C3-H9 | 120.69 | 120.87 | 120.88 | 120.6 |
| C4-C3-H9 | 120.24 | 120.06 | 120.05 | 120.6 |
| C3-C4-C5 | 121.23 | 121.05 | 121.03 | 121.18 |
| C3-C4-H10 | 119.55 | 119.72 | 119.72 | 119.4 |
| C5-C4-H10 | 119.21 | 119.22 | 119.23 | 119.4 |
| C4-C5-C6 | 121.08 | 121.09 | 121.08 | 121.48 |
| C4-C5-H11 | 119.48 | 119.36 | 119.37 | 119.3 |
| C6-C5-H11 | 119.42 | 119.53 | 119.53 | 119.3 |
| C1-C6-C5 | 117.35 | 117.45 | 117.49 | 117.05 |
| C1-C6-H12 | 121.4 | 120.34 | 121.35 | 121.5 |
| C5-C6-H12 | 121.23 | 121.2 | 121.15 | 121.5 |
| C8-C7-H14 | 128.51 | 128.3 | 128.27 | 125.1 |
| C8-C7-N15 | 109.73 | 110.2 | 110.18 | 109.75 |
| H14-C7-N15 | 121.74 | 121.48 | 121.53 | 125.1 |
| C2-C8-C7 | 106.43 | 106.32 | 106.34 | 106.56 |
| C2-C8-C16 | 127.34 | 127.61 | 127.54 | 128.18 |
| C7-C8-C16 | 126.21 | 126.05 | 126.1 | 125.24 |
| C1-N15-C7 | 109.75 | 109.33 | 109.33 | 109.28 |
| C1-N15-H13 | 125.24 | 125.58 | 125.6 | 125.4 |
| C7-N15-H13 | 125 | 125.07 | 125.05 | 125.4 |
| C8-C16-H17 | 115.82 | 115.88 | 115.79 | 120 |
| C8-C16-N28 | 122.52 | 123.57 | 122.68 | 119.98 |
| H17-C16-N28 | 121.64 | 121.53 | 121.51 | 120 |
| C19-C18-C20 | 118.01 | 118.14 | 118.1 | 119.8 |
| C19-C18-N28 | 117.72 | 118.03 | 118.04 | 118.31 |
| C20-C18-N28 | 124.21 | 123.77 | 123.79 | 122.9 |
| C18-C19-C21 | 121.15 | 121.1 | 121.1 | 121.61 |
| C18-C19-H22 | 118.29 | 118.68 | 118.67 | 119.2 |
| C21-C19-H22 | 120.54 | 120.2 | 120.21 | 119.2 |
| C18-C20-C23 | 121.11 | 121.07 | 121.09 | 120.09 |
| C18-C20-H24 | 119.62 | 119.82 | 119.86 | 120 |
| C23-C20-H24 | 119.22 | 119.07 | 119.01 | 117.56 |
| C19-C21-C25 | 120.02 | 120.03 | 120.09 | 120 |
| C19-C21-H26 | 119.99 | 119.83 | 119.78 | 119.8 |
| C25-C21-H26 | 119.97 | 120.12 | 120.11 | 119.8 |
| C20-C23-C25 | 120.02 | 120.01 | 120.07 | 120.45 |
| C20-C23-H27 | 121.12 | 120.95 | 120.92 | 119.8 |
| C25-C23-H27 | 118.84 | 119 | 119 | 119.8 |
| C21-C25-C23 | 119.62 | 119.57 | 119.47 | 120.46 |
| C21-C25-O29 | 122.81 | 122.66 | 122.69 | 122.57 |
| C23-C25-O29 | 117.55 | 177.76 | 117.82 | 116.97 |
| C16-N28-C18 | 119.95 | 119.94 | 120.01 | 120 |
| C25-O29-H30 | 108.9 | 110.81 | 110.56 | 109.5 |

Table3. Geometric dihedral angle of 1H-1MAP by B3LYP/6-31G(d, p), HF/ 6-31G(d,p) and HF/ 6-311G(d,p)

| Dihedral angle (°) | B3LYP/ 6-31G (d,p) | HF/ 6-31G (d,p) | HF/ 6-311G (d,p) | XRD [12] |
|---|---|---|---|---|
| C6-C1-C2-C3 | 0.0694 | -0.0914 | -0.0892 | 0.9 |
| C6-C1-C2-C8 | 179.98 | -179.9 | -179.98 | -177.38 |
| N15-C1-C2-C3 | -179.89 | 179.9 | 179.88 | 179.57 |
| N15-C1-C2-C8 | -0.0278 | -0.0054 | -0.004 | 1.29 |
| C2-C1-C6-C5 | -0.0244 | 0.0189 | 0.0166 | 0.33 |
| N15-C1-C6-C5 | 179.92 | -179.97 | -179.95 | -178.03 |
| C2-C1-N15-C7 | -0.0831 | 0.0643 | 0.0531 | -1.54 |
| C6-C1-N15-C7 | 179.96 | -179.94 | -179.97 | 177 |
| C1-C2-C3-C4 | -0.069 | 0.1076 | 0.1069 | -1.26 |
| C8-C2-C3-C4 | -179.95 | 179.98 | 179.96 | 176.42 |
| C1-C2-C8-C7 | 0.0359 | -0.0544 | -0.0459 | -0.58 |
| C1-C2-C8-C16 | -179.95 | -179.91 | -179.94 | 177.62 |
| C3-C2-C8-C7 | 179.93 | -179.93 | -179.91 | -178.47 |
| C3-C2-C8-C16 | -0.054 | 0.2007 | 0.1843 | -0.3 |
| C2-C3-C4-C5 | 0.0276 | -0.0559 | -0.0564 | 0.44 |
| C3-C4-C5-C6 | 0.0181 | -0.0177 | -0.0174 | 0.8 |
| C4-C5-C6-C1 | -0.0196 | 0.0361 | 0.0372 | -1.19 |
| N15-C7-C8-C2 | 0.0878 | 0.0957 | 0.08 | -0.35 |
| N15-C7-C8-C16 | 179.9 | 179.95 | 179.98 | -178.62 |
| C8-C7-N15-C1 | 0.1089 | -0.1024 | -0.0852 | 1.19 |
| C2-C8-C16-N28 | 177.3 | -176.52 | -176.52 | 179.45 |
| C7-C8-C16-N28 | -2.6781 | 3.4402 | 3.35921 | 177.29 |
| H17-C16-N28-C18 | -4.0076 | 2.5762 | 2.5314 | 0.9 |
| C20-C18-C19-H22 | -178.51 | 178.33 | 178.22 | -178.62 |
| N28-C18-C19-H22 | -0.8891 | 0.6671 | 0.7055 | -1.1 |
| C19-C18-C20-H24 | 176.16 | -176.37 | -176.38 | -179.42 |
| N28-C18-C20-H24 | -1.2961 | 1.1456 | 0.977 | -179.42 |
| C19-C18-N28-C16 | 148.01 | -141.56 | -141.31 | -146.25 |
| C20-C18-N28-C16 | -34.51 | 40.91 | 41.31 | 40.89 |
| C18-C20-C23-C25 | -0.0388 | -0.2463 | -0.2917 | -0.1 |
| C19-C21-C25-C23 | -0.2081 | 0.2594 | 0.2715 | 0.192 |
| C19-C21-C25-O29 | 179.28 | 179.54 | 179.54 | -178.26 |
| C20-C23-C25-C21 | 0.9918 | -0.783 | -0.7796 | 0.9 |
| C2O-C23-C25-O29 | -179.87 | 179.89 | 179.91 | -178.86 |

The optimized C19-H22, C20-H24, C21-H26 and C23-H27 bond distances in phenyl ring (Ph) moiety values are larger than the experimental C-H bond distance 0.9500Å of the reference molecule [13].

The optimized (Ph) C18-N28 bond distance for title compound computed by HF/6-31G (d,p), HF/6-311G(d,p) and B3LYP/6-31G(d,p), methods are 1.4078, 1.4084 and 1.4049Å respectively. On comparison with C-N bond distance 1.3712Å of experimental XRD value of reference compound and it has been observed that the computed values are remarkably greater than the experimental value.

The experimental bond distance of O-H is 0.8400Å in [13]. The computed O29-H30 bond distances for the title compound in HF and DFT methods show anomalously different from that of experimental bond distance of reference molecule.

The computed bond angles of C2-C1-N15 and C8-C7-N15 values are coinciding very well with experimental bond angles. The bond angle C6-C1-N15 closely related to experimental value by HF/6-31G(d,p) method only and other two methods deviate from experimental bond angles. The bond angles C8-C16-N28 and C20-C18-N28 are $1^0$ higher than experimental bond angles. For bond angle C19-C18-N28, HF methods show good agreement whereas B3LYP/6-31G(d,p)method $1^0$ lesser value than experimental bond angle[13].

The bond angles C2-C3-H9, C4-C3-H9, C3-C4-H10, C5-C4-H10, C4-C5-H11, C6-C5-H11, C1-C6-H12, C5-C6-H12, C8-C7-H14 for PhI are computed by B3LYP/6-31G(d,p) method stand closer to the experimental bond angles of reference molecule [13]. Computed from HF/6-31G(d,p) and HF/6-311G(d,p)  methods show much deviation from the experimental bond angles of similar moieties of the reference compound.

Out of these computed bond angles C19-C18-C20, C18-C19-C21, C18-C20-C23, C19-C21-C25, C20-C23-C25, C21-C25-C23 for Phenyl ring(Ph) moiety, C18-C19-C21, C19-C21-C25, C20-C23-C25 bond angles show coincide with experimental values, infact the remaining bond angles distinctly deviate from the experimental bond angles.

The bond angles C18-C19-H22, C21-C19-H22, C18-C20-H24, C23-C20-H24, C19-C21-H26, C25-C21-H26, C20-C23-H27, C25-C23-H27 for Phenyl ring (Ph) moiety are computed. Among the computed bond angles, C23-C20-H24, C20-C23-H27 bond angles appreciably deviate from the experimental values. However, the remaining bond angles coincide with very small deviation.

The optimized bond angles C1-N15-C7, C16-N28-C18 for both PhI and Phenyl ring (Ph)moiety are $109.75^0$, $119.95^0$ in B3LYP/6-31G(d,p), $109.33^0$, $119.94^0$ in HF/6-31G (d,p) and $109.33^0$, $120.01^0$ in HF/6-311G(d,p) respectively. Both HF and DFT methods coincide with experimental bond angles $109.28^0$, $120^0$.

The optimized bond angles C2-C1-C6, C1-C2-C3, C1-C2-C8, C3-C2-C8, C2-C3-C4, C3-C4-C5, C4-C5-C6, C1-C6-C5, C2-C8-C7, C2-C8-C16 for PhI are in agreement with experimental bond angles. The bond angles of C8-C16=N28 computed by HF and DFT methods for 1H-IMAP are remarkably lesser than that of reference compound [13].

Computed dihedral angles of 1H-IMAP are comparable with that of reference compound [13]. Theoretically computed dihedral angle for C18-C20-C23-C25 is $-0.0388^0$ in B3LYP/6-31G(d,p), $-0.2463^0$ in HF/6-31G(d,p), and $-0.2917^0$ in HF/6-311G(d,p), the corresponding experimental value of reference molecule is $-0.1^0$. Both the computed and experimental dihedral angles are negative. On comparing the computed and experimental dihedral angles are not coincides with one another.

On Comparing both the computed and experimental dihedral angles, it is observed only for C6-C1-C2-C8, N15-C1-C6-C5, C3-C2-C8-C7, C19-C18-C20-H24 group both experimental and computed values by HF method coincide with each other, but the other two dihedral angle  C1-C2-C8-C7 and C19-C18-N28-C16  values deviate from one another.

The optimized dihedral angles for N15-C7-C8-C16, C19-C21-C25-O29 groups are $179.9^0$, $179.28^0$ in B3LYP/6-31G(d,p), $179.95^0$, $179.54^0$ in HF/6-31G(d,p), $179.98^0$, $179.54^0$ in HF/6-311G(d,p) and the experimental dihedral angles are $-178.62^0$, $-178.26^0$. The computed dihedral angle values are positive, but the experimental values are negative. Both HF and DFT method show no agreement with the experimental dihedral angles of similar moieties of the reference compound [13].

## VIBRATIONAL ASSIGNMENT

The title molecule consists of 30 atoms so they have 84 normal vibrational modes which are IR active. According to theoretical calculation, the optimized geometry of the title molecule 1H–IMAP has C1 point group symmetry. Optimized ground state geometries and vibrational modes for studied molecule were obtained by HF and DFT (B3LYP) methods. The fundamental vibrational frequencies calculated for IH-IMAP at HF and B3LYP levels using the triple split valence basis set along with polarization function, 6-31G(d,p) and HF/6-311G(d,p) and observed FT-IR frequencies for various modes of vibrations have been collected in table(3).

Comparison of the frequencies calculated at HF and B3LYP with experimental values table (3) reveals the overestimation of the calculated vibrational modes due to neglect of anharmonicity in real system. Inclusion of electron correlation in Density Functional Theory to certain extends makes the frequency values smaller in comparison with the HF frequency data. Reduction in the computed harmonic vibrations, though basis set sensitive are only marginal as observed in the DFT values using 6-31G(d,p). Anyway not with standing the level of calculations, it is to scale down the calculated harmonic frequencies in order to experimental.

The calculated frequencies were scaled by factors 0.8992, 0.9051 and 0.955 for HF and DFT computation respectively. The resulting vibrational frequencies for the optimized geometries, the proposed vibrational assignments and available experimental Infrared frequencies are also given in table (3).

Vibrational modes are numbered from smallest to largest frequency. In the last columns are given a detailed description of the normal modes. The combined experimental and theoretical spectrum is given in figure(4).

## C-H vibration

The title molecule 1H-1MAP is an imine derivative and contains heterocyclic indole ring. Heteroaromatic systems exhibit C-H stretching vibrations in the region 3100–3000 cm$^{-1}$[16]. For PhI(Phenyl indole), the computed C-H stretching frequencies are assigned at 3137, 3036 cm$^{-1}$ for B3LYP/6-31G(d,p), 3095, 3001 cm$^{-1}$ for HF/6-31G(d,p) and 3094, 3002 cm$^{-1}$ for HF/6-311G(d,p). Among these methods, the mode 82 value obtained for B3LYP/6-31G(d,p) and mode 72 value obtained for HF methods are in agreement with experimental FT-IR band for the corresponding group at (modes 82, 75) 3170, 2979 cm$^{-1}$ for C-H stretching of PhI.

For all the aromatic compound the carbon–hydrogen stretching vibrations are observed in the region 3100-3000 cm$^{-1}$ [14, 15, 16]. Accordingly, in this range there are two calculated vibrations for Phenyl ring moiety (Ph) which are 3066, 3047 cm$^{-1}$ for B3LYP/6-31G(d,p), 3036, 3015 cm$^{-1}$for HF/6-31G(d,p) and 3035, 3015 cm$^{-1}$ for HF/6-311G(d,p). Among these methods, the B3LYP/6-31G(d,p) method vibrations are in agreement with experimental frequencies which are(modes 81, 77) 3105, 3044 cm$^{-1}$ and also literature value.
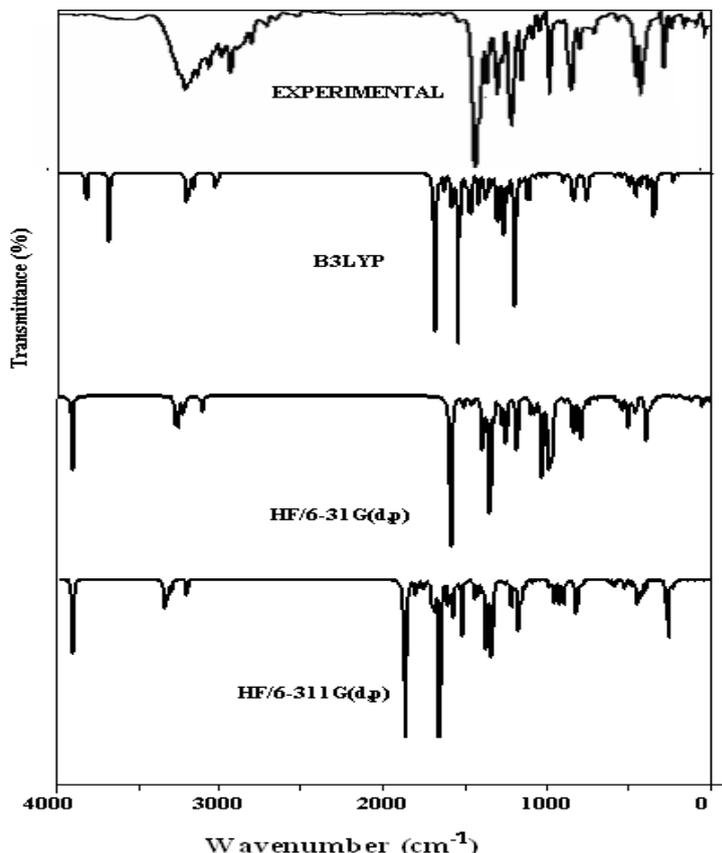


**Fig.2. Comparison of Experimental and Theoretical B3LYP, HF/6-31G (d,p) and HF/6-311G (d, p) FT-IR spectrum of 1H-IMAP.**
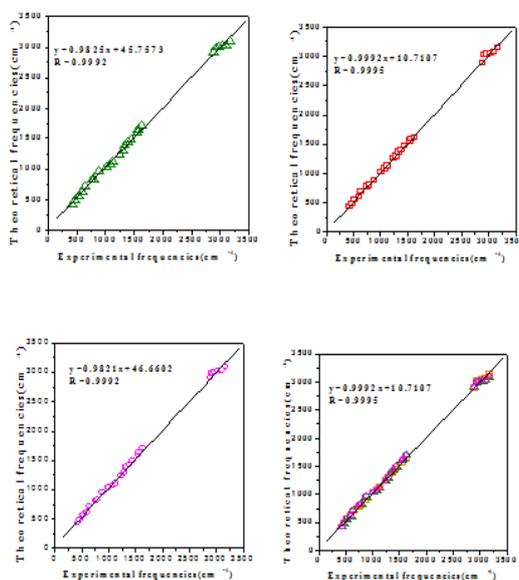
**Fig. 3. The graphical correlation between experimental and theoretical frequencies for IH-IMAP by B3LYP/6-31G(d,p), HF/6-31G(d,p) and HF/6-311G(d,p).**
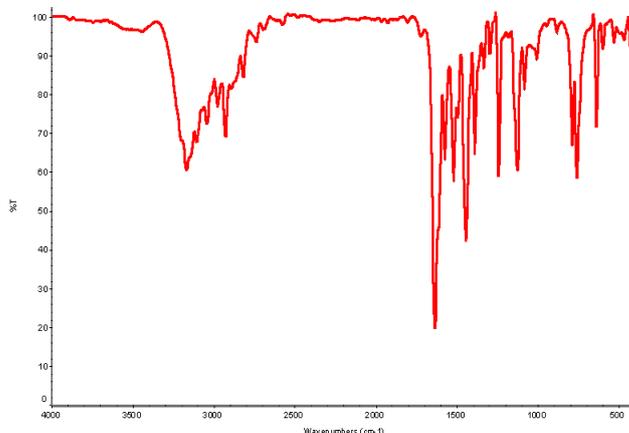


**Fig.4. Experimental FT-IR spectrum of 1H-IMAP**

**Table 4a: Vibrational wave numbers obtained for 1H-IMAP at B3LYP/6-31G(d,p), HF/6-31G(d,p) and HF/6-311G(d,p)**

| Mode | Experimental value | Calculated Frequencies cm-1 | | | HF/6-311G(d,p) | | HF/6-311G(d,p) | | Vibrational assignment |
|------|------|------|------|------|------|------|------|------|------|
| No | FT - IR | B3LYP/6-31 G (d,p) | HF/6-31 G(d,p) | HF/6-311 G(d,p) | IR Intensity | Raman Activity | Reduced mass | Force Constant | |
| 1 | – | 26 | 26 | 26 | 0.12 | 0.52 | 3.87 | 0 | τ(torsion) |
| 2 | – | 41 | 41 | 41 | 0.32 | 0.17 | 6.23 | 0 | τ(torsion) |
| 3 | – | 45 | 45 | 46 | 0.17 | 0.16 | 5.21 | 0 | τ(torsion) |
| 4 | – | 99 | 98 | 97 | 0.32 | 0.39 | 5.2 | 0.03 | τ(torsion) |
| 5 | – | 144 | 139 | 138 | 0.49 | 0.19 | 5.77 | 0.08 | τ(torsion) |
| 6 | – | 189 | 184 | 185 | 1.31 | 1.03 | 3.85 | 0.09 | ω C16-H17 |
| 7 | – | 205 | 203 | 203 | 1.02 | 0.06 | 5.08 | 0.15 | Ring breathing of PhI |
| 8 | – | 217 | 219 | 219 | 4.13 | 0.13 | 3.94 | 0.13 | ω -PhI |
| 9 | – | 220 | 225 | 226 | 0.57 | 0.05 | 4.36 | 0.16 | ω -PhI |
| 10 | – | 321 | 256 | 246 | 32.03 | 0.18 | 1.17 | 0.05 | ω of Ph & PhI |
| 11 | – | 329 | 323 | 323 | 0.45 | 0.27 | 4.73 | 0.35 | ω -OH |
| 12 | – | 360 | 367 | 368 | 6.76 | 0.05 | 4.84 | 0.47 | ω -OH |
| 13 | – | 386 | 395 | 394 | 10.76 | 0.18 | 2.84 | 0.31 | γ C-C of Ph |
| 14 | – | 408 | 415 | 412 | 13.63 | 0.05 | 1.97 | 0.24 | ω C-H of Ph |
| 15 | – | 412 | 421 | 423 | 1.28 | 0.34 | 2.94 | 0.38 | ω C-H of PhI |
| 16 | 427 | 425 | 426 | 426 | 0.08 | 0.01 | 2.63 | 0.34 | ω C-H of PhI + ω N15-H13 |
| 17 | – | 443 | 443 | 445 | 2.25 | 0.1 | 3.7 | 0.52 | ω 15N-13H of PhI |
| 18 | 468 | 480 | 482 | 484 | 5 | 0.14 | 7.1 | 1.2 | t-Ph& PhI |
| 19 | – | 485 | 490 | 491 | 1.46 | 0.01 | 4.63 | 0.8 | t-Ph& PhI |
| 20 | – | 519 | 536 | 537 | 4.6 | 0.07 | 2.83 | 0.59 | ω C-H of Ph |
| 21 | 531 | 551 | 559 | 561 | 1.39 | 0.28 | 4.43 | 1 | t-PhI |
| 22 | – | 560 | 571 | 574 | 1.35 | 0.02 | 3.15 | 0.74 | ω C-H of Ph |
| 23 | 601 | 607 | 612 | 615 | 0.11 | 0.52 | 6.48 | 1.76 | t-PhI |
| 24 | – | 615 | 621 | 624 | 0.14 | 0.06 | 2.86 | 0.8 | ω 15N-13H + ω 7C-14H |
| 25 | – | 627 | 636 | 639 | 0.14 | 0.51 | 6.36 | 1.87 | γ C-C of Ph |
| 26 | 640 | 690 | 714 | 719 | 2.66 | 0.42 | 3.84 | 1.43 | ω C-H of Ph |
| 27 | – | 721 | 731 | 734 | 1.39 | 0.27 | 5.52 | 2.14 | ω C-H of PhI |
| 28 | – | 730 | 741 | 743 | 4.76 | 1.67 | 5.39 | 2.14 | t (twisting) |
| 29 | – | 739 | 754 | 753 | 21.42 | 0 | 1.29 | 0.53 | t(twisting) |
| 30 | – | 742 | 764 | 769 | 0.6 | 0.04 | 3.96 | 1.69 | ω C-H of PhI |
| 31 | 761 | 776 | 812 | 812 | 11.04 | 1.59 | 5.21 | 2.47 | ω C-H of Ph |
| 32 | 790 | 797 | 824 | 824 | 1.28 | 0.23 | 1.26 | 0.62 | ω C-H of Ph |
| 33 | – | 803 | 843 | 844 | 14.97 | 0.91 | 2.07 | 1.06 | ω 7C-14H of PhI |
| 34 | – | 811 | 854 | 857 | 0.35 | 0.08 | 4.81 | 2.54 | ω C-H of Ph |
| 35 | – | 821 | 864 | 863 | 0.04 | 0.01 | 1.5 | 0.8 | ω C-H of PhI |
| 36 | – | 846 | 875 | 877 | 9.72 | 0.82 | 3.29 | 1.82 | γ -PhI |
| 37 | – | 861 | 895 | 897 | 2.73 | 0.23 | 1.46 | 0.84 | t-Ph |
| 38 | 886 | 886 | 953 | 953 | 0.27 | 0.1 | 1.4 | 0.92 | ω C-H of PhI |
| 39 | – | 899 | 954 | 957 | 0.3 | 0.02 | 1.36 | 0.89 | ω C-H of Ph |
| 40 | – | 907 | 972 | 976 | 0.05 | 0.15 | 1.34 | 0.92 | ω C-H of Ph |

For Phenyl ring moiety (Ph), the in-plane and out-of-plane deformation vibration normally observed in the region 1300-750 cm⁻¹ [14]. The C-H in plane bending vibration computed at (mode47) 1076 cm-1 for B3LYP/6-31G(d,p), 1074 cm⁻¹ by HF methods. Both HF and DFT shows very good agreement with experimental FT-IR band at 1083 cm⁻¹. The C-H out-of-plane bending vibration computed at (modes31, 32, 26) 797, 776, 690 cm⁻¹ for B3LY-6-31G(d,p)P, 714, 812, 824 cm⁻¹ for HF/6-31G(d,p) 719, 812, 824 cm⁻¹ for HF/6-311G(d,p). Among these methods, the B3LYP/6-31G(d,p) method values are closely related to FT-IR band at 790, 761 640 cm⁻¹.

For PhI (Phenyl indole), the C-H in-plane bending vibrations in aromatic heterocyclic compounds occur in the region between 1300 and 1000 cm^{-1} [16]. The C-H rocking mode obtained at(modes 65, 62, 61, 58, 49) 1465, 1402, 1358, 1294, 1127 cm^{-1}for B3LYP/6-31G(d,p), 1489, 1428, 1382, 1293, 1110 cm^{-1} for HF methods. On comparing them, the B3LYP/6-31G(d,p) method show very good agreement with experimental values of FI–IR band at 1445, 1391, 1336, 1296, 1127 cm^{-1}.

The C-H-out of plane bending for PhI(Phenyl indole), occur in the region between 1000 and 650 cm^{-1} [16]. The C-H wagging mode for PhI assigned at (modes16,38) 425, 886 cm^{-1} for B3LYP/6-31G(d,p), 426, 956 cm^{-1} for HF/6-31G(d,p) methods. Among these methods, the B3LYP/6-31G(d,p)method show good agreement with FI-IR band at 427, 886cm^{-1}.

**Table 4a: Vibrational wave numbers obtained for 1H-IMAP at B3LYP/6-31G (d,p), HF/6-31G(d,p) and HF/6-311G(d,p)**

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 41 | - | 929 | 990 | 990 | 0.01 | 0.02 | 1.3 | 0.91 | ω C-H of PhI |
| 42 | - | 955 | 993 | 993 | 0.26 | 0.13 | 2.53 | 1.8 | δC16-H17 |
| 43 | - | 977 | 999 | 997 | 1.2 | 1.23 | 2.17 | 1.56 | δ C-C of Ph |
| 44 | - | 995 | 1015 | 1016 | 0.55 | 1.68 | 1.61 | 1.19 | δ C-C of PhI |
| 45 | 1008 | 1029 | 1037 | 1038 | 5.07 | 4.05 | 3.91 | 3.03 | δ C-C of Ph |
| 46 | | 1063 | 1066 | 1060 | 9.03 | 0.86 | 2.05 | 1.66 | δ 15N-13H+δ 7C-14H of PhI |
| 47 | 1083 | 1076 | 1074 | 1074 | 26.14 | 1 | 1.53 | 1.27 | ρ C-H of PhI |
| 48 | | 1103 | 1108 | 1106 | 6.42 | 1.19 | 1.62 | 1.43 | ρ C-H of Ph |
| 49 | 1128 | 1127 | 1110 | 1108 | 11.81 | 0.48 | 1.95 | 1.73 | ρ C-H of PhI |
| 50 | - | 1132 | 1115 | 1115 | 2.93 | 0.49 | 1.46 | 1.3 | ρ C-H of Ph |
| 51 | - | 1144 | 1150 | 1151 | 2.05 | 2.11 | 1.12 | 1.07 | ρ O-H + ρ 21C-26H |
| 52 | - | 1186 | 1202 | 1202 | 0.55 | 7.25 | 3.24 | 3.37 | Ring breathing of Ph |
| 53 | - | 1209 | 1212 | 1215 | 0.4 | 0.56 | 1.88 | 2 | δ C-H of Ph |
| 54 | - | 1209 | 1219 | 1217 | 42.93 | 0.87 | 2.13 | 2.27 | ρ C-H of PhI |
| 55 | 1243 | 1245 | 1228 | 1229 | 25.76 | 5.42 | 1.76 | 1.91 | Ring breathing of Ph |
| 56 | - | 1262 | 1244 | 1242 | 2.77 | 2.95 | 2.48 | 2.75 | ρ C-H of Ph |
| 57 | - | 1281 | 1259 | 1255 | 3.83 | 0.88 | 3.99 | 4.52 | ρ C-H of PhI+ ρ C16-H17 |
| 58 | 1296 | 1294 | 1293 | 1293 | 5.45 | 2.3 | 2.59 | 3.12 | ρ C-H of PhI |
| 59 | - | 1311 | 1310 | 1312 | 8.04 | 0.18 | 1.4 | 1.73 | ν C-C of Ph |
| 60 | - | 1321 | 1320 | 1320 | 0.3 | 2.07 | 1.89 | 2.38 | ν C=C of PhI |
| 61 | 1336 | 1358 | 1382 | 1382 | 24.82 | 8.82 | 1.56 | 2.16 | ρ C-H of PhI+ ρ C16-H17 |
| 62 | 1391 | 1402 | 1428 | 1428 | 1.75 | 1.64 | 2.51 | 3.69 | ρ C-H of PhI |
| 63 | - | 1410 | 1436 | 1435 | 24.97 | 2.65 | 2.37 | 3.52 | ρ C-H of Ph |
| 64 | - | 1427 | 1456 | 1454 | 10.73 | 1.23 | 2.48 | 3.77 | ρ C-H of PhI |
| 65 | 1445 | 1465 | 1489 | 1487 | 10.82 | 3.34 | 2.79 | 4.45 | ρ C-H of PhI |
| 66 | - | 1477 | 1515 | 1512 | 84.52 | 11.13 | 2.73 | 4.5 | ρ C-H of Ph |
| 67 | | 1513 | 1544 | 1542 | 20.21 | 28.89 | 4.88 | 8.35 | ν C8=C7 of PhI |
| 68 | 1552 | 1554 | 1595 | 1593 | 2.61 | 6.57 | 5.62 | 10.29 | ν C=C of PhI |
| 69 | | 1559 | 1604 | 1604 | 3.79 | 2 | 6 | 11.11 | ν C=C of Ph |
| 70 | 1575 | 1585 | 1635 | 1633 | 0.52 | 14.44 | 5.74 | 11.04 | ν C=C of Ph |
| 71 | | 1598 | 1639 | 1637 | 5.68 | 14.29 | 5.85 | 11.28 | ν C=C of PhI |
| 72 | 1636 | 1614 | 1702 | 1698 | 100 | 100 | 8.02 | 16.66 | ν C16=N28+ ν C=C of Ph |
| 73 | 2888 | 2888 | 2905 | 2906 | 7 | 1.24 | 1.08 | 6.6 | ν C16-H17 |
| 74 | 2931 | 3020 | 2991 | 2992 | 8.13 | 7.93 | 1.09 | 7.02 | ν C-H of Ph(asym) |
| 75 | 2979 | 3036 | 3001 | 3002 | 0.23 | 2 | 1.08 | 7.04 | ν C-H of PhI(asym) |
| 76 | | 3042 | 3008 | 3010 | 1.6 | 7.95 | 1.09 | 7.1 | ν C-H of Ph |
| 77 | 3044 | 3047 | 3015 | 3015 | 2.52 | 2.56 | 1.08 | 7.12 | ν C-H of Ph |
| 78 | - | 3053 | 3019 | 3021 | 9.81 | 3.77 | 1.09 | 7.19 | ν C-H of PhI |
| 79 | - | 3062 | 3030 | 3031 | 6.26 | 18.14 | 1.09 | 7.26 | ν C-H of Ph |
| 80 | - | 3063 | 3032 | 3032 | 3.32 | 2.41 | 1.09 | 7.24 | ν C-H of PhI |
| 81 | 3105 | 3066 | 3036 | 3035 | 1.46 | 10.88 | 1.09 | 7.26 | ν C-H of Ph |
| 82 | 3170 | 3137 | 3095 | 3094 | 0.09 | 3.38 | 1.09 | 7.57 | ν 7C-14H of PhI |
| 83 | - | 3513 | 3533 | 3538 | 31.98 | 9.02 | 1.08 | 9.73 | ν 15N-13H |
| 84 | | 3651 | 3774 | 3791 | 29.61 | 7.59 | 1.06 | 11.03 | ν O-H |

The twisting mode for PhI occur at (mode21) 551, 559, 561 cm-1 for B3LYP/6-31G(d,p) , HF/6-31G(d,p) and HF/6-311G(d.p) respectively. Among these computational methods, the B3LYP/6-31G(d,p) method show good agreement with experimental FI-IR band at 531 cm^{-1}.

**C=C stretching vibration**

For Phenyl ring moiety (Ph), the ring carbon-carbon stretching vibrations occur in the region 1650-1400 cm^{-1} in benzene derivative varsanyi observed five bands 1625–1590, 1590–1575, 1540–1470, 1465–1430 and 1380–1280 cm^{-1}, in this region [15]. The vibrations 1636, 1575 cm^{-1} have been assigned to C=C bond stretching vibration by obtained at experimentally. The C=C stretching vibrations computed at (modes 70, 72) 1614, 1585 cm^{-1} for B3LYP/6-31G(d,p) 1702, 1635cm^{-1} for HF/6-31G(d,p) and 1698,

1633 cm$^{-1}$ for HF/6-311G(d,p). It is observed, the value obtained at B3LYP/6-31G(d,p) method shows very good agreement with experimental value.

For PhI(Phenyl indole), In aromatic heterocyclic compounds, the C=C stretching vibration occur in the region 1600 -1300 cm$^{-1}$ [16]. The theoretically computed C=C stretching vibration at (mode 68) 1554 cm$^{-1}$ for B3LYP/6-31G(d,p), 1595 cm$^{-1}$ for HF/6-311G(d,p). On comparing them, the B3LYP/6-31G(d,p) vibration shows good agreement with the experimental value of corresponding group.

### C–C Vibration

Vibrations C–C For B3LYP/6–31G(d,p), HF/6–31G(d,p), and HF / 6–311G(d,p), the C–C in plane bending for Phenyl ring moiety (Ph) is assigned at (mode43) 977, 999, and 997, respectively. There isn't any experimental evidence. Ph exhibits C–C out–of–plane bending at (modes13,25) 386, 627 cm$^{-1}$ for B3LYP/6–31G(d,p), 395, 636 cm-1 for HF/6–31G(d,p), and 394, 639 cm$^{-1}$ for HF/6–311G(d,p). The C–C in plane bending for PhI(Phenyl indole) is 1029 cm$^{-1}$ for B3LYP/6–31G(d,p), 1037 cm$^{-1}$ for HF/6–31G(d,p), and 1038 cm$^{-1}$ for HF/6–311G(d,p), respectively. The B3LYP/6-31G(d,p) technique, among these, shows good agreement with experimental assignment at 1008 cm$^{-1}$.

### C=N Stretching Vibration

The identification of C=N stretching vibration is not the easiest task, since the mixing of the several bonds are possible in this region Silverstein *et al* assigned C=N stretching absorption in the region 1689-1471 cm$^{-1}$ [16]. In the present work, mode (72) have been assigned to C=N stretching vibrations are 1702 cm$^{-1}$ for HF/6-31G(d,p), 1698 cm$^{-1}$ for HF/6-311G(d,p) and 1614 cm$^{-1}$ for B3LYP/6-31G(d,p) method respectively.

### N-H stretching vibration

Heteroaromatic compounds containing a N-H group exhibits N-H stretching absorption in the region 3500-3200 cm$^{-1}$ [16]. Indoles display very strong N-H stretching absorption between 3500 and 3450 cm$^{-1}$ while for the title compound the N-H stretching vibrations are assigned at (mode83) 3513 cm$^{-1}$ for B3LYP/6-31G(d,p), 3533 cm$^{-1}$ for HF/6-31G(d,p) and 3538 cm$^{-1}$ for HF/6-311G(d,p. The N-H out–of plane bending (wagging) occurs at (24) 615 cm$^{-1}$ for B3LYP/6-31G(d,p), at 612 cm$^{-1}$ for HF/6-31G and at 624 cm$^{-1}$ for HF-6-311G. The N-H in-plane bending computed at (mode46) 1063 cm$^{-1}$for B3LYP/6-31G(d,p), at 1066 cm$^{-1}$ for HF/-631G(d,p) and at 1060 for HF/6-311G (d,p).

### O-H stretching vibration

According to Silverstein [16] *et al*, the hydroxyl stretching occur above 3610 cm$^{-1}$ while the theoretically computed value at 3651 cm$^{-1}$ , 3770cm$^{-1}$ and 3791 cm$^{-1}$ (mode84) for B3LYP/6-31G(d,p), HF/6-31G(d,p) and HF/6-311G(d,p) respectively. B3LYP/6-31G(d,p) method shows very good agreement with literature data. The O-H wagging computed at 329 cm$^{-1}$, 360 cm$^{-1}$ (modes11,12) for B3LYP,323,367 cm$^{-1}$ for HF/6-31G(d,p) and 323, 368 cm$^{-1}$ for HF/6-311G(d,p). Computed vibrations for B3LYP/6-31G(d,p) coincide with experimental value.

### NLO properties

The first hyperpolarizability of the 1H-IMAP molecular system, as well as related properties ($\mu$, $\beta$, $\alpha_0$, and $\Delta\alpha$) have been calculated using the HF/6-31G (d,p),6-311G(d,p),andB3LYP/6-31G(d,p) methods

based on the finite field approach for 1H-IMAP.The energy of a system in the presence of an applied electric field is a function of the electric field. The first hyperpolarizability is a third rank tensor represented by a 3x3x3 matrix. Due to the Kleinman symmetry, the 27 components of a 3D matrix can be reduced to ten components. [17].The components of β are defined as the coefficients in the Taylor series expansion of the energy in the external electric field. When the external electric field is weak and homogenous this expansion becomes

$E=E_0-E_i\mu_i -1/2 \ \alpha_{ij} F_iF_j-1/6 \ \beta_{ijk} F_iF_j F_k-1/24\gamma_{ijkl} F_iF_j F_kF_l+.......$

Where $E_0$ is the energy of unperturbed molecules, $F_i$ is the field at the origin $\mu_i$, $\alpha_{ij}$, $\beta_{ijk}$ and $\gamma_{ijkl}$ are the components of the dipole moment, polarizability, first hyperpolarizability and the second hyperpolarizabilities, respectively. The static dipolemoment($\mu$), the mean polarizability ($\alpha_0$), the anisotropy of the polarizability ($\Delta\alpha$) and the mean hyperpolarizability ($\beta_0$) using x, y, z components they are defined as

$\mu =(\mu_x^2+\mu_y^2+\mu_z^2)^{1/2}$

$\alpha_0= (\alpha_{xx}+ \alpha_{yy} + \alpha_{zz})/3$

$\alpha = [(\alpha_{xx}- \alpha_{yy})^2 + (\alpha_{yy}- \alpha_{zz})^2 + (\alpha_{zz}- \alpha_{xx})^2 + 6 \ \alpha^2_{xx}]^{1/2}/ (2)^{1/2}$

$\beta_0=(\beta_x^2 +\beta_y^2 +\beta_z^2)$

$\beta_x= \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$

$\beta_y= \beta_{yyy} + \beta_{yxx} + \beta_{yzz}$

$\beta_z= \beta_{zzz} + \beta_{zxx} + \beta_{zyy}$

The first Hyperpolarizability of 1H-IMAP computed by ab inito and DFT methods are shown in the Table (4a-4c).

**Table 4a: The electric Dipole moments (Debye) and Dipole moment for 1H-IMAP were calculated using ab initio HF and DFT.**

|  | HF/6-31G(d.p) | HF/6-311G(d.p) | B3LYP/6-31G(d.p) |
|---|---|---|---|
| $\mu_x$ | 1.5743 | 1.6231 | 1.2771 |
| $\mu_y$ | 0.2546 | 0.2157 | -0.1053 |
| $\mu_z$ | 0.2324 | 0.2571 | 0.3135 |
| $\mu$ | 1.6115 | 1.6574 | 1.3192 |

Molecules with high hyperpolarizability do have in them planar D-π-A chromophores group, but the title compound is non-planar and non-conjugative system. Hence its hyperpolarizability value is of the order $1x10^{-30}$ esu [18].

**Table 5b: Calculated all β components and $\beta_{tot}$ ($x10^{-30}$) value of 1H-IMAP in (Debye-Ang **2) or $\beta_{tot}$ in esu.**

|  | HF/6-31G(d.p) | HF/6-311G(d.p) | B3LYP/6-31G(d.p) |
|---|---|---|---|
| $\beta_{xxx}$ | 43.0057 | 42.9576 | 42.7723 |
| $\beta_{xxy}$ | -49.3346 | -50.3101 | -47.8475 |
| $\beta_{xyy}$ | 13.5478 | 13.9914 | 14.6025 |
| $B_{yyy}$ | -6.0856 | -6.4816 | -7.7217 |
| $B_{xxz}$ | 53.9699 | 53.2946 | 51.8616 |
| $B_{xyz}$ | 3.4956 | 2.8863 | 2.6433 |
| $B_{yyz}$ | -9.7824 | -9.5379 | -8.3615 |
| $B_{xzz}$ | -25.0761 | -25.4599 | -23.0622 |
| $B_{yzz}$ | -0.2149 | -0.6915 | -0.3713 |
| $B_{zzz}$ | 1.236 | 1.3537 | 1.2446 |
| $\beta_{tot}$ | 78.418 | 79.2808 | 78.2841 |
|  | ($0.6774X 10^{-30}$esu) | ($0.6849X 10^{-30}$ esu) | ($0.6763X 10^{-30}$ esu) |

**Table 5c: The average polarizability for 1H-IMAP $\alpha_{tot}$ (Debye-Ang) or $\alpha_{tot}$ in esu**

| | HF/6-31G(d,p) | HF/6-311G(d,p) | B3LYP/6-31G(d,p) |
|---|---|---|---|
| $\alpha_{xx}$ | -90.554 | -91.3567 | -86.8599 |
| $\alpha_{xy}$ | 2.5219 | 2.147 | 0.5798 |
| $\alpha_{yy}$ | -91.5775 | -92.1646 | -91.122 |
| $\alpha_{xz}$ | -15.9157 | -15.4872 | -14.4108 |
| $\alpha_{yz}$ | 5.069 | 4.9703 | 4.4202 |
| $\alpha_{zz}$ | -111.598 | -113.4551 | -108.1888 |
| $\alpha_0$ | -97.9099 | -98.9921 | -93.7235 |
| | $(1.4510 \times 10^{-23} esu)$ | $(1.4670 \times 10^{-23} esu)$ | $(1.3889 \times 10^{-23} esu)$ |
| $\alpha_{tot}$ | 158.1848 | 159.685 | 157.6234 |
| | $(2.3442 \times 10^{-23} esu)$ | $(2.3665 \times 10^{-23} esu)$ | $(2.3359 \times 10^{-23} esu)$ |

## Conclusion

The structural properties of 4[(IH-indol-3yl) methylene amino]phenol were thoroughly investigated in this study using ab initio Hartree-Fock Theory and Density Functional Theory with B3LYP exchange correlation. The vibrational frequencies were computed, and the scaled values were compared to the experimental values.The XRD values were compared to the optimised geometric parameters such as bond angles, bond lengths, and dihedralangles. The measured and observed frequencies are found to agree well. The Non-Linear Optical properties are addressed theoretically. The electric dipolemoment ($\mu_{tot}$), the isotropic polarizability ($\alpha_{tot}$) and the hyperpolarizability($\beta_{tot}$) of the title compound are also studied

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